Modélisation et Analyse Mathématique d'Equations aux Dérivées Partielles Issues de la Physique et de la Biologie

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Comprendre, c'est accepter.
Lu dans Psychologies Magazine

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Avant-propos

La finalité de ce manuscrit est de présenter les résultats obtenus par l'auteure dans le cadre de son doctorat de Mathématiques effectué sous la direction de Prof. Laurent Desvillettes, au Centre des Mathématiques et de Leurs Applications à l'École Normale Supérieure de Cachan.

Le sujet de ce doctorat s'inscrit dans le vaste domaine des Équations aux Dérivées Partielles (EDP) issues des Sciences naturelles. Il comporte des résultats mathématiques d'Analyse des EDP ainsi que des aspects de modélisation. Il est constitué de deux parties indépendantes présentées ci-dessous.

Partie 1 : les systèmes de diffusion croisée en Dynamique des populations. Une question fondamentale en Biologie est de comprendre le comportement macroscopique d'une population de différentes espèces, en connaissant la nature des interactions entre individus. Les modèles classiques de réaction-diffusion supposent que les interactions influent sur la *croissance* (ou la mortalité) des individus (à travers la compétition, la prédation, etc.) ; mais récemment ont été développés de nombreux modèles qui prennent en compte des interactions affectant le *mouvement* des individus (attraction, répulsion, etc.). Les modèles résultants sont des systèmes fortement couplés (i.-e. le couplage entre équations se fait à travers les termes d'ordre deux au regard du nombre de dérivées), souvent non linéaires, pour lesquels l'analyse mathématique est un défi. Prenons l'exemple du système de ce type le plus utilisé, dit SKT, qui comporte des termes de diffusion croisée (qui modélisent la répulsion entre individus d'espèces différentes) : pour ce système pourtant très étudié, une question aussi fondamentale que l'existence de solutions fortes reste ouverte.

Dans ce manuscrit, on introduit une approche basée sur des extensions récentes de lemmes de dualité et sur des méthodes d'entropie. Grâce à cette approche, on démontre l'existence de solutions faibles dans un cadre général de systèmes de réaction-diffusion croisée (qui inclut notamment le système SKT), ainsi que, dans certains cas, des propriétés qualitatives des solutions (régularité, unicité, comportement au voisinage de zéro, approximation par un modèle microscopique).

Partie 2 : l'équation de Boltzmann en domaine borné. L'équation de Boltzmann, introduite en 1872 pour modéliser la dynamique des gaz raréfiés hors équilibre, a depuis été étudiée en profondeur par la communauté des spécialistes en EDP. Il existe de nombreux résultats autour de la question de l'existence de solutions fortes proches de l'équilibre ou du vide. Pourtant, très peu de résultats concernent l'existence de solutions fortes en domaine borné général, bien que cette situation soit la plus fréquente dans les applications. Une raison de la difficulté du problème est l'irruption de singularités le long des trajectoires rasant le bord du domaine.

Dans ce manuscrit, on présente une théorie précise de la régularité de l'équation de Boltzmann en domaine borné. Dans le cas où le domaine est convexe, on sait que les singularités sont confinées au bord. Dans ce cas, grâce notamment à l'introduction d'une *distance cinétique* qui compense ces singularités au bord, on montre des résultats de propagation de normes de Sobolev et de propagation $\mathscr{C}^1$. Dans le cas où le domaine n'est pas convexe, les singularités se propagent à l'intérieur du domaine et ont un impact bien plus sévère. Dans ce cas, on montre un résultat de propagation de régularité BV.

Liste des travaux rassemblés dans ce manuscrit

Les résultats présentés dans les Chapitres 4 à 8 sont des résultats originaux. Ils ont fait l'objet des publications décrites ci-dessous.

Le Chapitre 4 est le fruit d'une collaboration avec Laurent Desvillettes (CMLA, ENS Cachan & CNRS) ; il a été publié, sous le titre *New results for triangular reaction cross diffusion system*, dans le journal *Journal of Mathematical Analysis and Applications*.

Le Chapitre 5 est le fruit d'une collaboration avec Laurent Desvillettes (CMLA, ENS Cachan & CNRS), Thomas Lepoutre (INRIA, Université de Lyon & CNRS, & ICJ, Université Lyon 1) et Ayman Moussa (LJLL, UPMC Université Paris 06 & CNRS) ; il a été publié, sous le titre *On the entropic structure of reaction-cross diffusion systems*, dans le journal *Communications in Partial Differential Equations*.

Le Chapitre 6, fruit d'un travail autonome, a été soumis pour publication sous le titre *On reaction cross-diffusion systems with possible self-diffusion*.

Le Chapitre 7 est extrait d'un long article écrit en collaboration avec Yan Guo (DAM, Brown University), Chanwoo Kim (University of Wisconsin-Madison) et Daniela Tonon (CEREMADE, Université Paris-Dauphine). Plus précisément, cet article présente une théorie sur la régularité des solutions de l'équation de Boltzmann en domaine convexe avec différentes conditions de réflexion aux bords, et le Chapitre 7 présenté ici se focalise sur les résultats obtenus dans le cadre de conditions de réflexion *diffusive* aux bords. L'article, intitulé *Regularity of the Boltzmann equation in convex domains*, est reproduit dans son intégralité en annexe. Il a été soumis pour publication.

Le Chapitre 8 est le fruit d'une collaboration avec Yan Guo (DAM, Brown University), Chanwoo Kim (University of Wisconsin-Madison) et Daniela Tonon (CEREMADE, Université Paris-Dauphine) ; il a été soumis pour publication sous le titre *BV-regularity of the Boltzmann equation in non-convex domains.*

Première partie

Introduction

Chapitre 1

Généralités

Sommaire

Dans ce premier chapitre, on introduit des concepts assez généraux que l'on rencontre dans un large éventail de situations où l'on veut modéliser mathématiquement des phénomènes réels, et plus particulièrement lorsque ces derniers impliquent des systèmes composés d'un grand nombre de particules. Les deux chapitres suivants seront consacrés à l'introduction de deux problèmes particuliers qui s'inscrivent dans ce contexte : d'une part l'équation de Boltzmann pour l'évolution d'un gaz raréfié perturbé en domaine borné, et d'autre part les systèmes de réaction-diffusion croisée en Dynamique des populations.

1.1 Modélisation et EDP singulières

Un modèle mathématique est une description en langage mathématique d'un phénomène réel. Un modèle contient donc des informations sur le phénomène décrit. Du point de vue mathématique, ces informations peuvent prendre plusieurs aspects, par exemple quantitatifs (estimation par le calcul analytique ou par la simulation numérique de la valeur de certaines quantités) ou qualitatifs (conservation/croissance/décroissance de certaines quantités, comportement asymptotique, régularité ou singularité, stabilité, prédominance de certains phénomènes en jeu sur d'autres, effets de seuil, etc.). En conséquence, le travail d'analyse du modèle mathématique peut prendre plusieurs aspects (analytiques ou numériques), dont le plus fondamental est de s'assurer que les objets mathématiques utilisés sont bien définis, c'est-à-dire, que le modèle utilisé a un sens : quand on utilise des modèles EDP, cela revient à vérifier que les EDP utilisées possèdent bien une (unique) solution (problème *bien posé*).

Cette première tâche n'est pas aisée : d'une part, il n'existe pas pour les EDP de théorie générale pour l'existence et l'unicité des solutions. Le résultat le plus général dans cette direction est le théorème de Cauchy-Kowalevski, qui, si on le compare par exemple au théorème de Cauchy-Lipschitz pour l'existence et l'unicité des solutions des équations différentielles, présente deux limitations majeures : il fournit uniquement des solutions locales (et pas de critère simple pour que ces solutions soient globales) et il nécessite que les données (coefficients de l'équation, données initiales) soient analytiques réelles. A part dans quelques cas particuliers nécessitant de fortes hypothèses sur la régularité des données et/ou sur la structure de l'équation, la plupart des EDP recquièrent donc un travail pour démontrer l'existence de solutions. D'autre part, on sait que pour certaines EDP il n'existe *pas* de solution au sens classique : il faut donc pour ces EDP donner une nouvelle définition de la notion de solution. Cette nouvelle définition doit avoir de "bonnes" propriétés, à savoir, au moins : permettre de démontrer l'existence de solutions, et avoir des liens satisfaisants avec la notion de solution au sens classique. C'est dans ce contexte qu'est née la théorie des distributions : on pourra consulter à ce sujet le livre de L. Schwartz [83].

Dans ce manuscrit, c'est ce que l'on entend par EDP singulière : une EDP qui ne s'inscrit pas dans une théorie plus générale d'existence, et pour laquelle la notion de solution la plus adaptée, c'est-à-dire, celle qui donne *a priori* les résultats les plus probants, n'est pas la notion de solution classique.

1.2 Systèmes multi-particules

Lors de la modélisation mathématique d'un phénomène, il y a un conflit entre les deux idéaux d'une part d'*exhaustivité* du modèle (prendre en compte toute la "réalité" de l'objet modélisé) et d'autre part de *simplicité* mathématique (possibilité de résoudre les équations, et d'obtenir un maximum d'informations qualitatives et/ou quantitatives, analytiques et/ou numériques sur les solutions). Les choix qui découlent de ce conflit, inhérents au travail de modélisation, dépendent évidemment de la nature du phénomène étudié, mais aussi du contexte (usage auquel on destine les modèles, échelles caractéristiques [1] en jeu, etc). Ce choix est particulièrement délicat pour les systèmes complexes, qui, par définition [2], conduisent à des modèles mathématiques très coûteux, voire impossibles à résoudre.

Dans ce manuscrit, on s'intéresse à deux exemples qui relèvent d'un cas particulier de système complexe, les systèmes *multi-particules*. Ces systèmes sont composés d'un très grand nombre d'éléments identiques en interaction, qu'on appelle particules (ou individus).

Une situation typique pour les systèmes multi-particules est la suivante : on dispose d'un modèle standard pour les lois régissant les interactions entre particules (échelle dite *microscopique*), mais le système mathématique qui en découle est impossible à résoudre, compte-tenu du grand nombre d'équations

1. c'est-à-dire échelles de temps et d'espace (par exemple) auxquelles les phénomènes considérés ont une taille raisonnable et peuvent être observés.

2. On dit d'un phénomène que c'est un *système complexe* lorsqu'il peut être modélisé par un système composé d'un grand nombre d'entités en interaction, et que les nombreuses rétroactions qui découlent de ces interactions rendent le système imprévisible pour l'observateur.

couplées. Une direction possible est alors de chercher à décrire le système, non pas par l'état de chaque particule, mais par des quantités globales ou moyennées sur l'ensemble des particules (échelle dite *macroscopique*). Les particules du système étant identiques, ces informations macroscopiques suffisent dans de nombreux contextes à donner une description pertinente du phénomène étudié. Par exemple, pour modéliser un fluide, il est souvent plus efficace en pratique de le décrire par certaines quantités hydrodynamiques (densité, vitesse moyenne, température) plutôt que par l'état (position, vitesse, etc.) de chacune des molécules qui le composent. On peut aussi se placer à des échelles intermédiares, dites *mésoscopiques* : c'est le cas par exemple de l'équation de Boltzmann, qui modélise la dynamique des gaz raréfiés à une échelle intermédiaire entre l'échelle microscopique (molécules de gaz) et l'échelle macroscopique (hydrodynamique) : voir le Chapitre 3. Au Chapitre 2, on présente des systèmes de réaction-diffusion croisée pour la dynamique des populations de deux espèces en compétition (échelle macroscopique). Pour des raisons d'ordre mathématique et de modélisation, on introduit de plus un système de réaction-diffusion qui modélise le même phénomène à une échelle intérmédiaire [3] entre les échelles microscopique (individus) et macroscopique (populations de deux espèces).

Remarque 1.1. *Un problème fondamental lorsque l'on développe plusieurs modèles pour un phénomène, est, d'une part, de bien identifier les conditions pour lesquelles les modèles sont adaptés (les limites des modèles), et d'autre part, d'établir des liens précis et rigoureux entre les modèles : c'est une question de cohérence entre les différents modèles. S'il s'agit par exemple de modèles valables à différentes échelles, peut-on (et en quel sens) dériver les modèles de petite échelle large à partir des modèles d'échelle plus large ? A ce sujet, on ne peut pas ne pas mentionner le* $VI^{\grave{e}me}$ *problème de Hilbert, et en particulier sa déclinaison la plus connue, dans le cadre de la théorie cinétique des gaz : il s'agit de "développer mathématiquement les processus limitatifs, juste esquissés, qui mènent de la vision atomiste aux lois du mouvement du continu". Ce problème, énoncé en 1900 par D. Hilbert, est encore largement ouvert (voir par exemple [71]).*

Pour décrire les quantités de particules à une échelle macroscopique, on utilise la notion de densité. La densité de particules renseigne sur la quantité de particules du système par unité d'espace [4]. Elle dépend du point d'espace où on la regarde (et éventuellement d'autres variables, typiquement, le temps). Soit $u = u(x) \geq 0$ la densité d'individus d'une espèce au point d'espace x. Il y a plusieurs interprétations possibles pour $u(x)$, par exemple :
- on peut voir u directement comme une approximation : $u(x)\,\mathrm{d}x$ approche la quantité d'individus dans l'élément de volume (ou surface, etc.) $\mathrm{d}x$. Alors, pour toute partie ω de l'espace, $\int_\omega u(x)\,\mathrm{d}x$ est la quantitée approchée de particules contenues dans ω. Notons que c'est une *approximation* car $u(x)\,\mathrm{d}x$ peut ne pas être un nombre entier, contrairement au nombre de particules dans ω.
- on peut voir u comme un densité de probabilité : une particule étant fixée, $u(x)\,\mathrm{d}x$ est alors la probabilité que cette particule se trouve dans l'élément de volume (ou surface, etc.) $\mathrm{d}x$. Les particules étant toutes identiques, elles sont caractérisées par la même densité u, et ainsi la densité u renseigne sur la répartition probable des particules. Quand on ne s'intéresse pas uniquement à la répartition, mais aussi à la quantité totale de particules n, on "normalise" u pour qu'elle contienne aussi cette information : $n = \int u(x)\,\mathrm{d}x$ est la quantité totale de particules, et $u(x)/n$ est une densité de probabilité.

Remarque 1.2. *Un autre lien qui unit les problèmes mathématiques traités dans ce manuscrit est que leur traitement fait appel à la notion d'entropie. Cette notion, introduite orginellement dans le cadre de la théorie de l'information (Shannon, 1948) et de la thermodynamique (Clausius, 1865), caractérise les systèmes* irréversibles*. Du point de vue mathématique, cela se traduit par une fonction qui décroit le long du flot de l'équation d'évolution du système considéré, c'est-à-dire une fonction de Lyapunov. En EDP, c'est précisément cette fonction de Lyapunov qu'on appelle* entropie*, et on appelle* dissipation (d'entropie) *l'opposé de sa dérivée en temps, qui est donc une quantité positive. L'intérêt des fonctions de Lyapunov est de fournir des estimations sur les solutions et des informations sur leur comportement en temps long (en particulier, stabilité d'un équilibre). Ce qui fait la spécificité des méthodes d'entropie, c'est l'usage de l'information supplémentaire contenue dans la dissipation d'entropie. Les estimations ainsi obtenues peuvent être utiles pour démontrer la régularité des solutions, ou encore l'existence de solutions. Pour une introduction aux méthodes d'entropie en EDP, on pourra consulter par exemple [80] et [68].*

3. Au Chapitre 2 il n'est pas question de modèle à l'échelle de l'individu, donc on emploiera les termes *macroscopique* et *microscopique* pour désigner le système de réaction-diffusion croisée et le système de réaction-diffusion (plus précis), respectivement.

4. pour simplifier, mais cela peut être par extension un espace généralisé, par exemple l'espace des phases.

Chapitre 2

Introduction à la Partie II : les systèmes de diffusion croisée en Dynamique des populations

Sommaire

2.1 Introduction à la Dynamique des populations

La motivation générale en Dynamique des populations est de comprendre l'évolution de la quantité d'individus d'une certaine (ou de plusieurs) population. On considère une quantité $u = u(t) \geq 0$ qui représente la densité d'individus de la population au temps t, et on veut modéliser son évolution par une équation. Par exemple, si l'on adopte un point de vue déterministe [1] et si l'on prend en compte des temps continus $t \in \mathbb{R}$, on cherchera une équation différentielle, typiquement de la forme [2]

$$\mathrm{d}_t u(t) = f(t, u(t))\, u(t),$$

où $f(t, u(t))$ est le taux de croissance de la population (qui prend en compte natalité, mortalité et migration) au temps t, la fonction $f : \mathbb{R} \times \mathbb{R}_+ \mapsto \mathbb{R}$ étant à déterminer dans la phase de modélisation.

Le modèle le plus simple de ce type, dit modèle de Malthus, suppose que la croissance de la population est proportionnelle à la taille de la population. Autrement dit, le taux de croissance f est une constante. Si l'on note cette constante $r > 0$, le modèle s'écrit

Exemple 2.1 (Modèle de Malthus)**.**

$$\mathrm{d}_t u(t) = ru(t).$$

Ce modèle a tôt fait de montrer ses limites : en effet il implique une croissance exponentielle de la population, et par là ne prend pas en compte la possible saturation de l'environnement (liée à la compétition pour certaines ressources en quantité finie : nourriture, habitat, etc). Pour remédier à ce problème, on considèrera plutôt l'équation logistique :

Exemple 2.2 (Équation logistique)**.**

$$\mathrm{d}_t u(t) = ru(t)\left[1 - \frac{u(t)}{\kappa}\right].$$

Le terme $\kappa > 0$ est une constante strictement positive qui représente la capacité totale de l'environnement. En effet, quand à un temps t la densité de population $u(t)$ est supérieure au seuil κ, on a $\mathrm{d}_t u(t) = ru(t)\left[1 - \frac{u(t)}{\kappa}\right] \leq 0$ et ainsi la population décroit, signe que l'environnement est saturé (surpopulation). En revanche, quand la densité de population est inférieure au seuil κ, on a $\mathrm{d}_t u(t) = ru(t)\left[1 - \frac{u(t)}{\kappa}\right] \geq 0$ et ainsi la population croit. On remarque que dans les deux cas (pour une donnée initiale strictement positive), la densité de population $u(t)$ tend vers la capacité totale de l'environnement κ quand t tend vers l'infini. On remarque aussi que quand la population est peu importante, i.e. $u(t) \sim 0$, on a $\mathrm{d}_t u(t) = ru(t)\left[1 - \frac{u(t)}{\kappa}\right] \sim ru(t)$, et on retrouve le modèle de Malthus. Autrement dit, pour de petites populations on peut négliger l'effet concurrentiel, ce qui semble raisonnable du point de vue de la modélisation.

On peut bien sûr généraliser les modèles précédents en considérant non plus une unique population, mais un système composé de plusieurs populations, qu'on appèlera *système écologique*. Pour un nombre J ($J \in \mathbb{N}$) d'espèces différentes, notant $u_1 = u_1(t)$, ..., $u_J = u_J(t)$ les densités de population respectives de chacune des espèces, on est amené à considérer le système de taille J

$$\begin{cases} \mathrm{d}_t u_1(t) = f_1(t, u_1(t), \ldots, u_J(t))\, u_1(t), \\ \quad\vdots \\ \mathrm{d}_t u_J(t) = f_J(t, u_1(t), \ldots, u_J(t))\, u_J(t), \end{cases}$$

où les taux de croissance $f_i : \mathbb{R} \times \mathbb{R}_+ \mapsto \mathbb{R}$ de chacune des espèces i sont des fonctions à déterminer dans la phase de modélisation. La notion de système (écologique) implique des interactions entres les différentes espèces, ce qui se traduit mathématiquement par un couplage entre les équations du système (mathématique). Ainsi, l'évolution de la densité u_1 de la première espèce (par exemple) dépend aussi des densités des autres populations, ce qui modélise le fait que la présence d'individus des autres espèces a un impact sur la croissance de la première espèce (par exemple à travers la prédation, la compétition, la coopération, la prédation d'un concurrent, la coopération avec un prédateur, etc). Le modèle le plus classique dans ce contexte a été introduit simultanément par A. J. Lotka et V. Volterra en 1925 pour modéliser l'évolution de deux espèces dont l'une subit la prédation de l'autre ; il s'écrit

1. pas de hasard, ou bien un hasard négligé en un sens, par exemple après moyennisation de certaines quantités.
2. En considérant un second membre de cette forme, on suppose que la croissance est nulle quand la population est éteinte : pas de génération spontanée.

Exemple 2.3 (Système de Lotka-Volterra)**.**

$$\begin{cases} \mathrm{d}_t u_1(t) = [r_1 - r_b u_2(t)]\ u_1(t), \\ \mathrm{d}_t u_2(t) = -\ [r_2 - r_d u_1(t)]\ u_2(t), \end{cases}$$

où u_1 est la densité de proies, u_2 la densité de prédateurs, et r_1, r_2, r_b, r_d sont des constantes strictement positives. Le terme r_1 est le taux de croissance intrinsèque de la population de proies : en l'absence de prédateurs, i.e. quand $u_2 = 0$, celle-ci croit exponentiellement. Le terme r_2 est le taux de mortalité de la population de prédateurs : en l'absence de proies, i.e. quand $u_1 = 0$, celle-ci s'éteint. Les termes $-r_b u_2$ et $r_d u_1$ traduisent l'impact de la prédation sur le taux de croissance des proies et des prédateurs respectivement. Cela correspond naturellement à une contribution négative pour les proies, et positive pour les prédateurs. L'impact de la prédation sur la croissance de chacune des deux espèces est supposé proportionnel à la densité de proies et à la densité de prédateurs (produits $u_1 u_2$ dans les deux termes $-r_b u_2 u_1$ et $r_c u_2 u_1$).

Remarque 2.1. *Pour un ensemble assez large de valeurs des paramètres r_1, r_2, r_b, r_d, le système de Lotka-Volterra admet des solutions périodiques à quatre "phases" : au début de la phase 1, il y a peu de prédateurs, et beaucoup de proies donc le nombre de proies augmente, et le nombre de prédateurs aussi ; à partir d'un certain temps le nombre de prédateurs devient si élevé que les proies sont terrassées : le nombre de proies commence à diminuer (phase 2), jusqu'à ce qu'il devienne trop faible pour nourrir les prédateurs (alors en grand nombre) : on entre alors dans la phase 3 où proies et prédateurs diminuent en nombre ; quand le nombre de prédateurs est redevenu suffisamment faible, la population de proies croit de nouveau (phase 4), jusqu'à être suffisamment importante pour que la population de prédateurs croisse à nouveau : on retourne donc à la phase 1. Ce comportement oscillatoire est en quelque sorte la réponse dynamique à l'apparent paradoxe (statique) : "plus il y a de prédateurs, moins il y a de proies, mais moins il y a de proies, moins il y a de prédateurs".*

On peut tout à fait à partir du système de Lotka-Volterra proposer des variantes qui prennent en compte d'autres types d'interaction interspécifique, de la forme

$$\begin{cases} \mathrm{d}_t u_1(t) = [\sigma_1 r_1 + \sigma_b r_b u_2(t)]\ u_1(t), \\ \mathrm{d}_t u_2(t) = [\sigma_2 r_2 + \sigma_d r_d u_1(t)]\ u_2(t), \end{cases}$$

où r_1, r_2, r_b, r_d sont des constantes strictement positives, et où σ_1, σ_2, σ_b, σ_d sont dans $\{-1, 0, 1\}$. Les signes σ_1 et σ_2 renseignent sur le caractère obligatoire (essentiel à la survie) de la relation pour chacune des deux espèces, puisqu'ils indiquent le comportement (croissance, stagnation ou extinction) de chacune des deux espèces en l'absence de l'autre. Les signes σ_b et σ_d renseignent sur la nature bénéfique ou défavorable de la relation interspécifique, ce que l'on peut résumer dans le tableau (non exhaustif) suivant :

effet de l'interaction		pour la deuxième espèce : bénéfique $\sigma_d = +1$	neutre $\sigma_d = 0$	défavorable $\sigma_d = -1$
pour la première espèce :	bénéfique $\sigma_b = +1$	mutualisme	commensalisme	prédation/parasitisme
	neutre $\sigma_b = 0$		neutralisme	amensalisme
	défavorable $\sigma_b = -1$			compétition

Remarque 2.2. *Dans les exemples 2.2 et 2.3, les taux de croissance sont des fonctionnelles linéaires de u ou de u_1, u_2. Autrement dit, on suppose que l'interaction entre individus de la même ou de différentes populations (compétition intraspécifique pour l'exemple 2.2, prédation pour l'exemple 2.3) a un effet proportionnel à la densité de la population avec laquelle il y a interaction. Au début des années 1970, les biologistes F. J. Ayala, M. E. Gilpin et K. E. Justice ont montré dans [22] et [23] qu'il était parfois plus pertinent d'exprimer les taux de croissance avec des fonctionnelles non-linéaires, en prenant l'exemple de deux espèces de drosophiles en compétitions (intra et inter-spécifiques).*

Dans les appliations, il est souvent intéressant de considérer non plus seulement la taille totale d'une population, mais aussi sa répartition dans un environnement donné. C'est la cas par exemple si l'on veut observer spécifiquement des phénomènes de migration, de concentration, etc. On est amené à considérer un domaine Ω de l'espace $\mathbb{R}^m$ (l'environnement), où la dimension m vaut en général [3] 2 ou 3, et la quantité positive $u = u(t, x)$ qui est la valeur au temps t de la densité de population au point x de l'espace. On cherche alors une EDP [4] de la forme

$$\partial_t u(t, x) = \mathfrak{A}(t, x, u(t)),$$

où $\mathfrak{A}$ est un opérateur à déterminer dans la phase de modélisation, qui prend en compte à la fois la croissance et les déplacements de population. Cet opérateur prend comme arguments le temps t et le point x (l'environnement est muable et hétérogène) et la répartition de la population au temps t, $u(t, \cdot)$.

Le modèle de cette forme le plus étudié est le suivant.

Exemple 2.4 (Equation de Fisher-KPP)**.**

$$\partial_t u(t, x) - d\,\Delta_x u(t, x) = r\,u(t, x)\,(1 - u(t, x))\,,$$

Le terme de droite est similaire à celui de l'équation logistique : r est le taux de croissance de la population, et le terme quadratique $-u^2$ traduit un effet de saturation de l'environnement (de capacité totale prise égale à 1). Enfin, le paramètre d est une constante positive qui décrit la capacité des individus à diffuser, c'est-à-dire à se disperser de manière désordonnée dans l'espace.

On remarque pour l'équation de Fisher-KPP homogène (si on ne considère que des solutions indépendantes de x), $u = 0$ est une solution instable, et $u = 1$ est une solution stable. On peut en fait montrer avec la théorie des ondes progressives que pour une donnée initiale raisonnable (en particulier positive, non identiquement nulle sur le domaine mais pouvant être nulle sur une grande partie du domaine), la solution $u(t, x)$ se rapproche en un certain sens de l'état stationnaire stable 1 (sans le dépasser) quand t tend vers l'infini. On interprète ce comportement asymptotique comme le fait que la population colonise tout le territoire jusqu'à saturation.

Remarque 2.3. *L'équation de Fisher-KPP a été introduite en 1930 par R. A. Fisher, en l'occurence pour modéliser la propagation d'un gène A favorable dans une population. Dans ce contexte, la quantité $u(t, x)$ est la proportion d'individus de la population présentant le gène A au temps t et au point x, et satisfait $0 \le u(t, x) \le 1$. La saturation au seuil $u = 1$ s'interprète comme l'impossibilité pour u de dépasser la valeur 1 car c'est par définition une proportion. Le comportement asymptotique décrit précédemment modélise le fait que le gène A favorable se répand dans toute la population (ce qui est conforme à nos attentes du point de vue de la modélisation).*

Dans l'équation de Fisher-KPP, le terme $-d\Delta_x u$ décrit un cas particulier (milieu homogène) de phénomène de diffusion de Fick. La diffusion de Fick modélise un phénomène de migration qui a pour effet une tendance à rendre l'environnement homogène. Elle se décrit plus généralement sous la forme d'une

Exemple 2.5 (Équation de diffusion de Fick)**.**

$$\partial_t u(t, x) - \nabla_x \cdot [d(x)\,\nabla_x u(t, x)] = S(t, x),$$

où ici $u = u(t, x)$ représente la densité d'individus d'une espèce (biologique, chimique, etc) ayant tendance à diffuser, où $d(x) > 0$, le coefficient de diffusion, renseigne sur l'intensité du processus de diffusion, et où $S(t, x)$ représente une source d'individus. Quand le milieu est homogène (du moins en ce qui concerne la diffusion), la fonction $d(x)$ est une constante $d > 0$, on retrouve le terme $-d\Delta_x u$. Ce type de modèle a d'abord été dérivé empiriquement par A. Fick dans le cadre de la diffusion moléculaire. Toujours dans le même cadre, il a ensuite été montré par A. Einstein dans [19] que ce modèle pouvait être obtenu à partir d'un modèle de mouvement Brownien après un passage à la limite qui correspond à un changement d'échelle. En résumé, le résultat est le suivant : si à l'échelle microscopique on suppose que chaque particule (ou individu) se déplace de manière aléatoire en suivant un mouvement Brownien, alors

3. Il est souvent utile de considérer pour nos modèles des dimensions supérieures, voire arbitrairement grandes, dans des contextes où le paramètre x ne représente plus un point de l'espace, mais un autre paramètre (par exemple : trait phénotypique, âge, taille).

4. pour simplifier, mais, comme on le verra par la suite, on peut évidemment comme dans le cas précédent s'intéresser à des systèmes écologiques composés de différentes espèces, pour lesquels on utilisera des systèmes d'EDP.

à l'échelle macroscopique la densité de particules (ou individus) obéit à une équation de diffusion de Fick, où le coefficient de diffusion $d(x)$ est déterminé par les caractéristiques du mouvement microscopique.

Le concept de diffusion de Fick peut se décliner dans de nombreux contextes (par exemple : diffusion moléculaire en Physique-Chimie, mais aussi diffusion de la chaleur en Thermodynamique, propagation d'idées en Sciences humaines, diffusion dans l'espace des traits génotypiques par mutation génétique en Biologie, etc). En Dynamique des populations, on l'emploie pour modéliser à l'échelle de la population le mouvement spontané et aléatoire des individus dans l'espace. Comme on l'a vu avec l'exemple de l'équation de Fisher-KPP, il permet d'observer des phénomènes liés à la migration, comme, pour cet exemple, la colonisation du territoire.

2.2 Diffusion croisée en Dynamique des populations

On s'intéresse à présent à une classe de systèmes de la forme

$$\partial_t U(t,x) - \Delta_x[A(U(t,x))] = F(U(t,x)), \tag{2.1}$$

où $U = (u_1, \dots, u_J)$ est le vecteur composé des densités de population de J espèces distinctes, et A et F sont des fonctions de $\mathbb{R}_+^J$ à J composantes, A prenant des valeurs positives ($A(U) \in \mathbb{R}_+^I$). Le terme $F(U(t,x))$, dit *terme de réaction*[5], renseigne sur la croissance de population des différentes espèces. Comme dans les exemples précédents, on suppose qu'il n'y pas de génération spontanée, et on prend donc F de la forme

$$F(U) = (f_1(U)\, u_1, \dots, f_J(U)\, u_J).$$

Le terme $\Delta_x A(U(t,x))$, dit *terme de diffusion*, renseigne sur les déplacements des individus des différentes espèces.

Quand la différentielle de A, notée $\mathrm{D}A$, est une matrice (de taille J) diagonale, on peut réécrire le système

$$\begin{cases} \partial_t u_1(t,x) - \nabla_x \cdot [d_1(u_1(t,x))\, \nabla_x u_1(t,x)] = f_1(u_1(t,x), \dots, u_J(t,x))\, u_1(t,x), \\ \qquad \vdots \\ \partial_t u_J(t,x) - \nabla_x \cdot [d_J(u_J(t,x))\, \nabla_x u_J(t,x)] = f_J(u_1(t,x), \dots, u_J(t,x))\, u_J(t,x), \end{cases}$$

où on a noté d_i le $i \times i^{\text{ème}}$ terme de $\mathrm{D}A$. On a donc affaire à un système de J équations avec un terme de diffusion de Fick (comme dans l'Exemple 2.5), et le couplage entre les équations se fait uniquement via les termes de réaction. Autrement dit, pour une espèce i donnée, d'une part les individus se déplacent spontanément et aléatoirement avec une intensité $d_i(u_i)$, d'autre part la population croit avec un taux $f_i(U)$ qui dépend de la densité de population des différentes espèces. Cela signifie que la présence d'individus des autres espèces a un effet (seulement) sur la croissance de l'espèce i.

Ici, on s'intéresse justement au cas où la matrice $\mathrm{D}A$ n'est *pas* diagonale. Les termes du système (2.1) provenant des termes non diagonaux de $\mathrm{D}A$ sont appelés termes de *diffusion croisée*[6]. Le couplage entre les équations du système a alors lieu non seulement à travers les termes de réaction, mais aussi à travers les termes de diffusion. Cela signifie que, pour une espèce i, la présence d'individus des autres espèces a un effet non seulement sur la croissance de l'espèce i, mais aussi sur ses déplacements. Par exemple, si l'interaction avec une autre espèce i' est défavorable pour l'espèce i, une stratégie possible pour les individus de l'espèce i est de fuir[7] les individus de la population i'. Le couplage avec $u_{i'}$ dans le terme de diffusion de l'équation d'évolution de u_i permet de rendre compte de ce type de comportement. On présentera justement dans l'exemple suivant, très étudié, un système qui relève de ce cas.

Une des raisons de l'engouement mathématique pour ces types de systèmes est qu'ils présentent parfois des instabilités de Turing[8] avec formation de motifs (ou *patterns*). Ces motifs peuvent par exemple

5. La terminologie vient de la Chimie, où les systèmes de réaction-diffusion ont une place prépondérante. On y rencontre aussi des systèmes de diffusion croisée, voir par exemple [6].

6. Dans la littérature, le terme de *diffusion croisée* est parfois employé pour désigner des systèmes de la forme (plus générale) $\partial_t U - \nabla_x \cdot [B(U)\nabla_x U] = F(U)$, où la matrice B n'est pas diagonale.

7. Pour une interaction bénéfique avec un effet attractif, on regardera plutôt des systèmes de type Keller-Segel (pour le chimiotactisme). Ces systèmes, qui ne sont pas de la forme (2.1) (avec A à valeurs positives), sont aussi des systèmes d'équations d'évolution avec un couplage (en général triangulaire) dans les termes du second ordre qui modélisent le déplacement dans l'espace.

8. phénomène pouvant, dans les cas les plus intéressants, mener à une formation de motifs ; introduit par A. Turing en 1952 dans [51] pour modéliser la morphogénèse.

décrire des phénomènes de ségrégation entre plusieurs espèces en compétition. Il existe une littérature mathématique importante sur la question, qui démontre ces phénomènes (numériquement et/ou analytiquement) pour divers modèles particuliers de Dynamique des populations présentant de la diffusion croisée. Plus précisément, il est (en général) montré que l'instabilité est induite par la diffusion croisée, au sens où le système considéré s'écrit naturellement comme un système de réaction-diffusion classique présentant en plus un terme croisé dans la diffusion, et ce système de réaction-diffusion classique (sans le terme croisé) a un état d'équilibre stable, qui est cependant instable pour le système complet (avec terme de diffusion croisée). Pour ces questions, voir par exemple [4], [37], [32], [9] et les références mentionnées dans ces papiers.

Le système de réaction-diffusion croisée le plus populaire en Dynamique des populations a été introduit en 1979 par N. Shigesada, K. Kawasaki et E. Teramoto ([45]) pour modéliser l'évolution des populations de deux espèces en compétition avec un effet répulsif. Il s'écrit

Exemple 2.6 (Système de Shigesada-Kawasaki-Teramoto (SKT)).

$$\begin{cases} \partial_t u_1 - \Delta_x(d_1\, u_1 + d_\alpha\, u_1^2 + d_\beta\, u_1\, u_2) = u_1\,(r_1 - r_a\, u_1 - r_b\, u_2), \\ \partial_t u_2 - \Delta_x(d_2\, u_2 + d_\gamma\, u_2^2 + d_\delta\, u_1\, u_2) = u_2\,(r_2 - r_c\, u_2 - r_d\, u_1), \end{cases} \tag{2.2}$$

où les termes d_1, d_2, d_α, d_β, d_γ, d_δ, r_1, r_2, r_a, r_b, r_c, r_d, sont des constantes positives. Les quantités positives $u_1 = u_1(t,x)$ et $u_2 = u_2(t,x)$ sont les densités de population des deux espèces en compétition. Les termes de réaction modélisent la croissance des populations. Par analogie avec l'équation de Fisher-KPP, les termes $(r_1 - r_a\, u_1)$ et $(r_2 - r_c\, u_2)$ indiquent pour chacune des deux espèces l'effet néfaste sur le taux de croissance de la présence d'individus de la même espèce (compétition intra spécifique dans un environnement aux ressources limitées). Par analogie avec le système de Lotka-Volterra (généralisé) (2.1), les termes croisés $-r_b\, u_2$ et $-r_d\, u_1$ indiquent pour chacune des deux espèces l'effet néfaste sur le taux de croissance de la présence d'individus de l'autre espèce (compétition interspécifique). Les termes de diffusion modélisent le mouvement des individus. On reconnait des termes de diffusion linéaires $\Delta_x(d_1\, u_1)$ et $\Delta_x(d_2\, u_2)$, qui quantifient, comme dans l'équation de Fisher-KPP, la propension des individus de chacune des deux espèces à se disperser de manière aléatoire. Enfin, les termes produits dans le terme de diffusion : termes d'*auto-diffusion* $\Delta_x(d_\alpha\, u_1^2)$ et $\Delta_x(d_\gamma\, u_2^2)$ d'une part, et termes de diffusion croisée $\Delta_x(d_\beta\, u_1\, u_2)$ et $\Delta_x(d_\delta\, u_1\, u_2)$ d'autre part, modélisent l'effet répulsif entre les individus (respectivement de même espèce et d'espèces différentes), conséquence des compétitions (respectivement intra- et interspécifiques). On pourra interpréter ces termes grâce à la simple décomposition (formelle) suivante, par exemple pour la première équation :

$$\Delta_x\,[u_i\, u_1] = \underbrace{\nabla_x \cdot [u_1 \nabla_x u_i]}_{\text{transport}} + \underbrace{\nabla_x \cdot [u_i \nabla_x u_1]}_{\text{diffusion de Fick}}, \tag{2.3}$$

où $i \in \{1,2\}$. Le premier terme du membre de droite, replacé dans l'équation de u_1, s'interprète comme un terme de transport dans la direction $-\nabla_x u_i$, c'est-à-dire la meilleure direction (du moins localement) pour éviter la présence d'individus concurrents de la population i. Le second terme ci-dessus s'interprète comme une diffusion de Fick d'intensité u_i, et modélise donc une propension à se disperser de manière aléatoire d'autant plus grande que la présence d'individus de l'espèce i concurrente est forte. En résumé, les deux effets parallèles, d'une part fuite dans la direction optimale pour éviter les concurrents, d'autre part fuite dans des directions aléatoires liée proportionnellement à la présence des concurrents, traduisent un stratégie des individus de l'espèce 1 d'évitement des individus de l'espèce i (ou autrement dit, un effet répulsif des individus de l'espèce i sur les individus de l'espèce 1).

Le calcul formel (2.3), bien qu'utile pour interpréter en terme d'effet répulsif le système SKT, ne se veut pas une justification de ce modèle. En effet, si l'on veut modéliser un système écologique de deux espèces en compétition où sont présents les deux types d'effet répulsif présentés, on pourra considérer n'importe quelle combinaison des deux termes (terme de transport et terme de diffusion)

$$\lambda\, \nabla_x \cdot [u_1 \nabla_x u_i] + \mu\, \nabla_x \cdot [u_i \nabla_x u_1]\,,$$

pour λ, $\mu > 0$. Cette interprétation ne permet donc pas de justifier le choix du terme $\Delta_x[u_i\, u_1]$ dans le modèle SKT, qui revient à choisir $\lambda = \mu$ dans l'expression ci-dessus.

Une justification – d'un tout autre type – a été proposée par M. Iida, M. Mimura, et H. Ninomiya en 2006 dans [27]. Ils ont dérivé le système SKT (dans un cas particulier explicité par la suite) à partir d'un autre système qui modélise le même système écologique à une autre échelle. En partant du système qu'ils proposent et en passant à la limite correspondant au changement d'échelle approprié, ils retrouvent asymptotiquement le (cas particulier considéré du) système SKT (du moins, au niveau de calculs formels). Plus précisément, ils s'intéressent au cas le plus simple présentant de la diffusion croisée, à savoir le cas où $d_\delta = 0$ (cas dit *triangulaire* [9]), et où $d_\alpha = d_\delta = 0$. Au niveau de la modélisation, cela signifie que la compétition se manifeste par un effet répulsif uniquement de la deuxième espèce sur la première espèce. On a alors affaire au système suivant

$$\begin{cases} \partial_t u_1 - \Delta_x(d_1\, u_1 + d_\beta\, u_1\, u_2) = u_1\,(r_1 - r_a\, u_1 - r_b\, u_2), \\ \qquad\qquad \partial_t u_2 - d_2\,\Delta_x u_2 = u_2\,(r_2 - r_c\, u_2 - r_d\, u_1). \end{cases} \tag{2.4}$$

Nous décrivons à présent le système proposé par M. Iida, M. Mimura, et H. Ninomiya. Supposons que les individus de la première espèce (ceux qui ont tendance à fuir les individus de la deuxième espèce), soient en fait stressés en un sens par la présence des individus de la deuxième espèce, en ceci que leur tendance à se disperser augmente. On modélise cela par l'existence de deux états possibles pour l'espèce 1 : l'état A, qu'on appèlera état *au repos*, et l'état B, qu'on appèlera état *stressé*. Dans l'état A, les individus se dispersent peu ; dans l'état B, les individus se dispersent plus. Cet état de stress étant activé par la présence des individus de la deuxième espèce, le passage d'un état à l'autre dépend (uniquement) de la densité de population de la deuxième espèce. Enfin, on suppose que cet état de stress n'affecte pas la capacité des individus à se reproduire ou leur risque de décès : le taux de croissance de chacun des états est donc identique au taux de croissance de la population totale. Si l'on note u_A, u_B et u_2 les densités respectives des populations de l'espèce 1 dans l'état A, l'espèce 1 dans l'état B, et la deuxième espèce, on est amenés à considérer le système

$$\begin{cases} \partial_t u_A - d_A\,\Delta_x u_A = u_A\,(r_1 - r_a\,(u_A + u_B) - r_b\, u_2) + [k(u_2)u_B - h(u_2)u_A], \\ \partial_t u_B - d_B\,\Delta_x u_B = u_B\,(r_1 - r_a\,(u_A + u_B) - r_b\, u_2) - [k(u_2)u_B - h(u_2)u_A], \\ \;\partial_t u_2 - d_2\,\Delta_x u_2 = u_2\,(r_2 - r_c\, u_2 - r_d\,(u_A + u_B)). \end{cases} \tag{2.5}$$

Les termes d_A et d_B, qui quantifient la diffusion respectivement des états A et B, satisfont naturellement $0 < d_A < d_B$ (par définition des deux états). Conformément à ce qui a été décrit précédemment, les taux de croissance des états A et B sont formellement identiques à celui de la première espèce dans le modèle (2.4), à ceci près que la quantité u_1 a naturellement été remplacée par la quantité $u_A + u_B$ (pour chacun des deux modèles, il s'agit de la quantité totale de population de la première espèce). Le terme $[k(u_2)u_B - h(u_2)u_A]$ est le bilan des changements d'états : $h(u_2)$ et $k(u_2)$ sont respectivement les taux de passage de l'état A à l'état B et de l'état B à l'état A. Ces taux de passage sont des fonctions de u_2. Enfin, l'équation pour la densité u_2 de la deuxième espèce est identique à celle du modèle (2.4) (au changement de u_1 en $u_A + u_B$ près).

Analysons les unités des grandeurs de ce modèle : les quantités d_A, d_B, d_2 sont en unité d'aire par unité de temps (cela crorrespond à une vitesse de colonisation d'une aire) ; les quantités r_1 et r_2 sont en unité inverse d'unité de temps (vitesse de croissance) ; enfin $h(u_A)$ et $k(u_B)$ sont en unité inverse d'unité de temps (vitesse de changement d'état). Il semble raisonnable de supposer que les échelles de temps des trois phénomènes – dispersion, croissance, changement d'état – ne sont pas les mêmes. Supposons que les changements d'état s'effectuent dans un temps très court par rapport aux deux autres phénomènes. Les vitesses de changement d'état sont donc très grandes par rapport aux autres types de vitesse. Si l'on écrit le système en considérant comme unité de temps une échelle de temps caractéristique pour la croissance et la diffusion [10], les quantités d_A, d_B, d_2 et r_1, r_2 sont alors de taille raisonnable (ni grandes ni petites), alors que les quantités $h(u_2)$ et $k(u_2)$ sont très grandes. On les réécrit donc

$$h(u_2) = \frac{\tilde{h}(u_2)}{\epsilon}, \qquad k(u_2) = \frac{\tilde{k}(u_2)}{\epsilon}, \tag{2.6}$$

où $\tilde{h}(u_2)$ et $\tilde{k}(u_2)$ sont de taille raisonnable, et $\epsilon > 0$ est un petit paramètre qui quantifie le rapport d'échelle de temps entre le processus de changement d'état et les processus de diffusion et croissance.

9. Avec les notations de (2.1) la matrice DA est alors... triangulaire.

10. Plus précisément, on adopte une échelle de temps raisonnable pour observer la croissance, puis on choisit une échelle d'espace telle que les échelles d'espace et de temps adoptées soient raisonnables pour observer la diffusion.

Avec ces notations, on peut réécrire le système

$$\begin{cases} \partial_t u_A^\epsilon - d_A\,\Delta_x u_A^\epsilon = u_A^\epsilon\,(r_1 - r_a\,(u_A^\epsilon + u_B^\epsilon) - r_b\,u_2^\epsilon) + \dfrac{1}{\epsilon}[\tilde{k}(u_2^\epsilon)u_B^\epsilon - \tilde{h}(u_2^\epsilon)u_A^\epsilon], \\ \partial_t u_B^\epsilon - d_B\,\Delta_x u_B^\epsilon = u_B^\epsilon\,(r_1 - r_a\,(u_A^\epsilon + u_B^\epsilon) - r_b\,u_2^\epsilon) - \dfrac{1}{\epsilon}[\tilde{k}(u_2^\epsilon)u_B^\epsilon - \tilde{h}(u_2^\epsilon)u_A^\epsilon], \\ \partial_t u_2^\epsilon - d_2\,\Delta_x u_2^\epsilon = u_2^\epsilon\,(r_2 - r_c\,u_2^\epsilon - r_d\,(u_A^\epsilon + u_B^\epsilon)), \end{cases} \tag{2.7}$$

où on a explicité par un exposant la dépendance en le paramètre ϵ. Ce paramètre étant très petit, on voudrait le prendre nul : cela revient à supposer que le temps caractéristique des changements d'état est nul, autrement dit, les changements d'état sont instantanés. On s'intéresse donc à la limite du système quand ϵ tend vers zéro.

Asymptotique formelle quand $\epsilon \longrightarrow 0$. Nous présentons ici uniquement des calculs formels. On suppose que $(u_A^\epsilon, u_B^\epsilon, u_2^\epsilon)$ converge vers une limite (u_A, u_B, u_2) quand $\epsilon \longrightarrow 0$ et on se donne comme objectif de caractériser la limte (u_A, u_B, u_2) en explicitant le système d'EDP qu'elle vérifie. En multipliant par ϵ la première équation de (2.7), on peut directement passer à la limite $\epsilon \longrightarrow 0$ et obtenir

$$[\tilde{k}(u_2)u_B - \tilde{h}(u_2)u_A] = 0,$$

ce que l'on réécrit

$$\frac{u_A}{u_A + u_B} = \frac{\tilde{k}(u_2)}{\tilde{h}(u_2) + \tilde{k}(u_2)}, \qquad \frac{u_B}{u_A + u_B} = \frac{\tilde{h}(u_2)}{\tilde{h}(u_2) + \tilde{k}(u_2)}. \tag{2.8}$$

Cette réécriture apporte l'information suivante : à la limite $\epsilon = 0$, les taux d'individus stressés et au repos au sein de la première espèce sont des fonctions (explicites) de la densité de population de la deuxième espèce. A présent, si nous sommons les deux premières équations de (2.7), l'équation obtenue est formellement indépendante de ϵ : on peut donc prendre $\epsilon = 0$ pour obtenir

$$\partial_t(u_A + u_B) - \Delta_x(d_A u_A + d_B u_B) = (u_A + u_B)\,(r_1 - r_a\,(u_A + u_B) - r_b\,u_2).$$

Avec l'aide des taux d'individus stressés/au repos explicités précedemment, on peut réécrire le deuxième terme

$$\begin{aligned} \Delta_x(d_A u_A + d_B u_B) &= \Delta_x\left[\left(d_A \frac{u_A}{u_A + u_B} + d_B \frac{u_B}{u_A + u_B}\right)(u_A + u_B)\right] \\ &= \Delta_x\left[\left(d_A \frac{\tilde{k}(u_2)}{\tilde{h}(u_2) + \tilde{k}(u_2)} + d_B \frac{\tilde{h}(u_2)}{\tilde{h}(u_2) + \tilde{k}(u_2)}\right)(u_A + u_B)\right]. \end{aligned}$$

Enfin, on peut passer à la limite formellement dans la troisième équation de (2.7). On obtient finalement le système

$$\begin{cases} \partial_t u_1 - \Delta_x\left[\left(\dfrac{d_A\tilde{k}(u_2) + d_B\tilde{h}(u_2)}{\tilde{h}(u_2) + \tilde{k}(u_2)}\right)u_1\right] = u_1\,(r_1 - r_a\,u_1 - r_b\,u_2), \\ \partial_t u_2 - d_2\,\Delta_x u_2 = u_2\,(r_2 - r_c\,u_2 - r_d\,u_1), \end{cases} \tag{2.9}$$

où l'on a naturellement noté u_1 la densité de population de la première espèce, $u_1 = u_A + u_B$ (l'équation (2.8) permet de retrouver les quantités u_A, u_B). Pour un choix approprié des paramètres d_A, d_B et des fonctions $\tilde{h}$ et $\tilde{k}$, par exemple

$$d_A := d_1, \qquad d_B := d_1 + d_\beta \overline{u}, \qquad \tilde{h}(v) := d_\beta v, \qquad \tilde{k}(v) := d_\beta(\overline{u} - v),$$

où on a noté $\overline{u}$ une borne supérieure [11] de la densité u_2, on retrouve exactement le système SKT triangulaire (2.4). On a ainsi dérivé le modèle (2.4) à partir du modèle (2.5).

Remarque 2.4. *Pour les questions de modélisation sur le système SKT, voir [45] et [41]. Voir aussi [20] et [29] pour deux approches probabilistes.*

11. Ici, on suppose que cette quantité est bornée. On verra par la suite qu'un principe du maximum permet de le vérifier dans un cadre rigoureux.

Dans la suite, on s'intéresse à une version généralisée du système SKT. Dans le système SKT, les taux de croissance et les taux de diffusion (théoriques) sont exprimés par des fonctions linéaires de u_1 et u_2. En s'inspirant des idées développées par les biologistes M. E. Gilpin et F. J. Ayala (dans le contexte beaucoup plus simple mathématiquement du système de Lotka-Volterra, voir Remarque 2.2), on propose de remplacer ces fonctions linéaires par des fonctions plus générales de u_1 et u_2, plus précisément sous la forme

Exemple 2.7 (Système SKT généralisé).

$$\begin{cases} \partial_t u_1 - \Delta_x \left[(d_1 + d_\alpha\, u_1^\alpha + d_\beta\, u_2^\beta)\, u_1\right] = u_1\,(r_1 - r_a\, u_1^a - r_b\, u_2^b), \\ \partial_t u_2 - \Delta_x \left[\left(d_2 + d_\gamma\, u_2^\gamma + d_\delta\, u_1^\delta\right)\, u_2\right] = u_2\,(r_2 - r_c\, u_2^c - r_d\, u_1^d), \end{cases} \tag{2.10}$$

où les nouveaux paramètres α, β, γ, δ et a, b, c, d sont des constantes positives. Le choix d'utiliser des fonctions puissance se justifie par le souci d'éclaircir la présentation tout en conservant un large évantail de comportements possibles [12]. Ces puissances sont choisies positives car il est raisonnable de supposer que les effets des compétitions sont plus forts quand la présence des compétiteurs est accrue, et doivent donc être modélisés par des fonctions croissantes des densités de compétiteurs.

Dorénavant, tous les systèmes que nous considérerons serons de la forme (2.10), les constantes étant toutes prises positives, certaines pouvant être nulles, mais pas les constantes d_1 et d_2 qui seront toujours strictement positives [13]. On considèrera ce système dans un domaine borné, noté Ω, de $\mathbb{R}^m$ (l'environnement) et on ajoutera de plus les conditions aux bords de Neumann homogènes

$$\nabla_x u_1(t,x)\cdot n(x) = \nabla_x u_2(t,x)\cdot n(x) = 0 \quad \text{pour } (t,x) \in \mathbb{R}_+ \times \partial\Omega, \tag{2.11}$$

où on a noté $n(x)$ la normale unitaire extérieure au bord $\partial\Omega$ au point x. Cette condition traduit le fait que la population est confinée dans l'environnement.

2.3 Contexte mathématique

Comme mentionné précedemment, il existe une importante littérature traitant du comportement asymptotique et des solutions stationnaires (d'un point de vue numérique et/ou analytique) des systèmes de la forme (2.7), avec un intérêt particulier pour la formation de motifs. On renvoie par exemple à [4] et aux références citées.

Cependant, une question aussi fondamentale que l'existence de solutions globales pour ces systèmes n'est pas encore résolue. Une des causes de la difficulté de cette question est le couplage fort (c'est-à-dire au travers de termes d'ordre deux au regard du nombre de dérivées) entre les deux équations. En conséquence, il n'existe en général pas de principe du maximum pour ces systèmes.

Il existe bien une théorie d'existence locale (en temps) de solutions pour une gamme de systèmes incluant (2.20). Cette théorie a été développée par H. Amann dans la série de papiers [1], [2], [3]. Il y démontre (notamment) l'existence locale (en temps) de solutions fortes dans un certain espace de Sobolev ($\mathrm{W}^{1,p}$), et propose de plus un critère de prolongement de ces solutions fortes.

Pour ce qui est des solutions globales, on trouve dans la littérature des résultats d'existence uniquement dans des cas particuliers. La plupart des résultats traitent spécifiquement du système SKT original (2.2) et supposent des contraintes supplémentaires, généralement sur la dimension d'espace m ou sur la taille de la diffusion croisée (en des sens variés, mais qui peuvent typiquement revenir à supposer que les paramètres en facteur des termes de diffusions croisées d_β et d_δ sont plus petits qu'une certaine constante qui dépend d'autres données du problème - paramètres, domaine, etc). On renvoie aux introductions des Chapitres 4 et 5 pour une bibliographie détaillée (pour chacun des cas spécifiques triangulaire et non-triangulaire respectivement).

Les résultats présentés dans ce manuscrit reposent essentiellement sur des méthodes d'entropie et de dualité. Dans le cas non triangulaire $\beta\delta > 0$ (le cas triangulaire étant en un sens un peu plus simple car une des deux équations du système dispose alors d'un principe du maximum), L. Chen et A. Jüngel ont les premiers repéré une fonctionnelle de type entropique dans [8], en l'occurrence pour le système original (2.20). Cette méthode a été élargie au système SKT généralisé (sous certaines hypothèses sur les paramètres) par L. Desvillettes, Th. Lepoutre et A. Moussa dans [15]. Ici, on propose une analyse poussée

12. On verra que la plupart des résultats mathématiques pour ces systèmes présentés dans ce manuscrit sont en fait valables pour des fonctions plus générales, voir par exemple la Remarque 2.9.

13. C'est une condition d'ellipticité.

des conditions (c'est-à-dire, les hypothèses sur les paramètres) permettant l'existence d'une fonctionnelle de type entropique pour le système SKT généralisé. Grâce à cette analyse, on obtient des estimations d'entropie sous des conditions plus générales. Cette analyse est menée en détail au Chapitre 5. Les méthodes de dualité sont introduites dès à présent, dans la Section 2.4.

2.4 Lemme de dualité

On présente ici un outil mathématique primordial pour notre étude. Cet outil, attribué à M. Pierre, et souvent dénommé dans la littérature spécialisée *Lemme de dualité*, a été introduit dans [43] dans le cadre de systèmes de réaction-diffusion (voir aussi [42, 14]). Il s'est avéré par la suite d'une utilité cruciale dans le cadre des systèmes de diffusion croisée (voir par exemple [4, 15]).

Ce lemme concerne les équations de la forme

$$\begin{cases} \partial_t u - \Delta_x(Mu) = R(u) \text{ dans } [0,T]\times\Omega, \\ \nabla_x(Mu)\cdot n = 0 \text{ sur } [0,T]\times\partial\Omega, \end{cases} \tag{2.12}$$

où M est une fonction à valeurs positives. Il permet d'obtenir, (sous certaines conditions supplémentaires raisonnables sur M et R) pour toute solution positive u une borne de la forme

$$\left\|Mu^2\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\,[1+\|M\|_{\mathrm{L}^1([0,T]\times\Omega)}], \tag{2.13}$$

où C_T est une constante positive qui dépend uniquement du temps T et de données (paramètres et données initiales). Revenons à nos systèmes de la forme (2.10)–(2.11) et expliquons comment ce lemme peut être utile das notre cas. Les équations de u_1 et u_2 sont toutes deux de la forme précédente, avec (par exemple pour u_1) $M = M_1 := (d_1 + d_\alpha u_1^\alpha + d_\beta u_2^\beta) \ge 0$. Le Lemme de dualité fournit alors l'estimation *a priori* suivante

$$\left\|(d_1 + d_\alpha u_1^\alpha + d_\beta u_2^\beta)u_1^2\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\left[1+\left\|d_1 + d_\alpha u_1^\alpha + d_\beta u_2^\beta\right\|_{\mathrm{L}^1([0,T]\times\Omega)}\right],$$

d'où en particulier

$$\left\|u_1^{2+\alpha}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\left[1+\left\|u_1^\alpha + u_2^\beta\right\|_{\mathrm{L}^1([0,T]\times\Omega)}\right],$$

et en utilisant l'inégalité élémentaire (pour tout $\epsilon > 0$ et $u > 0$) $u^\alpha \le \epsilon u^{2+\alpha} + \frac{1}{\epsilon^{\alpha/2}}C(\alpha)$ et en prenant $\epsilon > 0$ suffisamment petit,

$$\left\|u_1^{2+\alpha}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\left[1+\left\|u_2^\beta\right\|_{\mathrm{L}^1([0,T]\times\Omega)}\right].$$

De même, pour u_2, on obtient l'estimation analogue

$$\left\|u_2^{2+\gamma}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\left[1+\left\|u_1^\delta\right\|_{\mathrm{L}^1([0,T]\times\Omega)}\right],$$

et donc en les additionnant on a finalement l'estimation

$$\left\|u_1^{2+\alpha}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} + \left\|u_2^{2+\gamma}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T\left[1+\left\|u_1^\delta\right\|_{\mathrm{L}^1([0,T]\times\Omega)} + \left\|u_2^\beta\right\|_{\mathrm{L}^1([0,T]\times\Omega)}\right].$$

On constate alors que pour un choix adapté des paramètres α, β, γ, δ, par exemple $\delta < 2+\alpha$ et $\beta < 2+\gamma$, on peut clore les deux estimations ci-dessus, et conclure l'estimation *a priori*

$$\left\|u_1^{2+\alpha}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T, \qquad \left\|u_2^{2+\gamma}\right\|_{\mathrm{L}^1([0,T]\times\Omega)} \le C_T.$$

Ces estimations permettent de prouver la non concentration des termes non-linéaires du système (2.10) (diffusion et réaction), sous des hypothèses supplémentaires sur les paramètres. Notons que ces estimations sont les seules informations dont nous disposons en général sur l'intégrabilité de u_1 et u_2 - mis à part le contrôle des masses $\sup_t \int_\Omega u_i \le C_T$ - et s'avèrent donc cruciales pour éviter la concentration.

On présente la version suivante du Lemme de dualité.

Lemme 2.1 (Lemme de dualité)**.** *Soit $T > 0$, Ω un domaine borné régulier de $\mathbb{R}^m$ ($m \geq 1$) et $u = u(t, x)$ une fonction régulière ($\mathscr{C}^2$) sur $[0, T] \times \Omega$, à valeurs positives, et vérifiant*

$$\begin{cases} \partial_t u - \Delta_x(Mu) \leq K \text{ dans } [0, T] \times \Omega, \\ \nabla_x(Mu) \cdot n = 0 \text{ sur } [0, T] \times \partial\Omega, \end{cases} \tag{2.14}$$

où $M = M(t, x)$ est une fonction régulière ($\mathscr{C}^1$) et à valeurs strictement positives sur $[0, T] \times \overline{\Omega}$, K est une constante positive, et $n = n(x)$ est la normale unitaire extérieure au bord $\partial\Omega$ au point x.

Alors u satisfait l'estimation

$$\left\| Mu^2 \right\|_{\mathrm{L}^1([0,T]\times\Omega)} \leq C(\Omega) \left\| u(0, .) \right\|_{\mathrm{L}^2(\Omega)} + 2[< u(0, .) > +KT] \left\| M \right\|_{\mathrm{L}^1([0,T]\times\Omega)} ,$$

où on a noté $C(\Omega) > 0$ la constante apparaissant dans l'inégalité de Poincaré-Wirtinger et $< \cdot >= |\Omega|^{-1} \int_\Omega \cdot$ l'opérateur moyenne sur Ω.

Démonstration. La preuve repose sur l'étude du problème adjoint

$$\begin{cases} \partial_t v + M\Delta_x v = -F \text{ dans } [0, T] \times \Omega, \\ \nabla_x v \cdot n = 0 \text{ sur } [0, T] \times \partial\Omega, \\ v(T, x) = 0 \text{ dans } [0, T] \times \Omega, \end{cases} \tag{2.15}$$

pour F une fonction régulière sur $[0, T] \times \overline{\Omega}$ à valeurs positives. Par des résultats classiques de la Théorie des équations linéaires paraboliques, ce problème adjoint possède une solution classique v à valeurs positives. Posons $u^0 = u(0, \cdot)$ et $v^0 = v(0, \cdot)$. La solution v du problème adjoint satisfait les estimations

$$\left\| \nabla_x v^0 \right\|_{\mathrm{L}^2(\Omega)} \leq \left\| \frac{F}{\sqrt{M}} \right\|_{\mathrm{L}^2([0,T]\times\Omega)} , \tag{2.16}$$

$$\left\| \sqrt{M} \Delta_x v \right\|_{\mathrm{L}^2([0,T]\times\Omega)} \leq \left\| \frac{F}{\sqrt{M}} \right\|_{\mathrm{L}^2([0,T]\times\Omega)} . \tag{2.17}$$

En effet, en multipliant l'équation (2.15) par $\Delta_x v$ puis en intégrant sur Ω en prenant en compte les conditions au bord pour v, nous obtenons

$$\begin{aligned} -\frac{1}{2} d_t \int_\Omega |\nabla_x v|^2 + \int_\Omega M(\Delta_x v)^2 &= -\int_\Omega F \Delta_x v \\ &\leq \int_\Omega \left(\frac{F^2}{2M} + \frac{M}{2} (\Delta_x v)^2 \right), \end{aligned}$$

où nous avons utilisé l'inégalité élémentaire $2\,ab \leq a^2 + b^2$ (pour tous a, $b \in \mathbb{R}$). Intégrons en temps, et utilisons à nouveau la condition $v(T, \cdot) = 0$ pour obtenir

$$\int_\Omega \left| \nabla_x v^0 \right|^2 + \int_0^T \int_\Omega M(\Delta_x v)^2 \leq \int_0^T \int_\Omega \frac{F^2}{M},$$

d'où (2.16) et (2.17).

Calculons alors

$$d_t \int_\Omega uv = \int_\Omega \partial_t u\, v + \int_\Omega u\, \partial_t v \leq \int_\Omega Kv - Fu,$$

qui après intégration en temps devient

$$\int_\Omega u(T, \cdot)\, v(T, \cdot) - \int_\Omega u^0 v^0 \leq K \int_0^T \int_\Omega v - \int_0^T \int_\Omega Fu,$$

que l'on réécrit en utilisant la condition sur v au temps T dans (2.15)

$$\int_0^T \int_\Omega Fu \leq K \int_0^T \int_\Omega v + \int_\Omega u^0 v^0. \tag{2.18}$$

Le premier membre se contrôle en écrivant $v(t) = \int_T^t \partial_t v$, d'où

$$\int_0^T \int_\Omega v \leq T \, \|\partial_t v\|_{\mathrm{L}^1([0,T]\times\Omega)}$$
$$\leq T \left\|\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \left\|\partial_t v/\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \quad \text{par l'inégalité de Cauchy-Schwarz.}$$

Or, en réécrivant l'équation satisfaite par v

$$\partial_t v/\sqrt{M} = -\sqrt{M}\Delta_x v - \frac{F}{\sqrt{M}},$$

on en déduit

$$\left\|\partial_t v/\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \leq \left\|\sqrt{M}\Delta_x v\right\|_{\mathrm{L}^2([0,T]\times\Omega)} + \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}$$
$$\leq 2\left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \quad \text{grâce à (2.17),}$$

et donc

$$\int_0^T \int_\Omega v \leq 2T \left\|\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}.$$

Il reste encore à estimer dans (2.18) le terme $\int_\Omega u^0 v^0$. Revenons à l'équation (2.15) pour écrire après intégration sur $[0,T]\times\Omega$

$$\int_\Omega v^0 = \int_0^T \int_\Omega (M\Delta_x v + F) \leq \int_0^T \int_\Omega \sqrt{M}\left(\sqrt{M}\,|\Delta_x v| + \frac{F}{\sqrt{M}}\right),$$

qui donne grâce à l'inégalité de Cauchy-Schwarz et à (2.17)

$$\int_\Omega v^0 \leq 2\left\|\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}. \tag{2.19}$$

Enfin, nous obtenons en utilisant l'inégalité de Poincaré-Wirtinger, (2.19) puis (2.16),

$$\int_\Omega u^0 v^0 = \int_\Omega u^0\left(v^0 - < v^0 >\right) + \int_\Omega < u^0 > v^0$$
$$\leq C(\Omega)\left\|u^0\right\|_{\mathrm{L}^2(\Omega)} \left\|\nabla_x v^0\right\|_{\mathrm{L}^2(\Omega)} + 2 < u^0 > \left\|\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}$$
$$\leq C(\Omega)\left\|u^0\right\|_{\mathrm{L}^2(\Omega)} \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} + 2 < u^0 > \left\|\sqrt{M}\right\|_{\mathrm{L}^2([0,T]\times\Omega)} \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}.$$

Revenant alors à (2.18), nous pouvons conclure que

$$\int_0^T \int_\Omega Fu = \int_0^T \int_\Omega \frac{F}{\sqrt{M}}\sqrt{M}u$$
$$\leq \left[C(\Omega)\left\|u^0\right\|_{\mathrm{L}^2(\Omega)} + 2[< u^0 > + KT]\,\|M\|_{\mathrm{L}^1([0,T]\times\Omega)}\right] \left\|\frac{F}{\sqrt{M}}\right\|_{\mathrm{L}^2([0,T]\times\Omega)}.$$

On a obtenu l'inégalité ci-dessus pour une fonction F régulière et positive quelconque. Par un argument de densité d'une part, et en constatant que u est positive d'autre part, on voit que cette inégalité est vérifiée pour toute fonction F telle que $F/\sqrt{M} \in \mathrm{L}^2([0,T]\times\Omega)$ (sans hypothèse sur le signe de F). Par dualité, cela revient à l'estimation cherchée. □

Remarque 2.5. *Dans les hypothèses du lemme, on peut autoriser le second membre de l'équation de u à être non borné, tant qu'il croît au plus linéairement en u. Avec cette hypothèse, on obtient alors une borne pour Mu^2 dans $\mathrm{L}^1([0,T]\times\Omega)$ avec croissance exponentielle en temps T.*

Remarque 2.6. *Quand M est supposée appartenir à $\mathrm{L}^\infty([0,T]\times\Omega)$ avec $0 < m_0 \le M(t,x) \le m_1$ pour tous $(t,x)\in[0,T]\times\Omega$, on déduit de ce lemme l'estimation suivante dans $\mathrm{L}^2([0,T]\times\Omega)$*

$$\|u\|_{\mathrm{L}^2([0,T]\times\Omega)} \le C_T(\Omega, m_0, m_1)\left[\|u(0,\cdot)\|_{\mathrm{L}^2(\Omega)} + K\right],$$

où la constante $C_T(\Omega,m_0,m_1)$ ne dépend que du domaine Ω, du temps T et des paramètres m_0, m_1. Dans ce cadre, un résultat perturbatif permet d'obtenir une estimation similaire dans $\mathrm{L}^{2+\eta}([0,T]\times\Omega)$ pour $\eta > 0$ suffisamment petit (dépendant uniquement de Ω, m_0 et m_1). Cette version dite "précisée" du lemme de dualité a été introduite par J. A. Cañizo, L. Desvillettes et K. Fellner dans [7] (dans le cadre de systèmes de réaction-diffusion provenant de la Chimie). Elle s'avère cruciale pour prouver la non concentration des termes de réaction quand ceux-ci s'expriment comme des fonctions quadratiques des inconnues. Dans notre étude, on l'utilisera pour traiter le système SKT triangulaire, par exemple (2.4) *: un principe du maximum permet d'obtenir une borne L^∞ pour u_2, ce qui permet d'appliquer le lemme de dualité précisé à l'équation de u_1 et ainsi obtenir un contrôle satisfaisant pour les termes de réaction.*

Remarque 2.7. *Une autre démonstration du Lemme 2.1 est possible, qui consiste à intégrer en temps l'équation de u, puis à multiplier le résultat par la quantité Mu, faisant apparaître dans le premier terme la quantité Mu^2. On pourra par exemple trouver dans le Chapitre 5 une version utilisant cette démonstration (dans un contexte semi-discret en temps, mais la preuve est facilement adaptable au contexte continu). Notons qu'il ne semble pas évident d'obtenir une version précisée avec cette technique de preuve.*

2.5 Notations, notions de solutions

Rappelons qu'on considère le système SKT généralisé avec conditions de Neumann homogènes au bord, qu'on munit de plus de données initiales $u_{1,in}$ et $u_{2,in}$ à valeurs positives :

$$\begin{cases} \partial_t u_1 - \Delta_x\left[(d_1 + d_\alpha\, u_1^\alpha + d_\beta\, u_2^\beta)\, u_1\right] = u_1\,(r_1 - r_a\, u_1^a - r_b\, u_2^b), & \text{dans } \mathbb{R}_+\times\Omega,\\ \partial_t u_2 - \Delta_x\left[(d_2 + d_\gamma\, u_2^\gamma + d_\delta\, u_1^\delta)\ u_2\right] = u_2\,(r_2 - r_c\, u_2^c - r_d\, u_1^d), & \text{dans } \mathbb{R}_+\times\Omega,\\ \nabla_x u_1\cdot n(x) = \nabla_x u_2\cdot n(x) = 0, & \text{sur } \mathbb{R}_+\times\partial\Omega,\\ u_1(0,\cdot) = u_{1,in}\ge 0, \quad u_2(0,\cdot) = u_{2,in}\ge 0, & \text{dans } \Omega. \end{cases} \tag{2.20}$$

Par commodité, on appèle D l'ensemble des paramètres du système,

$$\mathrm{D} := \{d_1, d_2, d_\alpha, d_\beta, d_\gamma, d_\delta, r_1, r_2, r_a, r_b, r_c, r_d, a, b, c, d, \alpha, \beta, \gamma, \delta\} \in (\mathbb{R}_+^*)^{16}\times\mathbb{R}_+^4. \tag{2.21}$$

Espaces fonctionnels. Rappelons les notations suivantes, pour Q un domaine régulier de $\mathbb{R}^m$ ou $\mathbb{R}^{m+1}$, et pour tout $1\le p<\infty$, tout $1\le q\le\infty$ et tout $k\in\mathbb{N}^*$,

$$\mathrm{L}^p(Q) = \{u :\ \int_Q |u|^p < \infty\}, \qquad \mathrm{L}^\infty(Q) = \{u :\ \sup_Q |u| < \infty\},$$
$$\mathrm{W}^{k,q}(Q) = \{u :\ u\in\mathrm{L}^q(Q), \nabla u\in\mathrm{L}^q(Q), \dots, \nabla^k u\in\mathrm{L}^q(Q)\}, \qquad \mathrm{H}^k(Q) = \mathrm{W}^{k,2}(Q),$$

où ∇ est à entendre au sens de la dérivation au sens des distributions, et selon la variable dans Q.

Pour Ω un domaine régulier et borné de $\mathbb{R}^m$, on note

$$\mathrm{L}^q_{\mathrm{loc}}(\mathbb{R}_+\times\overline{\Omega}) = \{u : \text{pour tout } T>0,\ u_{|[0,T]\times\Omega}\in\mathrm{L}^q([0,T]\times\Omega)\},$$

avec des notations analogues pour $\mathrm{W}^{k,q}_{\mathrm{loc}}(\mathbb{R}_+\times\overline{\Omega})$ et $\mathrm{H}^k_{\mathrm{loc}}(\mathbb{R}_+\times\overline{\Omega})$. Enfin, on note $\mathrm{H}^{-1}_m(\Omega)$ le dual de l'espace des fonctions de $\mathrm{H}^1(\Omega)$ ayant une valeur moyenne nulle sur Ω.

Notions de solutions. On décrit ci-dessous les différentes notions de solutions qui seront employées.

Définition 2.1 (Solution très faible)**.** *Soit Ω un domaine borné de $\mathbb{R}^m$ ($m\in\mathbb{N}^*$) et soit $\mathrm{D}\in(\mathbb{R}_+^*)^{16}\times\mathbb{R}_+^4$. Soient u_1^{in} et u_2^{in} des fonctions de $\mathrm{L}^1(\Omega)$ à valeurs positives. Pour u_1, u_2 deux fonctions de $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+\times\overline{\Omega})$ à valeurs positives, (u_1,u_2) est une **solution très faible** de* (2.20) *si (u_1,u_2) vérifie*

$$(r_a\, u_1^a + r_b\, u_2^b)\, u_1 \in \mathrm{L}^1_{loc}(\mathbb{R}_+\times\overline{\Omega}), \qquad (d_1 + d_\alpha u_1^\alpha + d_\beta u_2^\beta)\, u_1 \in \mathrm{L}^1_{loc}(\mathbb{R}_+\times\overline{\Omega}), \tag{2.22}$$
$$(r_c\, u_2^c + r_d\, u_1^d)\, u_2 \in \mathrm{L}^1_{loc}(\mathbb{R}_+\times\overline{\Omega}), \qquad (d_2 + d_\gamma u_2^\gamma + d_\delta u_1^\delta)\, u_2 \in \mathrm{L}^1_{loc}(\mathbb{R}_+\times\overline{\Omega}), \tag{2.23}$$

et pour toutes fonctions test $\psi_1,\ \psi_2 \in \mathscr{C}_c^1(\mathbb{R}_+;\mathscr{C}^2(\overline{\Omega}))$ *telles que* $\nabla_x \psi_i \cdot n = 0$ *au bord* $\partial\Omega$,

$$\begin{aligned}
&- \int_\Omega u_1^{in}(x)\,\psi_1(0,x)\ \mathrm{d}x - \int_0^\infty \int_\Omega u_1(t,x)\,\partial_t\psi_1(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
&- \int_0^\infty \int_\Omega \Delta_x\psi_1(t,x)\left[d_1 + d_\alpha u_1(t,x)^\alpha + d_\beta u_2(t,x)^\beta\right] u_1(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
= &\int_0^\infty \int_\Omega \psi_1(t,x)\,u_1(t,x)\left(r_1 - r_a u_1(t,x)^a - r_b u_2(t,x)^b\right)\ \mathrm{d}x\ \mathrm{d}t,
\end{aligned} \tag{2.24}$$

et

$$\begin{aligned}
&- \int_\Omega u_2^{in}(x)\,\psi_2(0,x)\ \mathrm{d}x - \int_0^\infty \int_\Omega u_2(t,x)\,\partial_t\psi_2(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
&- \int_0^\infty \int_\Omega \Delta_x\psi_2(t,x)\left[d_2 + d_\gamma u_2(t,x)^\gamma + d_\delta u_1(t,x)^\delta\right] u_2(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
= &\int_0^\infty \int_\Omega \psi_2(t,x)\,u_2(t,x)\left(r_2 - r_c u_2(t,x)^c - r_d u_1(t,x)^d\right)\ \mathrm{d}x\ \mathrm{d}t.
\end{aligned} \tag{2.25}$$

Définition 2.2 (Solution faible)**.** *Soit* Ω *un domaine borné de* $\mathbb{R}^m$ *(*$m \in \mathbb{N}^*$*) et soit* $\mathrm{D} \in (\mathbb{R}_+^*)^{16} \times \mathbb{R}_+^4$. *Soient* u_1^{in} *et* u_2^{in} *des fonctions de* $\mathrm{L}^1(\Omega)$ *à valeurs positives. Pour* u_1, u_2 *deux fonctions de* $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+ \times \overline{\Omega})$ *à valeurs positives,* (u_1, u_2) *est une* ***solution faible*** *de* (2.20) *si* (u_1, u_2) *vérifie*

$$(r_a\, u_1^a + r_b\, u_2^b)\, u_1 \ \in\ \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \qquad \nabla_x \left[(d_1 + d_\alpha u_1^\alpha + d_\beta u_2^\beta)\, u_1\right] \ \in\ \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \tag{2.26}$$

$$(r_c\, u_2^c + r_d\, u_1^d)\, u_2 \ \in\ \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \qquad \nabla_x \left[(d_2 + d_\gamma u_2^\gamma + d_\delta u_1^\delta)\, u_2\right] \ \in\ \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \tag{2.27}$$

et pour toutes fonctions test $\psi_1,\ \psi_2 \in \mathscr{C}_c^1(\mathbb{R}_+ \times \overline{\Omega})$

$$\begin{aligned}
&- \int_\Omega u_1^{in}(x)\,\psi_1(0,x)\ \mathrm{d}x - \int_0^\infty \int_\Omega u_1(t,x)\,\partial_t\psi_1(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
&- \int_0^\infty \int_\Omega \nabla_x\psi_1(t,x)\ \cdot \nabla_x\Big[(d_1 + d_\alpha u_1(t,x)^\alpha + d_\beta u_2(t,x)^\beta)\, u_1(t,x)\Big]\ \mathrm{d}x\ \mathrm{d}t \\
= &\int_0^\infty \int_\Omega \psi_1(t,x)\,u_1(t,x)\left(r_1 - r_a u_1(t,x)^a - r_b u_2(t,x)^b\right)\ \mathrm{d}x\ \mathrm{d}t,
\end{aligned} \tag{2.28}$$

et

$$\begin{aligned}
&- \int_\Omega u_2^{in}(x)\,\psi_2(0,x)\ \mathrm{d}x - \int_0^\infty \int_\Omega u_2(t,x)\,\partial_t\psi_2(t,x)\ \mathrm{d}x\ \mathrm{d}t \\
&- \int_0^\infty \int_\Omega \nabla_x\psi_2(t,x)\ \cdot \nabla_x\Big[(d_2 + d_\gamma u_2(t,x)^\gamma + d_\delta u_1(t,x)^\delta)\, u_2(t,x)\Big]\ \mathrm{d}x\ \mathrm{d}t \\
= &\int_0^\infty \int_\Omega \psi_2(t,x)\,u_2(t,x)\left(r_2 - r_c u_2(t,x)^c - r_d u_1(t,x)^d\right)\ \mathrm{d}x\ \mathrm{d}t.
\end{aligned} \tag{2.29}$$

On peut vérifier que dans chacune des deux définitions ci-dessus, les hypothèses sur les fonctions $u_{1,in}$, $u_{2,in}$, u_1, u_2, ψ_1, ψ_2 sont suffisantes pour que chacune des intégrales employées soit finie.

2.6 Le cas triangulaire : existence de solutions

Dans cette section on suppose qu'il y a de la diffusion croisée uniquement dans la deuxième équation, c'est-à-dire

$$\beta > 0,\ \delta = 0. \tag{2.30}$$

Dans ce cas, le couplage fort (c'est-à-dire le couplage à travers des termes d'ordre deux au regard du nombre de dérivées) entre u_1 et u_2 ne se fait que dans la première équation. La deuxième équation obéit à un principe du maximum, qui mène à une borne L^∞ pour u_2.

On présente des résultats d'existence de solutions faibles dans les deux cas (non exclusifs) suivants

$$(\alpha > 0,\ d < 2 + \alpha,\ a < 1 + \alpha) \text{ ou } (\alpha = 0,\ d \leq 2,\ a \leq 1), \tag{2.31}$$

$$(\alpha = \gamma = 0,\, \beta \geq 1,\, a > d). \tag{2.32}$$

Commentons les hypothèses ci-dessus. Une première constatation est qu'il n'y aucune hypothèse de petitesse sur les paramètres β, b et c, c'est-à-dire exactement les puissances de u_2 dans (2.20). En effet, grâce à la borne pour u_2 donnée par le principe du maximum, toute fonction régulière de u_2 est aussi bornée, et le comportement en l'infini des fonctions de u_2 apparaissant dans le système n'a aucune conséquence. L'hypothèse $\beta \geq 1$ est une hypothèse (technique) de régularité de la fonction $u \mapsto u^\beta$ en zéro, voir Remarque 2.9.

Pour le cas (2.31), le Lemme de dualité est crucial. On a vu à la section 2.4 que le Lemme de dualité (si applicable, ce qui sera vérifié au Chapitre 6) fournit une estimation pour $u_1^{2+\alpha}$ dans L^1. L'hypothèse $d < 2+\alpha$, $a < 1+\alpha$ dans (2.31) est exactement la condition sous laquelle cette estimation de dualité permet de contrôler les puissances de u_1 présentes dans la réaction, u_1^{1+a} et u_1^d. Dans le cas $\alpha = 0$, la version précisée (voir Remarque 2.6) du Lemme de dualité permet de considérer une inégalité large $d \leq 2$, $a \leq 1$.

Le cas (2.32) lui ne repose pas sur l'estimation de dualité mais principalement sur des méthodes d'entropie. L'idée est d'utiliser le signe du terme $r_a u_1^{1+a}$ pour obtenir un contrôle (qui dépend de a) sur l'intégrabilité de u_1, puis d'utiliser l'estimation obtenue pour contrôler le terme $r_d u_1^d u_2$.

On présente ci-dessous deux théorèmes d'existence de solutions faibles, le premier correspondant au cas (2.31), et le deuxième au cas (2.32). Dans le deuxième cas (2.32), on présente de plus des résultats de régularité, de stabilité et d'unicité.

Théorème 2.1 (T.). *Soit Ω un domaine borné régulier de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). On suppose que les paramètres (2.21) du système satisfont $\beta > 0$, $\delta = 0$ et la condition (2.31). Soient $u_{1,in}$, $u_{2,in}$ à valeurs positives et telles que $u_{1,in} \in \mathrm{L}^2(\Omega)$, $u_{2,in} \in \mathrm{L}^\infty(\Omega)$.*

Alors,
***i)** il existe $u_1 = u_1(t,x) \geq 0$, $u_2 = u_2(t,x) \geq 0$ telles que $(u_1,u_2) \in \mathrm{L}^{2+\alpha}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times \mathrm{L}^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et (u_1,u_2) est une solution faible du système (2.20) au sens de la Définition 2.2.*

De plus, cette solution (u_1,u_2) satisfait les estimations pour tout $T > 0$

$$\sup_{[0,T]\times\Omega} u_2 \leq \max\left\{\sup_\Omega u_{2,in}, \left(\frac{r_2}{r_c}\right)^{1/c}\right\}, \tag{2.33}$$

$$\int_0^T \int_\Omega u_1^{2+\alpha} \leq C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}), \tag{2.34}$$

$$\int_0^T \int_\Omega \left|\nabla_x[u_2^{p/2}]\right|^2 \leq C_p(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}) \qquad (\textit{pour tout } 0 < p < \infty), \tag{2.35}$$

$$\int_\Omega u_1(T) + \int_0^T \int_\Omega \left|\nabla_x[(1+u_1)^{\alpha/2}]\right|^2 \leq C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}) \qquad (\textit{si } \alpha > 0), \tag{2.36}$$

$$\int_\Omega u_1(T) + \int_0^T \int_\Omega |\nabla_x[\log(1+u_1)]|^2 \leq C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}) \qquad (\textit{si } \alpha = 0), \tag{2.37}$$

où la constante $C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D})$ dépend uniquement du domaine Ω (et de la dimension m), du temps T, des normes des données initiales $\|u_{1,in}\|_{\mathrm{L}^2(\Omega)}$ et $\|u_{2,in}\|_{\mathrm{L}^\infty(\Omega)}$ et du choix de paramètres D, et la constante $C_p(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D})$ dépend uniquement des mêmes quantités et du paramètre p.
Si $u_{1,in}$ satisfait de plus $u_{1,in}(x) > 0$ p.p. sur Ω et $\log u_{1,in} \in \mathrm{L}^1(\Omega)$, resp., si $u_{2,in}$ satisfait de plus $u_{2,in}(x) > 0$ p.p. sur Ω et $\log u_{2,in} \in \mathrm{L}^1(\Omega)$, alors pour tout $T > 0$

$$\begin{aligned} &\int_\Omega |\log u_1|(T) + d_1 \int_0^T \int_\Omega |\nabla_x[\log u_1]|^2 \leq \int_\Omega |\log u_{1,in}| + C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}), \\ \textit{resp.,} \quad &\int_\Omega |\log u_2|(T) + d_2 \int_0^T \int_\Omega |\nabla_x[\log u_2]|^2 \leq \int_\Omega |\log u_{2,in}| + C(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}). \end{aligned} \tag{2.38}$$

***ii)** Si $\alpha = 0$, on dispose des estimations supplémentaires, pour un certain $\nu = \nu(\Omega, u_{2,in}, \mathrm{D}) > 0$ qui dépend uniquement du domaine Ω (et m), de la norme $\|u_{2,in}\|_{\mathrm{L}^\infty(\Omega)}$ et des paramètres D, pour tout $T > 0$, et pour une certaine constante $C^1(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}) > 0$ qui dépend uniquement du domaine Ω (et m), du temps T, des normes $(\|u_{1,in}\|_{\mathrm{L}^2(\Omega)}, \|u_{2,in}\|_{\mathrm{L}^\infty(\Omega)})$ et des paramètres D,*

$$\int_0^T \int_\Omega u_1^{2+\nu} \leq C^1(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}). \tag{2.39}$$

iii) *Si $\gamma = 0$, en supposant de plus que $u_{2,in} \in \mathrm{W}^{2,q}(\Omega)$ pour un certain $q > 1$ tel que*

$$1 < q \leq (2+\alpha)/d \quad si\ \alpha > 0, \qquad 1 < q \leq (2+\nu)/d \quad si\ \alpha = 0,$$

(et en supposant de plus la condition de compatibilité $\nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$ si $q \geq 3$), on a l'estimation supplémentaire, pour tout $T > 0$,

$$\int_0^T \int_\Omega |\partial_t u_2|^q + \int_0^T \int_\Omega |\nabla_x^2 u_2|^q + \int_0^T \int_\Omega |\nabla_x u_2|^{2q} \leq C_q^2(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D}), \tag{2.40}$$

où la constante $C_q^2(\Omega, T, u_{1,in}, u_{2,in}, \mathrm{D})$ dépend uniquement du paramètre q, du domaine Ω (et de la dimension m), du temps T, des normes $(\|u_{1,in}\|_{\mathrm{L}^2(\Omega)}, \|u_{2,in}\|_{\mathrm{L}^\infty \cap \mathrm{W}^{2,q}(\Omega)})$ et des paramètres D.

Théorème 2.2 (Desvillettes, T.). *Soit Ω un domaine borné régulier de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). On suppose que les paramètres* (2.21) *du système satisfont $\beta > 0$, $\delta = 0$ et la condition* (2.32)*. Soient $u_{1,in}$, $u_{2,in}$ à valeurs positives et telles que $u_{1,in} \in \mathrm{L}^{p_0}(\Omega)$, $u_{2,in} \in \mathrm{L}^\infty(\Omega) \cap \mathrm{W}^{2,1+p_0/d}(\Omega)$ pour un certain $p_0 > 1$. Si $1 + p_0/d \geq 3$, on suppose de plus la condition de compatibilité "$\nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$".*

Alors,

i) *il existe $u_1 = u_1(t,x) \geq 0$, $u_2 = u_2(t,x) \geq 0$ telles que $(u_1, u_2) \in \mathrm{L}^{\max(1+a,d)}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times \mathrm{L}^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et (u_1, u_2) est une solution faible du système* (2.20) *au sens de la Définition 2.2.*

De plus, cette solution (u_1, u_2) satisfait les estimations pour tout $p \in]1, p_0]$ et tout $T > 0$

$$\sup_{(t,x)\in[0,T]\times\Omega} u_2(t,x) \leq \max\left(\|u_{2,in}\|_{\mathrm{L}^\infty(\Omega)}, \left[\frac{r_2}{r_c}\right]^{1/c} \right), \qquad \int_0^T \int_\Omega |\nabla_x u_2|^{2(1+p_0/d)} \leq C_T,$$

$$\int_0^T \int_\Omega u_1^{p_0+a} \leq C_T, \qquad \sup_{t\in[0,T]} \int_\Omega u_1^{p_0}(t) \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x (u_1^{p/2})|^2 \leq C_{T,p}\,,$$

où les constantes C_T et $C_{T,p}$ dépendent uniquement du domaine Ω (et de la dimension m), du temps T, des données initiales $(u_{1,in}, u_{2,in})$, du choix de paramètres D*, du paramètre p_0 et, pour $C_{T,p}$, du paramètre p.*

ii) *Si on suppose de plus que $\beta \geq 2$ et $u_{1,in} \in \mathrm{W}^{2,s_0}(\Omega)$, $u_{2,in} \in \mathrm{W}^{2,\frac{p_1+a}{d}}(\Omega)$ pour un certain $s_0 > 1 + m/2$ et un certain $p_1 \geq 2$, $p_1 > a(s_0 - 1)$, et que la condition de compatibilité "$\nabla_x u_{1,in} \cdot n = 0$ sur $\partial\Omega$" (resp. "$\nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$") est satisfaite si $s_0 \geq 3$ (resp. $\frac{p_1+a}{d} \geq 3$). Alors u_1 et u_2 sont des fonctions Höldériennes sur $\mathbb{R}_+ \times \bar{\Omega}$, et $\partial_t u_1$, $\partial_{x_i x_j} u_1 \in \mathrm{L}^{s_0}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, $\partial_{x_i} u_1 \in \mathrm{L}^2_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, $\partial_t u_2$, $\partial_{x_i x_j} u_2 \in \mathrm{L}^{(p_1+a)/d}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ ($i, j = 1..m$, et les dérivées sont à comprendre au sens des distributions).*

iii) *Enfin, si, en plus des hypothèses précédentes, les dérivées secondes de $u_{1,in}$, $u_{2,in}$ sont des fonctions Höldériennes sur Ω, et si les conditions de compatibilité "$\nabla_x u_{1,in} \cdot n = \nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$" sont satisfaites, alors $\partial_t u_1$, $\partial_{x_i x_j} u_1$, $\partial_{x_i} u_1$, $\partial_t u_2$, $\partial_{x_i x_j} u_2$ ($i, j = 1..m$) sont des fonctions Höldériennes sur $\mathbb{R}_+ \times \overline{\Omega}$.*

Dans ce cadre, et si de plus $b, d \geq 1$, on dispose du résultat de stabilité suivant : si $(u_{1,in}, u_{2,in})$ et $(u'_{1,in}, u'_{2,in})$ sont deux couples de données initiales (à valeurs positives) et telles que les normes L^∞ de leurs dérivées spatialles d'ordre zéro, d'odre un et d'ordre deux, ainsi que les normes Hölder d'ordre θ de leurs dérivées spatialles d'ordre deux sont majorées par une certaine constante $K > 0$ (pour un certain $\theta > 0$ fixé), alors tout couple de solutions faibles correspondantes (u_1, u_2), (u'_1, u'_2) au sens de la Définition 2.2, appartenant à $\mathrm{L}^{p_1+a}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times \mathrm{L}^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et telles que (pour tout $T > 0$)

$$\sup_{t\in[0,T]} \int_\Omega u_i^2(t) < +\infty \qquad and \qquad \int_0^T \int_\Omega |\nabla_x u_i|^2 < +\infty, \tag{2.41}$$

$$\sup_{t\in[0,T]} \int_\Omega u_i'^2(t) < +\infty \qquad and \qquad \int_0^T \int_\Omega |\nabla_x u'_i|^2 < +\infty \qquad for\ i = 1, 2, \tag{2.42}$$

satisfait (pour tout $T > 0$)

$$||u_1 - u'_1||_{\mathrm{L}^2([0,T]\times\Omega)} + ||u_2 - u'_2||_{\mathrm{L}^2([0,T]\times\Omega)} \leq C_{T,K} \left(||u_{1,in} - u'_{1,in}||_{\mathrm{L}^2(\Omega)} + ||u_{2,in} - u'_{2,in}||_{\mathrm{L}^2(\Omega)} \right),$$

où la constante $C_{T,K} > 0$ dépend uniquement de la constante K, du domaine Ω (et de la dimension m), des paramètres du système D*, du temps T et du paramètre θ.*

Il en découle un résultat d'unicité dans ce dernier cadre (unicité au sein des solutions faibles au sens de la Définition 2.2, appartenant à $\mathrm{L}^{p_1+a}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times \mathrm{L}^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et satisfaisant (2.41)*).*

Remarque 2.8. *Dans le premier cadre, on montre l'existence de solutions faibles. Dans le deuxième, on montre que ces solutions sont fortes, au sens où toutes les dérivées apparaissant dans les équations appartiennent à un espace $\mathrm{L}^p_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ pour un certain $p \in [1, \infty]$. Enfin, dans le dernier cadre, on montre que ces solutions sont classiques, au sens où toutes les dérivées apparaissant dans les équations sont continues. Le résultat de stabilité et d'unicité (au sein des solutions faibles satisfaisant certaines hypothèses de régularité supplémentaire) concerne le cas où les hypothèses sur les paramètres impliquent que toute solution faible est une solution classique.*

Remarque 2.9. *On se rapportera aux Chapitres 4 et 6 pour une liste d'extensions directes de ces résultats, permettant d'affaiblir les hypothèses sur les paramètres et sur la régularité des données initiales. Cependant, notons dès à présent l'extension suivante : les fonctions de lois de puissance "$u \mapsto u^\alpha$", "$u \mapsto u^a$" et "$u \mapsto u^d$" peuvent être remplacées par n'importe quelles fonctions continues sur $\mathbb{R}_+$, régulières ($\mathscr{C}^1$) et à valeurs strictement positives sur $\mathbb{R}_+^*$, et ayant le même comportement en l'infini, avec de plus une hypothèse de croissance pour la fonction remplaçant "$u \mapsto u^\alpha$". Grâce à la borne* (2.33)*, conséquence d'un principe du maximum pour la deuxième équation de* (2.10)*, les fonctions de lois de puissance "$u \mapsto u^\beta$", "$u \mapsto u^\gamma$", "$u \mapsto u^b$" et "$u \mapsto u^c$" peuvent être remplacées par n'importe quelles fonctions continues sur $\mathbb{R}_+$, régulières ($\mathscr{C}^1$) et à valeurs strictement positives sur $\mathbb{R}_+^*$, avec une croissance arbitraire en l'infini, sauf pour "$u \mapsto u^\gamma$" qui doit croître suffisamment pour garantir que le principe du maximum s'applique (diverger vers l'infini suffit), avec de plus une hypothèse de croissance pour la fonction remplaçant "$u \mapsto u^\gamma$" et, dans le cas du Théorème 2.2, de régularité ($\mathscr{C}^1$) en zéro pour la fonction remplaçant "$u \mapsto u^\beta$" (équivalent de la condition $\beta \geq 1$ dans l'hypothèse* (2.32)*). Sous ces hypothèses, les résultats d'existence des Théorèmes 2.1 et 2.2 sont valables, avec des adaptations évidentes des hypothèses et des estimations.*

La condition $\beta \geq 1$ dans le cas (2.32) *est technique, et sert à éviter des problèmes de singularité du terme $\nabla_x d_\beta u_1 u_2^\beta$ pour les petites valeurs de u_2. Dans le cas où $\beta < 1$, ce terme peut en fait être contrôlé grâce à une estimation du type* (2.35) *pour $p < 1$ (dont on peut montrer qu'elle est aussi valide dans ce cadre, c'est-à-dire sous l'hypothèse $\alpha = \gamma = 0$, $a > d$ à la place de l'hypothèse* (2.31)*). On s'attend donc à pouvoir en fait supprimer l'hypothèse $\beta \geq 1$ dans le Théorème 2.2, et même, conformént au paragraphe précédent, à pouvoir remplacer la fonction "$v \mapsto v^\beta$" par n'importe quelle fonction continue sur $\mathbb{R}_+$, et à valeurs strictement positives et $\mathscr{C}^1$ sur $\mathbb{R}_+^*$.*

La démonstration du Théorème 2.1 est l'objet du Chapitre 6. Elle repose sur des méthodes d'entropie ainsi que sur le Lemme de dualité. On trouvera la démonstration du Théorème 2.2 dans le Chapitre 4. Le résultat d'existence fait appel à des méthodes d'entropie et repose sur un résultat de perturbation singulière que l'on présente dans la Section ci-dessous. Les résultats de régularités "successives" sont quant à eux des conséquences de nos méthodes d'entropie et de résultats classiques de la Théorie des équations linéaires paraboliques.

2.7 Le cas triangulaire : un modèle microscopique

Dans le cas triangulaire sans auto-diffusion

$$\alpha = \gamma = \delta = 0, \tag{2.43}$$

et en supposant de plus

$$\beta \geq 1, \tag{2.44}$$

les solutions des théorèmes d'existence de la section précédente (avec une hypothèse de régularité supplémentaire sur $u_{2,in}$ dans le cas du Théorème 2.1) peuvent être obtenues à partir d'un résultat de perturbation singulière que l'on présente dans cette section. En s'inspirant de la démarche de M. Iida, M. Mimura et H. Ninomiya décrite à la Section 2.2, on propose un système de réaction-diffusion qui modélise le même système écologique à une autre échelle. On démontre le lien asymptotique entre le système de réaction-diffusion, dit "microscopique", et le système SKT généralisé. En particulier, on démontre une version rigoureuse de la limite formelle obtenue au paragraphe 2.2 dans le cadre du système SKT original.

Le système microscopique est le suivant

$$\begin{cases} \partial_t u_A^\epsilon - d_A\,\Delta_x u_A^\epsilon = u_A^\epsilon\,(r_1 - r_a\,(u_A^\epsilon + u_B^\epsilon)^a - r_b\,(u_2^\epsilon)^b) + \dfrac{1}{\epsilon}[k(u_2^\epsilon)u_B^\epsilon - h(u_2^\epsilon)u_A^\epsilon], & \text{dans } \mathbb{R}_+ \times \Omega, \\ \partial_t u_B^\epsilon - d_B\,\Delta_x u_B^\epsilon = u_B^\epsilon\,(r_1 - r_a\,(u_A^\epsilon + u_B^\epsilon)^a - r_b\,(u_2^\epsilon)^b) - \dfrac{1}{\epsilon}[k(u_2^\epsilon)u_B^\epsilon - h(u_2^\epsilon)u_A^\epsilon], & \text{dans } \mathbb{R}_+ \times \Omega, \\ \partial_t u_2^\epsilon - d_2\,\Delta_x u_2^\epsilon = u_2^\epsilon\,(r_2 - r_c\,(u_2^\epsilon)^c - r_d\,(u_A^\epsilon + u_B^\epsilon)^d), \quad \text{dans } \mathbb{R}_+ \times \Omega, \\ \nabla_x u_A^\epsilon \cdot n(x) = \nabla_x u_B^\epsilon \cdot n(x) = \nabla_x u_2^\epsilon \cdot n(x) = 0, \quad \text{sur } \mathbb{R}_+ \times \partial\Omega, \\ u_A^\epsilon(0,\cdot) = u_{A,in}^\epsilon \geq 0, \quad u_B^\epsilon(0,\cdot) = u_{B,in}^\epsilon \geq 0, \quad u_2^\epsilon(0,\cdot) = u_{2,in}^\epsilon \geq 0, \quad \text{dans } \Omega. \end{cases} \tag{2.45}$$

Les trois premières équations correspondent au système de Iida-Mimura-Ninomiya que l'on a généralisé à la manière de M. E. Gilpin et F. J. Ayala (i.-e. dans l'expression des taux de croissance, on a remplacé les fonctions linéaires en les inconnues par des fonctions puissances). Les taux de diffusion d_A et d_B satisfont

$$0 < d_A < d_B, \tag{2.46}$$

et les fonctions h et k sont dans $\mathscr{C}^1(\mathbb{R}_+)$ et satisfont pour tout $v \in [0, v_1]$

$$d_A + d_B\,\frac{h(v)}{h(v)+k(v)} = d_1 + d_\beta v^\beta, \qquad h(v) \geq h_0 > 0, \qquad k(v) \geq h_0 > 0, \tag{2.47}$$

où h_0 est une constante strictement positive, et où la constante $v_1 > 0$ est définie en (2.53). On pourra par exemple vérifier que le choix suivant de d_A, d_B, h et k convient (avec $h_0 = d_1/2$) :

$$d_A := d_1/2, \quad d_B := d_1 + d_\beta v_1^\beta, \quad h(v) := d_1/2 + d_\beta v^\beta, \quad k(v) := d_1/2 + d_\beta[v_1^\beta - v^\beta].$$

A ces trois équations, on a ajouté les conditions de Neumann homogènes au bord, ainsi que des conditions initiales régulières obtenues à partir de deux fonctions $u_{1,in}$ et $u_{2,in}$ à valeurs positives et intégrables, grâce au procédé de régularisation suivant. Soit $(\rho^\varepsilon)_{\varepsilon>0}$ un suite régularisante sur $\mathbb{R}^m$, et pour tout $\varepsilon > 0$, soit χ^ε une fonction de troncature, appartenant à $\mathscr{C}^\infty(\mathbb{R}^m, [0,1])$, et telle que

$$\chi^\varepsilon = 1 \text{ dans } \{x \in \Omega : d(x, \partial\Omega) > 2\varepsilon\}, \qquad \chi^\varepsilon = 0 \text{ hors de } \{x \in \Omega : d(x, \partial\Omega) > \varepsilon\}.$$

On définit alors

$$u_{A,in} := \frac{k(u_{2,in})}{h(u_{2,in}) + k(u_{2,in})}\,u_{1,in}, \qquad u_{B,in} := \frac{h(u_{2,in})}{h(u_{2,in}) + k(u_{2,in})}\,u_{1,in} \qquad \text{sur } \Omega, \tag{2.48}$$

que l'on prolonge par zéro sur $\mathbb{R}^m - \Omega$ (afin de pouvoir définir la convolée dans $\mathbb{R}^m$). On peut enfin définir sur Ω les données initiales régularisées

$$u_{A,in}^\varepsilon := (\chi^\varepsilon(u_{A,in} * \rho^\varepsilon) + \epsilon)|_\Omega, \quad u_{B,in}^\varepsilon := (\chi^\varepsilon(u_{A,in} * \rho^\varepsilon) + \varepsilon)|_\Omega, \quad u_{2,in}^\varepsilon := u_{2,in} + \varepsilon. \tag{2.49}$$

On montre alors que les solutions du système (2.45) convergent et qu'à la limite on retrouve le système (2.20). La notion de solution utilisée pour le système (2.45) est précisée dans la

Définition 2.3 (Solution forte)**.** *Soit Ω un domaine borné de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$), soit $\mathrm{D} \in (\mathbb{R}_+^*)^{16} \times \mathbb{R}_+^4$ et soient d_A, d_B satisfaisant* (2.46) *et h, k des fonctions de $\mathscr{C}^1(\mathbb{R}_+)$ satisfaisant* (2.47)*. Soient u_1^{in} et u_2^{in} des fonctions de $\mathrm{L}^1(\Omega)$ à valeurs positives. Soit $\varepsilon \in]0,1[$. Pour u_A^ϵ, u_B^ϵ, u_2^ϵ des fonctions de $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+ \times \overline{\Omega})$ à valeurs positives, $(u_A^\epsilon, u_B^\epsilon, u_2^\epsilon)$ est une **solution forte** de* (2.45) *si $(u_A^\epsilon, u_B^\epsilon, u_2^\epsilon)$ vérifie (pour i, $j = 1..m$)*

$$u_A^\epsilon \in \mathrm{L}_{loc}^{\max(1+a,d)}(\mathbb{R}_+ \times \overline{\Omega}), \qquad \partial_t u_A^\epsilon,\ \partial_{x_i,x_j} u_A^\epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \tag{2.50}$$

$$u_B^\epsilon \in \mathrm{L}_{loc}^{\max(1+a,d)}(\mathbb{R}_+ \times \overline{\Omega}), \qquad \partial_t u_B^\epsilon,\ \partial_{x_i,x_j} u_B^\epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \tag{2.51}$$

$$u_2^\epsilon \in \mathrm{L}^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \qquad \partial_t u_2^\epsilon,\ \partial_{x_i,x_j} u_2^\epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega}), \tag{2.52}$$

et le système (2.45) *est satisfait presque-partout dans $\mathbb{R}_+ \times \Omega$ (resp. $\mathbb{R}_+ \times \partial\Omega$, Ω), où les conditions initiales sont définies par* (2.48)–(2.49)*.*

Le comportement quand $\varepsilon \to 0$ des solutions fortes de (2.45) est décrit dans les deux théorèmes suivants, correspondant respectivement aux cas du Théorème 2.1 et du Théorème 2.2 (respectivement conditions (2.31) et (2.32)) sous les conditions supplémentaires (2.43), (2.44).

Théorème 2.3 (Desvillettes, T.). *Soit Ω un domaine borné de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). On suppose que les paramètres* (2.21) *satisfont $\alpha = \gamma = \delta = 0$, $\beta \geq 1$ et $d \leq 2$, $a \leq 1$. Soient d_A, d_B satisfaisant* (2.46) *et h, k des fonctions de $\mathscr{C}^1(\mathbb{R}_+)$ satisfaisant* (2.47). *Soient $u_{1,in}$, $u_{2,in}$ à valeurs positives et telles que $u_{1,in} \in \mathrm{L}^2(\Omega)$, $u_{2,in} \in \mathrm{L}^\infty(\Omega) \cap \mathrm{W}^{2,1+2/d}(\Omega)$ (en supposant de plus la condition de compatibilité $\nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$ si $1 + 2/d \geq 3$, i.-e., si $d \leq 1$).*

Alors, pour tout $\varepsilon \in]0,1[$, il existe un unique triplet de fonctions $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ à valeurs positives qui est solution du système (2.45) *au sens de la Définition 2.3.*

De plus, quand $\varepsilon \to 0$, $(u_A^\epsilon, u_B^\epsilon, u_2^\epsilon)$ converge, à l'extraction d'une sous-suite près, pour presque-tout $(t,x) \in \mathbb{R}_+ \times \Omega$ vers une limite (u_A, u_B, u_2) dont les trois composantes prennent des valeurs positives.

La quantité $(u_1, u_2) := (u_A + u_B, u_2)$ satisfait $\nabla_x u_1, \nabla_x(u_1\, u_2^\beta) \in \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et les estimations suivantes pour un certain $p \in]0,1[$ et $\eta > 0$ et pour tout $T > 0$,

$$\sup_{[0,T]\times\Omega} u_2 \leq \max\left\{\sup_\Omega u_{2,in}, \left(\frac{r_2}{r_c}\right)^{1/c}\right\} =: v_1, \tag{2.53}$$

$$\sup_{t\in[0,T]} \int_\Omega u_1(t) \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x(u_1^{p/2})|^2 \leq C_T, \tag{2.54}$$

$$\int_0^T \int_\Omega u_1^2 \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x u_2|^{2+\eta} \leq C_T, \tag{2.55}$$

où la constante C_T dépend uniquement du domaine Ω (et de la dimension m), du temps T, des données initiales $u_{1,in}$, $u_{2,in}$ et du choix de paramètres D.

Enfin, $h(u_2(t,x))\, u_A(t,x) = k(u_2(t,x))\, u_B(t,x)$ pour presque-tout $(t,x) \in \mathbb{R}_+ \times \Omega$, et (u_1, u_2) est une solution faible du système (2.10) *au sens de la Définition 2.2.*

Théorème 2.4 (Desvillettes, T.). *Soit Ω un domaine borné de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). On suppose que les paramètres* (2.21) *satisfont $\alpha = \gamma = \delta = 0$, $\beta \geq 1$ et $a > d$. Soient d_A, d_B satisfaisant* (2.46) *et h, k des fonctions de $\mathscr{C}^1(\mathbb{R}_+)$ satisfaisant* (2.47). *Soient $u_{1,in}$, $u_{2,in}$ à valeurs positives et telles que $u_{1,in} \in \mathrm{L}^{p_0}(\Omega)$, $u_{2,in} \in \mathrm{L}^\infty(\Omega) \cap \mathrm{W}^{2,1+p_0/d}(\Omega)$ pour un certain $p_0 > 1$ (en supposant de plus la condition de compatibilité $\nabla_x u_{2,in} \cdot n = 0$ sur $\partial\Omega$ si $1 + p_0/d \geq 3$).*

Alors, pour tout $\varepsilon \in]0,1[$, il existe un unique triplet de fonctions $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ à valeurs positives qui est solution du système (2.45) *au sens de la Définition 2.3.*

De plus, quand $\varepsilon \to 0$, $(u_A^\epsilon, u_B^\epsilon, u_2^\epsilon)$ converge, à l'extraction d'une sous-suite près, pour presque-tout $(t,x) \in \mathbb{R}_+ \times \Omega$ vers une limite (u_A, u_B, u_2) dont les trois composantes prennent des valeurs positives.

La quantité $(u_1, u_2) := (u_A + u_B, u_2)$ satisfait $\nabla_x u_1, \nabla_x(u_1\, u_2^\beta) \in \mathrm{L}^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et pour tout $T > 0$, la borne (2.53) *est satisfaite, ainsi que les estimations suivantes pour tout $p \in]1, p_0]$*

$$\sup_{t\in[0,T]} \int_\Omega u_1^{p_0}(t) \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x(u_1^{p/2})|^2 \leq C_{T,p}, \tag{2.56}$$

$$\int_0^T \int_\Omega u_1^{p_0+a} \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x u_2|^{2(1+p_0/d)} \leq C_T\,, \tag{2.57}$$

où les constantes C_T et $C_{T,p}$ dépendent uniquement du domaine Ω (et de la dimension m), du temps T, des données initiales $(u_{1,in}, u_{2,in})$, du choix de paramètres D, *du paramètre p_0 et, pour $C_{T,p}$, du paramètre p.*

Enfin, $h(u_2(t,x))\, u_A(t,x) = k(u_2(t,x))\, u_B(t,x)$ pour presque-tout $(t,x) \in \mathbb{R}_+ \times \Omega$, et (u_1, u_2) est une solution faible du système (2.10) *au sens de la Définition 2.2.*

La démonstration des Théorèmes 2.3 et 2.4 se trouve dans le Chapitre 4, ainsi que la démonstration de leurs conséquences directes en terme d'existence de solutions (incluses dans les Théorèmes 2.1 et 2.2). Les démonstrations reposent sur des méthodes d'entropie, et pour le Théorème 2.3, sur le Lemme de dualité.

2.8 Le cas non-triangulaire

On présente des résultats d'existence de solutions très faibles pour le système SKT généralisé "complet" (non-triangulaire) sous la condition sur les paramètres de diffusion croisée

$$0 < \delta < 1/\beta < 1. \tag{2.58}$$

Pour simplifier, on se place dans un contexte sans auto-diffusion

$$\alpha = \gamma = 0. \tag{2.59}$$

Enfin, on suppose que les paramètres de réaction satisfont

$$a < 1,\ b < \beta + c/2,\ d < 2. \tag{2.60}$$

L'hypothèse $0 < \beta\delta < 1$ dans (2.58) est une hypothèse fondamentale sur la structure des termes de diffusion qui permet, après une réécriture appropriée du système, d'obtenir une fonctionnelle de type entropique. Cette fonctionnelle de type entropique a été repérée dans le cas particulier $0 < \beta < 1$, $0 < \delta < 1$ par L. Desvillettes, Th. Lepoutre et A. Moussa dans [15], où elle a été employée pour obtenir des résultats d'existence : ici, on se place donc naturellement dans le cadre non traité dans [15], à savoir le cas où un des paramètres de diffusion croisée est strictement plus grand que 1, d'où (sans perte de généralité) (2.58).

La condition (2.59) vise uniquement à simplifier la présentation des résultats. Tous les résultats présentés sont maintenus en présence d'auto-diffusion, et mieux encore, la présence d'auto-diffusion permet en général de considérer un ensemble de paramètres encore plus large (mais long à décrire !) : voir la Section 5.5.1 du Chapitre 5.

Enfin, l'hypothèse (2.60) permet de contrôler les termes de réaction. On reconnait [14] la condition $a < 1$, $d < 2$ qui permet de contrôler les termes u_1^{1+a} et $u_1^d u_2$ grâce au Lemme de dualité. La condition $b < \beta + c/2$ permet de contrôler le terme $u_2^b u_1$ grâce à une estimation d'entropie, que l'on retrouve dans l'estimation (2.63). Cette même estimation permet de contrôler le terme u_2^{1+c} sans hypothèse sur le paramètre c (on "utilise" le signe de u_2^{1+c} pour obtenir un contrôle - qui dépend de c - sur l'intégrabilité de u_2).

Nos résultats d'existence de solution sont décrits dans le

Théorème 2.5 (Desvillettes, Lepoutre, Moussa, T.)**.** *Soit Ω un domaine borné régulier de $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). On suppose que les paramètres* (2.21) *du système satisfont* (2.58)–(2.60)*. Soient $u_{1,in}$, $u_{2,in}$ à valeurs positives et telles que $u_{1,in} \in (\mathrm{L}^1 \cap \mathrm{H}_m^{-1})(\Omega)$, $u_{2,in} \in (\mathrm{L}^\beta \cap \mathrm{H}_m^{-1})(\Omega)$.*

Alors, il existe $u_1 = u_1(t,x) \geq 0$, $u_2 = u_2(t,x) \geq 0$ telles que $(u_1, u_2) \in \mathrm{L}^2_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times \mathrm{L}^{\beta+c}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ et (u_1, u_2) est une solution très faible du système (2.20) *au sens de la Définition 2.1.*

De plus, cette solution (u_1, u_2) satisfait les estimations pour tout $T > 0$

$$\int_0^T \int_\Omega (u_1 + u_2)\,(u_1^\delta u_2 + u_2^\beta u_1 + u_1 + u_2)\, \mathrm{d}x\ \mathrm{d}t \leq C_T, \tag{2.61}$$

$$\sup_{t\in[0,T]} ||u_i(t,\cdot)||_{\mathrm{L}^1(\Omega)} \leq e^{r_i T} ||u_i^{in}||_{\mathrm{L}^1(\Omega)}, \tag{2.62}$$

$$\begin{aligned} &\sup_{t\in[0,T]} \int_\Omega u_2(t,\cdot)^\beta + \int_0^T \int_\Omega u_2^\beta\ \left(u_1^d + u_2^c\right)\ \mathrm{d}x\,\mathrm{d}t \\ &+ \int_0^T \int_\Omega \left\{ |\nabla u_1^{\delta/2}|^2 + |\nabla u_2^{\beta/2}|^2 + \left|\nabla \sqrt{u_1^\delta\, u_2^\beta}\right|^2 \right\} \mathrm{d}x\,\mathrm{d}t \\ &\qquad\qquad \leq K_T\,(1 + \|u_1^{in}\|_{\mathrm{L}^1(\Omega)} + \|u_2^{in}\|^\beta_{\mathrm{L}^{\gamma_2}(\Omega)}). \end{aligned} \tag{2.63}$$

où la constante K_T dépend uniquement du domaine Ω (et de la dimension m), du temps T et du choix de paramètres D, et la constante C_T dépend uniquement des mêmes quantités et des normes des données initiales $\|u_{1,in}\|_{\mathrm{H}_m^{-1}(\Omega)}$ et $\|u_{2,in}\|_{\mathrm{H}_m^{-1}(\Omega)}$.

Remarque 2.10. *Comme pour les théorèmes précédents, on peut remplacer les fonctions de loi de puissance en u_1 et u_2 par des fonctions continues plus générales ayant le même comportement en l'infini, sous des hypothèses adéquates de régularité, monotonie et convexité. Notons que grâce aux estimations ci-dessus, u_1 est en fait une solution faible (de la première équation du système). Voir le Chapitre 5 pour plus de détails et pour d'autres extensions permettant de considérer un évantail de paramètres plus large.*

14. comme dans l'hypothèse (2.31) pour le cas triangulaire.

On trouvera la démonstration du Théorème 2.5 dans le Chapitre 5. Les outils essentiels de la démonstration sont le Lemme de dualité et l'exploitation d'une structure entropique cachée. On trouvera aussi dans le Chapitre 5 de nombreuses explications et extensions concernant cette structure entropique. De plus, d'un point de vue plus technique, la démonstration repose sur l'introduction d'un schéma semi-discret en temps qui permet d'approximer le système (2.20). De manière très résumée, on peut dire que cette approximation semi-discrète se comporte bien vis-à-dis des estimations d'entropie et de dualité, ce qui n'est pas évident vu leur nature très différente. Elle s'avère donc tout à fait adaptée à notre système, et on peut aussi s'attendre à ce qu'elle convienne à d'autres types de systèmes pour lesquels on aurait des estimations d'entropie et de dualité. Voilà pourquoi, dans le Chapitre 5, ce schéma est introduit et étudié (existence et régularité des solutions, estimations de dualité) dans un contexte abstrait assez général (pour I espèces distinctes, $I \in \mathbb{N}^*$).

2.9 Conclusion et perspectives

Pour une large gamme de systèmes de diffusions croisées pour deux espèces en compétition, on a établi des résultats d'existence de solution, ainsi que, dans certains cas, des propriétés qualitatives (régularité, stabilité, comportement au voisinage de zéro, approximation par un modèle microscopique) et un résultat d'unicité. On présente ici quelques questions dans le prolongement de ces résultats.

Autour du problème bien posé. L'existence de solutions au système (2.20) pour des paramètres ne satisfaisant pas nos hypothèses (ou le cas original (2.2)) reste un problème ouvert. Par exemple, dans le cas non triangulaire, si les paramètres de diffusion croisée β et δ vérifient $\beta\delta > 1$, alors la structure d'entropie se brise, et, pire encore, il est possible que la matrice de diffusion A dégénère, au sens où on peut *a priori* (i.-e. à moins de connaître de - surprenantes - bornes particulières dans L^∞ sur les solutions) avoir $\det(D(A))(u_1, u_2) < 0$ en certains points, et il est alors impossible d'obtenir une entropie convexe. Peut-on tout de même trouver une entropie non-convexe ?

Pour ce qui est de l'unicité, on a obtenu un résultat dans un cas particulier du cas triangulaire où les solutions faibles obtenues s'avèrent être assez régulières et, en particulier, des solutions fortes. La question de l'unicité est donc largement ouverte, et c'est une question difficile compte tenu du peu de régularité des solutions obtenues en général (solutions faibles, voire très faibles).

Plus généralement, il reste de nombreuses propriétés à interroger pour mieux comprendre le comportement qualitatif de ces systèmes : comportement au voisinage de zéro (dans l'esprit des estimations (2.38)), comportement en temps long, éventuel gain de régularité en temps court.

Entropie, dualité et existence. Grâce au Lemme de dualité, on a développé une méthode assez systématique pour les systèmes de diffusion croisée (généraux) présentant une fonctionnelle de type entropique. On peut espérer adapter cette méthode pour de nouveaux systèmes de diffusion croisée, sous réserve qu'ils possèdent une structure entropique : le problème revient donc à trouver une fonctionnelle de type entropique pour ces nouveaux systèmes. On peut par exemple considérer des systèmes de taille J pour J espèces avec $J \geq 3$ (on trouvera des travaux dans cette direction dans [29, 31]), ou encore des interactions légèrement différentes (par exemple, un modèle de type prédateur-proie avec diffusion croisée).

Problèmes d'approximation. Dans le cas général, trouver un procédé d'approximation convenable est un problème qui peut amener à des constructions complexes. Le schéma semi-discret introduit au Chapitre 5 nous permet de résoudre ce problème pour de nombreux cas (i.-e. pour de nombreux choix de paramètres). Cependant, il reste des cas où on connaît des estimations *a priori* satisfaisantes sur les solutions, mais où ce procédé ne convient pas : typiquement, dans le cas triangulaire sans auto-diffusion dans la deuxième équation, les propriétés du noyau de la chaleur fournissent des bornes *a priori* sur les dérivées de la deuxième inconnue. Dans les cas où ces estimations s'avèrent cruciales pour l'obtention de compacité sur la deuxième inconnue, il est nécessaire que le procédé d'approximation se comporte bien vis-à-vis de ces estimations : ce n'est pas le cas du schéma semi-discret.

Dans le cas triangulaire sans auto-diffusion (aucune), un procédé d'approximation "intuitif" nous est donné par le système microscopique. La démonstration de la limite singulière du système microscopique ne s'adapte pas facilement, par exemple au cas avec auto-diffusion dans une (quelconque) des deux équations. On peut se demander s'il est possible d'adapter la démonstration pour la faire fonctionner dans des cas plus généraux. Une autre direction serait construire de nouveaux modèles microscopiques pour lesquels on peut démontrer une limite singulière liée à nos systèmes de diffusions croisées. L'idée serait de fournir des informations sur le comportement qualitatif des solutions (du système de diffusion croisée).

Finalement, il reste des cas pour lesquels on a de bonnes estimations *a priori*, mais pour lesquels il reste à trouver un procédé d'approximation satisfaisant.

Chapitre 3

Introduction à la Partie III : l'équation de Boltzmann en domaine borné

Sommaire

3.1 Équation de Boltzmann

L'équation de Boltzmann a été introduite en 1872 par J. C. Maxwell et L. Boltzmann pour modéliser l'évolution des gaz raréfiés. Elle se situe à une échelle intermédiaire, dite *mésoscopique*, entre l'échelle microscopique, à laquelle le gaz est représenté par un grand nombre de molécules en interaction obéissant aux lois de la mécanique de Newton, et l'échelle macroscopique, à laquelle le gaz est représenté par un milieu continu dont la densité obéit aux lois de la mécanique des fluides. D'un côté, la modélisation à l'échelle microscopique mène à des calculs extrêmement complexes et coûteux compte tenu du grand nombre de molécules à prendre en compte ; de l'autre, la modélisation à l'échelle macroscopique peut s'avérer trop grossière [1], et faillit à expliquer certains phénomènes physiques subtils comme le fluage thermique. L'échelle mésoscopique permet des modèles de complexité et précision intermédiaires. On propose dans cette section une brève introduction à l'équation de Boltzmann : aspects de modélisation et présentation de quelques propriétés élémentaires. On trouvera une introduction complète par exemple dans [63].

3.1.1 La théorie cinétique

Pour simplifier, on suppose que le gaz considéré est constitué de particules monoatomiques identiques. On suppose aussi pour le moment que le gaz évolue dans tout l'espace $\mathbb{R}^3$. A l'échelle mésoscopique, le gaz est décrit par une équation cinétique, c'est-à-dire une équation d'évolution dont l'inconnue est la densité (en espace-vitesse) de particules $F = F(t,x,v) \geq 0$ au point x à la vitesse v, prise au temps t. Autrement dit, pour un élément de volume $\mathrm{d}x$ et un élément de volume $\mathrm{d}v$, la quantité $F(t,x,v)\,\mathrm{d}x\,\mathrm{d}v$ représente la quantité de particules qui au temps t sont situées dans l'élément de volume (centré au point x) $x + \mathrm{d}x$ et ont une vitesse dans l'élément de volume (centré en v) $v + \mathrm{d}v$.

On peut alors définir formellement les quantités macroscopiques (observables) locales suivantes :
- la densité macroscopique locale $n = n(t,x)$:

$$n(t,x) = \int_{\mathbb{R}^3} F(t,x,v)\,\mathrm{d}v,$$

- la vitesse macroscopique locale $u = u(t,x)$:

$$n(t,x)\,u(t,x) = \int_{\mathbb{R}^3} v\,F(t,x,v)\,\mathrm{d}v,$$

- la température cinétique $T(t,x)$:

$$n(t,x)\,T(t,x) = \frac{1}{3}\int_{\mathbb{R}^3} (v-u(t,x))^2\,F(t,x,v)\,\mathrm{d}v.$$

(Certaines constantes physiques on été adimensionnées et prises égales à 1.)

Si les particules ne sont soumises à aucune force extérieure et qu'on ne prend pas en compte leurs interactions entre elles, elles se déplacent linéairement à vitesse constante. Une particule qui au temps initial $t = 0$ est à la position x et est propulsée à la vitesse v va donc se déplacer le long de la trajectoire linéaire $\{(t, x + v\,t),\ t \geq 0\}$. À un temps $t > 0$, la quantité $F(t,x,v)$ de particules au point x ayant pour vitesse v est donc exactement la quantité (constante) qui a parcouru la trajectoire $\{(s, x - v(t-s)),\ s \in [0,t]\}$, et en particulier

$$F(t,x,v) = F(0, x - v\,t, v). \tag{3.1}$$

En en déduit, après dérivation par rapport au temps t,

$$\forall t \geq 0,\ \forall x, v \in \mathbb{R}^3, \qquad \partial_t F(t,x,v) + v \cdot \nabla_x F(t,x,v) = 0. \tag{3.2}$$

Cette équation est appelée *équation de transport libre.*

3.1.2 Opérateur de collision

On veut à présent prendre en compte les interactions entre les particules du gaz. Lorsque deux particules passent à proximité l'une de l'autre, le potentiel d'interaction entre les deux particules fait dévier celles-ci de leur trajectoire. Par abus de langage, on appelle ce phénomène collision. On fait les hypothèses de modélisation suivantes :

1. Autrement dit, l'approximation n'est valable que sous certaines limitations, à savoir, dans un régime d'équilibre thermodynamique.

Collisions binaires. On ne considère que les collisions entre deux particules. Cela signifie que le gaz est suffisamment peu dense pour que l'on puisse négliger les collisions entre trois particules (ou plus).

Collisions instantanées. Cela signifie que les déviations de trajectoires significatives ont lieu sur une durée et sur une distance négligeables devant les échelles de temps et, respectivement, d'espace d'observation. On traduit cela mathématiquement par l'hypothèse que chaque collision a lieu en un point x de l'espace et à un temps t. Si on appelle v et v_* les vitesses de deux particules sur le point d'entrer en collision, chacune des deux particules va donc prendre instantanément au temps t et au point x une nouvelles vitesse, disons v' et, respectivement, v'_*.

Collisions élastiques. Les collisions conservent la quantité de mouvement et l'énergie cinétique. Cela s'écrit (on a simplifié par la masse des particules, identiques) :

$$v + v_* = v' + v'_* \qquad \text{et} \qquad |v|^2 + |v_*|^2 = |v'| + |v'_*|^2.$$

Ces égalités sont équivalentes à l'existence d'un vecteur unitaire $\omega \in \mathrm{S}^2$ tel que

$$v' = v + [(v_* - v)\cdot\omega]\,\omega, \qquad v'_* = v_* - [(v_* - v)\cdot\omega]\,\omega. \tag{3.3}$$

On a donc une paramétrisation dans S^2 des vitesses postcollisionnelles (v', v'_*) en fonction des vitesses précollisionnelles (v, v_*). En particulier, lors de la collision sont conservées le module de la vitesse relative des deux particules ainsi que le module de sa composante dans la direction de la déviation ω, c'est-à-dire,

$$|v' - v'_*| = |v - v_*|, \qquad \left|\frac{v' - v'_*}{|v' - v' *|}\cdot\omega\right| = \left|\frac{v - v_*}{|v - v *|}\cdot\omega\right|. \tag{3.4}$$

Collisions microréversibles. Cette hypothèse implique que la probabilité que deux particules de vitesses précollisionnelles (v, v_*) prennent lors d'une collision les vitesses postcollisionnelles (v', v'_*) est la même que la probabilité que deux particules de vitesses précollisionnelles (v', v'_*) prennent lors d'une collision les vitesses postcollisionnelles (v, v_*).

Chaos moléculaire. Cette hypothèse signifie que les interactions entre deux particules fixées (directes ou indirectes [2]) sont extrêmement diluées dans l'ensemble des collisions que chacune subit, de sorte que lors d'une collision entre ces deux particules, on peut négliger leurs interactions précédentes. Autrement dit, le mouvement de deux particules sur le point d'entrer en collision n'est pas corrélé.

Fixons une vitesse $v \in \mathbb{R}^3$. On appelle $Q_{loss}(F,F)(t,x,v)$ la quantité de particules qui, ayant la vitesse v (au temps t et au point x) en changent (du fait d'une collision avec une particule de vitesse v_*). Grâce aux hypothèses précédentes, l'opérateur Q_{loss} prend la forme

$$Q_{loss}(F,F)(t,x,v) = \iint_{\mathbb{R}^3\times\mathbb{S}^2} F(t,x,v_*)\,F(t,x,v)\,B\left(|v - v_*|, \left|\frac{v - v_*}{|v - v *|}\cdot\omega\right|\right)\,\mathrm{d}\omega\,\mathrm{d}v_*,$$

où la fonction $B : \left(|v - v_*|, \left|\frac{v-v_*}{|v-v*|}\cdot\omega\right|\right) \mapsto B\left(|v - v_*|, \left|\frac{v-v_*}{|v-v*|}\cdot\omega\right|\right)$, liée à la section efficace de collision, renseigne sur la probabilité que deux particules de vitesses précollisionnelles (v, v_*) prennent lors d'une collision les vitesses postcollisionnelles (v', v'_*).

De la même manière, si on appelle $Q_{gain}(F,F)(t,x,v')$ la quantité de particules qui (au temps t et au point x) prennent la vitesse v' (du fait d'une collision avec une particule de vitesse v_*), on a

$$Q_{gain}(F,F)(t,x,v') = \iint_{\mathbb{R}^3\times\mathbb{S}^2} F(t,x,v_*)\,F(t,x,v)\,B\left(|v - v_*|, \left|\frac{v - v_*}{|v - v *|}\cdot\omega\right|\right)\,\mathrm{d}\omega\,\mathrm{d}v_*,$$

où, dans l'intégrale, v est définie par les relations (3.3).

Quitte à changer la notation v' en v, et v'_* en v_* (autrement dit, (v, v_*) désigne maintenant les vitesses post-collisionnelles), on obtient en utilisant à nouveau les relations (3.3) puis les relations (3.4)

$$\begin{aligned} Q_{gain}(F,F)(t,x,v) &= \iint_{\mathbb{R}^3\times\mathbb{S}^2} F(t,x,v'_*)\,F(t,x,v')\,B\left(|v' - v'_*|, \left|\frac{v' - v'_*}{|v' - v' *|}\cdot\omega\right|\right)\,\mathrm{d}\omega\,\mathrm{d}v_* \\ &= \iint_{\mathbb{R}^3\times\mathbb{S}^2} F(t,x,v'_*)\,F(t,x,v')\,B\left(|v - v_*|, \left|\frac{v - v_*}{|v - v *|}\cdot\omega\right|\right)\,\mathrm{d}\omega\,\mathrm{d}v_*. \end{aligned}$$

2. par exemple, si une des deux particules entre en collision avec une troisième particule ayant interagi avec la deuxième.

On écrit le bilan des collisions

$$Q(F,F)(t,x,v) \quad := \quad Q_{gain}(F,F)(t,x,v) - Q_{loss}(F,F)(t,x,v).$$

et on peut finalement écrire l'opérateur de collision Q sous la forme (la dépendance en (t,x) est sous-entendue)

$$Q(F,F)(v) = \iint_{\mathbb{R}^3\times\mathbb{S}^2} [F(v'_*)\,F(v') - F(v_*)\,F(v)]\,B\left(|v-v_*|, \left|\frac{v-v_*}{|v-v*|}\cdot\omega\right|\right)\,\mathrm{d}\omega\,\mathrm{d}v_*.$$

Remarquons que l'opérateur de collision n'agit que sur la variable de vitesse, c'est-à-dire, $Q(F,F)$ ne dépend du temps et de l'espace qu'à travers F.

On fera pour l'opérateur de collision les hypothèses simplificatrices suivantes : B s'écrit

$$B\left(|v-v_*|, \left|\frac{v-v_*}{|v-v*|}\cdot\omega\right|\right) = |v-v_*|^\kappa\,q_0\left(\left|\frac{v-v_*}{|v-v*|}\cdot\omega\right|\right),$$

avec

$$0 \le \kappa \le 1 \quad \text{(potentiel dur)},$$
$$0 \le q_0(a) \le C|\cos a| \quad \text{(troncature angulaire)}.$$

Ces hypothèses classiques ont un intérêt mathématique : elles permettent de simplifier ou expliciter certains calculs.

Finalement, l'équation de Boltzmann s'écrit

$$\partial_t F(t,x,v) + v\cdot\nabla_x F(t,x,v) = Q(F,F)(t,x,v). \tag{3.5}$$

3.1.3 Quelques propriétés

On énonce ici quelques propriété fondamentales de l'équation de Boltzmann.

Conservation de certains moments. En multipliant par le vecteur $(1, v, |v|^2)$ chaque terme de l'équation de Boltzmann et en intégrant sur l'ensemble des vitesses $v\in\mathbb{R}^3$ et dans tout l'espace $\mathbb{R}^3$, on montre formellement la conservation des quantités macroscopiques suivantes :
- la masse totale

$$\int_{\mathbb{R}^3} n(t,x,v)\,\mathrm{d}x = \int_{\mathbb{R}^3} n(0,x,v)\,\mathrm{d}x,$$

- la quantité de mouvement

$$\int_{\mathbb{R}^3} n(t,x)\,u(t,x)\,\mathrm{d}x = \int_{\mathbb{R}^3} n(0,x)\,u(0,x)\,\mathrm{d}x,$$

- l'énergie

$$\int_{\mathbb{R}^3} E(t,x)\,\mathrm{d}x = \int_{\mathbb{R}^3} E(0,x)\,\mathrm{d}x,$$

où $E = n\,(|u|^2 + 3T)$, et où les quantités n, u et T ont été définies au 3.1.1.

Distribution Maxwellienne. Soit $n = n(t,x) \ge 0$ et $T = T(t,x) > 0$ deux fonctions à valeurs positives, et $u = u(t,x)$ à valeurs dans $\mathbb{R}^3$. On définit la *distribution Maxwellienne locale* $\mu_{n,u,T}$ de densité n, de vitesse macroscopique u et de température T par (certaines quantités sont adimensionnées)

$$\mu_{n,u,T}(t,x,v) = \frac{n(t,x)}{(2\pi\,T(t,x))^{3/2}} e^{-|v-u(t,x)|^2/2T(t,x)}. \tag{3.6}$$

On a alors la propriété formelle suivante : pour toute fonction $F = F(t,x,v) \ge 0$, on a l'inégalité

$$\forall t\ge 0,\ \forall x\in\mathbb{R}^3, \qquad \int_{\mathbb{R}^3} Q(F,F)(t,x,v)\,\log F(t,x,v)\,\mathrm{d}v \;\le\; 0 \tag{3.7}$$

avec égalité si et seulement si F est une distribution Maxwellienne locale. De cette propriété on déduit formellement :

$$\forall F = F(t,x,v)\ge 0, \qquad Q(F,F) = 0 \;\Leftrightarrow\; F \text{ est une densité Maxwellienne locale.}$$

En particulier, toute distribution Maxwellienne $\mu_{n,u,T}$ stationnaire et homogène (i.-e. on prend n, u et T constantes) vérifie $\partial_t\mu_{n,u,T} + v\cdot\nabla_x\mu_{n,u,T} = 0 = Q(\mu_{n,u,T},\mu_{n,u,T})$ et fournit donc une solution particulière de l'équation de Boltzmann.

Théorème H. Une autre conséquence de la propriété (3.7) est le Théorème H de Boltzmann. On définit l'entropie H par

$$\forall t \geq 0, \qquad H(t) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} F(t,x,v) \, \log F(t,x,v) \, \mathrm{d}v \, \mathrm{d}x.$$

Alors, si $F = F(t,x,v) \geq 0$ est une solution de l'équation de Boltzmann, on a formellement

$$\mathrm{d}_t H(t) = \int_{\mathbb{R}^3} Q(F,F) \, \log F(t,x,v)(t,x,v) \, \mathrm{d}v \, \mathrm{d}x \leq 0,$$

avec égalité si et seulement si F est une distribution Maxwellienne.

Le Théorème H joue un rôle fondamental dans l'analyse de l'équation de Boltzmann. Formellement, il indique que l'effet des collisions est de faire tendre le gaz à se comporter en temps long selon une loi de densité de distribution Maxwellienne. D'un point de vue physique, il traduit l'irréversibilité de l'équation de Boltzmann.

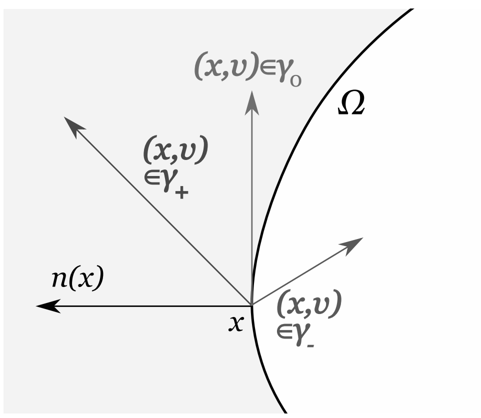
3.2 Conditions au bord

Dans la plupart des applications, le gaz rencontre des objets solides, voire évolue dans un espace confiné. Il faut alors prendre en compte dans notre modèle les collisions des particules de gaz avec les parois en présence (dont on verra qu'elles ont un effet radical sur le comportement mathématique de la densité de gaz). Ici on considère le cas d'un gaz confiné, et on note Ω le domaine borné de $\mathbb{R}^3$ dans lequel le gaz évolue. A l'intérieur du domaine, le gaz satisfait l'équation de Boltzmann. L'objectif de cette section est de rappeler quelques éléments de modélisation de l'interaction du gaz avec les parois du domaine. Pour plus de détails, voir par exemple [62] et les références citées.

Soit un point $x \in \partial\Omega$ sur le bord du domaine. On appelle $n = n(x)$ la normale au bord au point x dirigée vers l'extérieur. Une particule au point x ayant la vitesse v se dirige vers l'extérieur du domaine (donc vers le solide) si $v \cdot n(x) > 0$. Au contraire, elle se dirige vers l'intérieur du domaine (s'éloigne du solide) si $v \cdot n(x) < 0$. Enfin, la particule est dite rasante si elle se dirige tangentiellement au bord, c'est-à-dire si $v \cdot n(x) = 0$. Les particules rasantes au point $x \in \partial\Omega$ peuvent être dirigées vers l'intérieur ou l'extérieur du domaine suivant que le point x est un point de (stricte) convexité ou de (stricte) concavité, d'inflexion, etc., du bord. Il est utile d'introduire les définitions suivantes :

$$\begin{aligned}
\gamma_+ &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) > 0\}, \qquad &\text{(bord sortant)}\\
\gamma_- &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) < 0\}, \qquad &\text{(bord entrant)}\\
\gamma_0 &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) = 0\}, \qquad &\text{(bord rasant)}
\end{aligned}$$

qui sont représentées sur le schéma suivant.



Généralement, pour une équation cinétique, on impose une condition au bord définissant le flux sur le bord entrant, de la forme

$$\forall t \geq 0, \, \forall (x,v) \in \gamma_-, \qquad F(t,x,v) = g(t,x,v), \tag{3.8}$$

où g est une fonction à préciser. Physiquement, cela implique que la présence du bord ne se traduit directement que sur les particules qui viennent de toucher le bord. Autrement dit, la dynamique des particules sortantes (donc "avant" collision avec le bord) est définie uniquement par les phénomènes en jeu à l'intérieur du domaine. Il est parfois utile de considérer le cas où on connait exactement le flux entrant : c'est le cas par exemple si on injecte du gaz dans un domaine. La fonction $g = g(t, x, v)$ est alors donnée, et on parle simplement de *condition entrante (donnée)* au bord. Mais dans de nombreux cas on devra modéliser les collisions des particules (sortantes) avec le bord du domaine pour définir le flux entrant. La fonction $g = g(t, x, v)$ s'écrit alors comme une fonctionnelle du flux sortant $F_{|\gamma_+}$ (fonctionnelle à préciser dans la phase de modélisation), et on parle de *condition de réflexion* au bord. On détaille ce cas ci-dessous.

On suppose qu'une particule heurtant la paroi au point x avec la vitesse v dirigée vers la paroi ($v \cdot n(x) > 0$) rebondit au même point instantanément [3] avec une nouvelle vitesse v', et on note $p(v \to v')$ la densité de probabilité que la particule ayant la vitesse v prenne au moment du rebond la vitesse v'. Si on appelle $\mathrm{d}t$ un élément réel et $\mathrm{d}\sigma(x)$ un élément de surface autour du point $x \in \partial\Omega$, la quantité de particules heurtant entre le temps t et le temps $t + \mathrm{d}t$ l'élement de surface $\mathrm{d}\sigma(x)$ avec la vitesse v vaut

$$F(t, x, v)\, |v \cdot n(x)|\, \mathrm{d}\sigma(x)\, \mathrm{d}t.$$

De même, la quantité de particules émergeant entre le temps t et le temps $t + \mathrm{d}t$ de l'élement de surface $\mathrm{d}\sigma(x)$ avec la vitesse v' vaut

$$F(t, x, v')\, |v' \cdot n(x)|\, \mathrm{d}\sigma(x)\, \mathrm{d}t.$$

Cette quantité est exactement le nombre de particules qui après rebond entre t et $t + \mathrm{d}t$ en un point de $\mathrm{d}\sigma(x)$ prennent la vitesse v', et s'exprime donc par

$$F(t, x, v')\, |v' \cdot n(x)|\, \mathrm{d}\sigma(x)\, \mathrm{d}t = \int_{v:\, v \cdot n(x) > 0} p(v \to v') F(t, x, v) |v \cdot n(x)|\, \mathrm{d}\sigma(x)\, \mathrm{d}v\, \mathrm{d}t.$$

En simplifiant par $\mathrm{d}\sigma(x)\, \mathrm{d}t$, on obtient

$$F(t, x, v')\, |v' \cdot n(x)| = \int_{v:\, v \cdot n(x) > 0} p(v \to v') F(t, x, v) |v \cdot n(x)|\, \mathrm{d}v. \tag{3.9}$$

Comme $p(v \to \cdot)$ est une densité de probabilité sur $\{v' : v' \cdot n(x) < 0\}$, on a $\int_{v':\, v' \cdot n(x) < 0} p(v \to v')\, \mathrm{d}v' = 1$, et donc, en intégrant en v' l'égalité ci-dessus, on obtient (formellement) la *conservation de la masse* au point x :

$$\int_{v':\, v' \cdot n(x) < 0} F(t, x, v')\, |v' \cdot n(x)|\, \mathrm{d}v' = \int_{v:\, v \cdot n(x) > 0} F(t, x, v)\, |v \cdot n(x)|\, \mathrm{d}v.$$

Autrement dit, la quantité de particules sortantes au point x et au temps t est égale à la quantité de particules entrantes au point x et au temps t : c'est une conséquence de l'hypothèse d'instantanéité des collisions avec le bord.

Il reste à déterminer la fonction $p(v \to v')$. Plusieurs types de réflexion au bord sont généralement considérées :

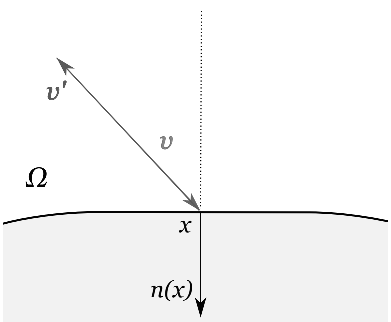


FIGURE 3.1 – Réflexion inverse

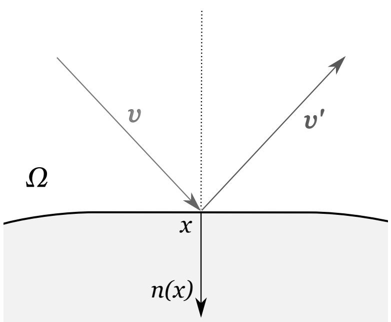


FIGURE 3.2 – Réflexion spéculaire

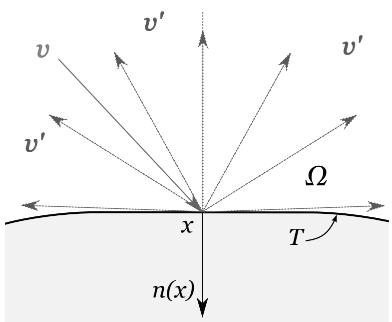


FIGURE 3.3 – Réflexion diffusive

3. Plus précisément, on suppose que la paroi absorbe la particule et la relâche en un temps suffisamment court devant les durées d'observation pour être négligé, et à un point suffisamment proche de x devant la taille du domaine.

Réflexion inverse. On suppose qu'une particule à vitesse v rebondit (systématiquement) avec la vitesse $-v$, c'est-à-dire

$$p(v \to v') = \delta_0(v + v'),$$

où on a noté δ_0 la distribution de Dirac au point 0. En réinsérant dans (3.9), on trouve que la condition de réflexion inverse s'écrit

$$\forall t \geq 0,\, \forall (x,v) \in \gamma_-, \qquad F(t,x,v) = F(t,x,-v). \tag{3.10}$$

Réflexion spéculaire. Physiquement, la réflexion spéculaire est obtenue si on considère que le bord est parfaitement élastique, et que la pression exercée au moment du choc avec une particule est dirigée selon la normale au point du choc. Alors, une particule à vitesse v rebondit (systématiquement) symétriquement par rapport à la normale au bord (comme une boule de billard), c'est-à-dire

$$p(v \to v') = \delta_0(v' - v + 2\,(v \cdot n(x))n(x)).$$

En réinsérant dans (3.9), on trouve que la condition de réflexion spéculaire s'écrit

$$\forall t \geq 0,\, \forall (x,v) \in \gamma_-, \qquad F(t,x,v) = F(t,x,v - 2\,(v \cdot n(x))n(x)). \tag{3.11}$$

Réflexion diffusive. La réflexion diffusive permet d'introduire de l'aléa, au sens où la vitesse après choc n'est pas entièrement déterminée par la vitesse avant choc et la géométrie du bord. Cet aléa modélise les nombreuses approximations, liées par exemple à l'hypothèse d'un bord lisse et d'épaisseur nulle (de co-dimension 1), c'est-à-dire à la non-prise en compte de chacune des molécules de la paroi (position et vitesse). On suppose que la paroi est à l'équilibre, de température constante notée T. En particulier, on néglige l'effet des collisions des particules de gaz sur l'état de la paroi. On suppose

$$p(v \to v') = c_\mu \mu_T(v')|v' \cdot n(x)|,$$

où $\mu_T = \mu_{1,0,T}(v)$ est une distribution Maxwellienne (3.6) de densité unitaire, de vitesse macroscopique nulle et de température T, et où c_μ est une constante positive définie de sorte que $p(v \to v')$ est bien une densité de probabilité sur $\{v' : v' \cdot n(x) < 0\}$, c'est-à-dire

$$c_\mu \int_{v' :\, v' \cdot n(x) < 0} \mu_T(v')|v' \cdot n(x)|\, \mathrm{d}v' = 1.$$

En réinsérant dans (3.9), on trouve que la condition de réflexion diffusive s'écrit

$$\forall t \geq 0,\, \forall (x,v) \in \gamma_-, \qquad F(t,x,v) = c_\mu \mu_T(v) \int_{u :\, u \cdot n(x) > 0} F(t,x,u)\,(u \cdot n(x))\, \mathrm{d}u. \tag{3.12}$$

Ce choix implique que le flux sortant est à la température T. Physiquement, cela signifie que la paroi "transmet" sa température au gaz au moment de la collision.

Réflexion de Maxwell. Le modèle le plus pertinent du point de vue physique est de considérer une combinaison de la condition de réflexion spéculaire et de la condition de réflexion diffusive : c'est la condition de réflexion de Maxwell, qui s'écrit

$$\begin{aligned} \forall t \geq 0,\, \forall (x,v) \in \gamma_-, \qquad F(t,x,v) =& (1-\alpha)F(t,x,v - 2\,(v \cdot n(x))n(x)) \\ &+ \alpha c_\mu \mu_T(v) \int_{u :\, u \cdot n(x) > 0} F(t,x,u)\,(u \cdot n(x))\, \mathrm{d}u, \end{aligned} \tag{3.13}$$

où $\alpha \in]0,1[$ est le coefficient d'accommodation. Le coefficient d'accommodation α étant proche de 1, la condition de réflexion diffusive, plus simple mathématiquement, est souvent prise pour approximer la condition de réflexion de Maxwell. Ce sera notre cas ici : à l'exception de la Remarque 3.2 et du premier paragraphe de la Section 3.7.2, dans tout ce Chapitre il sera toujours question de réflexion diffusive au bord.

Remarque 3.1. *La distribution Maxwellienne μ_T satisfait chacune des conditions de réflexions au bord présentées ci-dessus (avec $T > 0$ la température du bord dans les cas de réflexions diffusive et de Maxwell, et avec $T > 0$ quelconque dans les cas de réflexions inverse et spéculaire). Pour chacun des types de réflexions au bord introduits ci-dessus, on a donc une solution (sationnaire et homogène) de l'équation de Boltzmann avec conditions au bord, fournie par la distribution Maxwellienne μ_T.*

3.3 Contexte mathématique

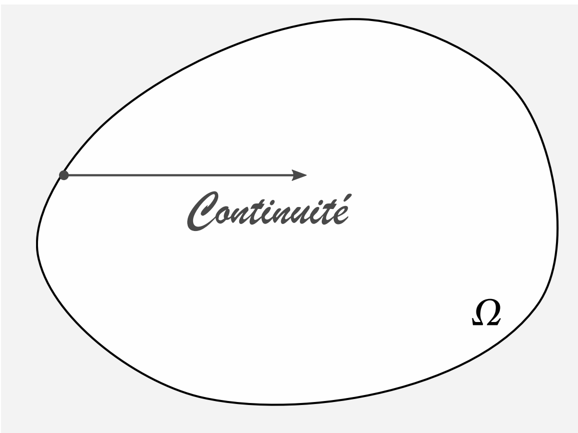
On présente dans cette section l'état de l'art pour les questions de l'existence et de la régularité de l'équation de Boltzmann en domaine borné avec condition de réflexion diffusive au bord. Il existe dans la littérature de nombreux résultats dans des domaines particuliers (non nécessairement bornés, typiquement dans le demi-espace, dans une boule ou entre deux plateaux) : on pourra consulter une bibliographie détaillée dans le livre de Y. Sone [86]. Concernant un domaine borné général, de nombreux résultats concernent l'existence de solutions ayant (*a priori*) une régularité très faible (plus précisément, des solutions renormalisées de DiPerna-Lions) : on pourra consulter à ce sujet [78, 61, 57, 58, 82], ainsi que [63] qui contient une bibliographie sur cette question. Une autre direction concerne des solutions plus fortes dans un cadre perturbatif au voisinage de l'équilibre Maxwellien : ces méthodes ont été introduites dans le cadre de domaines avec une géométrie particulière par J.-P. Guiraud [72] et S. Ukai [87] (voir aussi [88, 84]) puis développées dans le cadre de domaines bornés généraux par Y. Guo [75]. C'est dans cette direction que cette thèse s'inscrit [4].

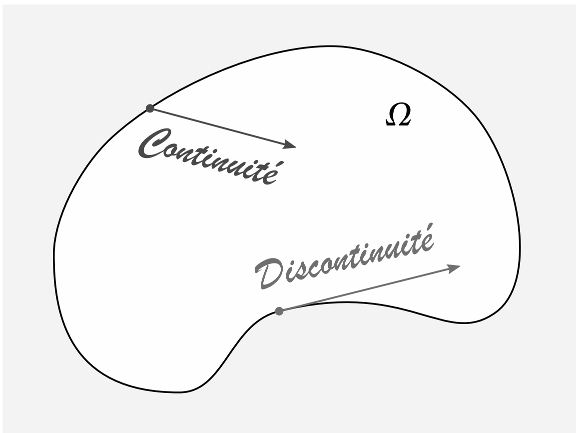
L'existence de solutions fortes globales proches de l'équilibre a été établie en 2010 par Y. Guo dans [75]. Il y démontre notamment les résultats suivants, pour une donnée initiale proche d'une distribution Maxwellienne globale :
- l'existence d'une unique solution globale forte dans un certain espace L^∞ (en espace-vitesse) avec un poids en vitesse adéquat,
- la relaxation de la solution vers l'équilibre Maxwellien avec une vitesse exponentielle,
- dans le cas où le domaine Ω est strictement convexe, la continuité de la solution (en espace-vitesse) à part au bord rasant, pour tout temps (si la donnée initiale a la même continuité).

D'autre part, C. Kim a montré en 2011 dans [81] que dans le cas d'un domaine non convexe, une singularité sévère pouvait apparaître. Plus précisément, on peut résumer son résultat de la manière suivante : si Ω est un domaine (strictement) non convexe, soit $x_0 \in \partial\Omega$ un point de non-convexité du bord et soit v_0 une vitesse tangente au bord au point x_0 et dirigée vers l'intérieur du domaine, alors on peut trouver une donnée initiale régulière ($\mathscr{C}^\infty$) proche de l'équilibre Maxwellien, et telle que
- il existe une unique solution globale issue de cette donnée initiale,
- la solution devient discontinue (en espace-vitesse) au point (x_0, v_0) au bout d'un certain temps fini t_0,
- la discontinuité se propage à l'intérieur du domaine, le long de la trajectoire linéaire issue de (x_0, v_0) (c'est à dire $\{x_0 + v_0\, t \in \Omega,\, t \geq 0\}$).

De plus, si (x, v) est un point du bord rasant suffisamment proche de (x_0, v_0), alors la solution est discontinue (en espace-vitesse) au point (x, v) au temps t_0, et la discontinuité se propage le long de la trajectoire linéaire issue de (x, v).

Pour Ω un domaine borné régulier, on peut donc résumer les résultats de régularité obtenus par Y. Guo et C. Kim par le schéma suivant, selon que le domaine Ω est ou non convexe.





4. Comparons avec la théorie de l'équation de Boltzmann dans tout l'espace. Pour résumer, il existe trois directions principales qui mènent à une théorie d'existence (globale) de solutions :
-l'étude de solutions fortes proches du vide ($F \sim 0$), qui consiste en un sens à négliger l'effet des collisions,
-l'étude de solutions fortes proches de l'équilibre Maxwellien ($F \sim \mu_T$),
-l'étude de solutions renormalisées.
Un intérêt de l'étude autour de l'équilibre Maxwellien est le lien avec l'hydrodynamique. La théorie des solutions renormalisées permet l'existence de solutions dans un cadre très large, mais le prix à payer est la régularité extrêmement faible des solutions, qui mène en particulier à des problèmes d'unicité. On pourra consulter par exemple [63] autour de ces questions.

Dans les deux cas (convexe/non convexe), les singularités peuvent apparaître uniquement au bord rasant γ_0. La différence essentielle réside en le fait que dans le cas strictement convexe, les trajectoires linéaires issues du bord rasant sont réduites à des points (elles "sortent" du domaine instantanément), alors que dans le cas strictement non convexe, certaines de ces trajectoires (précisément, celles issues du bord rasant aux points de concavité ou d'inflexion du bord) traversent l'intérieur du domaine. Dans ce deuxième cas, la singularité formée au bord rasant se propage alors à l'intérieur du domaine, le long des trajectoires rasantes.

Dans ce contexte, il est naturel de se demander quelle est la régularité de la solution dans chacun des deux cas convexe/non convexe. Peut-on prouver une certaine régularité des dérivées de la solution ? La difficulté pour répondre à cette question est le traitement de la condition au bord en interaction avec l'opérateur de transport. En particulier, comment définir au bord la dérivée en espace de la solution dans la direction normale au bord ? Heuristiquement, on se propose d'utiliser l'équation de Boltzmann "jusqu'au bord", c'est-à-dire $\partial_t F + v \cdot \nabla_x F = Q(F, F)$ sur le bord. Si on note n la normale au bord et (τ_1, τ_2, n) une base orthonormée, on obtient $\partial_n F = (v \cdot n)^{-1}\{Q(F, F) - \partial_t F - \sum_i (v \cdot \tau_i)\partial_{\tau_i} F\}$. Remarquons la singularité en $(v \cdot n)^{-1}$! L'équation d'évolution de la différentielle en vitesse (obtenue heuristiquement en différenciant l'équation de Boltzmann par rapport à la variable vitesse) étant couplée avec la différentielle en espace, on s'attend à ce que cette singularité se répercute sur la différentielle en vitesse de la solution. En revanche, notons que la dérivée en temps est découplée des autres dérivées, et satisfait un problème avec condition au bord très similaire à celui de la solution (identique à l'opérateur de collision près, qui est alors "linéarisé" autour de la solution F). Le traitement de la dérivée en temps est donc plus classique : il est analogue à celui de la solution elle-même.

Dans le cas où le domaine n'est pas convexe, une difficulté supplémentaire est de définir les traces sur le bord rasant, qui demandent donc un traitement spécifique. Compte tenu de la propagation de discontinuité le long des trajectoires rasantes, les espaces fonctionnels considérés doivent être suffisamment faibles pour contenir des fonctions discontinues (sur un ensemble de codimension 1, voir Chapitre 8) : cela exclut donc les espaces de Sobolev faisant intervenir un nombre entier de derivées, auxquels on préfèrera l'espace BV.

Dans ce manuscrit, on présente les résultats suivants : on étudie d'abord au Chapitre 7 le cas convexe, pour lequel on montre la propagation d'une régularité de type Sobolev pour la solution, à l'ajout d'un "poids" près qu'on appèle *distance cinétique*. Cette distance cinétique permet de mesurer précisément la sévérité de la singularité au bord rasant. De plus, on obtient la propagation de la régularité $\mathscr{C}^1$ en dehors du bord rasant. Dans le cas non convexe, on montre au Chapitre 8 la propagation de la régularité BV pour la solution. Pour chacun des deux cas, on indique en quoi ces résultats sont optimaux.

Remarque 3.2. *Les résultats de Y. Guo présentés ci-dessus (existence, comportement asymptotique, régularité) sont en fait établis pour les quatre types de conditions au bord usuelles : condition rentrante, réflexion diffusive, réflexion spéculaire et inverse. De même, les résultats de C. Kim (formation et propagation de discontinuité en domaine non convexe) sont en fait établis pour les trois types de conditions au bord : condition rentrante, réflexion diffusive et inverse. En Annexe on présente aussi des résultats de régularité $\mathscr{C}^1$ (en dehors du bord rasant) des solutions pour les trois types de conditions de réflexion au bord (diffusive, spéculaire, inverse) : voir Section 3.7.2.*

3.4 Hypothèses, notations et théorème d'existence

On considère un domaine Ω borné et régulier, c'est-à-dire qu'il existe une fonction ξ régulière ($\mathscr{C}^3$) sur $\mathbb{R}^3$ telle que

$$\Omega := \{x \in \mathbb{R}^3 : \xi(x) < 0\} \tag{3.14}$$

est borné. On a alors les égalités

$$\partial\Omega = \{x \in \mathbb{R}^3 : \xi(x) = 0\}, \qquad \overline{\Omega} = \{x \in \mathbb{R}^3 : \xi(x) \leq 0\}.$$

On dira que Ω est strictement convexe si pour tout $x \in \overline{\Omega}$,

$$\sum_{i,j} \partial_{ij}\xi(x)\zeta_i\zeta_j \geq C_\xi |\zeta|^2 \quad \text{pour tout} \quad \zeta \in \mathbb{R}^3. \tag{3.15}$$

On rappelle les notations suivantes : $n = n(x)$ est la normale au bord au point $x \in \partial\Omega$, et

$$\begin{aligned}
\gamma_+ &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) > 0\},\\
\gamma_- &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) < 0\},\\
\gamma_0 &= \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : v \cdot n(x) = 0\}.
\end{aligned}$$

On appelle μ la distribution Maxwellienne globale de vitesse macroscopique nulle et de température $T = 1$ (pour simplifier) renormalisée, $\mu(v) = e^{-|v|^2/2}$, et on définit f par

$$F(t,x,v) = \sqrt{\mu(v)}\, f(t,x,v).$$

Le problème de Cauchy avec condition diffusive au bord se réécrit alors

$$\begin{cases}
\partial_t f + v \cdot \nabla_x f + \nu[\sqrt{\mu} f] f = \Gamma_{\mathrm{gain}}(f,f), & \text{dans } \mathbb{R}_+ \times \Omega \times \mathbb{R}^3,\\
f_{|t=0} = f^0, & \text{dans } \Omega \times \mathbb{R}^3,\\
f_{|\gamma_-} = c_\mu \sqrt{\mu(v)} \displaystyle\int_{u\cdot n(x)>0} \sqrt{\mu(u)} f(u) u \cdot n(x)\, \mathrm{d}u, & \text{dans } \mathbb{R}_+ \times \gamma_-,
\end{cases} \tag{3.16}$$

avec

$$\begin{aligned}
\nu[\sqrt{\mu} f] &= Q_{\mathrm{loss}}(\sqrt{\mu} f, 1) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} |v-u|^\kappa \{\sqrt{\mu}(u) f(u)\} q_0\left(\left|\tfrac{v-u}{|v-u|} \cdot \omega\right|\right) \mathrm{d}\omega\, \mathrm{d}u \geq 0,\\
\Gamma_{\mathrm{gain}}(f,f) &= \tfrac{Q_{\mathrm{gain}}(\sqrt{\mu} f, \sqrt{\mu} f)}{\sqrt{\mu(v)}} = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} |v-u|^\kappa \{\sqrt{\mu}(u) f(u') f(v')\} q_0\left(\left|\tfrac{v-u}{|v-u|} \cdot \omega\right|\right) \mathrm{d}\omega\, \mathrm{d}u,
\end{aligned}$$

où $v' = v + [(u-v)\cdot\omega]\,\omega$, $u' = u - [(u-v)\cdot\omega]\,\omega$, et où on suppose

$$0 \leq \kappa \leq 1 \quad \text{(potentiel dur)}, \qquad 0 \leq q_0(a) \leq C|\cos a| \quad \text{(troncature angulaire)}. \tag{3.17}$$

Espaces fonctionnels. On note, pour $1 \leq p < \infty$, et pour $u = u(x,v)$ une fonction sur $\Omega \times \mathbb{R}^3$,

$$\begin{aligned}
\|u\|_{\mathrm{L}^p} &= \left(\iint_{\Omega\times\mathbb{R}^3} |u|^p\right)^{1/p}, & \|u\|_{\mathrm{L}^\infty} &= \sup\nolimits_{\Omega\times\mathbb{R}^3} |u|,\\
\|u\|_{\mathrm{W}^{1,p}} &= \|u\|_{\mathrm{L}^p} + \|\nabla_{x,v} u\|_{\mathrm{L}^p}, & \|u\|_{BV} &= \|u\|_{\mathrm{L}^1} + V(u),
\end{aligned}$$

où $V(u)$ est la variation totale de u sur $\Omega \times \mathbb{R}^3$,

$$V(u) = \sup\Big\{ \iint_{\Omega\times\mathbb{R}^3} u \,\mathrm{div}_{x,v}\varphi \,\mathrm{d}x\,\mathrm{d}v : \varphi \in \mathscr{C}_c^1(\Omega\times\mathbb{R}^3; \mathbb{R}^3\times\mathbb{R}^3),\ |\varphi| \leq 1\Big\}.$$

Pour $E = \mathrm{L}^p$, L^∞, $\mathrm{W}^{1,p}$, BV, on note naturellement $E = E(\Omega\times\mathbb{R}^3) = \{u :\ \|u\|_E < \infty\}$.

Sur le bord $\gamma = \partial\Omega \times \mathbb{R}^3$, on introduit la mesure

$$\mathrm{d}\gamma = |v \cdot n(x)|\ \mathrm{d}\sigma(x)\,\mathrm{d}v, \tag{3.18}$$

où σ est la mesure de Lebesgue sur $\partial\Omega$. On définit naturellement les normes associées pour $1 \leq p < \infty$, et pour $u = u(x,v)$ une fonction sur γ,

$$|u|_{\gamma,p} = \left(\int_\gamma |u|^p\,\mathrm{d}\gamma\right)^{1/p}.$$

Notation. On écrit $X \lesssim Y$ quand il existe une constante $C > 0$ (indépendante de X et Y) telle que $X \leq CY$. On écrit $X \lesssim_\alpha Y$ dans la même situation quand on veut préciser que la constante $C = C(\alpha)$ dépend du paramètre α. De plus, quand on indique une dépendance en temps t sous la forme $X \lesssim_t Y$ (ou $X \lesssim_{t,\alpha} Y$), la constante $C = C(t)$ (ou $C = C(t,\alpha)$) peut être choisie continue et croissante en t.

Enfin, pour tout $v \in \mathbb{R}^3$, on note $\langle v\rangle = \sqrt{1+|v^2|}$.

Théorème d'existence. On présente d'abord un résultat d'existence de solutions locales (en temps), qui s'avèrent être globales dans un régime proche de l'équilibre Maxwellien. Ce résultat vaut pour un domaine Ω borné quelconque (sans hypothèse de convexité). Si le domaine est convexe, on obtient de plus la continuité de la dérivée temporelle de la solution.

Théorème 3.1 (Existence (Guo, Kim, Tonon, T.)). *Soit Ω un domaine borné et régulier de $\mathbb{R}^3$. On suppose* (3.17)*. Soit $0 < \theta' < \theta < 1/4$ et $f_0 \geq 0$ une donnée initiale satisfaisant*

$$||e^{\theta|v|^2} f_0||_\infty < +\infty. \tag{3.19}$$

Alors,
i) il existe $T_* = T_*(||e^{\theta|v|^2} f_0||_\infty) > 0$ tel qu'il existe une unique solution $f \geq 0$ de (3.16) *sur $[0,T_*)\times\Omega\times\mathbb{R}^3$ telle que pour tout $0 \leq t < T_*$,*

$$||e^{\theta'|v|^2} f(t)||_\infty \lesssim_t P(||e^{\theta|v|^2} f_0||_\infty), \tag{3.20}$$

pour un certain polynôme P.

ii) Soit $0 \leq \bar{\theta} < \frac{1}{4}$. Si $e^{\bar{\theta}|v|^2}\partial_t f_0 := e^{\bar{\theta}|v|^2} \frac{-v\cdot\nabla_x F_0 + Q(F_0,F_0)}{\sqrt{\mu}} \in \mathrm{L}^\infty(\Omega\times\mathbb{R}^3)$ et si f_0 satisfait la condition de compatibilité au bord

$$f_0(x,v) = c_\mu\sqrt{\mu(v)} \int_{n(x)\cdot u>0} f_0(x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \qquad \textit{pour tout } (x,v)\in\gamma_-, \tag{3.21}$$

alors pour tout $0 \leq t < T_*$,

$$||e^{\bar{\theta}|v|^2}\partial_t f(t)||_\infty \lesssim_t P(||e^{\bar{\theta}|v|^2}\partial_t f_0||_\infty) + P(||e^{\theta|v|^2} f_0||_\infty), \tag{3.22}$$

pour un certain polynôme P.

iii) Si Ω est strictement convexe (3.15) *et si f_0 est continue et satisfait la condition de compatibilité* (3.21)*, alors f est continue en dehors du bord rasant γ_0.*

Enfin, si $||e^{\theta|v|^2}(f_0 - \sqrt{\mu})||_\infty \ll 1$ alors $T_* = +\infty$, c'est-à-dire, les résultats précédents sont vrais pour tout $t \geq 0$.

Ce théorème est à comparer avec le théorème d'existence et de continuité (cas convexe) de Y. Guo, [75], qui se place dans un cadre perturbatif autour d'une distribution Maxwellienne globale et qui prend en compte un poids polynomial en vitesse (et non pas exponentiel). La démonstration, qui repose sur les méthodes de la démonstration de Y. Guo, se trouve au Chapitre 7.

3.5 Propagation de régularité de Sobolev en domaine convexe

On suppose dans toute cette section que le domaine Ω considéré est convexe (3.15). On présente deux Théorèmes de propagation de régularité de type Sobolev et $\mathscr{C}^1$, et on commente l'optimalité de ces résultats.

Théorème 3.2 (Propagation $\mathrm{W}^{1,p}$, $1 < p < 2$ (Guo, Kim, Tonon, T.)). *Soit Ω un domaine borné régulier convexe* (3.15) *de $\mathbb{R}^3$. On suppose* (3.17)*. Soit $0 < \theta < 1/4$, $1 < p < 2$ et $f_0 \geq 0$ une donnée initiale satisfaisant* (3.19)*, $f_0 \in \mathrm{W}^{1,p}(\Omega\times\mathbb{R}^3)$ et la condition de compatibilité* (3.21)*. On considère $T_* = T_*(||e^{\theta|v|^2} f_0||_\infty) > 0$ et f l'unique solution de* (3.16) *sur $[0,T_*)\times\Omega\times\mathbb{R}^3$ fournis par le Théorème 3.1.*

Alors, $f \in \mathrm{L}^\infty_{loc}([0,T_*);\mathrm{W}^{1,p}(\Omega\times\mathbb{R}^3))$ et, pour tout $0 \leq t < T_*$,

$$||\nabla_{x,v} f(t)||_p^p + \int_0^t |\nabla_{x,v} f(s)|_{\gamma,p}^p \mathrm{d}s \lesssim_t ||\nabla_{x,v} f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty), \tag{3.23}$$

pour un certain polynôme P.

On rappelle que si $||e^{\theta|v|^2}(f_0 - \sqrt{\mu})||_\infty \ll 1$ alors $T_* = +\infty$; en particulier, les résultats précédents sont alors vrais pour tout $t \geq 0$.

La démonstration du Théorème 3.2 se trouve au Chapitre 7.

La Proposition suivante indique que la restriction $p < 2$ semble être optimale, au sens où on s'attend à ce que le résultat ne s'étende pas au cas $p = 2$. On exhibe en effet un contre-exemple pour le problème (plus simple) de transport libre avec réflexion diffusive au bord, dans le cas particulier où le domaine considéré est la boule unité.

Proposition 3.1 (Explosion $\mathrm{W}^{1,2}$ (Guo, Kim, Tonon, T.))**.** *Soit $B(0;1) := \{x \in \mathbb{R}^3 : |x| < 1\}$. Alors, il existe une donnée initiale $f_0(x,v) \geq 0$ infiniment dérivable et à support compact dans $B(0;1) \times B(0;1)$ telle que la solution f du système*

$$\begin{aligned} &\partial_t f + v \cdot \nabla_x f = 0, \quad \text{dans } \mathbb{R}_+ \times \Omega \times \mathbb{R}^3, \quad f|_{t=0} = f_0, \quad \text{dans } \Omega \times \mathbb{R}^3, \\ &f(t,x,v)|_{\gamma_-} = c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u > 0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \quad \text{dans } \mathbb{R}_+ \times \gamma_-, \end{aligned} \tag{3.24}$$

vérifie

$$\int_0^1 \int_{\gamma_-} |\nabla_x f(s,x,v)|^2 \mathrm{d}\gamma \mathrm{d}s \;=\; +\infty. \tag{3.25}$$

En particulier, l'estimation (3.23) du Théorème 3.2 échoue pour $p = 2$.

Il ne parait donc pas raisonnable d'espérer obtenir pour l'équation de Boltzmann des estimations de Sobolev dans des espaces $\mathrm{W}^{1,p}$ avec $p \geq 2$ sur l'ensemble du domaine, bord inclus. Plus précisément, la démonstration de la Proposition 3.1 fait apparaître une singularité au le bord rasant γ_0, à l'origine de l'explosion (3.25). On propose donc dans la suite des estimations de Sobolev dans des espaces $\mathrm{W}^{1,p}$ avec $p \geq 2$ qui sont valables en dehors du bord rasant.

Pour cela, on introduit une *distance cinétique* qui compense la singularité au bord. La *distance cinétique* est une fonction régulière qui s'annule exactement sur l'ensemble singulier (le bord rasant). On la définit par

Définition 3.1 (Distance cinétique)**.** *Pour $(x,v) \in \bar{\Omega} \times \mathbb{R}^3$,*

$$\alpha(x,v) := |v \cdot \nabla\xi(x)|^2 - 2\{v \cdot \nabla^2\xi(x) \cdot v\}\xi(x) \geq 0. \tag{3.26}$$

Grâce à l'hypothèse de stricte convexité (3.15), il est facile de vérifier qu'on a bien

$$\alpha(x,v) = 0 \quad \Leftrightarrow \quad (x,v) \in \gamma_0.$$

On présente dans la suite des estimations de Sobolev pondérées par une certaine puissance de la distance cinétique. Grâce à la propriété de la distance cinétique de s'annuler exactement sur l'ensemble singulier, pondérer les normes de Sobolev par la distance cinétique permet d'effacer exactement la singularité. Les estimations nous donnent une information exacte sur la régularité de Sobolev en dehors de l'ensemble singulier, ainsi qu'une estimation précise de la sévérité de la singularité au bord rasant.

Théorème 3.3 (Propagation $\mathrm{W}^{1,p}$ pondéré, $p \geq 2$ (Guo, Kim, Tonon, T.))**.** *Soit Ω un domaine borné régulier convexe* (3.15) *de $\mathbb{R}^3$. On peut alors choisir $\varpi > 0$ tel que*

$$\varpi > \sup_{(x,v)\in\Omega\times\mathbb{R}^3} \frac{2v\{v \cdot \nabla^3\xi(x) \cdot v\}\xi(x)}{\alpha(x,v)\,\langle v\rangle}.$$

On suppose (3.17) *et $\kappa > 0$. Soit $0 < \theta < 1/4$, $2 \leq p < \infty$, $\frac{p-2}{2p} < \beta < \frac{p-1}{2p}$, et $f_0 \geq 0$ une donnée initiale satisfaisant* (3.19) *et la condition de compatibilité* (3.21)*. On considère $T_* = T_*(||e^{\theta|v|^2} f_0||_\infty) > 0$ et f l'unique solution de* (3.16) *sur $[0,T_*) \times \Omega \times \mathbb{R}^3$ fournis par le Théorème 3.1. Alors,*

i) si $\alpha^\beta \nabla_{x,v} f_0 \in \mathrm{L}^p(\Omega\times\mathbb{R}^3)$, alors $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_{x,v} f \in \mathrm{L}^\infty_{loc}([0,T_*);\mathrm{L}^p(\Omega\times\mathbb{R}^3))$ et, pour tout $0 \leq t < T_*$,

$$||e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_{x,v} f(t)||_p^p + \int_0^t |e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_{x,v} f(s)|_{\gamma,p}^p \mathrm{d}s \lesssim_t ||\alpha^\beta\nabla_{x,v} f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty),$$

pour un certain polynôme P.

ii) Si $\alpha^{1/2}\nabla_{x,v} f_0 \in \mathrm{L}^\infty(\Omega \times \mathbb{R}^3)$*, alors* $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v} f \in \mathrm{L}^\infty([0,T_*); \mathrm{L}^\infty(\Omega\times\mathbb{R}^3))$ *et, pour tout* $0 \le t < T_*$*,*

$$||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v} f(t)||_\infty \ \lesssim_t \ ||\alpha^{1/2}\nabla_{x,v} f_0||_\infty + P(||e^{\theta|v|^2} f_0||_\infty).$$

iii) Enfin, si $\alpha^{1/2}\nabla_{x,v} f_0 \in \mathscr{C}^0(\bar\Omega \times \mathbb{R}^3)$ *et si* f_0 *satisfait de plus la condition de compatibilité d'ordre supérieur*

$$v\cdot\nabla_x f_0 - \Gamma(f_0,f_0) = c_\mu\sqrt{\mu}\int_{n\cdot u>0}\{u\cdot\nabla_x f_0 - \Gamma(f_0,f_0)\}\sqrt{\mu}\{n\cdot u\}\mathrm{d}u \qquad \textit{sur } \gamma_-\cup\gamma_0,$$

alors f *est* $\mathscr{C}^1$ *en dehors du bord rasant* γ_0*.*

On rappelle que si $||e^{\theta|v|^2}(f_0-\sqrt{\mu})||_\infty \ll 1$ *alors* $T_* = +\infty$ *; en particulier, les résultats précédents sont alors vrais pour tout* $t \ge 0$*.*

La démonstration du Théorème 3.3 se trouve au Chapitre 7. Elle exploite notamment une propriété essentielle d'invariance de la distance cinétique α le long des caractéristiques : voir l'Introduction du Chapitre 7.

Pour conclure sur le cas convexe, nous mentionnons le résultat suivant : dans le cas où le domaine considéré est la boule unité $B(0;1)$, il est possible de construire une donnée initiale régulière telle qu'au bout d'un certain temps t, la différentielle seconde de la solution $\nabla^2_{t,x,v} f(t)$ n'est pas dans $\mathrm{L}^1(\gamma, \mathrm{d}\gamma)$. Voir l'Annexe du Chapitre 7.

3.6 Propagation de régularité BV en domaine non convexe

Dans le cas où Ω n'est pas convexe, on a vu que les solutions pouvaient développer en temps fini des discontinuités sur (un sous-ensemble ouvert de) l'ensemble des trajectoires rasantes. Or, on peut montrer que cet ensemble est de codimension 1 :

Proposition 3.2 (Dimension de l'ensemble singulier)**.** *Soit* Ω *un domaine non convexe : il existe un point* $x_0 \in \partial\Omega$ *et* $v \in \mathbb{R}^3$ *tels que*

$$\sum_{i,j}\partial_{ij}\xi(x)v_iv_j < 0. \tag{3.27}$$

Alors, l'ensemble singulier

$$\mathfrak{S}_{\mathrm{B}} := \{(x,v)\in\bar\Omega\times\mathbb{R}^3 : n(x_{\mathbf{b}}(x,v))\cdot v = 0\},$$

où $x_{\mathbf{b}}(x,v)$ *est le* point de sortie arrière *(de la trajectoire issue de* (x,v)*),*

$$x_{\mathbf{b}}(x,v) := x - t_{\mathbf{b}}(x,v)v; \qquad t_{\mathbf{b}}(x,v) := \inf\{s>0 : \ x - sv \notin \Omega\},$$

est de co-dimension 1 dans $\Omega\times\mathbb{R}^3$*.*

En conséquence, la régularité BV est la meilleure régularité (standard) que l'on puisse espérer pour les solutions. On présente ci-dessous un résultat de régularité BV.

Théorème 3.4 (Propagation BV (Guo, Kim, Tonon, T.))**.** *Soit* Ω *un domaine borné régulier de* $\mathbb{R}^3$*. On suppose* (3.17)*. Soit* $0<\theta<1/4$ *et* $f_0 \ge 0$ *une donnée initiale satisfaisant* (3.19)*,* $f_0 \in BV(\Omega\times\mathbb{R}^3)$ *et la condition de compatibilité* (3.21)*. On considère* $T_* = T_*(||e^{\theta|v|^2}f_0||_\infty) > 0$ *et* f *l'unique solution de* (3.16) *sur* $[0,T_*)\times\Omega\times\mathbb{R}^3$ *fournis par le Théorème 3.1.*

Alors, $f \in \mathrm{L}^\infty_{loc}([0,T_*); BV(\Omega\times\mathbb{R}^3))$ *et, pour tout* $0 \le t < T_*$*,* $\nabla_{x,v} f(t)\mathrm{d}\gamma$ *est une mesure de Radon notée* σ_t *sur* $\partial\Omega\times\mathbb{R}^3$*, et*

$$||f(t)||_{BV} + \int_0^t |\sigma_s(\partial\Omega\times\mathbb{R}^3)|\,\mathrm{d}s \ \lesssim_t \ ||f_0||_{BV} + P(||e^{\theta|v|^2}f_0||_\infty), \tag{3.28}$$

pour un certain polynôme P*.*

On rappelle que si $||e^{\theta|v|^2}(f_0-\sqrt{\mu})||_\infty \ll 1$ *alors* $T_* = +\infty$ *; en particulier, les résultats précédents sont alors vrais pour tout* $t \ge 0$*.*

La démonstration des deux résultats se trouve dans le Chapitre 8. La démonstration du Théorème 3.4 repose sur la mise en place d'une fonction de troncature sur un petit voisinage des trajectoires rasantes, qui permet d'éviter les singularités et d'obtenir des estimations $\mathrm{W}^{1,1}$ pour la solution (uniformes en la taille du voisinage). Notons que la construction de ce voisinage et l'estimation de sa petitesse s'avèrent assez technique, car il n'est pas possible de définir ce voisinage formellement. Après passage à la limite dans les estimations $\mathrm{W}^{1,1}$ obtenues quand la taille du petit voisinage tend vers zéro, on obtient les estimations BV désirées.

3.7 Conclusion et perspectives

3.7.1 Résultats

Le tableau ci-dessous reprend l'ensemble des résultats de propagation de régularité obtenus.

Dans un domaine convexe	Dans un domaine non convexe
$\mathscr{C}^0$ hors de γ_0 [75] $\mathrm{W}^{1,p}$ pour $1 < p < 2$ $\cancel{\mathrm{W}^{1,2}}$: *Contre-ex. pour l'éq. de transport* $\mathrm{W}^{1,p}$ pondéré pour $p \in [2, \infty]$ $\mathscr{C}^1$ hors de γ_0 $\cancel{\mathrm{W}^{2,1}}$: *Contre-ex.*	$\cancel{\mathscr{C}^0}$: *Discontinuité formée sur γ_0 et propagée le long des trajectoires rasantes* [81] Propagation BV

On a donc une théorie bien élaborée de la propagation de régularité pour l'équation de Boltzmann (avec potentiel dur et cut-off angulaire) dans un domaine borné régulier quelconque avec réflexion diffusive au bord.

3.7.2 Pour aller plus loin

On présente dans cette section plusieurs questions dans la continuité des résultats obtenus.

Autres types de conditions au bord. On a vu en Remarque 3.2 que les résultats d'existence de solutions et, en domaine convexe, de propagation de continuité [75] étaient aussi valables lorsque l'on prend pour condition au bord une des deux autres conditions de réflexion classiques : réflexion spéculaire (3.11), réflexion inverse (3.10). Dans le cadre du travail collaboratif incluant les résultats du Chapitre 7, Y. Guo et C. Kim ont de plus démontré, pour chacun de ces deux types de réflexion au bord, des résultats de propagation de régularité $\mathscr{C}^1$ en dehors de γ_0 dans le cas d'un domaine convexe. Ces résultats sont analogues à celui présenté au *iii)* du Théorème 3.3 dans le cas de la réflexion diffusive, et comme lui reposent sur l'usage de la distance cinétique α (mais avec un exposant différent pour chacun des types de réflexion). On trouvera l'énoncé et la démonstration de ces résultats dans l'Annexe.

Une première série de questions en continuité directe est d'interroger la possibilité d'obtenir des résultats de propagation analogues à ceux obtenus pour la réflexion diffusive : propagation BV en domaine non convexe, propagation $\mathrm{W}^{1,p}$ en domaine convexe, éventuellement pondérée pour p supérieur à une valeur critique p_0. Cette valeur critique vaut-elle alors $p_0 = 2$ comme dans le cas de la réflexion diffusive ? Ces questions ouvertes sont intéressantes pour la complétude de la théorie mathématique.

Une deuxième série de questions concerne la possibilité de combiner nos méthodes (entre elles ou avec d'autres) : par exemple, si on considère les conditions aux bords de Maxwell (3.13) (combinaison des conditions de réflexion spéculaire et diffusive), peut-on obtenir des résultats de propagation de régularité analogues aux cas diffusif et spéculaire ? Cette question ouverte est d'autant plus importante que les conditions aux bords de Maxwell sont les plus réalistes du point de vue de la Physique. Autre exemple, qu'advient-il dans le cas où le domaine considéré n'est pas borné ? Sachant que la question de la régularité dans tout l'espace est largement résolue, avec existence de solutions infiniment dérivables (proches d'une distribution Maxwellienne globale), est-il possible de combiner les méthodes du cas d'un domaine borné avec celles du cas de tout l'espace pour obtenir des résultats en domaine non borné ? Cette question est importante car la plupart des applications concernent un gaz évoluant autour d'un objet, donc dans un domaine non borné (typiquement, le complémentaire d'un domaine borné convexe).

Température variable. On a jusqu'ici considéré le cas d'un domaine de température homogène (prise pour simplifier égale à 1). Pourtant, on sait que les variations de température du bord peuvent être à l'origine de phénomènes physiques comme le *fluage thermique*[5], qui a de nombreuses applications particulièrement intéressantes (par exemple en ingénierie spatiale). Du point de vue mathématique, le cas d'un bord inhomogène est beaucoup plus compliqué à analyser. L'existence même d'une solution stationnaire reste un enjeu, par opposition au cas homogène pour lequel une solution stationnaire explicite est donnée par la distribution Maxwellienne globale μ. En conséquence, les méthodes d'existence de solutions dans un cadre perturbatif (solutions proches de μ) pour le cas homogène n'ont pas d'équivalent *a priori* dans le cas inhomogène, et la question de l'existence de solutions au problème d'évolution dans le cas inhomogène reste ouverte. Voir [67] pour une revue bibliographique.

Le résultat le plus complet, dû à R. Esposito, Y. Guo, C. Kim et R. Marra [67], concerne le cas où l'amplitude des variations de température du bord est petite (en ce sens, il s'agit d'un résultat perturbatif du cas homogène). Dans ce cadre, pour un domaine borné général, ils obtiennent l'existence et l'unicité d'une solution stationnaire, et l'existence, l'unicité et la stabilité (convergence exponentielle vers la solution du problème stationnaire) d'une solution du problème d'évolution (pour une donnée initiale proche de la solution stationnaire). De plus, ils montrent la continuité de la solution hors de γ_0 dans le cas où le domaine est convexe.

Le problème est encore largement ouvert quand la température du bord varie (régulièrement) avec une amplitude quelconque.

Bord à géométrie singulière. Les résultats de cette thèse, associés aux résultats de C. Kim [81] et de Y. Guo [75], délivrent une description précise des singularités occasionnées par la présence d'un bord totalement régulier. On a une description dans le cas d'un domaine régulier strictement convexe, et une autre dans le cas d'un domaine régulier strictement non-convexe.

Une première question est d'interroger la régularité dans le cas limite, c'est-à-dire quand le domaine est convexe mais non strictement convexe. (On peut prendre pour cas typique un domaine régulier convexe dont une partie du bord est plate, par exemple, un cube aux angles arrondis). Pour avoir une intuition de le la sévérité des singularités dans ce cas, on peut comparer la taille du domaine singulier $\mathfrak{S}_{\mathrm{B}}$ dans les trois cas :

	Domaine strictement convexe	Cas limite	Domaine non convexe
Co-dimension de $\mathfrak{S}_{\mathrm{B}}$	2	2	1

On s'attend donc à obtenir dans le cas limite "convexe - non strictement" la même régularité que dans le cas strictement convexe.

Une autre direction[6] d'analyse envisageable est de regarder (dans le cas convexe ou non) comment se propagent les singularités à partir d'un point singulier du bord, c'est-à-dire un point $x \in \partial\Omega$ auquel la fonction ξ définissant le domaine Ω (3.14) n'est pas régulier (par exemple, un angle).

5. mouvement de gaz provoqué par un gradient de température, en l'absence de gradient de pression. Voir [64, 85] et références citées.

6. Notons, dans le même esprit, les travaux [55, 56] (voir aussi [86]) qui se penchent, d'un point de vue mathématique et/ou numérique, sur la propagation de singularités à partir d'une singularité présente dans la donnée (par exemple, température) au bord (sur un bord régulier), et les travaux [60, 59, 66] qui explorent mathématiquement la propagation de singularité à partir d'une singularité présente dans la condition initiale (dans tout l'espace, pour l'équation de Boltzmann homogène). Voir [81] pour une bibliographie détaillée sur ces questions.

Deuxième partie

Systèmes de diffusion croisée en Dynamique des populations

Chapitre 4

The triangular reaction-cross diffusion system : a microscopic approach

Abstract

This Chapter is taken from the paper [17] in collaboration with L. Desvillettes. We present an approach based on entropy and duality methods for "triangular" reaction cross diffusion systems of two equations, in which cross diffusion terms appear only in one of the equations. Thanks to this approach, we recover and extend many existing results on the classical "triangular" Shigesada-Kawasaki-Teramoto model. Our results rely on the introduction of an approximating reaction-diffusion system (without cross-diffusion) which models the same dynamics at a microscopic scale.

Sommaire

4.1 Introduction

4.1.1 Context

Reaction cross diffusion equations naturally appear in physics (cf. [6] for example) as well as in population dynamics. We are interested here in the study of a class of systems first introduced by Shigesada, Kawasaki, and Teramoto (cf. [45]). Those systems aim at modeling the repulsive effect of populations of two different species in competition, and are possibly leading to the apparition of patterns (cf. [28]).

The unknowns are the quantities $u := u(t,x) \geq 0$ and $v := v(t,x) \geq 0$. They represent the number densities of the two considered species (say, species 1 and species 2). They depend on the time variable $t \in \mathbb{R}_+$ and the space variable $x \in \Omega$. Hereafter, Ω is a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^* := \mathbb{N}-\{0\}$) and we denote by $n = n(x)$ its unit normal outward vector at point $x \in \partial\Omega$. The original model of [45] writes

$$\begin{cases} \partial_t u - \Delta_x(d_u\, u + d_{11}\, u^2 + d_{12}\, u\, v) = u\,(r_u - r_a\, u - r_b\, v) & \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t v - \Delta_x(d_v\, v + d_{21}\, u\, v + d_{22}\, v^2) = v\,(r_v - r_c\, v - r_d\, u) & \text{in } \mathbb{R}_+ \times \Omega, \\ \nabla_x u \cdot n = \nabla_x v \cdot n = 0 & \text{on } \mathbb{R}_+ \times \partial\Omega. \end{cases} \tag{4.1}$$

The coefficients $r_u, r_v > 0$ are the growth rates in absence of other individuals, $r_a, r_b, r_c, r_d > 0$ correspond to the logistic inter- and intraspecific competition effects, and $d_u, d_v > 0$ are the diffusion rates. The coefficients $d_{ij} \geq 0$ ($i,j = 1,2$) represent the repulsive effect : individuals of species i increase their diffusion rate in presence of individuals of their own species when $d_{ii} > 0$ (self diffusion) or of the other species when $d_{ij} > 0$ ($i \neq j$, cross diffusion).

In the sequel, we shall only consider the case when $d_{21} = 0$ and $d_{12} > 0$, which is sometimes called "triangular". In such a situation, the second equation is coupled to the first one only through the competition (reaction) term while the first one is coupled to the second one through both diffusion and competition terms (the fully coupled system when $d_{21} > 0$ and $d_{12} > 0$ has a quite different mathematical structure, cf. [8] and [15] for example). We shall also only focus on the case when no self diffusion appears (that is $d_{11} = d_{22} = 0$) since this case is the most studied one : note however that the presence of self-diffusion (that is, $d_{11} > 0$ and/or $d_{22} > 0$) usually helps to obtain better bounds on the solution. As a consequence, our results are expected to hold when self-diffusion is present.

Under the extra assumptions detailed above, the Shigesada-Kawasaki-Teramoto system writes

$$\begin{cases} \partial_t u - \Delta_x(d_u\, u + d_{12}\, u\, v) = u\,(r_u - r_a\, u - r_b\, v) & \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t v - d_v\, \Delta_x v = v\,(r_v - r_c\, v - r_d\, u) & \text{in } \mathbb{R}_+ \times \Omega, \\ \nabla_x u \cdot n = \nabla_x v \cdot n = 0 & \text{on } \mathbb{R}_+ \times \partial\Omega. \end{cases} \tag{4.2}$$

Following [27], this system can be seen as the formal singular limit of a reaction diffusion system which writes

$$\begin{cases} \partial_t u_A^\epsilon - d_u\, \Delta_x u_A^\epsilon = [r_u - r_a\,(u_A^\epsilon + u_B^\epsilon) - r_b\, v^\epsilon]\, u_A^\epsilon + \dfrac{1}{\epsilon}[k(v^\epsilon)\, u_B^\epsilon - h(v^\epsilon)\, u_A^\epsilon] & \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t u_B^\epsilon - (d_u + d_B)\, \Delta_x u_B^\epsilon = [r_u - r_a\,(u_A^\epsilon + u_B^\epsilon) - r_b\, v^\epsilon]\, u_B^\epsilon - \dfrac{1}{\epsilon}[k(v^\epsilon)\, u_B^\epsilon - h(v^\epsilon)\, u_A^\epsilon] & \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t v^\epsilon - d_v\, \Delta_x v^\epsilon = [r_v - r_c\, v^\epsilon - r_d\,(u_A^\epsilon + u_B^\epsilon)]\, v^\epsilon & \text{in } \mathbb{R}_+ \times \Omega, \\ \nabla_x u_A^\epsilon \cdot n = \nabla_x u_B^\epsilon \cdot n = \nabla_x v^\epsilon \cdot n = 0 & \text{on } \mathbb{R}_+ \times \partial\Omega, \end{cases} \tag{4.3}$$

where $d_B > 0$, and h, k are two (continuous) functions from $\mathbb{R}_+$ to $\mathbb{R}_+$ satisfying (for all $v \geq 0$) the identity

$$d_B\, \frac{h(v)}{h(v) + k(v)} = d_{12}\, v.$$

The limit holds (at the formal level) in the following sense : if u_A^ε, u_B^ε, and v^ε are solutions to system (4.3) (with ε-independent initial data), the quantity $(u_A^\varepsilon + u_B^\varepsilon, v^\varepsilon)$ converges towards (u, v), where u and v are solutions to system (4.2). Note that this asymptotics can be biologically meaningful : when $\varepsilon > 0$, the system (4.3) represents a microscopic model in which the species u can be found in two states (the quiet state u_A and the stressed state u_B), and the individuals of this species switch from one state to the other one with a "large" rate (proportional to $1/\varepsilon$).

4.1.2 Main results

We present in this paper results for the existence, uniqueness and stability of a large class of systems including (4.2). More precisely, we relax the assumption stating that the competition terms are logistic (quadratic), and replace it with the assumption stating that the competition terms are given by power laws (the powers being suitably chosen). We also relax the assumption stating that the cross diffusion term is quadratic (that is, proportional to $u\,v$) and replace it by the more general assumption stating that it writes $u\,\phi(v)$ (with $\phi \in C^1(\mathbb{R}_+)$, and ϕ nonnegative).

Hence, we shall consider the system

$$\partial_t u - \Delta_x(d_u\,u + u\,\phi(v)) = u\,(r_u - r_a\,u^a - r_b\,v^b) \qquad \text{in } \mathbb{R}_+ \times \Omega, \tag{4.4}$$

$$\partial_t v - d_v\,\Delta_x v = v\,(r_v - r_c\,v^c - r_d\,u^d) \qquad \text{in } \mathbb{R}_+ \times \Omega, \tag{4.5}$$

with homogeneous Neumann boundary conditions

$$\nabla_x u \cdot n = \nabla_x v \cdot n = 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega, \tag{4.6}$$

and initial data

$$u(0,\cdot) = u_{in}, \qquad v(0,\cdot) = v_{in} \qquad \text{in } \Omega. \tag{4.7}$$

The functions $u_{in} := u_{in}(x) \ge 0$ and $v_{in} := v_{in}(x) \ge 0$ are defined on Ω and assumed to be nonnegative. In cases in which we want to prove that the solutions are strong, they will sometimes be required to satisfy the following compatibility conditions on the boundary

$$\nabla_x u_{in} \cdot n = 0 \qquad \text{on } \partial\Omega, \tag{4.8}$$

$$\nabla_x v_{in} \cdot n = 0 \qquad \text{on } \partial\Omega. \tag{4.9}$$

In our theorems, we shall consider parameters in (4.4)-(4.5) which satisfy the

Assumption A : $d_u, d_v > 0$, $r_u, r_v, r_a, r_b, r_c, r_d > 0$, $a, b, c, d > 0$, and $\phi := \phi(v) \ge 0$, $\phi \in C^1(\mathbb{R}_+)$.

We now specify what is meant by a weak solution in our theorems.

We recall the following notation : for $p \in [1, \infty[$,

$$L^p_{\text{loc}}(\mathbb{R}_+ \times \overline{\Omega}) := \{u = u(t,x) : \text{for all } T > 0,\ \int_0^T \int_\Omega |u(t,x)|^p\,dxdt < \infty\}.$$

Definition 4.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$). Let u_{in}, v_{in} be two nonnegative functions lying in $L^1(\Omega)$, and d_u, d_v, $r_u, r_v, r_a, r_b, r_c, r_d$, $a, b, c, d > 0$, $\phi := \phi(v)$ be parameters satisfying assumption A.*

A pair of functions (u, v) such that $u := u(t,x) \ge 0$ and $v := v(t,x) \ge 0$, lying moreover in $L^{\max(1+a,d)}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ is a **weak solution** *of (4.4)-(4.7) if $\nabla_x u$, $\nabla_x v$, $\nabla_x [\phi(v)\,u]$ lie in $L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ and, for all test functions ψ_1, $\psi_2 \in C^1_c(\mathbb{R}_+ \times \overline{\Omega})$, the following identities hold :*

$$-\int_0^\infty \int_\Omega (\partial_t \psi_1) u - \int_\Omega \psi_1(0,\cdot)\,u_{in} + \int_0^\infty \int_\Omega \nabla_x \psi_1 \cdot \nabla_x [(d_u + \phi(v))u] = \int_0^\infty \int_\Omega \psi_1 u (r_u - r_a\,u^a - r_b\,v^b),$$

$$-\int_0^\infty \int_\Omega (\partial_t \psi_2)\,v - \int_\Omega \psi_2(0,\cdot)\,v_{in} + d_v \int_0^\infty \int_\Omega \nabla_x \psi_2 \cdot \nabla_x v = \int_0^\infty \int_\Omega \psi_2\,v\,(r_v - r_c\,v^c - r_d\,u^d).$$

Note that all terms in the previous identities are well-defined under our assumptions on u_{in}, v_{in}, u, v, ψ_1, ψ_2, ϕ.

We propose two theorems, corresponding to the respective cases $d < a$ and $a \le d$. The first one writes :

Theorem 4.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$). We suppose that Assumption A on the coefficients of system (4.4) – (4.5) holds, together with the extra assumption $d < a$. Finally, we consider initial data $u_{in} \ge 0$, $v_{in} \ge 0$, such that $u_{in} \in L^{p_0}(\Omega)$, $v_{in} \in L^\infty(\Omega) \cap W^{2,1+p_0/d}(\Omega)$ for some $p_0 > 1$. If $1 + p_0/d \ge 3$, we also assume the compatibility condition (4.9).*

Then, there exists a (global, with nonnegative components) weak solution (u,v) *of system (4.4) – (4.7) in the sense of Definition 4.1 [In particular,* $(u,v) \in L^{\max(1+a,d)}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ *and* $\nabla_x u$, $\nabla_x v$, $\nabla_x [\phi(v)\, u]$ *lie in* $L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$*].*

Moreover, this solution satisfies for all $p \in]1, p_0]$ *and all* $T > 0$,

$$\sup_{(t,x)\in[0,T]\times\Omega} v(t,x) \le \max\left(||v_{in}||_{L^\infty(\Omega)}, \left[\frac{r_v}{r_c}\right]^{1/c}\right), \qquad \int_0^T \int_\Omega |\nabla_x v|^{2(1+p_0/d)} \le C_T,$$

$$\int_0^T \int_\Omega u^{p_0+a} \le C_T, \qquad \sup_{t\in[0,T]} \int_\Omega u^{p_0}(t) \le C_T, \qquad \int_0^T \int_\Omega |\nabla_x (u^{p/2})|^2 \le C_{T,p}\,,$$

for some positive constants C_T *and* $C_{T,p}$ *depending only on the initial data* u_{in} *and* v_{in}*, the domain* Ω *(and the dimension* N*), the parameters of the system (4.4)–(4.5), the time* T*, the parameter* p_0 *and, for* $C_{T,p}$*, the parameter* p*.*

We suppose in addition to the previous assumptions that $\phi \in C^2(\mathbb{R}_+)$, $u_{in} \in W^{2,s_0}(\Omega)$, $v_{in} \in W^{2,\frac{a+p_1}{d}}(\Omega)$ *for some* $s_0 > 1 + N/2$ *and some* $p_1 \ge 2$, $p_1 > a(s_0 - 1)$*, and that compatibility conditions* (4.8) *(resp.* (4.9)*) hold when* $s_0 \ge 3$ *(resp.* $\frac{a+p_1}{d} \ge 3$*). Then* (u,v) *is Hölder continuous on* $\mathbb{R}_+ \times \overline{\Omega}$*, and* $\partial_t u$, $\partial_{x_i x_j} u \in L^{s_0}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, $\partial_{x_i} u \in L^2_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, $\partial_t v$, $\partial_{x_i x_j} v \in L^{(a+p_1)/d}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ *(*$i,j = 1..N$*, and the derivatives are taken in the sense of distributions). Note that since* u *is Hölder, we know that* $u \in L^{p_1+a}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$*.*

Finally, if (in addition to the previous assumptions) ϕ *has Hölder continuous second order derivatives on* $\mathbb{R}_+$*, if* u_{in}, v_{in} *have Hölder continuous second order derivatives on* $\overline{\Omega}$*, and if compatibility conditions* (4.8)–(4.9) *are satisfied, then* u, v *have Hölder continuous first order time derivatives and Hölder continuous second order space derivatives on* $\mathbb{R}_+ \times \overline{\Omega}$*.*

In this last setting, and provided that $b, d \ge 1$*, the following stability estimate holds : if* $(u_{1,in}, v_{1,in})$ *and* $(u_{2,in}, v_{2,in})$ *are two sets of initial data with nonnegative components and such that the* L^∞ *norms of their zeroth, first and second order spatial derivatives and the* α*-Hölder norms of their second spatial derivatives are bounded by some constant* $K > 0$ *(for some fixed* $\alpha > 0$*), then any corresponding weak solutions* (u_1, v_1), (u_2, v_2) *in the sense of Definition 4.1, lying in* $L^{p_1+a}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ *and such that (for any* $T > 0$*)*

$$\sup_{t\in[0,T]} \int_\Omega u_i^2(t) < +\infty \qquad \text{and} \qquad \int_0^T \int_\Omega |\nabla_x u_i|^2 < +\infty \qquad \text{for } i = 1,\, 2, \tag{4.10}$$

satisfy (for any $T > 0$*)*

$$||u_1 - u_2||_{L^2([0,T]\times\Omega)} + ||v_1 - v_2||_{L^2([0,T]\times\Omega)} \le C'_T \left(||u_{1,in} - u_{2,in}||_{L^2(\Omega)} + ||v_{1,in} - v_{2,in}||_{L^2(\Omega)}\right),$$

for some positive constant C'_T *depending only on the constant* K*, the domain* Ω *(and the dimension* N*), the parameters of the system (4.4)–(4.5), the time* T *and the parameter* α*. As a consequence, uniqueness holds in this last setting (among weak solutions in the sense of Definition 4.1 lying in* $L^{a+p_1}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ *and satisfying* (4.10)*).*

Remark 4.1. *The first setting provides global weak solutions. In the second setting, those solutions are shown to be strong, in the sense that all derivatives appearing in the equations lie in some* L^p *with* $p \in [1, \infty]$*. Finally, in the last setting, those solutions are shown to be classical, in the sense that all derivatives appearing in the equations are continuous. Stability and uniqueness (in the class of weak solutions satisfying some extra regularity) holds when the assumptions on the parameters imply that weak solutions are classical solutions.*

Then, our second theorem writes

Theorem 4.2. *Let* Ω *be a smooth bounded domain of* $\mathbb{R}^N$ *(*$N \in \mathbb{N}^*$*). We suppose that Assumption A on the coefficients of system (4.4) – (4.5) holds. We moreover suppose that* $a \le d$, $a \le 1$, $d \le 2$*. Finally, we consider initial data* $u_{in} \ge 0$, $v_{in} \ge 0$ *such that* $u_{in} \in L^2(\Omega)$, $v_{in} \in L^\infty(\Omega) \cap W^{2,1+2/d}(\Omega)$*. If* $1 + 2/d \ge 3$ *(i.e.* $d \le 1$*), we also assume the compatibility condition* (4.9)*.*

Then, there exists a (global, with nonnegative components) weak solution (u, v) of system (4.4) – (4.7) in the sense of Definition 4.1 [In particular, $(u, v) \in L^{\max(1+a,d)}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^{\infty}_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ and $\nabla_x u$, $\nabla_x v$, $\nabla_x [\phi(v)\, u]$ lie in $L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$].

Moreover, this solution satisfies for some $p > 0$ and $\eta > 0$ and for all $T > 0$,

$$\sup_{(t,x)\in[0,T]\times\Omega} v(t,x) \le \max\left(||v_{in}||_{L^\infty(\Omega)}, \left[\frac{r_v}{r_c}\right]^{1/c} \right), \qquad \int_0^T \int_\Omega |\nabla_x v|^{2+\eta} \le C_T,$$

$$\int_0^T \int_\Omega u^2 \le C_T, \qquad \sup_{t\in[0,T]} \int_\Omega u(t) \le C_T, \qquad \int_0^T \int_\Omega |\nabla_x (u^{p/2})|^2 \le C_T\,,$$

for some positive constant C_T depending only on the initial data u_{in} and v_{in}, the domain Ω (and the dimension N), the parameters of the system (4.4)–(4.5) and the time T.

4.1.3 Singular perturbation

The existence theorems presented above are consequences of propositions showing the convergence in a singular perturbation problem. This problem is analogous to system (4.3) in the case of the Shigesada-Kawasaki-Teramoto model. It writes, in $\mathbb{R}_+ \times \Omega$:

$$\begin{cases} \partial_t u^\epsilon_A - d_A\, \Delta_x u^\epsilon_A = [r_u - r_a\,(u^\epsilon_A + u^\epsilon_B)^a - r_b\,(v^\epsilon)^b]\, u^\epsilon_A + \dfrac{1}{\epsilon}\,[k(v^\epsilon)\, u^\epsilon_B - h(v^\epsilon)\, u^\epsilon_A], \\ \partial_t u^\epsilon_B - (d_A + d_B)\, \Delta_x u^\epsilon_B = [r_u - r_a\,(u^\epsilon_A + u^\epsilon_B)^a - r_b\,(v^\epsilon)^b]\, u^\epsilon_B - \dfrac{1}{\epsilon}\,[k(v^\epsilon)\, u^\epsilon_B - h(v^\epsilon)\, u^\epsilon_A], \\ \partial_t v^\epsilon - d_v\, \Delta_x v^\epsilon = [r_v - r_c\,(v^\epsilon)^c - r_d\,(u^\epsilon_A + u^\epsilon_B)^d]\, v^\epsilon, \end{cases} \tag{4.11}$$

where h and k lie in $C^1(\mathbb{R}_+)$ and satisfy, for some $h_0 > 0$,

$$d_A + d_B\, \frac{h(v)}{h(v) + k(v)} = d_u + \phi(v), \qquad h(v) \ge h_0, \qquad k(v) \ge h_0, \qquad \text{for all } v \in \mathbb{R}_+. \tag{4.12}$$

The existence of h and k in $C^1(\mathbb{R}_+)$ satisfying (4.12) is a part of the proof of Theorems 4.1 and 4.2.

We add homogeneous Neumann boundary conditions

$$\nabla_x u^\epsilon_A \cdot n = \nabla_x u^\epsilon_B \cdot n = \nabla_x v^\epsilon \cdot n = 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega. \tag{4.13}$$

We also add initial data to (4.11), (4.13) thanks to a regularization process that we now describe. Let $(\rho^\varepsilon)_{\varepsilon>0}$ be a family of mollifiers on $\mathbb{R}^N$, and for all $\varepsilon > 0$, let χ^ε be a cutoff function (given by Urysohn's lemma) lying in $C^\infty(\mathbb{R}^N)$, and satisfying

$$\begin{aligned} 0 \le \chi^\varepsilon \le 1 \text{ in } \mathbb{R}^N, \qquad & \chi^\varepsilon = 1 \quad \text{inside} \quad \{x \in \Omega : d(x, \partial\Omega) > 2\varepsilon\}, \\ & \chi^\varepsilon = 0 \quad \text{outside} \quad \{x \in \Omega : d(x, \partial\Omega) > \varepsilon\}. \end{aligned}$$

Then, given two nonnegative functions (lying in $L^1(\Omega)$) u_{in}, v_{in}, we define

$$u_{A,in} := \frac{k(v_{in})}{h(v_{in}) + k(v_{in})}\, u_{in}, \qquad u_{B,in} := \frac{h(v_{in})}{h(v_{in}) + k(v_{in})}\, u_{in} \qquad \text{on } \Omega, \tag{4.14}$$

and extend by zero those functions on $\mathbb{R}^N - \Omega$ (so that the convolution on $\mathbb{R}^N$ can be used).

We therefore add to (4.11), (4.13) the regularized initial data (defined on Ω) :

$$\begin{aligned} u^\varepsilon_A(0,\cdot) = u^\varepsilon_{A,in} := (\chi^\varepsilon(u_{A,in} * \rho^\varepsilon) + \epsilon)|_\Omega, \quad u^\varepsilon_B(0,\cdot) = u^\varepsilon_{B,in} := (\chi^\varepsilon(u_{A,in} * \rho^\varepsilon) + \varepsilon)|_\Omega, \\ v^\varepsilon(0,\cdot) = v^\varepsilon_{in} := v_{in} + \varepsilon. \end{aligned} \tag{4.15}$$

We shall use in our propositions related to the system (4.11), (4.13), (4.15) the

Assumption B : $d_A, d_B, d_u, d_v > 0$, $r_u, r_v, r_a, r_b, r_c, r_d > 0$, $a, b, c, d > 0$. The functions ϕ, h and k lie in $C^1(\mathbb{R}_+)$ and satisfy (4.12).

For the singular perturbation problem with a given $\varepsilon \in]0, 1[$, we shall consider strong solutions defined in the following way :

Definition 4.2. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$). We suppose that Assumption B on the coefficients of system (4.11), (4.13), (4.15) holds, and that u_{in}, v_{in} are two nonnegative functions lying in $L^1(\Omega)$. We finally consider $\varepsilon \in]0,1[$.*

A set of nonnegative functions $(u_A^\epsilon, u_B^\epsilon, v^\epsilon)$ such that $u_A^\epsilon := u_A^\epsilon(t,x)$, $u_B^\epsilon := u_B^\epsilon(t,x)$ lie in $L^{\max(1+a,d)}_{loc}$ $(\mathbb{R}_+ \times \overline{\Omega})$, and $v^\epsilon := v^\epsilon(t,x)$ lie in $L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, will be called a **strong solution** *of (4.11), (4.13), (4.15) if $\partial_t u_A^\epsilon$, $\partial_t u_B^\epsilon$, $\partial_t v^\epsilon$ and $\partial_{x_i,x_j} u_A^\epsilon$, $\partial_{x_i,x_j} u_B^\epsilon$, $\partial_{x_i,x_j} v^\epsilon$ (i, $j = 1..N$) lie in $L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ and equations* (4.11), (4.13) *and* (4.15) *are satisfied almost everywhere in $\mathbb{R}_+ \times \Omega$ (resp. $\mathbb{R}_+ \times \partial\Omega$, Ω).*

Our results concerning the behavior when $\varepsilon \to 0$ of the strong solutions of system (4.11), (4.13), (4.15) are summarized in the two following propositions (corresponding to the respective cases $d < a$ and $d \geq a$) :

Proposition 4.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$). We suppose that Assumption B on the coefficients of system (4.11), (4.13), (4.15) holds, and assume moreover that $d < a$. Finally, we consider initial data $u_{in} \geq 0$, $v_{in} \geq 0$ such that $u_{in} \in L^{p_0}(\Omega)$, $v_{in} \in L^\infty(\Omega) \cap W^{2,1+p_0/d}(\Omega)$ for some $p_0 > 1$. If $1 + p_0/d \geq 3$, we also assume the compatibility condition* (4.9).

Then, for any $\varepsilon \in]0,1[$, there exists a strong (global, with nonnegative components) solution $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ in the sense of Definition 4.2 to system (4.11), (4.13), (4.15).

Moreover, when $\varepsilon \to 0$, $(u_A^\epsilon, u_B^\epsilon, v^\epsilon)$ converges, up to extraction of a subsequence, for almost every $(t,x) \in \mathbb{R}_+ \times \Omega$ to a limit (u_A, u_B, v) such that $u_A \geq$, $u_B \geq 0$, $v \geq 0$. Furthermore, the quantity v satisfies the bound

$$0 \leq v(t,x) \leq \max\left(||v_{in}||_{L^\infty(\Omega)}, \left[\frac{r_v}{r_c}\right]^{1/c} \right) \qquad \text{for a.e.} \quad (t,x) \in \mathbb{R}_+ \times \Omega, \tag{4.16}$$

and the quantity $(u,v) := (u_A + u_B, v)$ satisfies $\nabla_x u, \nabla_x(u\,\phi(v)) \in L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$, and for all $p \in]1, p_0]$, $T > 0$,

$$\sup_{t\in[0,T]} \int_\Omega u^{p_0}(t) \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x (u^{p/2})|^2 \leq C_{T,p}, \tag{4.17}$$

$$\int_0^T \int_\Omega u^{p_0+a} \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x v|^{2(1+p_0/d)} \leq C_T\,, \tag{4.18}$$

for some positive constants C_T and $C_{T,p}$ depending only on the initial data u_{in} and v_{in}, the domain Ω (and the dimension N), the parameters of the system (4.11)*, the time T, the parameter p_0 and, for $C_{T,p}$, the parameter p.*

Finally, $h(v(t,x))\,u_A(t,x) = k(v(t,x))\,u_B(t,x)$ for a.e. $(t,x) \in \mathbb{R}_+ \times \Omega$, and (u,v) is a (global, with nonnegative components) weak solution of system (4.4) – (4.7) in the sense of Definition 4.1.

Proposition 4.2. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$). We suppose that Assumption B on the coefficients of system (4.11), (4.13), (4.15) holds, and assume moreover that $a \leq d$, $a \leq 1$, $d \leq 2$. Finally, we consider initial data $u_{in} \geq 0$, $v_{in} \geq 0$ such that $u_{in} \in L^2(\Omega)$, $v_{in} \in L^\infty(\Omega) \cap W^{2,1+2/d}(\Omega)$. If $1 + 2/d \geq 3$ (i.e. $d \leq 1$), we also assume the compatibility condition* (4.9).

Then, for any $\varepsilon \in]0,1[$, there exists a strong (global, with nonnegative components) solution $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ in the sense of Definition 4.2 to system (4.11), (4.13), (4.15).

Moreover, when $\varepsilon \to 0$, $(u_A^\epsilon, u_B^\epsilon, v^\epsilon)$ converges, up to extraction of a subsequence, for almost every $(t,x) \in \mathbb{R}_+ \times \Omega$ to a limit (u_A, u_B, v) such that $u_A \geq 0$, $u_B \geq 0$, $v \geq 0$. The explicit L^∞ estimate on v given by (4.16) also holds. Furthermore, the quantity $(u,v) := (u_A + u_B, v)$ satisfies $\nabla_x u, \nabla_x(u\,\phi(v)) \in L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ and for some $p > 0$ and $\eta > 0$ (and all $T > 0$),

$$\sup_{t\in[0,T]} \int_\Omega u(t) \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x (u^{p/2})|^2 \leq C_T, \tag{4.19}$$

$$\int_0^T \int_\Omega u^2 \leq C_T, \qquad \int_0^T \int_\Omega |\nabla_x v|^{2+\eta} \leq C_T, \tag{4.20}$$

for some positive constant C_T depending only on the initial data u_{in} and v_{in}, the domain Ω (and the dimension N), the parameters of the system (4.4)–(4.5) and the time T.

Finally, $h(v(t,x))\,u_A(t,x) = k(v(t,x))\,u_B(t,x)$ for a.e. $(t,x) \in \mathbb{R}_+ \times \Omega$, and (u,v) is a (global, with nonnegative components) weak solution of system (4.4) – (4.7) in the sense of Definition 4.1.

4.1.4 Direct extensions

In the following remarks, we discuss some direct extensions of the results stated above.

Remark 4.2. *Theorems 4.1 and 4.2 use classical parabolic ($W^{2,1}_s$ with the notations of [33]) estimates. For the sake of simplicity, we chose to use a non-optimal version of those estimates, formulated below in Proposition 4.4. Note that the assumptions could be somewhat improved (see [33]) in Theorems 4.1 and 4.2 : first, the estimates do not require a full compatibility condition on the boundary $\partial\Omega$ in the critical case $s = 3$; secondly, some of the initial data assumed to belong to $W^{2,s}(\Omega)$ in our theorems and propositions can be assumed to belong only to the fractional Sobolev space $W^{2-2/s,s}(\Omega)$.*

Remark 4.3. *In the case of Theorem 4.2, the compactness of the nonlinear reaction terms u^{1+a} and u^d is obtained thanks to an L^p estimate for some $p > 2$ given by a duality lemma. Notice first that this enables to treat coefficients $a = 1 + \eta$ and $d = 1 + \eta$ when $\eta > 0$ is smaller than some (small) constant. Secondly, the duality lemma (stated in Lemma 4.4) for initial data in $L^2(\Omega)$ holds in fact for initial data in $L^{2-\eta}(\Omega)$ when $\eta > 0$ is also smaller than some (small) constant. This allows to replace in Theorem 4.2 the assumption $u_{in} \in L^2(\Omega)$ by the weaker assumption $u_{in} \in L^{2-\eta}(\Omega)$.*

Remark 4.4. *Since (as we shall see later on), v satisfies a maximum principle in Theorems 4.1 and 4.2, those theorems can easily be extended in the case when the functions $v \mapsto r_b\, v^b$ and $v \mapsto r_c\, v^c$ are replaced by any smooth functions of v (with an arbitrary growth when $v \to \infty$). The functions $u \mapsto r_a\, u^a$ and $u \mapsto r_d\, u^d$ can also be replaced by smooth functions in Theorems 4.1 and 4.2, provided that those functions behave in the same way as $u \mapsto r_a\, u^a$ and $u \mapsto r_d\, u^d$ when $u \to \infty$.*

Remark 4.5. *In the last setting of Theorem 4.1, a minimum principle for v allows to replace the assumption stating that ϕ'' is locally Hölder continuous on $[0, +\infty[$ by the assumption stating that ϕ'' is locally Hölder continuous on $]0, +\infty[$, provided that the initial datum for v is bounded below by a strictly positive constant.*

4.1.5 In the literature

The model (4.1) was proposed by Shigesada, Kawasaki and Teramoto in [45]. For modeling issues, see also [41]. As far as mathematical analysis is concerned, two directions have been widely investigated in the literature : a series of papers focuses on steady-states and stability (patterns are shown to appear ; see [27] and the references therein) ; other works concern existence, smoothness and uniqueness of solutions.

The local (in time) existence was established by Amann : in his series of papers [1, 2, 3], he proved a general result of existence of local (in time) solutions for parabolic systems, including (4.1) and (4.4)-(4.5).

The global (in time) existence has then been proved under various assumptions. One of the difficulties which arises is related to the use of Sobolev inequalities in parabolic estimates, which only provides results in low dimension. Indeed, for the well studied triangular quadratic case (that is, (4.1) with $d_{21} = 0$), most papers allowing strong cross diffusion (that is, when no restriction is imposed on d_{12}) only deal with low dimensions : for results in dimension 1, see [37], [38] and [46]. In [53], Yagi showed the global existence in dimension 2 in the presence of self diffusion, and Lou, Ni and Wu obtained it in [34] without condition on self diffusion, together with a stability result. Choi, Lui and Yamada first got rid of the restriction on the dimension in [10] (without self diffusion in the second equation), provided that the cross diffusion coefficient d_{12} is sufficiently small. In a following paper [11], they removed the smallness assumption on the cross diffusion in the presence of self diffusion in the first equation. However, in the presence of self diffusion in the second equation, they require that the dimension is lower than 6. Finally, Phan improved this result up to dimension lower than 10 in [49], and in any dimension under the assumption that the self diffusion dominates the cross diffusion in [50]. For the quadratic system (4.2) without self diffusion, our Theorem 4.2 gives the existence of global solutions in any dimension, without restriction on the strength of the cross diffusion.

When it comes to systems with general reaction terms of the form (4.4)-(4.5), Pozio and Tesei first showed the existence (in any dimension) of global solutions under some strong assumption on the reaction coefficients in [44]. This assumption was relaxed in [54] by Yamada, who obtained the existence of global strong solutions under the assumption $a > d$, which is exactly our assumption in Theorem 4.1. The main differences between our work (in the case $a > d$) and [54] are the following : first, our Theorem 4.1 allows singular initial data leading to weak solutions (and provides results very close to those of [54] when initial data are smooth). Then our method, based on simple energy estimates, presents a unifying proof for a wide range of parameters including both the quadratic case and the case $a > d$. Finally, the approximating system that we use leads to self-contained proofs without reference to abstract existence theorems. Note also that (for general reaction terms) Wang got similar results in [52] in the presence of self diffusion in the first equation, under a condition (depending on the dimension) of smallness of the parameter d w.r.t. the parameter a.

Systems of reaction diffusion equations such as (4.3) were introduced by Iida, Mimura and Ninomiya in [27] to approximate cross diffusion systems, in particular from the point of view of stability. The convergence of the stationary problem was explored by Izuhara and Mimura in [28], both numerically and theoretically. In [12], Conforto and Desvillettes showed the convergence of the solutions of (4.3) towards a solution of the system (4.2) in dimension one. Our paper generalizes their result to a wider set of admissible reaction terms and in any dimension. Note finally that Murakawa obtained similar results for a class of non triangular systems in [40].

Note : After submission of this article, Hoang, Nguyen and Phan released the paper [26]. Therein, they obtain global smooth solutions in any dimension of space for the quadratic case (system (4.1) with $d_{21} = 0$) in the presence of self diffusion in the first equation. Their result relies on new nonlinear parabolic estimates (that they establish) and uses the regularizing effect of the presence of the self diffusion.

The *a priori* estimates obtained thanks to our methods (duality lemma and entropy functional in L^p spaces) still hold in the case when self-diffusion is present. However, it is not obvious whether or not the singular perturbation method that we use can be extended to this case.

The rest of our paper is structured as follows : Propositions 4.1 and 4.2 are proven in Section 4.2. Then, Section 4.3 is devoted to the proof of Theorems 4.1 and 4.2.

4.2 Proof of the convergence of the singularly perturbed equations

We begin with the

Proof of Proposition 4.1. We fix $T > 0$, and shall write from now on (for any $q \in [1, \infty]$) $L^q := L^q([0, T] \times \Omega)$. In the proof of this proposition and of the following proposition, the constant $C_T > 0$ only depends on the parameters d_A, d_B, d_u, d_v, $r_u, r_v, r_a, r_b, r_c, r_d$, a, b, c, d, the domain Ω, the initial data u_{in}, v_{in}, the functions ϕ, h and k, and the time T. It may also depends on the parameters p and q used later. In this proposition, it also depends on the parameter p_0 in the initial datum. In particular, all the estimates are uniform w.r.t $\epsilon \in]0, 1[$, unless stated otherwise.

We first observe that for a given $\varepsilon \in]0, 1[$, standard theorems for reaction-diffusion equations show the existence of a (global, nonnegative for each component) strong solution $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ in the sense of Definition 4.2 to system (4.11), (4.13), (4.15). Moreover, these solutions satisfy

$$\begin{aligned} &\|\partial_t u_A^\varepsilon\|_q,\ \|\partial_t u_B^\varepsilon\|_q,\ \|\partial_{x_i x_j} u_A^\varepsilon\|_q,\ \|\partial_{x_i x_j} u_B^\varepsilon\|_q \le \mu_{T,\varepsilon} \qquad \text{for } i,\ j = 1..N, \text{ for all } q > 1, \\ &\qquad\qquad \|\partial_t v^\varepsilon\|_{1+p_0/d},\ \|\partial_{x_i x_j} v^\varepsilon\|_{1+p_0/d} \le \mu_{T,\varepsilon} \quad \text{for } i,\ j = 1..N, \\ &\nu^1_{T,\varepsilon} \ge u_A^\varepsilon(t,x) \qquad \nu^1_{T,\varepsilon} \ge u_B^\varepsilon(t,x) \qquad \nu^1_{T,\varepsilon} \ge v^\varepsilon(t,x) \ge \nu^0_{T,\varepsilon} > 0 \quad \text{a.e. } (t,x) \in [0,T] \times \Omega, \end{aligned} \tag{4.21}$$

where the constants $\mu_{T,\varepsilon} > 0$, $\nu^1_{T,\varepsilon} > 0$, $\nu^0_{T,\varepsilon} > 0$ depend on ε and the other parameters, including T, and the last inequality is a direct consequence of the minimum principle. We refer to [13] for complete proofs.

We now establish three lemmas stating the (uniform w.r.t. $\varepsilon \in]0, 1[$) *a priori* estimates for this solution $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$.

Lemma 4.1. *Under the assumptions of Proposition 4.1, the following (uniform w.r.t $\varepsilon \in]0, 1[$) estimates hold :*

$$\sup_{0 \le t \le T} \int_\Omega (u_A^\epsilon + u_B^\epsilon)(t) \le C_T; \qquad \|u_A^\epsilon + u_B^\epsilon\|_{L^{1+a}} \le C_T. \tag{4.22}$$

Proof of Lemma 4.1. The quantity $u_A^\epsilon + u_B^\epsilon$ satisfies the equation

$$\partial_t(u_A^\epsilon + u_B^\epsilon) - \Delta_x[M^\epsilon(u_A^\epsilon + u_B^\epsilon)] = [r_u - r_a(u_A^\epsilon + u_B^\epsilon)^a - r_b(v^\epsilon)^b](u_A^\epsilon + u_B^\epsilon) \le C_T, \tag{4.23}$$

where $M^\epsilon = \frac{d_A u_A^\epsilon + (d_A+d_B)u_B^\epsilon}{u_A^\epsilon + u_B^\epsilon}$. We integrate w.r.t. space and time to get

$$\sup_{0\le t\le T} \int_\Omega (u_A^\epsilon + u_B^\epsilon)(t) \le \int_\Omega (u_{A,in}^\epsilon + u_{B,in}^\epsilon) + C_T \le C_T, \tag{4.24}$$

so that

$$\sup_{0\le t\le T} \int_\Omega (u_A^\epsilon + u_B^\epsilon)(t) + r_a \int_0^T \int_\Omega (u_A^\epsilon + u_B^\epsilon)^{1+a} \le \int_\Omega (u_{A,in}^\epsilon + u_{B,in}^\epsilon) + r_u \int_0^T \int_\Omega (u_A^\epsilon + u_B^\epsilon) \le C_T. \tag{4.25}$$

□

Lemma 4.2. *Under the assumptions of Proposition 4.1, for all* $1 < q \le 1 + p_0/d$, *the following (uniform w.r.t* $\varepsilon \in]0,1[$*) estimates hold :*

$$\|v^\epsilon\|_{L^\infty} \le C_T; \qquad \|\nabla_x v^\epsilon\|^2_{L^{2q}} \le C_T\,(1 + \|(u_A^\epsilon + u_B^\epsilon)^d\|_{L^q}); \qquad \|\partial_t v^\epsilon\|_{L^q} \le C_T\,(1 + \|(u_A^\epsilon + u_B^\epsilon)^d\|_{L^q}). \tag{4.26}$$

Proof of Lemma 4.2. The first estimate is a consequence of the maximum principle for the equation satisfied (in the strong sense) by v^ε. More precisely, this maximum principle writes

$$0 \le v^\varepsilon(t,x) \le \max\left(||v_{in}||_{L^\infty(\Omega)} + \varepsilon, \left[\frac{r_v}{r_c}\right]^{1/c} \right) \qquad \text{for a.e.} \quad (t,x) \in \mathbb{R}_+ \times \Omega. \tag{4.27}$$

We can then apply the maximal regularity result for the heat equation (satisfied by v^ε when the reaction term is considered as given) in order to get the third estimate (note that we use here the assumption on v_{in}, since $v_{in}^\varepsilon = v_{in} + \varepsilon$). The same bound also holds for $\partial_{x_i x_j} v^\epsilon$, so that interpolating with the first estimate, the second estimate holds. □

We now write down a (uniform w.r.t. $\varepsilon \in]0,1[$) bound obtained thanks to the use of a Lyapounov-like (entropy) functional :

Lemma 4.3. *Under the assumptions of Proposition 4.1, for all* $p \in]1, p_0]$, *the following inequalities hold :*

$$\sup_{t\in[0,T]} \int_\Omega (u_A^\epsilon + u_B^\epsilon)^p(t) \le C_T\,(1 + \|u_A^\epsilon + u_B^\epsilon\|^{p+d}_{L^{p+d}}), \tag{4.28}$$

$$\|u_A^\epsilon + u_B^\epsilon\|^{p+a}_{L^{p+a}} \le C_T\,(1 + \|u_A^\epsilon + u_B^\epsilon\|^{p+d}_{L^{p+d}}), \tag{4.29}$$

$$\|\nabla_x (u_A^\epsilon)^{p/2}\|^2_{L^2} + \|\nabla_x (u_B^\epsilon)^{p/2}\|^2_{L^2} + \frac{1}{\epsilon}\|(h(v^\epsilon)u_A^\epsilon)^{p/2} - (k(v^\epsilon)u_B^\epsilon)^{p/2}\|^2_{L^2} \le C_T\,(1 + \|u_A^\epsilon + u_B^\epsilon\|^{p+d}_{L^{p+d}}). \tag{4.30}$$

Proof of Lemma 4.3. We define the following entropy for any $p > 0$ (with $p \ne 1$) :

$$\mathscr{E}^\epsilon(t) = \int_\Omega h(v^\epsilon)^{p-1} \frac{(u_A^\epsilon)^p}{p}(t) + \int_\Omega k(v^\epsilon)^{p-1} \frac{(u_B^\epsilon)^p}{p}(t) \qquad (=: \mathscr{E}_A^\epsilon(t) + \mathscr{E}_B^\epsilon(t)). \tag{4.31}$$

We compute the derivative (note that in the computation below all integrals lie in $L^1([0,T])$ thanks to the properties (4.21) ; therefore the computation holds for a.e. $t \in [0,T]$) :

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_A^\epsilon(t) &= \int_\Omega \partial_t \{h(v^\epsilon)^{p-1}\frac{(u_A^\epsilon)^p}{p}\}(t) \\ &= \frac{p-1}{p}\int_\Omega \partial_t v^\epsilon h'(v^\epsilon) h(v^\epsilon)^{p-2} (u_A^\epsilon)^p + \int_\Omega \partial_t u_A^\epsilon (u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1} \\ &= \frac{p-1}{p}\int_\Omega \partial_t v^\epsilon h'(v^\epsilon) h(v^\epsilon)^{p-2} (u_A^\epsilon)^p + \int_\Omega [r_u - r_a(u_A^\epsilon + u_B^\epsilon)^a - r_b(v^\epsilon)^b](u_A^\epsilon)^p h(v^\epsilon)^{p-1} \\ &\quad + \frac{1}{\epsilon}\int_\Omega [k(v^\epsilon)u_B^\epsilon - h(v^\epsilon)u_A^\epsilon](u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1} + d_A \int_\Omega \Delta_x u_A^\epsilon (u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1}, \end{aligned} \tag{4.32}$$

where the last term is estimated by integrating by part (and using the inequality $2|ab| \le a^2+b^2$) in the case when $p>1$:

$$
\begin{aligned}
& d_A \int_\Omega \Delta_x u_A^\epsilon (u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1} \\
&= -\, d_A\,(p-1)\int_\Omega |\nabla_x u_A^\epsilon|^2 (u_A^\epsilon)^{p-2} h(v^\epsilon)^{p-1} - d_A\,(p-1)\int_\Omega \nabla_x u_A^\epsilon\cdot\nabla_x h(v^\epsilon)(u_A^\epsilon)^{p-1}h(v^\epsilon)^{p-2} \\
&\le -\,\frac{d_A}{2}\,(p-1)\int_\Omega |\nabla_x u_A^\epsilon|^2 (u_A^\epsilon)^{p-2} h(v^\epsilon)^{p-1} + \frac{d_A}{2}\,(p-1)\int_\Omega |\nabla_x h(v^\epsilon)|^2 (u_A^\epsilon)^{p} h(v^\epsilon)^{p-3} \\
&= -\,2\,d_A\,\frac{(p-1)}{p^2}\int_\Omega |\nabla_x (u_A^\epsilon)^{p/2}|^2 h(v^\epsilon)^{p-1} + \frac{(p-1)}{2}\,d_A\int_\Omega |\nabla_x v^\epsilon|^2 (u_A^\epsilon)^p (h'(v^\epsilon))^2 h(v^\epsilon)^{p-3}.
\end{aligned}
\tag{4.33}
$$

Similarly, we get for u_B^ϵ (still for a.e. $t\in[0,T]$),

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_B^\epsilon(t) \le{}& \frac{p-1}{p}\int_\Omega \partial_t v^\epsilon k'(v^\epsilon)k(v^\epsilon)^{p-2}(u_B^\epsilon)^p \\
&+\int_\Omega [r_u - r_a(u_B^\epsilon+u_B^\epsilon)^a - r_b(v^\epsilon)^b](u_B^\epsilon)^p k(v^\epsilon)^{p-1} - \frac{1}{\epsilon}\int_\Omega [k(v^\epsilon)u_B^\epsilon - h(v^\epsilon)u_A^\epsilon](u_B^\epsilon)^{p-1}k(v^\epsilon)^{p-1} \\
&-2(d_A+d_B)\frac{p-1}{p^2}\int_\Omega |\nabla_x (u_B^\epsilon)^{p/2}|^2 k(v^\epsilon)^{p-1} \\
&+\frac{p-1}{2}(d_A+d_B)\int_\Omega |\nabla_x v^\epsilon|^2 (u_B^\epsilon)^p (k'(v^\epsilon))^2 k(v^\epsilon)^{p-3}.
\end{aligned}
\tag{4.34}
$$

We add the two estimates and integrate w.r.t time to get (still for any $p>1$)

$$
\begin{aligned}
&\int_\Omega \left[h(v^\epsilon)^{p-1}\frac{(u_A^\epsilon)^p}{p}(T) + k(v^\epsilon)^{p-1}\frac{(u_B^\epsilon)^p}{p}(T)\right] \\
&+2\,d_A\,\frac{p-1}{p^2}\int_0^T\int_\Omega |\nabla_x (u_A^\epsilon)^{p/2}|^2 h(v^\epsilon)^{p-1} + 2\,(d_A+d_B)\,\frac{p-1}{p^2}\int_0^T\int_\Omega |\nabla_x (u_B^\epsilon)^{p/2}|^2 k(v^\epsilon)^{p-1} \\
&+\frac{1}{\epsilon}\int_0^T\int_\Omega [k(v^\epsilon)u_B^\epsilon - h(v^\epsilon)u_A^\epsilon][(u_B^\epsilon)^{p-1}k(v^\epsilon)^{p-1} - (u_A^\epsilon)^{p-1}h(v^\epsilon)^{p-1}] \\
&+r_a\int_0^T\int_\Omega (u_A^\epsilon+u_B^\epsilon)^a[(u_A^\epsilon)^p h(v^\epsilon)^{p-1} + (u_B^\epsilon)^p k(v^\epsilon)^{p-1}] \\
&\le \int_\Omega \left[h(v_{in}^\epsilon)^{p-1}\frac{(u_{A,in}^\epsilon)^p}{p} + k(v_{in}^\epsilon)^{p-1}\frac{(u_{A,in}^\epsilon)^p}{p}\right] \\
&+\frac{p-1}{p}\int_0^T\int_\Omega \partial_t v^\epsilon[h'(v^\epsilon)h(v^\epsilon)^{p-2}(u_A^\epsilon)^p + k'(v^\epsilon)k(v^\epsilon)^{p-2}(u_B^\epsilon)^p] \\
&+r_u\int_0^T\int_\Omega \left[(u_A^\epsilon)^p h(v^\epsilon)^{p-1} + (u_B^\epsilon)^p k(v^\epsilon)^{p-1}\right] \\
&+\frac{p-1}{2}\int_0^T\int_\Omega [d_A(u_A^\epsilon)^p(h'(v^\epsilon))^2h(v^\epsilon)^{p-3} + (d_A+d_B)(u_B^\epsilon)^p(k'(v^\epsilon))^2k(v^\epsilon)^{p-3}]|\nabla_x v^\epsilon|^2.
\end{aligned}
\tag{4.35}
$$

Let us estimate the right-hand side of inequality (4.35) under the assumptions of the lemma : the first term is finite since $p\le p_0$. Thanks to the maximum principle for the density v^ϵ (obtained in Lemma 4.2) and the regularity of the functions h and k in Assumption B, the terms $h(v^\epsilon)$, $h'(v^\epsilon)$ and $k(v^\epsilon)$, $k'(v^\epsilon)$ are uniformly bounded in L^∞. We then can estimate the third term with Hölder's inequality. Indeed,

$$
\begin{aligned}
&\left|\int_0^T\int_\Omega \left[(u_A^\epsilon)^p h(v^\epsilon)^{p-1} + (u_B^\epsilon)^p k(v^\epsilon)^{p-1}\right]\right| \\
\le\;& ||h(v^\epsilon)^{p-1} + k(v^\epsilon)^{p-1}||_{L^\infty}\,||u_A^\epsilon+u_B^\epsilon||_{L^p}^p \le C_T\,(1+\|u_A^\epsilon+u_B^\epsilon\|_{L^{p+d}}^{p+d}).
\end{aligned}
$$

The second and the last terms are estimated thanks to Hölder's inequality and bounds given by Lemma 4.2. More precisely, for the second term, we get

$$
\begin{aligned}
&\left|\frac{p-1}{p}\int_0^T\int_\Omega \partial_t v^\epsilon[h'(v^\epsilon)h(v^\epsilon)^{p-2}(u_A^\epsilon)^p + k'(v^\epsilon)k(v^\epsilon)^{p-2}(u_B^\epsilon)^p]\right| \\
&\le \|h'(v^\epsilon)h(v^\epsilon)^{p-2} + k'(v^\epsilon)k(v^\epsilon)^{p-2}\|_{L^\infty}\|\partial_t v^\epsilon\|_{L^{1+p/d}}\|(u_A^\epsilon+u_B^\epsilon)^p\|_{L^{1+d/p}} \\
&\le C_T\,(1+\|u_A^\epsilon+u_B^\epsilon\|_{L^{p+d}}^{p+d}),
\end{aligned}
\tag{4.36}
$$

and for the last term, we get

$$\begin{aligned}
&\left| \frac{p-1}{2} \int_0^T \int_\Omega [d_A (u_A^\epsilon)^p (h'(v^\epsilon))^2 h(v^\epsilon)^{p-3} + (d_A+d_B)(u_B^\epsilon)^p (k'(v^\epsilon))^2 k(v^\epsilon)^{p-3}] |\nabla_x v^\epsilon|^2 \right| \\
&\leq (p/2) \, \|h'(v^\epsilon)^2 h(v^\epsilon)^{p-3} + k'(v^\epsilon)^2 k(v^\epsilon)^{p-3}\|_{L^\infty} \| \, |\nabla_x v^\epsilon|^2 \|_{L^{1+p/d}} \|(u_A^\epsilon + u_B^\epsilon)^p\|_{L^{1+d/p}} \\
&\leq C_T \, (1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p+d}}^{p+d}),
\end{aligned} \tag{4.37}$$

thanks to Lemma 4.2.

The terms of the left-hand side of (4.35) being all nonnegative, they are all bounded by the quantity $(1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p+d}}^{p+d})$. We then obtain the estimates announced in the lemma by using the lower bound of h and k (remember Assumption B), and the following elementary inequality for all positive x, y : $(x-y)\,(x^{p-1} - y^{p-1}) \geq C_p \, |x^{p/2} - y^{p/2}|^2$, where $C_p > 0$ is a constant depending on p (remember that $p \in]1, p_0]$). □

We now turn back to the proof of Proposition 4.1.

As a first consequence of Lemma 4.3, we can improve the Lebesgue space in which we get a uniform (w.r.t. ε) estimate for $u_A^\epsilon + u_B^\epsilon$. Taking $p = p_0$ in (4.29) and using Hölder's inequality (remember that $d < a$), we see that

$$\|u_A^\epsilon + u_B^\epsilon\|_{L^{p_0+a}}^{p_0+a} \leq C_T \, (1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p_0+d}}^{p_0+d}) \leq C_T \, (1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p_0+a}}^{p_0+d}),$$

so that

$$\|u_A^\epsilon + u_B^\epsilon\|_{L^{p_0+a}} \leq C_T. \tag{4.38}$$

Let us combine estimate (4.38) and Lemma 4.2 with $q = 1 + p_0/d > 1$ to get

$$\|\nabla_x v^\epsilon\|_{L^{2\,(1+p_0/d)}}^2 \leq C_T, \qquad \|\partial_t v^\epsilon\|_{L^{1+p_0/d}} \leq C_T. \tag{4.39}$$

Then, from Aubin's lemma (see Theorem 5 in [47]), we can extract a subsequence - still called $(v^\epsilon)_\epsilon$ - which converges towards a limit v a.e. :

$$v^\epsilon(t,x) \to v(t,x) \qquad \text{almost everywhere on } [0,T] \times \Omega, \tag{4.40}$$

and such that

$$\nabla_x v^\epsilon \rightharpoonup \nabla_x v \qquad \text{weakly in} \qquad L^{2\,(1+p_0/d)} \quad \text{(and therefore in)} \quad L^1. \tag{4.41}$$

Thanks to this passage to the limit, the function v automatically lies in L^∞, and is nonnegative. Passing to the limit in estimate (4.27), we get estimate (4.16). Finally, $\nabla_x v \in L^{2\,(1+p_0/d)}$.

Recall now eq. (4.23) for $u_A^\epsilon + u_B^\epsilon$. Notice that the reaction term in (4.23) is uniformly bounded in L^λ with $\lambda = \frac{p_0+a}{1+a} > 1$, thanks to estimate (4.38). As a consequence, $\partial_t(u_A^\epsilon + u_B^\epsilon)$ in (4.23) is uniformly bounded in $L^\lambda([0,T], W^{-2,\lambda})$. Furthermore, let us choose some p in the interval $]1, p_0[$ and $\zeta = \zeta(p) \in]0,1[$ such that $(2-p)\,\frac{1+\zeta}{1-\zeta} < p_0 + a$. Then for $C = A$ or B, Hölder's inequality implies

$$\begin{aligned}
\| \, |\nabla_x u_C^\epsilon|^{1+\zeta} \, \|_{L^1} &\leq \int_0^T \int \Big[|u_C^\epsilon|^{p/2-1} \, |\nabla_x u_C^\epsilon| \Big]^{1+\zeta} \; |u_C^\epsilon|^{(1-p/2)\,(1+\zeta)} \\
&\leq \left(\int_0^T \int \Big[|u_C^\epsilon|^{p/2-1} \, |\nabla_x u_C^\epsilon| \Big]^2 \right)^{\frac{1+\zeta}{2}} \left(\int_0^T \int \Big[|u_C^\epsilon|^{(2-p)\,\frac{1+\zeta}{1-\zeta}} \Big] \right)^{\frac{1-\zeta}{2}} \\
&\leq (2/p)^{1+\zeta} \, ||\nabla_x (u_C^\epsilon)^{p/2}||_{L^2}^{1+\zeta} \left(\int_0^T \int \Big[|u_C^\epsilon|^{(2-p)\,\frac{1+\zeta}{1-\zeta}} \Big] \right)^{\frac{1-\zeta}{2}} \leq C_T,
\end{aligned} \tag{4.42}$$

thanks to Lemma 4.3 and estimate (4.38).

We therefore can apply Aubin's lemma to extract a subsequence (still called $(u_A^\epsilon + u_B^\epsilon)_\epsilon$) which converges towards a limit u a.e. :

$$u_A^\epsilon(t,x) + u_B^\epsilon(t,x) \to u(t,x) \qquad \text{almost everywhere on } [0,T] \times \Omega. \tag{4.43}$$

Thanks to estimate (4.38) and Fatou's lemma, we know that $u \in L^{a+p_0}$. Moreover, $u \geq 0$ a.e. thanks to the passage to the limit a.e., and $\nabla_x u \in L^{1+\zeta}$ for some $\zeta > 0$ small enough, thanks to estimate (4.42).

We now use the following elementary inequality : for any $p \in]0, 2[$, there exists a constant $C_p > 0$ (which depends only on p) such that

$$\forall x \in \mathbb{R}_+, \qquad |x - 1| \leq C_p\, |x^{p/2} - 1| \times |x^{1-p/2} + 1|. \tag{4.44}$$

Taking p in the interval $]1, \min\{p_0, 2\}[$, we see that

$$\begin{aligned}
&\int_0^T \int_\Omega |k(v^\epsilon) u_B^\epsilon - h(v^\epsilon) u_A^\epsilon| \\
&\leq C_p \int_0^T \int_\Omega |(u_B^\epsilon k(v^\epsilon))^{p/2} - (u_A^\epsilon h(v^\epsilon))^{p/2}| \times [(u_B^\epsilon k(v^\epsilon))^{1-p/2} + (u_A^\epsilon h(v^\epsilon))^{1-p/2}] \\
&\leq C_p \left(\int_0^T \int_\Omega |(u_B^\epsilon k(v^\epsilon))^{p/2} - (u_A^\epsilon h(v^\epsilon))^{p/2}|^2 \right)^{1/2} \left(\int_0^T \int_\Omega [(u_B^\epsilon k(v^\epsilon))^{1-p/2} + (u_A^\epsilon h(v^\epsilon))^{1-p/2}]^2 \right)^{1/2} \\
&\leq \sqrt{\epsilon}\, C_T,
\end{aligned} \tag{4.45}$$

thanks to Lemma 4.3. Then, $u_B^\epsilon\, k(v^\epsilon) - u_A^\epsilon\, h(v^\epsilon)$ converges to 0 in L^1, and therefore, up to a subsequence,

$$h(v^\epsilon(t,x))\, u_A^\epsilon(t,x) - k(v^\epsilon(t,x))\, u_B^\epsilon(t,x) \to 0 \qquad \text{a. e. on } [0,T] \times \Omega. \tag{4.46}$$

Thanks to the convergences (4.40), (4.43) and (4.46), we can compute

$$u_A^\epsilon(t,x) = \frac{k(v^\epsilon)\,(u_A^\epsilon + u_B^\epsilon) + [h(v^\epsilon)\, u_A^\epsilon - k(v^\epsilon)\, u_B^\epsilon]}{h(v^\epsilon) + k(v^\epsilon)} \to \frac{k(v)\, u}{h(v) + k(v)} =: u_A(t,x) \qquad \text{a. e. on } [0,T] \times \Omega, \tag{4.47}$$

and similarly, a. e. on $[0,T] \times \Omega$

$$u_B^\epsilon(t,x) = \frac{h(v^\epsilon)\,(u_A^\epsilon + u_B^\epsilon) - [h(v^\epsilon)\, u_A^\epsilon - k(v^\epsilon)\, u_B^\epsilon]}{h(v^\epsilon) + k(v^\epsilon)} \to \frac{h(v)\, u}{h(v) + k(v)} =: u_B(t,x) \qquad \text{a. e. on } [0,T] \times \Omega. \tag{4.48}$$

Up to another extraction, we see that, thanks to estimate (4.42), for $C = A, B$,

$$\nabla_x u_C^\epsilon \rightharpoonup \nabla_x u_C \qquad \text{weakly in} \qquad L^1. \tag{4.49}$$

Extracting again subsequences, we can perform this proof on $[0, 2T]$, $[0, 3T]$, ..., so that by Cantor's diagonal argument,

$$u_A^\epsilon(t,x) \to u_A(t,x), \quad u_B^\epsilon(t,x) \to u_B(t,x), \quad v^\epsilon(t,x) \to v(t,x) \tag{4.50}$$

for a.e. $(t,x) \in \mathbb{R}_+ \times \Omega$, where u_A, u_B, v are defined on $\mathbb{R}_+ \times \Omega$. It is clear that $u_A, u_B, v \geq 0$ a.e. Remembering the definition of u_A and u_B, we also see that $h(v)\, u_A = k(v)\, u_B$ a.e., and $u_A, u_B \in L^{a+p_0}$. Finally, we recall that $v \in L^\infty$.

Let us now show (4.17). Thanks to the uniform (in ε) estimates (4.28), (4.30) and (4.38), we have for all $p \in]1, p_0]$,

$$\sup_{t \in [0,T]} \int_\Omega u^p(t) \leq C_T \qquad \text{and} \qquad \int_0^T \int_\Omega |\nabla_x u_A^{p/2}|^2 + |\nabla_x u_B^{p/2}|^2 \leq C_T, \tag{4.51}$$

where we have used Fatou's lemma for the first inequality and Kakutani's Theorem applied to the reflexive space L^2 for the second inequality. Remembering that $u = \frac{h(v)+k(v)}{k(v)}\, u_A$, we can see that for all $p \in]1, p_0]$,

$$\nabla_x \left(u^{p/2} \right) = \overbrace{u_A^{p/2}}^{\in L^{2(1+a/p_0)}} \overbrace{\left[\left(\frac{h+k}{k} \right)^{p/2} \right]'(v)}^{\in L^\infty} \overbrace{\nabla_x v}^{\in L^{2(1+p_0/d)}} + \overbrace{\left(\frac{h(v)+k(v)}{k(v)} \right)^{p/2}}^{\in L^\infty} \overbrace{\nabla_x \left(u_A^{p/2} \right)}^{\in L^2} \in L^2.$$

In order to conclude the proof of Proposition 4.1, it only remains to check that $(u,v) = (u_A + u_B, v)$ is a weak solution of (4.4)–(4.7) in the sense of Definition 4.1.

Let ψ_1, $\psi_2 \in C_c^1(\mathbb{R}_+ \times \overline{\Omega})$ be test functions. Multiplying all terms of the two first equations of (4.23) by ψ_1, multiplying all terms of equation (4.11) by ψ_2, and integrating on $\mathbb{R}_+ \times \Omega$, we get

$$\begin{aligned} -\int_0^\infty \int_\Omega \partial_t\psi_1\,(u_A^\epsilon + u_B^\epsilon) - \int_\Omega \psi_1(0,\cdot)\,(u_{A,in}^\epsilon + u_{B,in}^\epsilon) + \int_0^\infty \int_\Omega \nabla_x\psi_1 \cdot \nabla_x(M^\epsilon\,(u_A^\epsilon + u_B^\epsilon)) \\ = \int_0^\infty \int_\Omega \psi_1\,(u_A^\epsilon + u_B^\epsilon)\,(r_u - r_a\,(u_A^\epsilon + u_B^\epsilon)^a - r_b\,(v^\epsilon)^b), \end{aligned} \tag{4.52}$$

$$\begin{aligned} -\int_0^\infty \int_\Omega \partial_t\psi_2\, v^\epsilon - \int_\Omega \psi_2(0,\cdot)\, v_{in}^\epsilon + d_v \int_0^\infty \int_\Omega \nabla_x\psi_2 \cdot \nabla_x v^\epsilon \\ = \int_0^\infty \int_\Omega \psi_2\, v^\epsilon\,(r_v - r_c\,(v^\epsilon)^c - r_d\,(u_A^\epsilon + u_B^\epsilon)^d). \end{aligned} \tag{4.53}$$

Note that thanks to (4.50),

$$\partial_t\psi_1\,(u_A^\epsilon + u_B^\epsilon) \to (\partial_t\psi_1)\,u,$$

for a.e. $(t,x) \in \mathbb{R}_+ \times \Omega$, and $\psi_1\,(u_A^\epsilon + u_B^\epsilon)$ is bounded (uniformly w.r.t. $\varepsilon \in]0,1[$) in L^{p_0+a} thanks to (4.38), so that

$$-\int_0^\infty \int_\Omega \partial_t\psi_1\,(u_A^\epsilon + u_B^\epsilon) \to -\int_0^\infty \int_\Omega (\partial_t\psi_1)\,u. \tag{4.54}$$

In the same way, since v^ε is uniformly bounded w.r.t. $\varepsilon \in]0,1[$, (4.50) and (4.41) imply that

$$-\int_0^\infty \int_\Omega \partial_t\psi_2\, v^\epsilon \to -\int_0^\infty \int_\Omega \partial_t\psi_2\, v, \quad d_v \int_0^\infty \int_\Omega \nabla_x\psi_2 \cdot \nabla_x v^\epsilon \to d_v \int_0^\infty \int_\Omega \nabla_x\psi_2 \cdot \nabla_x v, \tag{4.55}$$

Then, we observe that $\psi_1\,(u_A^\epsilon + u_B^\epsilon)\,(r_u - r_a\,(u_A^\epsilon + u_B^\epsilon)^a - r_b\,(v^\epsilon)^b)$ is bounded (uniformly w.r.t. $\varepsilon \in]0,1[$) in $L^{\frac{p_0+a}{1+a}}$ thanks to (4.38), so that (4.50) implies that

$$\int_0^\infty \int_\Omega \psi_1\,(u_A^\epsilon + u_B^\epsilon)\,(r_u - r_a\,(u_A^\epsilon + u_B^\epsilon)^a - r_b\,(v^\epsilon)^b) \to \int_0^\infty \int_\Omega \psi_1\, u\,(r_u - r_a\, u^a - r_b\, v^b). \tag{4.56}$$

In the same way, $\psi_2\, v^\epsilon\,(r_v - r_c\,(v^\epsilon)^c - r_d\,(u_A^\epsilon + u_B^\epsilon)^d)$ is bounded (uniformly w.r.t. $\varepsilon \in]0,1[$) in $L^{\frac{p_0+a}{d}}$, so that

$$\int_0^\infty \int_\Omega \psi_2\, v^\epsilon\,(r_v - r_c\,(v^\epsilon)^c - r_d\,(u_A^\epsilon + u_B^\epsilon)^d) \to \int_0^\infty \int_\Omega \psi_2\, v\,(r_v - r_c\, v^c - r_d\, u^d). \tag{4.57}$$

According to the definition of $u_{A,in}^\epsilon$ and $u_{B,in}^\epsilon$, it is clear that $u_{A,in}^\epsilon \to u_{A,in}$ a.e. on Ω, and $u_{B,in}^\epsilon \to u_{B,in}$ a.e. on Ω, so that $u_{A,in}^\epsilon + u_{B,in}^\epsilon \to u_{in}$ a.e. on Ω. But $u_{in} \in L^{p_0}(\Omega)$, so that $u_{A,in}$ and $u_{B,in}$ also lie in $L^{p_0}(\Omega)$, and $u_{A,in}^\epsilon, u_{B,in}^\epsilon$ are bounded (uniformly w.r.t. $\varepsilon \in]0,1[$) in $L^{p_0}(\Omega)$. Then

$$\int_\Omega \psi_1(0,\cdot)\,(u_{A,in}^\epsilon + u_{B,in}^\epsilon) \to \int_\Omega \psi_1(0,\cdot)\,u. \tag{4.58}$$

In the same way, observing that v_{in}^ε is bounded (uniformly w.r.t. $\varepsilon \in]0,1[$) in $L^\infty(\Omega)$, we see that

$$-\int_\Omega \psi_2(0,\cdot)\, v_{in}^\epsilon \to -\int_\Omega \psi_2(0,\cdot)\, v_{in}. \tag{4.59}$$

It remains to study the convergence of $\nabla_x\psi_1 \cdot \nabla_x[M^\varepsilon\,(u_A^\varepsilon + u_B^\varepsilon)]$. But $M^\varepsilon\,(u_A^\varepsilon + u_B^\varepsilon) = d_A\, u_A^\varepsilon + (d_A + d_B)\, u_B^\varepsilon$, so that $M^\varepsilon\,(u_A^\varepsilon + u_B^\varepsilon) \to d_A\, u_A + (d_A + d_B)\, u_B = d_A\, u + d_B\, u_B = d_A\, u + d_B\, \frac{h(v)\,u}{h(v)+k(v)} = (d_u + \phi(v))\,u$ a.e. on $\mathbb{R}_+ \times \Omega$. Then, using the convergence (4.49),

$$\int_0^\infty \int_\Omega \nabla_x\psi_1 \cdot \nabla_x[M^\varepsilon\,(u_A^\varepsilon + u_B^\varepsilon)] \to \int_0^\infty \int_\Omega \nabla_x\psi_1 \cdot \nabla_x[(d_u + \phi(v))\,u]. \tag{4.60}$$

Note that this automatically implies the estimate $\nabla_x(\phi(v)\,u) \in L^1$. It is however possible to directly get it by using estimate (4.42) and the fact that $\nabla_x v \in L^{2(1+p_0/d)}$. Indeed, one can get a slightly better estimate :

$$\nabla_x\,[(d_u + \phi(v))u] = \overbrace{(d_u + \phi(v))}^{\in L^\infty}\ \overbrace{\nabla_x u}^{\in L^{1+\zeta}} + \overbrace{u}^{\in L^{p_0+a}}\ \overbrace{\nabla_x\phi(v)}^{\in L^{2(1+p_0/d)}} \ \in\ L^{1+\zeta'} \qquad \text{for some } \zeta,\, \zeta' > 0.$$

This concludes the proof of Proposition 4.1. □

We now turn to the

Proof of Proposition 4.2. As in Proposition 4.1, we recall that for a given $\varepsilon \in]0,1[$, standard theorems for reaction-diffusion equations imply the existence of a (global, nonnegative for each component) strong solution $(u_A^\varepsilon, u_B^\varepsilon, v^\varepsilon)$ in the sense of Definition 4.2, to system (4.11), (4.13), (4.15). Moreover, properties (4.21) hold with $p_0 = 2$. We again refer to [13] for complete proofs.

Note first that the estimates of Lemmas 4.1 and 4.2 still hold under the assumptions of Proposition 4.2, with $p_0 = 2$ in the case of Lemma 4.2.

More precisely, the following (uniform w.r.t. $\varepsilon \in]0,1[$) estimates hold, the proofs being identical to those of Lemmas 4.1 and 4.2 :

$$\sup_{0\le t\le T} \int_\Omega (u_A^\epsilon + u_B^\epsilon)(t) \le C_T; \qquad \|u_A^\epsilon + u_B^\epsilon\|_{L^{1+a}} \le C_T, \tag{4.61}$$

and for all $1 < q \le 1 + 2/d$,

$$\|v^\epsilon\|_{L^\infty} \le C_T; \qquad \|\nabla_x v^\epsilon\|_{L^{2q}}^2 + \|\partial_t v^\epsilon\|_{L^q} \le C_T \,(1 + \|(u_A^\epsilon + u_B^\epsilon)^d\|_{L^q}). \tag{4.62}$$

In fact, estimate (4.27) still holds (it is the explicit version of the first part of (4.62)).

As a consequence, for all $p \in]0,1[$, taking $q = 1 + p/d \le 1 + 2/d$,

$$\|\,|\nabla_x v^\epsilon|^2\|_{L^{1+p/d}} \le C_T \,(1 + \|(u_A^\epsilon + u_B^\epsilon)^d\|_{L^{1+p/d}}); \qquad \|\partial_t v^\epsilon\|_{L^{1+p/d}} \le C_T \,(1 + \|(u_A^\epsilon + u_B^\epsilon)^d\|_{L^{1+p/d}}). \tag{4.63}$$

We now introduce a duality lemma in the spirit of the one used in [7] :

Lemma 4.4. *We consider $T > 0$, Ω a bounded regular open set of $\mathbb{R}^N$ $(N \in \mathbb{N}^*)$, and a function $M := M(t,x)$ satisfying*

$$0 < m_0 \le M(t,x) \le m_1 \qquad \text{for } t \in [0,T] \text{ and } x \in \Omega, \tag{4.64}$$

for some constants $m_0, m_1 > 0$. Then, one can find $p^* > 2$ such that for all $r \in [2, p^*[$, there exists a constant $C_T > 0$ depending only on Ω, N, T, and the constants m_0, m_1, r, such that for any initial datum u_{in} in $L^2(\Omega)$ and any $K > 0$, all nonnegative strong solutions $u \in L^r([0,T]\times\Omega)$ of the system

$$\begin{cases} \partial_t u - \Delta_x(Mu) \le K \text{ in } [0,T]\times\Omega, \\ u(0,x) = u_{in}(x) \text{ in } \Omega, \\ \nabla_x(Mu)(t,x)\cdot n(x) = 0 \text{ on } [0,T]\times\partial\Omega, \end{cases} \tag{4.65}$$

satisfy

$$\|u\|_{L^r([0,T]\times\Omega)} \le C_T \,\left(\|u_{in}\|_{L^2(\Omega)} + K\right). \tag{4.66}$$

Proof of Lemma 4.4. It relies on the study of the dual problem

$$\begin{cases} \partial_t v + M\Delta_x v = -f \text{ in } [0,T]\times\Omega, \\ v(T,x) = 0 \text{ in } \Omega, \\ \nabla_x v(t,x)\cdot n(x) = 0 \text{ on } [0,T]\times\partial\Omega, \end{cases} \tag{4.67}$$

for f a nonnegative function in $L^{r'}([0,T]\times\Omega)$, with $\frac{1}{r} + \frac{1}{r'} = 1$.

Using the notations of [7], we define the constant $C_{m,q} > 0$ for $m > 0$, $q \in]1,2]$ as the best constant in the parabolic estimate

$$\|\Delta_x w\|_{L^q([0,T]\times\Omega)} \le C_{m,q}\, \|g\|_{L^q([0,T]\times\Omega)}, \tag{4.68}$$

where g is any function in $L^q([0,T]\times\Omega)$ and w is the solution of the backward heat equation

$$\begin{cases} \partial_t w + m\,\Delta_x w = g \text{ in } [0,T]\times\Omega, \\ w(T,x) = 0 \text{ in } \Omega, \\ \nabla_x w(t,x)\cdot n(x) = 0 \text{ on } [0,T]\times\partial\Omega. \end{cases} \tag{4.69}$$

Let $r \ge 2$, $q = r' \le 2$ and let f be any smooth function defined on $[0,T]\times\Omega$. We consider the solution v of system (4.67). Notice that thanks to the minimum principle, v is nonnegative. Then, from Lemma

2.2 and Remark 2.3 in [7], there exists a constant C_T depending only on Ω, N, T and m_0, m_1, q such that v satisfies

$$\|\Delta_x v\|_{L^q} \leq C_T \, \|f\|_{L^q}, \tag{4.70}$$

and

$$\|v(0,\cdot)\|_{L^2(\Omega)} \leq C_T \, \|f\|_{L^q}, \tag{4.71}$$

provided that $q > 2\frac{N+2}{N+4}$ and

$$C_{\frac{m_0+m_1}{2},q} \, \frac{m_1 - m_0}{2} < 1. \tag{4.72}$$

Let us first assume that condition (4.72) holds for some fixed $q \in]2\frac{N+2}{N+4}, 2]$. Then we compute (for a.e. $t \in [0,T]$)

$$\frac{d}{dt} \int_\Omega u(t)v(t) \leq K \int_\Omega v(t) - \int_\Omega u(t) f(t), \tag{4.73}$$

so that integrating w.r.t. time, and using the condition $v(T,\cdot) = 0$,

$$\int_0^T \int_\Omega uf \leq K \int_0^T \int_\Omega v + \int_\Omega u_{in} \, v(0,\cdot). \tag{4.74}$$

The first term is estimated with (4.70) :

$$\int_0^T \int_\Omega v = -\int_0^T \int_\Omega \int_t^T \partial_t v = \int_0^T \int_\Omega \int_t^T (f + M\Delta_x v) \tag{4.75}$$

$$\leq T \left(\int_0^T \int_\Omega [f + m_1 |\Delta_x v|] \right) \leq T^{1+1/p} \, |\Omega|^{1/p} \, (1 + m_1 C_T) \, \|f\|_{L^q},$$

and the second term with (4.71) :

$$\int_\Omega u_{in} \, v(0,\cdot) \leq \|u_{in}\|_{L^2(\Omega)} \, \|v(0,\cdot)\|_{L^2(\Omega)} \leq C_T \, \|f\|_{L^q} \, \|u_{in}\|_{L^2(\Omega)}. \tag{4.76}$$

Recombining those estimates, we get

$$\int_0^T \int_\Omega u \, f \leq C_T \left(K + \|u_{in}\|_{L^2(\Omega)} \right) \|f\|_{L^q}, \tag{4.77}$$

which, by duality, gives estimate (4.66) (note that it is sufficient to show the previous bound for smooth f, since all functions of L^q can be approximated by such smooth functions in the L^q norm).

It remains to check that there exists an interval $[2, p^*[$ in which any r satisfies condition (4.72) with $q = r'$. This is done in [7]. □

We now come back to the proof of Proposition 4.2.

As in the proof of Proposition 4.1, we add the two equations and get

$$\partial_t(u_A^\epsilon + u_B^\epsilon) - \Delta_x[M^\epsilon(u_A^\epsilon + u_B^\epsilon)] = [r_u - r_a(u_A^\epsilon + u_B^\epsilon)^a - r_b(v^\epsilon)^b](u_A^\epsilon + u_B^\epsilon), \tag{4.78}$$

with

$$M^\epsilon = \frac{d_A u_A^\epsilon + (d_A + d_B) u_B^\epsilon}{u_A^\epsilon + u_B^\epsilon}.$$

Then $d_A \leq M^\epsilon \leq d_A + d_B$, and

$$[r_u - r_a(u_A^\epsilon + u_B^\epsilon)^a - r_b(v^\epsilon)^b] \, (u_A^\epsilon + u_B^\epsilon) \leq \sup_{w \geq 0} [r_u - r_a \, w^a] \, w = \left(\frac{r_u}{(1+a)\, r_a} \right)^{1/a} := K.$$

We can apply Lemma 4.4 to eq. (4.78), with M replaced by M^ε, u replaced by $u_A^\varepsilon + u_B^\varepsilon$, and u_{in} replaced by $u_{A,in}^\varepsilon + u_{B,in}^\varepsilon$. Note that for any $\varepsilon > 0$, $u_A^\varepsilon + u_B^\varepsilon$ is a strong solution of eq. (4.78).

Lemma 4.4 implies that for some $p^* > 2$,

$$||u_A^\varepsilon + u_B^\varepsilon||_{L^{p^*}} \leq C_T. \tag{4.79}$$

Using estimates (4.79) and (4.62), we see that when $p \in]0, p^* - d]$,

$$\| \nabla_x v^\epsilon \|_{L^{2\,(1+p/d)}} \le C_T; \qquad \|\partial_t v^\epsilon\|_{L^{1+p/d}} \le C_T. \tag{4.80}$$

Thanks to estimates (4.62), (4.80), we can extract from $(v^\epsilon)_{\epsilon>0}$ a subsequence (still denoted $(v^\epsilon)_{\epsilon>0}$) which converges a.e. towards some $v \in L^\infty$, and such that $\nabla_x v^\epsilon$ converges weakly in $L^{2\,(1+p/d)}$ (and therefore in L^1) towards $\nabla_x v$.

Recalling definition (4.31) and computation (4.32) in the case when $p \in]0, \inf(1, p^* - d)[$, we use the inequality (for a.e. $t \in [0, T]$)

$$-d_A \int_\Omega \Delta_x u_A^\epsilon (u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1} = -4\, d_A\, \frac{(1-p)}{p^2} \int_\Omega |\nabla_x[(u_A^\epsilon)^{p/2}]|^2 h(v^\epsilon)^{p-1}$$
$$-d_A\,(1-p) \int_\Omega (u_A^\epsilon)^{p-1} h'(v^\epsilon)\, h(v^\epsilon)^{p-2}\, \nabla_x u_A^\epsilon \cdot \nabla_x v^\epsilon$$
$$\le -2\, d_A\, \frac{(1-p)}{p^2} \int_\Omega |\nabla_x[(u_A^\epsilon)^{p/2}]|^2 h(v^\epsilon)^{p-1} + \frac{(1-p)}{2}\, d_A \int_\Omega |\nabla_x v^\epsilon|^2 (u_A^\epsilon)^p (h'(v^\epsilon))^2 h(v^\epsilon)^{p-3},$$

and the corresponding inequality for u_B^ε (with d_A replaced by $d_A + d_B$) and get the estimate

$$\begin{aligned}
&\int_\Omega \left[h(v_{in}^\epsilon)^{p-1} \frac{(u_{A,in}^\epsilon)^p}{p} + k(v_{in}^\epsilon)^{p-1} \frac{(u_{B,in}^\epsilon)^p}{p} \right] \\
&+ 2\, d_A \frac{1-p}{p^2} \int_0^T \int_\Omega |\nabla_x[(u_A^\epsilon)^{p/2}]|^2 h(v^\epsilon)^{p-1} + 2\,(d_A + d_B) \frac{1-p}{p^2} \int_0^T \int_\Omega |\nabla_x[(u_B^\epsilon)^{p/2}]|^2 k(v^\epsilon)^{p-1} \\
&- \frac{1}{\epsilon} \int_\Omega [k(v^\epsilon) u_B^\epsilon - h(v^\epsilon) u_A^\epsilon][(u_B^\epsilon)^{p-1} k(v^\epsilon)^{p-1} - (u_A^\epsilon)^{p-1} h(v^\epsilon)^{p-1}] \\
&\le \int_\Omega \left[h(v^\epsilon)^{p-1} \frac{(u_A^\epsilon)^p}{p}(T) + k(v^\epsilon)^{p-1} \frac{(u_B^\epsilon)^p}{p}(T) \right] \\
&+ \frac{1-p}{p} \int_0^T \int_\Omega \partial_t v^\epsilon [h'(v^\epsilon) h(v^\epsilon)^{p-2} (u_A^\epsilon)^p + k'(v^\epsilon) k(v^\epsilon)^{p-2} (u_B^\epsilon)^p] \\
&- \int_0^T \int_\Omega [r_u - r_a (u_A^\epsilon + u_B^\epsilon)^a - r_b (v^\epsilon)^b][(u_A^\epsilon)^p h(v^\epsilon)^{p-1} + (u_B^\epsilon)^p k(v^\epsilon)^{p-1}] \\
&+ \frac{1-p}{2} \int_0^T \int_\Omega [d_A (u_A^\epsilon)^p (h'(v^\epsilon))^2 h(v^\epsilon)^{p-3} + (d_A + d_B)(u_B^\epsilon)^p (k'(v^\epsilon))^2 k(v^\epsilon)^{p-3}] |\nabla_x v^\epsilon|^2.
\end{aligned} \tag{4.81}$$

Note that in estimate (4.81), the first and third terms of the r.h.s. are clearly bounded (w.r.t. $\varepsilon \in]0, 1[$) thanks to estimates (4.61), (4.62), and (4.79) (remember that $p \in]0, 1[$).

The second term is estimated thanks to the following inequality (remember that $p \in]0, \inf(1, p^* - d)[$, and that estimates (4.79), (4.80) hold) :

$$\begin{aligned}
&\left| \frac{1-p}{p} \int_0^T \int_\Omega \partial_t v^\epsilon [h'(v^\epsilon) h(v^\epsilon)^{p-2} (u_A^\epsilon)^p + k'(v^\epsilon) k(v^\epsilon)^{p-2} (u_B^\epsilon)^p] \right| \\
&\le \|h'(v^\epsilon) h(v^\epsilon)^{p-2} + k'(v^\epsilon) k(v^\epsilon)^{p-2}\|_{L^\infty} \|\partial_t v^\epsilon\|_{L^{1+p/d}} \|(u_A^\epsilon + u_B^\epsilon)^p\|_{L^{1+d/p}} \\
&\le C_T\,(1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p+d}}^{p+d}) \le C_T.
\end{aligned} \tag{4.82}$$

Finally, the last term is estimated thanks to the inequality (we still use $p \in]0, \inf(1, p^* - d)[$, and estimates (4.79), (4.80)) :

$$\begin{aligned}
&\left| \frac{1-p}{2} \int_0^T \int_\Omega [d_A (u_A^\epsilon)^p (h'(v^\epsilon))^2 h(v^\epsilon)^{p-3} + (d_A + d_B)(u_B^\epsilon)^p (k'(v^\epsilon))^2 k(v^\epsilon)^{p-3}] |\nabla_x v^\epsilon|^2 \right| \\
&\le (p/2)\, \|h'(v^\epsilon)^2 h(v^\epsilon)^{p-3} + k'(v^\epsilon)^2 k(v^\epsilon)^{p-3}\|_{L^\infty} \|\, |\nabla_x v^\epsilon|^2 \|_{L^{1+p/d}} \|(u_A^\epsilon + u_B^\epsilon)^p\|_{L^{1+d/p}} \\
&\le C_T\,(1 + \|u_A^\epsilon + u_B^\epsilon\|_{L^{p+d}}^{p+d}) \le C_T.
\end{aligned} \tag{4.83}$$

Finally, we end up with the following (uniform w.r.t. $\varepsilon \in]0,1[$) estimates (for $p \in]0, \inf(1, p^* - d)[$) :

$$\int_0^T \int_\Omega |\nabla_x[(u_A^\epsilon)^{p/2}]|^2 h(v^\epsilon)^{p-1} \le C_T, \qquad \int_0^T \int_\Omega |\nabla_x[(u_B^\epsilon)^{p/2}]|^2 k(v^\epsilon)^{p-1} \le C_T, \tag{4.84}$$

and

$$-\frac{1}{\epsilon} \int_\Omega [k(v^\epsilon)u_B^\epsilon - h(v^\epsilon)u_A^\epsilon]\,[(u_B^\epsilon)^{p-1}k(v^\epsilon)^{p-1} - (u_A^\epsilon)^{p-1}h(v^\epsilon)^{p-1}] \le C_T. \tag{4.85}$$

Remembering that h, k lie in $C^1(\mathbb{R}_+)$, and that v^ϵ is uniformly bounded (thanks to estimate (4.62)), we see that estimate (4.84) implies (for $p \in]0, \min(1, p^* - d)[$), the bound

$$||\nabla_x[(u_A^\varepsilon)^{p/2}]||_{L^2} \le C_T, \qquad ||\nabla_x[(u_B^\varepsilon)^{p/2}]||_{L^2} \le C_T. \tag{4.86}$$

Then, using the elementary inequality (for $p \in]0,1[$)

$$\forall x, y \in \mathbb{R}, \qquad -(x-y)\,(x^{p-1} - y^{p-1}) \ge C_p\,|x^{p/2} - y^{p/2}|^2,$$

where $C_p > 0$ is a constant (only depending on p), we obtain (for $p \in]0, \min(1, p^* - d)[$),

$$||(h(v^\varepsilon)\,u_A^\varepsilon)^{p/2} - (k(v^\varepsilon)\,u_B^\varepsilon)^{p/2}||_{L^2} \le C_T\,\sqrt{\varepsilon}.$$

Moreover, thanks to estimate (4.79), eq. (4.78) implies that $\partial_t(u_A^\varepsilon + u_B^\varepsilon)$ is bounded in $L^\lambda([0,T], W^{-2,\lambda})$ with $\lambda = \frac{p^*}{1+a} > 1$ (remember that $a \le 1$). Finally, for $C = A, B$, we still can use the computation of estimate (4.42) and get, for $p \in]0, \min(1, p^* - d)[$, and selecting $\zeta = \zeta(p) \in]0,1[$ such that $(2-p)\,\frac{1+\zeta}{1-\zeta} < 1$, thanks to the bounds (4.84) and (4.79),

$$\|\,|\nabla_x u_C^\epsilon|^{1+\zeta}\,\|_{L^1} \le (2/p)^{1+\zeta}\,||\nabla_x(u_C^\epsilon)^{p/2}||_{L^2}^{1+\zeta}\,\left(\int_0^T \int \left[|u_C^\epsilon|^{(2-p)\,\frac{1+\zeta}{1-\zeta}}\right]\right)^{\frac{1-\zeta}{2}} \le C_T. \tag{4.87}$$

We can therefore use Aubin's lemma and extract a subsequence from $(u_A^\epsilon + u_B^\epsilon)_\epsilon$ (we keep the notation $(u_A^\epsilon + u_B^\epsilon)_\epsilon$ for this subsequence) which converges towards a limit u (lying in L^2, and nonnegative) for a.e. $(t,x) \in [0,T] \times \Omega$.

Using the elementary inequality (4.44), inequality (4.45) still holds when $p \in]0, \min(1, p^* - d)[$, and implies the convergences (4.46), (4.47), (4.48), (4.50) [with $a + p_0$ replaced by p^*]. Moreover, thanks to estimate (4.87), the convergence (4.49) also holds.

Then, as in Proposition 4.1, u_A, u_B, v are defined on $\mathbb{R}_+ \times \Omega$, and $u_A, u_B, v \ge 0$ a.e. Moreover, $h(v)\,u_A = k(v)\,u_B$ a.e., and $u_A, u_B \in L^{p^*}$. Finally, we recall that $v \in L^\infty$.

Let us now show (4.19). Thanks to the uniform (in ε) estimates (4.61) and (4.86), we get for all $p \in]0, \min(1, p^* - d)[$,

$$\sup_{t\in[0,T]} \int_\Omega u(t) \le C_T \qquad \text{and} \qquad \int_0^T \int_\Omega \left(|\nabla_x u_A^{p/2}|^2 + |\nabla_x u_B^{p/2}|^2\right) \le C_T, \tag{4.88}$$

where we have used Fatou's lemma for the first inequality and Kakutani's Theorem applied to the reflexive space L^2 for the second inequality. We also recall that $\nabla_x v \in L^{2(1+p/d)}$ for all $p \in]0, p^* - d]$. Using the identity, $u = \frac{h(v)+k(v)}{k(v)}\,u_A$, we see that for some $p > 0$ small enough

$$\nabla_x\left(u^{p/2}\right) = \overbrace{u_A^{p/2}}^{\in L^{2p^*/p}}\;\overbrace{\left[\left(\frac{h+k}{k}\right)^{p/2}\right]'(v)}^{\in L^\infty}\;\overbrace{\nabla_x v}^{\in L^{2(1+p/d)}} + \overbrace{\left(\frac{h(v)+k(v)}{k(v)}\right)^{p/2}}^{\in L^\infty}\overbrace{\nabla_x\left(u_A^{p/2}\right)}^{\in L^2} \in L^2,$$

since (using $d \le 2 < p^*$) $\frac{1}{2p^*/p} + \frac{1}{2(1+p/d)} = \frac{p}{2p^*} + \frac{1}{2(1+p/d)} = \frac{1}{2} - \frac{p}{2}(\frac{1}{d} - \frac{1}{p^*}) + o_{p\to 0}(p) < \frac{1}{2}$ (remember that we take $p > 0$ small enough).

We now briefly indicate how to pass to the limit in the various terms appearing in the approximate equations (4.52) and (4.53). Using estimate (4.79), the uniform boundedness of v^ε in L^∞ and the weak convergence of $\nabla_x v^\epsilon$, we get (4.54) and (4.55).

The same estimates imply that $\psi_1\,(u^\epsilon_A+u^\epsilon_B)\,(r_u-r_a\,(u^\epsilon_A+u^\epsilon_B)^a-r_b\,(v^\epsilon)^b)$ is bounded in $L^{\frac{p^*}{1+a}}$, and $\psi_2\,v^\epsilon\,(r_v-r_c\,(v^\epsilon)^c-r_d\,(u^\epsilon_A+u^\epsilon_B)^d)$ is bounded in $L^{\frac{p^*}{d}}$, so that we get (4.56), (4.57).

We know that $u^\epsilon_{A,in}+u^\epsilon_{B,in}\to u_{in}$ a.e. on Ω. But $u_{in}\in L^2(\Omega)$, so that $u_{A,in}$ and $u_{B,in}$ also lie in $L^2(\Omega)$, and $u^\epsilon_{A,in},u^\epsilon_{B,in}$ are bounded (uniformly w.r.t. ε) in $L^2(\Omega)$, so that we get (4.58), (4.59).

Finally, the weak convergence (in L^1) of $\nabla_x u^\epsilon_C$ towards $\nabla_x u_C$ (for $C=A,B$) implies the convergence (4.60), and the estimate $\nabla_x[\phi(v)\,u]\in L^1$.

This concludes the proof of Proposition 4.2. □

4.3 Proof of existence, regularity and stability

In this section, we prove the Theorems 4.1 and 4.2.

Proof of Theorem 4.1. First step : existence

We use the notation $v_1:=\max\left(||v_{in}||_{L^\infty(\Omega)},\left[\frac{r_v}{r_c}\right]^{1/c}\right)$. Thanks to a smooth cutoff function $\chi(v)$ ($\chi(v)=1$ for $0\le v\le v_1$, $\chi(v)=0$ for $v\ge 2v_1$ and $0\le\chi(v)\le 1$ for all $v\ge 0$), we define $\phi_B(v):=\chi(v)\,\phi(v)$ for all $v\ge 0$. Since ϕ_B is a continuous function with compact support, it is bounded by some positive constant ϕ_1.

Thanks to Assumption A satisfied by the parameters of Theorem 4.1, we see that $d_u,d_v,r_u,r_v,r_a,r_b,r_c,r_d$, a,b,c,d satisfy Assumption B of Proposition 4.1. Then we define $d_A:=d_u/2$, $d_B:=d_u+\phi_1$, so that they also satisfy Assumption B (that is, they are strictly positive). Finally we define the functions h,k thanks to $h(v):=d_u/2+\phi_B(v)$, $k(v):=d_u/2+\phi_1-\phi_B(v)$. It is clear that $h,k\in C^1(\mathbb{R}_+)$ (because $\phi\in C^1(\mathbb{R}_+)$ and χ is smooth). Moreover $h(v)\ge d_u/2>0$, $k(v)\ge d_u/2>0$, and $d_A+d_B\frac{h(v)}{h(v)+k(v)}=d_u+\phi_B(v)$. As a consequence, Assumption B is fulfilled except that $\phi(v)$ is replaced by $\phi_B(v)$.

Moreover, the extra assumptions on the parameters ($d<a$) and on the initial data ($u_{in}\in L^{p_0}(\Omega)$, $v_{in}\in L^\infty(\Omega)\cap W^{2,1+p_0/d}(\Omega)$ for some $p_0>1$) are the same in Theorem 4.1 and Proposition 4.1.

Then, Proposition 4.1 ensures that there exists a weak solution to system (4.4)–(4.7) with $\phi(v)$ replaced by $\phi_B(v)$. Moreover, this solution (u,v) has nonnegative components, and for all $p\in]1,p_0]$, $T>0$,

$$\int_0^T\int_\Omega u^{p_0+a}\le C_T\qquad \int_0^T\int_\Omega|\nabla_x v|^{2(1+p_0/d)}\le C_T,$$
$$\sup_{t\in[0,T]}\int_\Omega u^{p_0}(t)\le C_T,\qquad \int_0^T\int_\Omega|\nabla_x u^{p/2}|^2\le C_T. \tag{4.89}$$

Finally, $\nabla_x u,\nabla_x(u\,\phi(v))\in L^1_{\text{loc}}(\mathbb{R}_+\times\overline{\Omega})$.

We also know that the bound $0\le v(t,x)\le v_1$ holds. By definition of ϕ_B, we then have $\phi_B(v(t,x))=\phi(v(t,x))$ for all $t\ge 0$, $x\in\Omega$, so that (u,v) is in fact a weak solution of (4.4)–(4.7), and this ends the proof of existence in Theorem 4.1.

Second step : regularity, first part

We fix $T>0$. Recall $p_1\ge 2$, $p_1>a(s_0-1)$. By assumption, u_{in} lies in $W^{2,s_0}(\Omega)$ with $s_0>1+N/2$, so that using a Sobolev embedding, u_{in} lies in $L^{p_1}(\Omega)$. We also know (thanks to our assumptions) that $v_{in}\in W^{2,1+p_1/d}(\Omega)$. The results of the first step can therefore be obtained with p_0 replaced by p_1 : in particular, estimate (4.89) with p_0 replaced by p_1 implies that $\int_0^T\int_\Omega u^{p_1+a}\le C_T$ and

$$\sup_{t\in[0,T]}\int_\Omega u^2(t)<+\infty\qquad;\qquad\int_0^T\int_\Omega|\nabla_x u|^2<+\infty. \tag{4.90}$$

We now define $q_0:=(a+p_1)/d>s_0$. Using the maximal regularity for the (weak solutions of the) heat equation, we get (remember that v lies in L^∞)

$$\|\partial_t v\|_{L^{q_0}}\le C_T\,(1+\|u^d\|_{L^{q_0}})\le C_T,\qquad \|\nabla_x^2 v\|_{L^{q_0}}\le C_T\,(1+\|u^d\|_{L^{q_0}})\le C_T. \tag{4.91}$$

Using embedding results (see for example Lemma 3.3 in Chapter II of [33]) and the fact that $q_0 > 1 + N/2$, we see that v is Hölder continuous on $[0,T] \times \overline{\Omega}$.

This shows that v has the smoothness required in the theorem.

Similarly, $\partial_t \phi(v) = \phi'(v)\, \partial_t v$ and $\nabla_x^2 \phi(v) = \phi''(v)\, |\nabla_x v|^2 + \phi'(v) \nabla_x^2 v$ lie in L^{q_0}, so that $\phi(v)$ is also Hölder continuous on $[0,T] \times \overline{\Omega}$. We then rewrite the equation satisfied by u as

$$\partial_t u - \nabla_x \cdot [A(t,x)\, \nabla_x u + B(t,x) u] + C(t,x)\, u = 0, \tag{4.92}$$

where $A = d_u + \phi(v)$ is Hölder continuous on $[0,T] \times \overline{\Omega}$, $B = \nabla_x \phi(v)$ lies in L^{2q_0}, and $C = -r_u + r_a u^a + r_b v^b$ lies in $L^{1+p_1/a}$. Note furthermore that $\nabla_x A = \nabla_x \phi(v)$ lies in L^{2q_0} and $\nabla_x \cdot B = \Delta_x \phi(v)$ lies in L^{q_0}.

We now recall two classical theorems from the theory of linear parabolic equations (see for example Theorem 5.1 in Chapter III of [33] for the first one, and Theorem 9.1 and its corollary in Chapter IV of [33] for the second one) :

Proposition 4.3. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$), $T > 0$ and $u_{in} \in L^2(\Omega)$. Consider the system*

$$\begin{aligned} \partial_t u - \nabla_x \cdot [A(t,x)\, \nabla_x u + B(t,x) u] + C(t,x)\, u = 0 \quad &\text{in } [0,T] \times \Omega, \\ \nabla_x u(t,x) \cdot n(x) = 0 \quad \text{on } [0,T] \times \partial\Omega, \qquad u(0,\cdot) = u_{in} \quad &\text{in } \Omega, \end{aligned} \tag{4.93}$$

where the coefficients satisfy : $A := A(t,x) > 0$ is continuous on $[0,T] \times \overline{\Omega}$, $B := B(t,x)$ lies in $(L^{N+2})^N$, and $C := C(t,x)$ lies in $L^{1+N/2}$.

A function $u := u(t,x)$ is said to be a weak solution of (4.93) *(in the V_2 sense) if u satisfies* (4.90) *and, for all test functions $\psi \in C_c^1([0,T[\times\overline{\Omega})$, the following identity holds :*

$$-\int_0^\infty \int_\Omega (\partial_t \psi)\, u - \int_\Omega \psi(0,\cdot)\, u_{in} + \int_0^\infty \int_\Omega [A\, \nabla_x u + B\, u] \cdot \nabla_x \psi + \int_0^\infty \int_\Omega C\, u\, \psi = 0.$$

Notice that all terms in the previous identity are well defined when u, ψ, A, B, C satisfy the assumptions of Proposition 4.3 (cf. estimate (3.4) in Chapter II of [33]).

Then system (4.93) *has at most one weak solution (in the V_2 sense).*

Proposition 4.4. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$), $s > 1 + N/2$ and $T > 0$. Consider the system*

$$\begin{aligned} \partial_t u - A(t,x)\, \Delta_x u + B_1(t,x) \cdot \nabla_x u + C_1(t,x)\, u = 0 \quad &\text{in } [0,T] \times \Omega, \\ \nabla_x u(t,x) \cdot n(x) = 0 \quad \text{on } [0,T] \times \partial\Omega, \qquad u(0,\cdot) = u_{in} \quad &\text{in } \Omega, \end{aligned} \tag{4.94}$$

where the coefficients satisfy : $A := A(t,x) > 0$ is continuous on $[0,T] \times \overline{\Omega}$, $B_1 := B_1(t,x)$ lies in $(L^r)^N$ for some $r > \max(s, N+2)$, and $C_1 := C_1(t,x)$ lies in $L^{r'}$ for some $r' > s$. Suppose also that $u_{in} \in W^{2,s}(\Omega)$ (and, if $s \geq 3$, that the compatibility condition $\nabla_x u_{in}(x) \cdot n(x) = 0$ on $\partial\Omega$ holds).

A function $u := u(t,x)$ is said to be a strong solution of (4.94) *(in the $W_s^{1,2}$ sense) if $\partial_t u$ and $\partial^2_{x_i x_j} u$ lie in L^s (for $i,j = 1..N$) and system* (4.94) *is satisfied almost everywhere in $[0,T] \times \Omega$ (resp. $[0,T] \times \partial\Omega$, resp. Ω).*

Then, system (4.94) *has a unique strong solution u (in the $W_s^{1,2}$ sense). Furthermore, u is Hölder continuous on $[0,T] \times \overline{\Omega}$.*

A direct consequence of these two propositions is given by the

Corollary 4.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^N$ ($N \in \mathbb{N}^*$), $s > 1 + N/2$ and $T > 0$. We assume that u_{in}, A, B, C, $B_1 := -B - \nabla_x A$ and $C_1 := C - \nabla_x \cdot B$ satisfy the requirements of Propositions 4.3 and 4.4.*

Then any weak solution u of system (4.93)*, or equivalently system* (4.94)*, (in the V_2 sense) is a strong solution (in the $W_s^{1,2}$ sense). In particular, $\partial_t u$ and $\partial^2_{x_i x_j} u$ lie in L^s (for $i,j = 1..N$). Furthermore, u is Hölder continuous on $[0,T] \times \overline{\Omega}$.*

Remark 4.6. *Proposition 4.4 (and therefore Corollary 4.1) furthermore provides upper bounds for the L^s norms of the derivatives $\partial_t u$ and $\partial^2_{x_i x_j} u$ (for $i,j = 1..N$). It can be checked in the proof in [33] that these upper bounds only depend on the initial datum u_{in}, the domain Ω (and the dimension N), the time T, the parameters s, r and r', the norms $\|B_1\|_{L^r}$ and $\|C_1\|_{L^{r'}}$, the positive quantities $\min_{[0,T]\times\overline{\Omega}} A$ and $\max_{[0,T]\times\overline{\Omega}} A$ and the modulus of continuity of A on $[0,T] \times \overline{\Omega}$.*

We now come back to the second step of the proof of Theorem 4.1. Using Corollary 4.1 with $s = s_0$, we see that u has the smoothness required in the theorem. This concludes the second step of the proof of Theorem 4.1, that is the first part of the study of regularity.

Third step : regularity, second part

We now assume that ϕ (resp. u_{in}, v_{in}) have α-Hölder continuous second order derivatives on $\mathbb{R}_+$ (resp. $\overline{\Omega}$) for some $\alpha \in]0,1[$. We fix $T > 0$.

We already know that u and v are Hölder continuous on $[0,T] \times \overline{\Omega}$. It is then clear that in eq. (4.5), the reaction term is Hölder continuous on $[0,T] \times \overline{\Omega}$. Thanks to standard results in the theory of linear parabolic equations (see for example Theorem 5.3 in Chapter IV of [33]), $\partial_t v$ and $\nabla_x^2 v$ are also Hölder continuous on $[0,T] \times \overline{\Omega}$. Writing eq. (4.4) in its form (4.94), we see that the coefficients A, $B_1 := -B - \nabla_x A$ and $C_1 := C - \nabla_x \cdot B$ are Hölder continuous on $[0,T] \times \overline{\Omega}$ (note that we use here the Hölder continuity of ϕ''). The same result for linear parabolic equations implies that $\partial_t u$ and $\nabla_x^2 u$ are Hölder continuous on $[0,T] \times \overline{\Omega}$. Furthermore, we obtain bounds for the β-Hölder norms on $[0,T] \times \overline{\Omega}$ (for some $\beta > 0$) of $\partial_t v$, $\nabla_x^2 v$, $\partial_t u$ and $\nabla_x^2 u$ and for the L^∞ norms of v, $\partial_t v$, $\nabla_x v$, $\nabla_x^2 v$, u, $\partial_t u$, $\nabla_x u$ and $\nabla_x^2 u$ which depend only on the initial data u_{in} and v_{in}, the domain Ω (and the dimension N), the parameters of the system (4.4)–(4.5), the time T and the parameter α.

This concludes the second step of the study of the regularity.

Fourth step : stability and uniqueness

We still assume that ϕ (resp. u_{in}, v_{in}) have α-Hölder continuous second order derivatives on $\mathbb{R}_+$ (resp. $\overline{\Omega}$). We pick up some $K > 0$ such that the L^∞ norms of the zeroth, first and second order spatial derivatives and the α-Hölder norms of the second order derivatives of u_{in}, v_{in} are bounded by K.

Let (u_1, v_1) and (u_2, v_2) be two weak solutions of (4.4)-(4.7) in the sense of Definition 4.1 satisfying the assumptions of the theorem. Notice that by assumption u_1, $u_2 \in L^{p_1+a}$. Moreover, (4.90) with $u = u_1$, u_2 holds. Therefore the computations of the second and third steps are valid for $(u,v) = (u_1,v_1)$, (u_2,v_2). This implies that these solutions (u_1, v_1) and (u_2, v_2) are continuous (and even Hölder continuous) functions on $[0,T] \times \overline{\Omega}$, and so are their space gradients $\nabla_x u_i$ and $\nabla_x v_i$. Furthermore, these quantities are bounded in L^∞ by a constant $C_T > 0$ depending only on K, the domain Ω (and the dimension N), the parameters of the system (4.4)–(4.5), the time T and the parameter α.

For any function $(u,v) \mapsto F(u,v)$, we write $\overline{F(u,v)} = \frac{F(u_1,v_1)+F(u_2,v_2)}{2}$.

We substract the equations satisfied by (u_2, v_2) to the equations satisfied by (u_1, v_1), and get

$$\begin{aligned}
&\partial_t(u_1 - u_2) - \Delta_x[(d_A + \overline{\phi(v)})\,(u_1 - u_2)] - \Delta_x[(\phi(v_1) - \phi(v_2))\,\overline{u}] \\
&\qquad = [r_v - r_a\,\overline{u^a} - r_b\,\overline{v^b}]\,(u_1 - u_2) - [r_a\,(u_1^a - u_2^a) + r_b\,(v_1^b - v_2^b)]\,\overline{u}, \\
&\partial_t(v_1 - v_2) - d_v\,\Delta_x(v_1 - v_2) \\
&\qquad = [r_v - r_c\,\overline{v^c} - r_d\,\overline{u^d}]\,(v_1 - v_2) - [r_c\,(v_1^c - v_2^c) + r_d\,(u_1^d - u_2^d)]\,\overline{v}.
\end{aligned} \tag{4.95}$$

We multiply the first equation by the difference $u_1 - u_2$ and integrate w.r.t. space and time. We get the identity

$$\begin{aligned}
&\frac{1}{2}\int_\Omega (u_1 - u_2)^2(T) \\
&+ \int_0^T \int_\Omega (d_A + \overline{\phi(v)})\,|\nabla_x(u_1 - u_2)|^2 + \int_0^T \int_\Omega (u_1 - u_2)\nabla_x(u_1 - u_2)\cdot\nabla_x(\overline{\phi(v)}) \\
&+ \int_0^T \int_\Omega (\phi(v_1) - \phi(v_2))\nabla_x(u_1 - u_2)\cdot\nabla_x\overline{u} + \int_0^T \int_\Omega \overline{u}\,\nabla_x(u_1 - u_2)\cdot\nabla_x[\phi(v_1) - \phi(v_2)] \\
&= \frac{1}{2}\int_\Omega (u_1 - u_2)^2(0) + \int_0^T \int_\Omega [r_v - r_a\overline{u^a} - r_b\overline{v^b}]\,(u_1 - u_2)^2 \\
&\quad - \int_0^T \int_\Omega (u_1 - u_2)\,[r_a\,(u_1^a - u_2^a) + r_b\,(v_1^b - v_2^b)]\,\overline{u}.
\end{aligned} \tag{4.96}$$

In the left-hand side of this identity, the two first terms are nonnegative. The other terms are controlled thanks to the smoothness of the functions $(\overline{u}, \overline{v})$ and their space gradients (and the elementary inequality $2ab \le a^2 + b^2$). We detail below their treatment : the third term of (4.96) is controlled by

$$\begin{aligned}\Big|\int_0^T \int_\Omega (u_1 - u_2)\,\nabla_x(u_1 - u_2)\cdot\nabla_x(\overline{\phi(v)})\Big| &\le C_T \int_0^T \int_\Omega |u_1 - u_2|\,|\nabla_x(u_1 - u_2)| \\ &\le \frac{d_A}{4}\int_0^T \int_\Omega |\nabla_x(u_1 - u_2)|^2 + C_T \int_0^T \int_\Omega |u_1 - u_2|^2,\end{aligned} \tag{4.97}$$

the fourth term of (4.96) is controlled by

$$\begin{aligned}&\left|\int_0^T \int_\Omega (\phi(v_1) - \phi(v_2))\,\nabla_x(u_1 - u_2)\cdot\nabla_x\overline{u}\right| \\ &\le \frac{d_A}{4}\int_0^T \int_\Omega |\nabla_x(u_1 - u_2)|^2 + C_T \int_0^T \int_\Omega |\phi(v_1) - \phi(v_2)|^2,\end{aligned} \tag{4.98}$$

and the fifth term of (4.96) is controlled by

$$\begin{aligned}&\left|\int_0^T \int_\Omega \overline{u}\,\nabla_x(u_1 - u_2)\cdot\nabla_x[\phi(v_1) - \phi(v_2)]\right| \\ &\le \frac{d_A}{4}\int_0^T \int_\Omega |\nabla_x(u_1 - u_2)|^2 + C_T \int_0^T \int_\Omega |\nabla_x[\phi(v_1) - \phi(v_2)]|^2,\end{aligned} \tag{4.99}$$

where moreover

$$\begin{aligned}\int_0^T \int_\Omega |\nabla_x[\phi(v_1) - \phi(v_2)]|^2 &= \int_0^T \int_\Omega |\overline{\phi'(v)}\,\nabla_x(v_1 - v_2) + (\phi'(v_1) - \phi'(v_2))\,\nabla_x\overline{v}|^2 \\ &\le C_T \int_0^T \int_\Omega |\nabla_x(v_1 - v_2)|^2 + C_T \int_0^T \int_\Omega |\phi'(v_1) - \phi'(v_2)|^2.\end{aligned} \tag{4.100}$$

It remains to control the last term of the right-hand side :

$$\begin{aligned}-\int_0^T \int_\Omega (u_1 - u_2)\,[r_a\,(u_1^a - u_2^a) + r_b\,(v_1^b - v_2^b)]\,\overline{u} &\le r_b \int_0^T \int_\Omega |u_1 - u_2|\,|v_1^b - v_2^b|\,\overline{u} \\ &\le C_T \int_0^T \int_\Omega |u_1 - u_2|^2 + C_T \int_0^T \int_\Omega |v_1^b - v_2^b|^2.\end{aligned} \tag{4.101}$$

Thanks to those estimates, the identity (4.96) becomes

$$\begin{aligned}\int_\Omega (u_1 - u_2)^2(T) \le \int_\Omega (u_1 - u_2)^2(0) + C_T \Bigg(\int_0^T \int_\Omega (u_1 - u_2)^2 + \int_0^T \int_\Omega |\phi(v_1) - \phi(v_2)|^2 \\ + \int_0^T \int_\Omega |\phi'(v_1) - \phi'(v_2)|^2 + \int_0^T \int_\Omega |\nabla_x(v_1 - v_2)|^2 + \int_0^T \int_\Omega |v_1^b - v_2^b|^2\Bigg).\end{aligned} \tag{4.102}$$

We now multiply the second equation of (4.95) by the difference $v_1 - v_2$ and integrate w.r.t. space and time. We get

$$\begin{aligned}&\frac{1}{2}\int_\Omega (v_1 - v_2)^2(T) + d_v \int_0^T \int_\Omega |\nabla_x(v_1 - v_2)|^2 \\ &= \frac{1}{2}\int_\Omega (v_1 - v_2)^2(0) \\ &+ \int_0^T \int_\Omega [r_v - r_c\,\overline{v^c} - r_d\,\overline{u^d}]\,(v_1 - v_2)^2 - \int_0^T \int_\Omega (v_1 - v_2)\,[r_c\,(v_1^c - v_2^c) + r_d\,(u_1^d - u_2^d)]\,\overline{v} \\ &\le \frac{1}{2}\int_\Omega (v_1 - v_2)^2(0) + C_T\Big(\int_0^T \int_\Omega (v_1 - v_2)^2 + \int_0^T \int_\Omega |u_1^d - u_2^d|^2\Big).\end{aligned} \tag{4.103}$$

We combine the two energy estimates (4.102) and (4.103) :

$$\int_\Omega (u_1-u_2)^2(T) + \int_\Omega (v_1-v_2)^2(T) \le \int_\Omega (u_1-u_2)^2(0) + \int_\Omega (v_1-v_2)^2(0)$$
$$+ C_T \Bigg(\int_0^T \int_\Omega (u_1-u_2)^2 + \int_0^T \int_\Omega (v_1-v_2)^2 \tag{4.104}$$
$$+ \int_0^T \int_\Omega |u_1^d - u_2^d|^2 + \int_0^T \int_\Omega |\phi(v_1)-\phi(v_2)|^+ \int_0^T \int_\Omega |v_1^b - v_2^b|^2 + \int_0^T \int_\Omega |\phi'(v_1)-\phi'(v_2)|^2 \Bigg).$$

Since ϕ'' is continuous on $\mathbb{R}_+$, the applications ϕ and ϕ' are locally Lipschitz on $\mathbb{R}_+$. The assumption $b \ge 1, d \ge 1$ ensures that the applications $v \mapsto v^b$ and $u \mapsto u^d$ are also locally Lipschitz on $\mathbb{R}_+$. Therefore

$$\int_\Omega (u_1-u_2)^2(T) + \int_\Omega (v_1-v_2)^2(T) \le \int_\Omega (u_1-u_2)^2(0) + \int_\Omega (v_1-v_2)^2(0) \tag{4.105}$$
$$+ C_T \left(\int_0^T \int_\Omega (u_1-u_2)^2 + \int_0^T \int_\Omega (v_1-v_2)^2 \right),$$

and we can conclude thanks to Gronwall's lemma.

Note that thanks to the minimum principle, the assumption $b \ge 1, d \ge 1$ can be relaxed if the initial data u_{in} and v_{in} are bounded below by a strictly positive constant.

This concludes the study of stability (and uniqueness), and ends the proof of Theorem 4.1.

□

Proof of Theorem 4.2. We use again the notation $v_1 := \max\left(||v_{in}||_{L^\infty(\Omega)}, \left[\frac{r_v}{r_c}\right]^{1/c} \right)$. We also introduce a smooth cutoff function $\chi(v)$ ($\chi(v) = 1$ for $0 \le v \le v_1$, $\chi(v) = 0$ for $v \ge 2v_1$ and $0 \le \chi(v) \le 1$ for all $v \ge 0$), together with $\phi_B(v) := \chi(v)\,\phi(v)$ (for all $v \ge 0$), and an upper bound ϕ_1 for ϕ_B.

Thanks to Assumption A satisfied by the parameters of Theorem 4.2, we see that the parameters $d_u, d_v,\ r_u, r_v, r_a, r_b, r_c, r_d,\ a, b, c, d$ satisfy Assumption B of Proposition 4.2. Then we define, as in the proof of Theorem 4.1, $d_A := d_u/2$, $d_B := d_u + \phi_1$, so that they satisfy Assumption B, and the functions h, k thanks to $h(v) := d_u/2 + \phi_B(v)$, $k(v) := d_u/2 + \phi_1 - \phi_B(v)$. It is clear that $h, k \in C^1(\mathbb{R}_+)$ and $h(v) \ge d_u/2 > 0$, $k(v) \ge d_u/2 > 0$, and $d_A + d_B \frac{h(v)}{h(v)+k(v)} = d_u + \phi_B(v)$. As a consequence, Assumption B is fulfilled except that $\phi(v)$ is replaced by $\phi_B(v)$.

Moreover, the extra assumptions on the parameters ($d \ge a$, $a \le 1$, $d \le 2$) and on the initial data ($u_{in} \in L^2(\Omega)$, $v_{in} \in L^\infty(\Omega) \cap W^{2,1+2/d}(\Omega)$) are the same in Theorem 4.2 and Proposition 4.2.

Then, Proposition 4.2 ensures that there exists a weak solution to system (4.4)–(4.7) with $\phi(v)$ replaced by $\phi_B(v)$. Moreover, this solution (u, v) has nonnegative components and lies in $L^2_{\text{loc}}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{\text{loc}}(\mathbb{R}_+ \times \overline{\Omega})$. We also know that for some $p > 0$, u satisfies (4.19). Moreover, we know that $\nabla_x v \in L^{2+\eta}_{\text{loc}}(\mathbb{R}_+ \times \overline{\Omega})$, $\nabla_x u, \nabla_x(u\,\phi(v)) \in L^1_{\text{loc}}(\mathbb{R}_+ \times \overline{\Omega})$, for some $\eta > 0$.

Finally, we know that the bound $0 \le v(t,x) \le v_1$ holds, so that by definition of ϕ_B, we see that $\phi_B(v(t,x)) = \phi(v(t,x))$ for all $t \ge 0$, $x \in \Omega$. Then, (u, v) is in fact a weak solution of (4.4)–(4.7). This ends the proof of Theorem 4.2. □

Chapitre 5

Reaction-cross diffusion systems : entropic structure

Abstract

This Chapter is taken from the paper [16] in collaboration with L. Desvillettes, Th. Lepoutre and A. Moussa. It is devoted to the study of systems of reaction-cross diffusion equations arising in Population dynamics. New results of existence of weak solutions are presented, allowing to treat systems of two equations in which one of the cross diffusion terms is convex, while the other one is concave. The treatment of such cases involves a general study of the structure of Lyapunov functionals for cross diffusion systems, and the introduction of a new approximation scheme, which provides simplified proofs of existence.

Sommaire

5.1 Introduction

5.1.1 The system

All the systems that we are going to tackle in this study take the following form

$$\partial_t u_i - \Delta[a_i(u_1,\dots,u_I)\,u_i] = r_i(u_1,\cdots,u_I)\,u_i, \text{ on } \mathbb{R}_+\times\Omega, \text{ for } i=1,\dots,I, \tag{5.1}$$

where $a_i, r_i : \mathbb{R}^I \to \mathbb{R}$, the unknown being here the family of I nonnegative functions $u_1,\dots,u_I$. Here and hereafter, Ω is a bounded open set of $\mathbb{R}^d$, whose unit normal outward vector at point $x\in\partial\Omega$ is denoted by $n=n(x)$. The system is completed with initial conditions given by a family of functions $u_1^{in},\dots,u_I^{in}$, and homogeneous Neumann boundary conditions, that is $\partial_n u_i := \nabla u_i\cdot n = 0$ on $\mathbb{R}_+\times\partial\Omega$ for $i=1,\dots,I$.

Introducing the vectorial notations $U := (u_1,\dots,u_I)$ and $U^{in} := (u_1^{in},\dots,u_I^{in})$, and denoting by A and R the maps $A : U\mapsto (a_i(U)\,u_i)_i$ and $R : U \mapsto (r_i(U)\,u_i)_i$, the previous system (5.1) can be summarized in the vectorial equations

$$\partial_t U - \Delta[A(U)] = R(U), \text{ on } \mathbb{R}_+\times\Omega, \tag{5.2}$$

$$\partial_n U = 0, \text{ on } \mathbb{R}_+\times\partial\Omega, \tag{5.3}$$

$$U(0) = U^{in}, \text{ on } \Omega. \tag{5.4}$$

Such systems have received a lot of attention lately (cf. [8], [15], for example). Their origin is to be found in the seminal paper [45], where one typical example (now known in the literature as the SKT system) is introduced : namely, $I=2$, and A, R are given by affine functions :

$$a_1(u_1,u_2) = d_1 + d_{11}\,u_1 + d_{12}\,u_2, \qquad a_2(u_1,u_2) = d_2 + d_{21}\,u_1 + d_{22}\,u_2,$$

$$r_1(u_1,u_2) = R_1 - R_{11}\,u_1 - R_{12}\,u_2, \qquad r_2(u_1,u_2) = R_2 - R_{21}\,u_1 - R_{22}\,u_2.$$

The corresponding equations model the evolution of individuals belonging to two species in competition, which increase their diffusion rate in order to avoid the individuals of the other (or the same) species. This evolution can lead to the formation of patterns when $t\to\infty$ (cf. [45]). There is an important literature on the question of existence of global classical solutions to the SKT systems (but only for particular cases). To summarize the approach, one can prove local existence of classical solutions using Amann's theorem [3] and the difficulty relies then in the proof of bounds on the solutions in suitable Sobolev spaces to prevent blow up. The works in this direction always have restrictions on the coefficients (typically no cross diffusion is introduced for one of the species, cf. for example [17]) and/or on dimension. In particular, it is worth noticing that existence of global classical solutions to the full SKT system (that is, when all coefficients are positive) remains a challenging open problem except in dimension 1.

Our work however deals with the existence of global weak solutions for which an important step forward was made by Chen and Jüngel in [8]. They indeed showed that a hidden Lyapunov-style (also called entropy) functional (that is, a Lyapunov functional if the terms r_1, r_2 are neglected) exists for this system without restriction on coefficients such as strong self diffusion for instance. Their entropy is based on the following remark : the SKT system can be rewritten under the following form, setting $d_{ij}=1$ for simplification

$$\partial_t U = \partial_t\begin{pmatrix}u_1\\u_2\end{pmatrix} = \nabla\cdot\underbrace{\begin{pmatrix}(d_1+2u_1+u_2)u_1 & u_1u_2\\ u_1u_2 & (d_2+u_1+2u_2)u_2\end{pmatrix}}_{Z(u_1,u_2)}\begin{pmatrix}\nabla\log u_1\\ \nabla\log u_2\end{pmatrix} + R(U).$$

Noticing that the matrix Z is positive definite, multypling the equation by $(\log u_1,\, \log u_2)$ and integrating over space, one obtains a bound of type

$$\frac{d}{dt}\int_\Omega\Big[u_1\log u_1 + u_2\log u_2\Big] + \int_\Omega \begin{pmatrix}\nabla\log u_1 & \nabla\log u_2\end{pmatrix} Z(u_1,u_2)\begin{pmatrix}\nabla\log u_1\\ \nabla\log u_2\end{pmatrix}$$

$$\leq C\left(1+\int_\Omega\Big[u_1\log u_1 + u_2\log u_2\Big]\right),$$

where the term involving gradients is strictly positive.

In [15], this structure was shown to be robust enough to treat functions a_1, a_2 such as

$$a_1(u_1, u_2) = d_1 + d_{11}\, u_1^{\delta_{11}} + d_{12}\, u_2^{\delta_{12}}, \qquad a_2(u_1, u_2) = d_2 + d_{21}\, u_1^{\delta_{21}} + d_{22}\, u_2^{\delta_{22}}, \tag{5.5}$$

when $\delta_{12} \in]0,1[$ and $\delta_{21} \in]0,1[$. A tool coming out of the reaction-diffusion theory (namely, duality lemmas, cf. [43]) was also introduced in the context of cross diffusion type systems in [5] and [4]. It was then used, associated with the entropy structure in [15], in order to extend the range of systems that could be treated. This tool gives an additional estimate, namely (when suitable assumptions are made on R),

$$\Big(\sum_i u_i\Big)\Big(\sum_j a_j(U)\, u_j\Big) \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+, \mathrm{L}^1(\Omega)).$$

This bound can be crucial, especially when the gradients controlled by the entropy are very weak. In particular, in many cases, this extra bound is useful for getting uniform integrability of reaction terms.

In this paper, we investigate more deeply the structure of systems like (5.1), in order to exhibit as much as possible the conditions which enable the existence of Lyapunov-style functionals. Subsection 5.3.2 is directly devoted to this study. As an application, we show that cross-diffusion terms like (5.5) can be treated as soon as the product $\delta_{12}\,\delta_{21}$ belongs to $]0,1[$, thus significantly enlarging the conditions described in [15].

Another difficulty appearing in many works on equations involving cross diffusion is the difficulty, once *a priori* estimates have been established, to write down an approximation scheme which implies existence. An important issue comes from the fact that the entropy structure and the duality estimates are of very different nature. Therefore it is difficult to build an approximation that preserves both properties. In [8] and related works, the entropy induces a better integrability, or even boundedness in [29, 30], making the use of duality estimates unnecessary. In [15], the approximation procedure is inspired from [8] and duality is proved to be satisfied *a posteriori* (in fact at some intermediate step). This is related to a lack of robustness of the Lyapunov-style functionals (it is indeed difficult to extend them to the approximate system). We therefore present in this paper a new approximation scheme which is definitely easier to grasp than those presented in [8] or [15]. Indeed, we use a time-discretized version of the equation for which existence can be obtained thanks to a standard (Schauder-type) fixed-point theorem, and which conserves the structure of the time-continuous equation from the viewpoint of *a priori* estimates. As a consequence, the passage to the limit when the discretization step goes to 0 is not much more difficult than the passage to the limit in a sequence of solutions to the equation (that is, the weak stability of the equation). Note that a related (yet different) time-discrete approximation was recently used (together with a regularization) in the context of cross-diffusion systems in [29].

5.1.2 Assumptions

Throughout this study, we will state and prove results necessitating one or several of the following assumptions on the parameters of (5.1) :

H1 The functions a_i and r_i are continuous from $\mathbb{R}_+^I$ to $\mathbb{R}$.

H2 For all i, a_i is lower bounded by some positive constant $\alpha > 0$, and r_i is upper bounded by a positive constant $\rho > 0$. That is $a_i(U) \geq \alpha > 0$, $r_i(U) \leq \rho$ for all $U \in \mathbb{R}_+^I$.

H3 A is a homeomorphism from $\mathbb{R}_+^I$ to itself.

The set of all these assumptions will be invoked at the beginning of each statement (if needed) by writing (**H**). Assumption **H3** will be of utmost importance during the establishment of our approximation scheme. Assumptions **H1** and **H2** are usually easily checked and appear quite natural. It is however less clear to understand what type of systems satisfies **H3**. We explain in Remark 5.1 why **H3** can also often be easily checked in our framework.

5.1.3 Notations

Since we will always work on $Q_T := [0,T] \times \Omega$, we will simply denote by $\mathrm{L}^p_t(\mathrm{L}^q_x)$ the corresponding evolution spaces and we will use the same convention for Sobolev spaces H^ℓ and $\mathrm{W}^{\ell,p}$ (for $\ell \in \mathbb{N}, p \in [1,\infty]$). Cones of nonnegative functions will be denoted by a $+$ subscript, for instance $\mathrm{L}^\infty(\Omega)_+$ is the cone of all essentially bounded nonnegative functions. For $p \in [1,\infty[$, we will sometimes use the notation L^{p^+} to speak of the set of all L^q functions with $q > p$. We define also the space $\mathrm{H}^1_m(\Omega)$ of $\mathrm{H}^1(\Omega)$ functions having zero mean. Its dual is denoted by $\mathrm{H}^{-1}_m(\Omega)$. For any space of functions defined on Ω whose gradient has a well-defined trace on $\partial\Omega$ (such as $\mathrm{H}^2(\Omega)$ or $\mathscr{C}^\infty(\overline{\Omega})$ for instance), we add the subscript ν (the former spaces becoming then $\mathrm{H}^2_\nu(\Omega)$ and $\mathscr{C}^\infty_\nu(\overline{\Omega})$) when we wish to consider the subspaces of functions satisfying the homogeneous Neumann boundary condition.

Given a normed space X, we will always denote by $\|\cdot\|_X$ its norm, except for L^p spaces for which we often write $\|\cdot\|_p$. The symbol $|\cdot|$ will always represent the Euclidian norm (but possibly in different dimensions depending of the context), whereas $|\cdot|_1$ will be the Manhattan norm. Finally, given two vectors $X = (x_i)_i$ and $Y = (y_i)_i$ of $\mathbb{R}^I$, we write $X \le Y$ whenever $x_i \le y_i$ for all i. We extend this order relation to $\mathbb{R}^I$ valued functions $f(X)$ and write, for a real number c, $f(X) \le c$ when $f(X) \le C = (c, \dots, c)$. The same convention is used for $<$. The set of nonnegative numbers is denoted $\mathbb{R}_+$ and the set of strictly positive numbers is denoted $\mathbb{R}_+^*$.

5.1.4 Entropic structure

The key of our approach is the notion of entropy for systems of the form (5.2). We define this notion here.

Definition 5.1 (Entropy)**.** *Consider $D \subset \mathbb{R}^I$ an open set. A real valued function $\Phi \in \mathscr{C}^2(D)$ is called an* entropy *on D for the system* (5.2) *if it is nonnegative, and if, for all $X \in D$, $\mathrm{D}^2(\Phi)\mathrm{D}(A)(X)$ is positive-semidefinite (in the sense of symmetric matrices, that is, its symmetric part is positive-semidefinite).*

Section 5.3 will be devoted to the study of typical entropies in the case of two species, but let us immediately explain how entropies (in the sense of the above definition) naturally provide estimates. For the sake of simplicity, we assume here that $R = 0$. Suppose that an entropy Φ exists for the system (5.2). Then, if U is solution of (5.2) (with $R = 0$), a formal computation gives (with $\langle\ ,\ \rangle$ the usual scalar product in $\mathbb{R}^I$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Phi(U) = \int_\Omega \langle \nabla\Phi(U), \Delta[A(U)]\rangle = -\sum_{j=1}^d \int_\Omega \langle \partial_j U, \mathrm{D}^2\Phi(U)\mathrm{D}(A)(U)\partial_j U\rangle \le 0,$$

where the last inequality comes from the fact that Φ is an entropy. Therefore, $\Phi(U)$ is a Lyapunov functional of the system. Furthermore, an integration w.r.t. time gives the estimate

$$\int_\Omega \Phi(U)(T) + \int_0^T \sum_{j=1}^d \int_\Omega \langle \partial_j U, \mathrm{D}^2\Phi(U)\mathrm{D}(A)(U)\partial_j U\rangle = \int_\Omega \Phi(U(0)). \tag{5.6}$$

As we shall explain in Section 5.3, this estimate often yields crucial bounds on the gradient of the solution U.

We give here two examples of systems of the form (5.2) (presented here in the case when $R = 0$) which satisfy assumptions **(H)**, and for which a nontrivial entropy exists.

Example 1. The first example consists in a two-species systems where A is given by (5.5) and (for suitable parameters $d_i > 0, \delta_{ij} > 0$ described in Section 5.5)

$$\partial_t u_1 - \Delta[u_1\,(d_1 + d_{11}\,u_1^{\delta_{11}} + d_{12}\,u_2^{\delta_{12}})] = 0,$$
$$\partial_t u_2 - \Delta[u_2\,(d_2 + d_{21}\,u_1^{\delta_{21}} + d_{22}\,u_2^{\delta_{22}})] = 0.$$

Example 2. The second example is the following three-species system :

$$\partial_t u_1 - \Delta[u_1\,(d_1 + u_2^s + u_3^s)] = 0,$$
$$\partial_t u_2 - \Delta[u_2\,(d_2 + u_1^s + u_3^s)] = 0,$$
$$\partial_t u_3 - \Delta[u_3\,(d_3 + u_1^s + u_2^s)] = 0,$$

where $0 < s < 1/\sqrt{3}$ (and $d_1, d_2, d_3 > 0$).

These two examples will be studied separately in Section 5.5. More precisely, we will present nontrivial entropies for these systems and we will explain how those entropies can be used in order to obtain the existence of solutions.

Remark 5.1. *In our examples we will always consider convex entropies which satisfy the stronger condition that* $\mathrm{D}^2(\Phi)\mathrm{D}(A)$ *is a positive-definite matrix. This implies that* $\det(\mathrm{D}^2(\Phi)\mathrm{D}(A)) > 0$ *and* $\det(\mathrm{D}^2(\Phi)) \geq 0$*, so that* $\det(\mathrm{D}(A)) > 0$*. But if the system* (5.2) *satisfies Assumptions* ***H1*** *and* ***H2*** *(which are easily checked), then the positivity of* $\det(\mathrm{D}(A))$ *allows to show* ***H3*** *under quite general assumptions (see Subsection 5.6.1). Therefore in this context* ***H3*** *can also easily be checked.*

5.1.5 Main application

Though the examples presented above have their own interest, the main application of the methods developed in this work is a new theorem of existence of (very) weak solutions for systems with the same structure as in [15], but with parameters in an enlarged space :

$$\partial_t u_1 - \Delta\Big[u_1\,(d_1 + u_2^{\gamma_2})\Big] = u_1\,(\rho_1 - u_1^{s_{11}} - u_2^{s_{12}}), \quad \text{on } \mathbb{R}_+ \times \Omega \tag{5.7}$$

$$\partial_t u_2 - \Delta\Big[u_2\,(d_2 + u_1^{\gamma_1})\Big] = u_2\,(\rho_2 - u_2^{s_{22}} - u_1^{s_{21}}), \quad \text{on } \mathbb{R}_+ \times \Omega \tag{5.8}$$

$$\partial_n u = \partial_n v = 0, \quad \text{on } \mathbb{R}_+ \times \partial\Omega. \tag{5.9}$$

We introduce the

Definition 5.2 ((Very) Weak solution)**.** *We consider* $d_1, d_2 > 0$*,* $\rho_1, \rho_2 > 0$*,* $\gamma_1, \gamma_2 > 0$*, and* $s_{ij} > 0$ *(*$i, j = 1, 2$*). Let* u_1^{in}*,* u_2^{in} *be two nonnegative functions in* $\mathrm{L}^1(\Omega)$*. For* u_1*,* u_2 *two nonnegative functions in* $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+, \mathrm{L}^1(\Omega))$*, we say that* (u_1, u_2) *is a (very) weak solution of* (5.7)–(5.9) *with initial conditions* (u_1^{in}, u_2^{in}) *if* (u_1, u_2) *satisfies*

$$u_1\,[u_1^{s_{11}} + u_2^{s_{12}} + u_2^{\gamma_2}] \,+\, u_2\,[u_1^{s_{21}} + u_2^{s_{22}} + u_1^{\gamma_1}] \,\in\, \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+, \mathrm{L}^1(\Omega)), \tag{5.10}$$

and for any ψ_1*,* $\psi_2 \in \mathscr{C}^1_c(\mathbb{R}_+; \mathscr{C}^2_\nu(\overline{\Omega}))$*,*

$$\begin{aligned} &- \int_\Omega u_1^{in}(x)\,\psi_1(0,x)\;\mathrm{d}x - \int_0^\infty \int_\Omega u_1(t,x)\,\partial_t\psi_1(t,x)\;\mathrm{d}x\;\mathrm{d}t \\ &- \int_0^\infty \int_\Omega \Delta\psi_1(t,x)\,\Big[d_1 + u_2(t,x)^{\gamma_2}\Big]\,u_1(t,x)\;\mathrm{d}x\;\mathrm{d}t \\ = &\int_0^\infty \int_\Omega \psi_1(t,x)\,u_1(t,x)\,\big(\rho_1 - u_1(t,x)^{s_{11}} - u_2(t,x)^{s_{12}}\big)\;\mathrm{d}x\;\mathrm{d}t, \end{aligned} \tag{5.11}$$

and

$$\begin{aligned} &- \int_\Omega u_2^{in}(x)\,\psi_2(0,x)\;\mathrm{d}x - \int_0^\infty \int_\Omega u_2(t,x)\,\partial_t\psi_2(t,x)\;\mathrm{d}x\;\mathrm{d}t \\ &- \int_0^\infty \int_\Omega \Delta\psi_2(t,x)\,\Big[d_2 + u_1(t,x)^{\gamma_1}\Big]\,u_2(t,x)\;\mathrm{d}x\;\mathrm{d}t \\ = &\int_0^\infty \int_\Omega \psi_2(t,x)\,u_2(t,x)\,\big(\rho_2 - u_2(t,x)^{s_{22}} - u_1(t,x)^{s_{21}}\big)\;\mathrm{d}x\;\mathrm{d}t. \end{aligned} \tag{5.12}$$

Our theorem writes

Theorem 5.1. *Let* Ω *be a smooth (*$\mathscr{C}^2$*) bounded open subset of* $\mathbb{R}^d$ *(*$d \geq 1$*). Consider* $\gamma_2 > 1$*,* $0 < \gamma_1 < 1/\gamma_2$ *and* $\rho_i > 0$*,* $s_{ij} > 0$*,* $d_i > 0$*,* $i, j = 1, 2$*, with* $s_{11} < 1$*,* $s_{12} < \gamma_2 + s_{22}/2$ *and* $s_{21} < 2$*. Let* $U^{in} := (u_1^{in}, u_2^{in}) \in (\mathrm{L}^1 \cap \mathrm{H}_m^{-1})(\Omega) \times (L^{\gamma_2} \cap \mathrm{H}_m^{-1})(\Omega)$ *be a couple of nonnegative initial data.*

Then, there exists a couple $U := (u_1, u_2)$ *of nonnegative functions which is a (very) weak solution to* (5.7)–(5.9) *in the sense of Definition 5.2, and satisfies, for all* $s > 0$*,*

$$\int_0^s \int_\Omega (u_1 + u_2)\,(u_1^{\gamma_1} u_2 + u_2^{\gamma_2} u_1 + u_1 + u_2)\;\mathrm{d}x\;\mathrm{d}t \leq D_s, \tag{5.13}$$

$$\sup_{t\in[0,s]} ||u_i(t,\cdot)||_{\mathrm{L}^1(\Omega)} \leq e^{\rho_i s}||u_i^{in}||_{\mathrm{L}^1(\Omega)}, \tag{5.14}$$

$$\sup_{t\in[0,s]}\int_\Omega u_2(t,\cdot)^{\gamma_2}+\int_0^s\int_\Omega u_2^{\gamma_2}\ (u_1^{s_{21}}+u_2^{s_{22}})\ \mathrm{d}x\,\mathrm{d}t$$
$$+\int_0^s\int_\Omega\Big\{|\nabla u_1^{\gamma_1/2}|^2+|\nabla u_2^{\gamma_2/2}|^2+\Big|\nabla\sqrt{u_1^{\gamma_1}\,u_2^{\gamma_2}}\Big|^2\Big\}\ \mathrm{d}x\,\mathrm{d}t \tag{5.15}$$
$$\leq K_s\,(1+\|u_1^{in}\|_{\mathrm{L}^1(\Omega)}+\|u_2^{in}\|^{\gamma_2}_{\mathrm{L}^{\gamma_2}(\Omega)}).$$

The positive constants K_s and D_s used above only depend on s, Ω and the data of the equations (ρ_i, d_i, γ_i, s_{ij}). The constant D_s in (5.13) also depends on $\|U^{in}\|_{\mathrm{H}_m^{-1}(\Omega)^2}$. Both functions $s\mapsto D_s$ and $s\mapsto K_s$ may be chosen continuous and belong in particular to $\mathrm{L}^\infty_{\mathrm{loc}}(\mathbb{R}_+)$.

Remark 5.2. *We consider in this theorem the case $\gamma_2>1$, $\gamma_1<1$, which falls outside of the scope of the systems studied in [15].*

Note that Theorem 5.1 and its proof still hold when one adds some positive constants in front of the non-linearities.

A more technical aspect concerns the self-diffusion, that we have chosen to disregard in this theorem. As it was the case in [15], adding self-diffusion terms tends in fact here to facilitate the study of the system, and it gives rise to extra estimates on the gradients of the densities. Details can be found in Subsection 5.5.1

Note also that Theorem 5.1 may be generalized to the case when power rate diffusion coefficients are replaced by mere functions $a_{ij}(u_i)$, with ad hoc *assumptions of regularity/monoticity/concavity on the functions a_{ij}. An extension to reaction coefficients R different from power laws is also certainly possible.*

The condition $s_{12}<\gamma_2+s_{22}/2$ is in fact not optimal. It can be improved using different interpolations. As it will be seen, we have (A) $\int_0^T\int_\Omega u_1^{\max(2,s_{21})}u_2^{\gamma_2}<\infty$, (B) $\int_0^T\int_\Omega u_2^{\gamma_2+s_{22}}<\infty$ and (C) $\int_0^T\int_\Omega u_1^{\gamma_1}u_2^2<\infty$. Interpolating between (A) and (B) leads to the condition $s_{12}<\gamma_2+s_{22}(1-1/\max(2,s_{21}))$ while interpolating between (A) and (C) leads to the condition $s_{12}<2-(2-\gamma_2)(1-\gamma_1)/(\max(2,s_{21})-\gamma_1)$. All in all, we get the sufficient condition

$$s_{12}<\max\bigg(\gamma_2+s_{22}/2,\gamma_2+s_{22}(1-1/s_{21}),2-(2-\gamma_2)(1-\gamma_1)/2-\gamma_1),$$
$$2-(2-\gamma_2)(1-\gamma_1)/(s_{21}-\gamma_1)\bigg).$$

In this formula, the four different expressions can lead to the best condition on s_{12}, depending on the coefficients $s_{21},s_{22},\gamma_1,\gamma_2$. For instance : if $s_{21}=1,s_{22}=2,\gamma_2=2$, the best condition is given by the first expression ; if $s_{21}=4,s_{22}=2,\gamma_2=2$, the best condition is given by the second expression, if $s_{21}=1,s_{22}=1/5,\gamma_2=3/2$, the best condition is given by the third expression, if $s_{21}=4,s_{22}=1/5,\gamma_2=3/2$, the best condition is given by the fourth expression.

Thanks to estimates (5.13) *and* (5.15)*, it is sometimes possible (that is, under extra assumptions on the parameters γ_i,s_{ij}) that the quantity $\nabla\{[d_1+u_2^{\gamma_2}]u_1\}$ (resp. $\nabla\{[d_2+u_1^{\gamma_1}]u_2\}$) lies in the space $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^1(\Omega))$, so that u_1 is actually a weak solution of* (5.7) *(resp. u_2 is a weak solution of* (5.8)*) in the sense that in the weak formulation* (5.11) *we can replace $-\iint\Delta\psi_1[d_1+u_2^{\gamma_2}]u_1$ by $\iint\nabla\psi_1\cdot\nabla\{[d_1+u_2^{\gamma_2}]u_1\}$ for all $\psi_1\in\mathscr{C}^1_c(\mathbb{R}_+;\mathscr{C}^2_\nu(\overline{\Omega}))$, and therefore by a density argument enlarge the set of test functions ψ_1 to $\mathscr{C}^1_c(\mathbb{R}_+;\mathscr{C}^1_\nu(\overline{\Omega}))$ (resp. a similar formulation for u_2). Note in particular that (thanks to estimates* (5.13) *and* (5.15)*) $u_1^{1-\gamma_1/2}\,u_2^{\gamma_2/2}\in\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^2(\Omega))$, $u_1\,u_2^{\gamma_2/2}\in\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^2(\Omega))$, $\nabla[u_1^{\gamma_1/2}\,u_2^{\gamma_2/2}]\in\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^2(\Omega))$, $\nabla[u_2^{\gamma_2/2}]\in\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^2(\Omega))$, so that $\nabla[u_1\,u_2^{\gamma_2}]=\nabla[(u_1^{\gamma_1/2}\,u_2^{\gamma_2/2})^{2/\gamma_1}\times(u_2^{\gamma_2\,(1-1/\gamma_1)})]\in\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^1(\Omega))$, and u_1 is always a weak solution of* (5.7).

5.1.6 Structure of the paper

We begin by introducing and studying a general (that is, for I species, with any $I\geq 1$) semi-discrete scheme in Section 5.2. More precisely, we prove the existence of a solution for the discretized system and we show estimates satisfied by the solution (some of them are uniform in the time step and some are not). Section 5.3 is devoted to the study of the hidden entropy structure for a class of two-species cross-diffusion systems including (5.7)–(5.9). We prove Theorem 5.1 in Section 5.4. We then present two examples of systems on which our methods can be used (Examples 1 and 2) in Section 5.5, in order to show the range of applications of these methods. Finally, the Appendix (Section 5) gathers some technical lemmas : we discuss assumption **H3**, and we recall some classical results : Leray Schauder fixed point Theorem, some elliptic estimates and a version of the Nonlinear Aubin-Lions Lemma. Sections 5.2 and 5.3 are independent, whereas the proof of Theorem 5.1 in Section 5.4 uses the results of Section 5.2 and relies on the entropy structure detailed in Section 5.3. Section 5.5 extends ideas developed in Sections 5.2 to 5.4.

5.2 Semi-discrete scheme

We begin here the presentation of general statements which will be used in the proof of Theorem 5.1. More precisely, we intend in this section to introduce a semi-discrete implicit scheme to approximate multi-dimensional systems of the form (5.1). Although many breakthroughs occurred in the mathematical understanding of cross-diffusion systems in the recent years (see [8, 15] and the references therein), the approximation procedure of these systems frequently leads to intricate or technical methods. The main reason is that the hidden entropy structure often relies on functionals defined on nonlinear subspaces of $\mathbb{R}^I$ ($\mathbb{R}^I_+$ for instance), and a condition as simple as "u_i is nonnegative" is not easily kept during the approximation process.

The scheme is based on the following semi-discretization ($1 \leq k \leq N-1$, $N = T/\tau$, $T > 0$)

$$\begin{aligned} \frac{U^k - U^{k-1}}{\tau} - \Delta[A(U^k)] = R(U^k), \text{ on } \Omega, \\ \partial_n A(U^k) = 0, \text{ on } \partial\Omega. \end{aligned} \tag{5.16}$$

We introduce the

Definition 5.3 (Strong solution). (**H**). *Let $\tau > 0$ and $U^{k-1} \in \mathrm{L}^\infty(\Omega)^I_+$. We say that a nonnegative vector-valued function U^k is a strong solution of* (5.16) *if U^k lies in $\mathrm{L}^\infty(\Omega)^I$, $A(U^k)$ lies in $\mathrm{H}^2_\nu(\Omega)^I$ and the first equation in* (5.16) *is satisfied almost everywhere on Ω.*

Our results concerning this scheme are summarized in the

Theorem 5.2 (**H**). *Let Ω be a bounded open set of $\mathbb{R}^d$ with smooth boundary. Fix $T > 0$ and an integer N large enough such that $\rho\tau < 1/2$, where $\tau := T/N$ and ρ is the positive number defined in* **H2**. *Fix $\eta > 0$ and a vector-valued function $\mathrm{L}^\infty(\Omega)^I \ni U^0 \geq \eta$. Then there exists a sequence of positive vector-valued functions $(U^k)_{1\leq k\leq N-1}$ in $\mathrm{L}^\infty(\Omega)^I$ which solve* (5.16) *(in the sense of Definition 5.3). Furthermore, it satisfies the following estimates : for all $k \geq 1$ and $p \in [1, \infty[$,*

$$U^k \in \mathscr{C}^0(\overline{\Omega})^I, \tag{5.17}$$

$$U^k \geq \eta_{A,R,\tau} \text{ on } \overline{\Omega}, \tag{5.18}$$

$$A(U^k) \in \mathrm{W}^{2,p}_\nu(\Omega)^I, \tag{5.19}$$

where $\eta_{A,R,\tau} > 0$ is a positive constant depending on the maps A and R and τ, and

$$\max_{0\leq k\leq N-1} \int_\Omega U^k \leq 2^{2\rho\tau N} \int_\Omega U^0, \tag{5.20}$$

$$\sum_{k=1}^{N-1} \tau \int_\Omega \left(\rho U^k - R(U^k)\right) \leq 2^{2\rho\tau N} \int_\Omega U^0, \tag{5.21}$$

$$\sum_{k=0}^{N-1} \tau \int_\Omega \left(\sum_{i=1}^I u_i^k\right)\left(\sum_{i=1}^I a_i(U^k) u_i^k\right) \leq C(\Omega, U^0, A, \rho, N\tau), \tag{5.22}$$

where $C(\Omega, U^0, A, \rho, N\tau)$ is a positive constant depending only on Ω, A, ρ, $N\tau$ and $\|U^0\|_{\mathrm{L}^1\cap\mathrm{H}^{-1}_m(\Omega)}$.

Remark 5.3. *Estimates* (5.17)–(5.19) *strongly depend on τ. In particular, they will be lost when we pass to the limit $\tau \to 0$ during the proof of existence of global solutions in Section 5.4. These estimates are however crucial in order to perform rigorous computations and obtain uniform estimates on the scheme.*

Consider $T > 0$ as fixed. Estimates (5.20) *and* (5.21) *do not depend on τ, since $\tau N = T$. Estimate* (5.22) *is in fact also uniform w.r.t. τ, in the sense that it yields a limiting estimate in the limit $\tau \to 0$.*

Remark 5.4. *The main feature of the discretization* (5.16) *is its ability to preserve the entropy structure xhen it exists. Indeed, assume for the sake of simplicity that $R = 0$; then if $\Phi \in \mathscr{C}^2(\mathbb{R}_+^* \times \mathbb{R}_+^*)$ is a convex entropy in the sense of Definition 5.1, multiplying* (5.16) *by $\tau \Phi'(U^k)$ and integrating by parts leads to the following estimate, for all $1 \leq \ell \leq N$*

$$\int_\Omega \Phi(U^\ell) + \sum_{k=1}^{\ell} \tau \int_\Omega \sum_{j=1}^{d} \langle \partial_j U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\partial_j U^k \rangle \leq \int_\Omega \Phi(U^0),$$

where we used the convexity of Φ and the regularity estimates (5.17)–(5.19) *to make the computations rigorous. This estimate can be seen as the "discretized" version of estimate* (5.6)*. It will be rigorously proven in Proposition 5.5 on the specific system used in our main application.*

The proof of the existence of the family $(U^k)_k$ solving (5.16) is done in Subsection 5.2.1. The proof of the various estimates is done in Subsection 5.2.2.

5.2.1 Existence theory for the scheme

We plan in this section to build step by step a family $(U^k)_{1 \leq k \leq N-1}$ solution of (5.16) (for a given U^0, bounded and nonnegative). For simplicity, we drop the subscripts and rewrite the scheme (5.16) with the notations $U := U^k$ and $S := U^{k-1}$:

$$\begin{aligned} U - \tau\Delta[A(U)] &= S + \tau R(U) \qquad && \text{on } \Omega, \\ \partial_n A(U) &= 0 && \text{on } \partial\Omega. \end{aligned} \tag{5.23}$$

The existence of the family $(U^k)_{1 \leq k \leq N-1}$ is a consequence of the iterated use of the following Theorem

Theorem 5.3 (H). *Let Ω be a bounded open set of $\mathbb{R}^d$ with smooth boundary. If $S \in \mathrm{L}^\infty(\Omega)_+^I$, then for all $\tau > 0$ such that $\rho\tau < 1/2$, there exists $U \in \mathrm{L}^\infty(\Omega)_+^I$ which is a strong solution of* (5.23) *(in the sense of Definition 5.3). Furthermore, this solution satisfies (for some $C(\Omega, I\|S\|_\infty)$ only depending on Ω and $I\|S\|_\infty$) the estimate*

$$\|U\|_\infty \leq \frac{1}{\alpha\tau} C(\Omega, I\|S\|_\infty).$$

The proof of Theorem 5.3 is based on a fixed point method that we present in Subsection 5.2.1.

Fixed point

Proof of Theorem 5.3 : Our aim is to apply the Leray-Schauder fixed point Theorem (see Theorem 5.4 of the Appendix). In order to do so, we start by defining, for $U \in \mathrm{L}^\infty(\Omega)^I$,

$$\overline{M}(U) := \max\left\{ \frac{M_{p,\Omega}}{2\rho}, \frac{2 + \tau \max_{i=1\cdots n} \|r_i(U)\|_\infty}{\alpha} \right\},$$

where $p > d/2$ is fixed and $M_{p,\Omega}$ is the constant defined in Lemma 5.5. The quantity $\overline{M}(U)$ is well defined because r_i is assumed to be continuous (so that $r_i(U) \in \mathrm{L}^\infty(\Omega)$). The definition of $\overline{M}(U)$ and the fact that $\rho\tau < 1/2$ imply the two following inequalities (almost everywhere on Ω)

$$\overline{M}(U) > \tau M_{p,\Omega},$$
$$\overline{M}(U)A(U) - U + \tau R(U) \geq 0,$$

where the second (vectorial) inequality has to be understood coordinates by coordinates.

Consider now the following maps (here both A and R are extended to continuous functions on $\mathbb{R}^I$ by parity) :

$$\begin{aligned} \Psi : \mathrm{L}^\infty(\Omega)^I &\longrightarrow \mathrm{L}^\infty(\Omega)_+^I \times (\tau M_{p,\Omega}, +\infty) \\ U &\longmapsto (S + \overline{M}(U)A(U) - U + \tau R(U), \overline{M}(U)), \end{aligned}$$

$$\begin{aligned} \Theta : \mathrm{L}^\infty(\Omega)_+^I \times (\tau M_{p,\Omega}, +\infty) &\longrightarrow \mathrm{L}^\infty(\Omega)_+^I \\ (U, M) &\longmapsto (M\mathrm{Id} - \tau\Delta)^{-1} U, \end{aligned}$$

$$\begin{aligned} \Phi : \mathrm{L}^\infty(\Omega)_+^I &\longrightarrow \mathrm{L}^\infty(\Omega)_+^I \\ U &\longmapsto A^{-1}(U), \end{aligned}$$

where the inverse operator in the definition of Θ has to be understood with homogeneous Neumann boundary conditions on $\partial\Omega$ and in the strong sense (that is, $\Theta(U,M) \in \mathrm{H}^2_\nu(\Omega)^I$ and $(M\mathrm{Id}-\tau\Delta)(\Theta(U,M)) = U$ a.e. on Ω).

Notice that for all M, $\Theta(\cdot, M)$ indeed sends $\mathrm{L}^\infty(\Omega)^I$ to $\mathrm{L}^\infty(\Omega)^I$ thanks to Lemma 5.5 of the Appendix, since $p > d/2$, and remembering Sobolev embedding $\mathrm{W}^{2,p}(\Omega) \hookrightarrow \mathrm{L}^\infty(\Omega)$. Using the maximum principle, we also can see that $\Theta(\cdot, M)$ preserves the nonnegativity of the components, so that $\Theta(\mathrm{L}^\infty(\Omega)^I_+ \times (\tau M_{p,\Omega}, +\infty)) \subset \mathrm{L}^\infty(\Omega)^I_+$.

We can therefore consider the mapping $\Phi\circ\Theta\circ\Psi$, and it is clear that any fixed point of this mapping will give us a solution of the discretized system (5.23). We hence plan to apply the Leray-Schauder Theorem to prove the existence of such a fixed point. We consider for this purpose the map $\Lambda(\sigma, \cdot) := \Phi \circ \sigma\Theta \circ \Psi$. We obviously have $\Lambda(0, \cdot) = 0$. Let us first check the continuity and compactness of Λ, and then look for a uniform estimate for the fixed points of the applications $\Lambda(\sigma, \cdot)$, to prove that $\Lambda(1, \cdot) = \Phi \circ \Theta \circ \Psi$ indeed has a fixed point.

Compactness and continuity of Λ.

Lemma 5.1. (**H**) *The map $\Lambda : [0,1] \times \mathrm{L}^\infty(\Omega)^I \to \mathrm{L}^\infty(\Omega)^I$ is compact and continuous.*

Proof. Thanks to the Heine-Cantor Theorem and the continuity of A, R and A^{-1} (see assumptions **H**), we see that both Φ and Ψ are continuous. It is hence sufficient to prove the continuity and compactness of $\sigma\Theta$ from $[0,1] \times \mathrm{L}^\infty(\Omega)^I_+ \times (\tau M_{p,\Omega}, +\infty)$ to $\mathrm{L}^\infty(\Omega)^I_+$. The compactness of this mapping is a straightforward consequence of Lemma 5.5 of the Appendix together with the corresponding Sobolev embeddings.

For the continuity, let us define $\tilde{U} := \Theta(U, M)$. By maximum principle, we see that

$$\|\tilde{U}\|_\infty \le \frac{\|U\|_\infty}{M} \le \frac{\|U\|_\infty}{\tau M_{p,\Omega}}.$$

Furthermore, for given $(U, M), (U', M')$, defining similarly $\tilde{U}' := \Theta(U', M')$, we can write

$$M(\tilde{U} - \tilde{U}') - \tau\Delta(\tilde{U} - \tilde{U}') = (U - U') + (M' - M)\tilde{U}', \quad \partial_n(\tilde{U} - \tilde{U}') = 0.$$

Still by maximum principle, we immediately get

$$\begin{aligned}\|\tilde{U} - \tilde{U}'\|_\infty &\le \frac{1}{M}\left(\|U - U'\|_\infty + |M' - M|\|\tilde{U}'\|_\infty\right)\\ &\le \frac{1}{\tau M_{p,\Omega}}\left(\|U - U'\|_\infty + |M' - M|\frac{\|U'\|_\infty}{\tau M_{p,\Omega}}\right),\end{aligned}$$

which yields the continuity of the application Θ, and thereby of the application Λ. □

Estimates on fixed points of $\Lambda(\sigma, \cdot)$.

In order to apply the Leray-Schauder fixed-point Theorem 5.4, we need an *a priori* estimate (uniform in σ) on the fixed points of $\Lambda(\sigma, \cdot)$. The fixed point equation is rewritten as

$$\overline{M}(U)A(U) - \tau\Delta[A(U)] = \sigma(S + \overline{M}(U)A(U) - U + \tau R(U)).$$

We prove the

Lemma 5.2. (**H**) *For any $\sigma \in [0,1]$, any fixed point $U \in \mathrm{L}^\infty(\Omega)^I$ of $\Lambda(\sigma, .)$ satisfies*

$$\int_\Omega |A(U)|_1 \le C(\Omega, I\|S\|_\infty).$$

Proof. Notice first that such fixed points are necessarily nonnegative, so that $R(U) \le \rho U$ (assumption **H2**) and

$$|A(U)|_1 = \sum_{i=1}^I a_i(U)u_i \in \mathrm{H}^2_\nu(\Omega).$$

The equations associated to the fixed point imply the following vectorial inequality :

$$\overline{M}(U)(1-\sigma)A(U)+\sigma(1-\tau\rho)U-\tau\Delta[A(U)]\le\sigma S,\qquad\text{a.e. on }\Omega.$$

Summing up each coordinate of this inequality, we get

$$\overline{M}(U)(1-\sigma)|A(U)|_1+\sigma(1-\tau\rho)|U|_1-\tau\Delta|A(U)|_1\le\sigma|S|_1,\qquad\text{a.e. on }\Omega,\tag{5.24}$$

which, after multiplication by $|A(U)|_1$ and integration on Ω, leads to

$$\begin{aligned}(1-\sigma)\int_\Omega\bar{M}(U)|A(U)|_1^2+\sigma(1-\rho\tau)\int_\Omega|A(U)|_1|U|_1+\tau\int_\Omega|\nabla|A(U)|_1|^2\\ \le\sigma\int_\Omega|S|_1|A(U)|_1\,.\end{aligned}$$

For $\sigma=0$, we have $U=0=A(U)$, otherwise we get

$$(1-\rho\tau)\int_\Omega|A(U)|_1|U|_1\le\int_\Omega|S|_1|A(U)|_1\le I\|S\|_\infty\int_\Omega|A(U)|_1,$$

whence, since $\rho\tau<1/2$,

$$\int_\Omega|A(U)|_1|U|_1\le 2I\|S\|_\infty\int_\Omega|A(U)|_1.\tag{5.25}$$

Thanks to the continuity of A, we see that for all $R>0$, there exists $C_1(R)>0$ such that

$$|U|_1\le R\Longrightarrow|A(U)|_1\le C_1(R),$$

so that small values of U will be handled. On the other hand, we have

$$\int|A(U)|_1|U|_1\ge\int_{|U|_1\ge R}|A(U)|_1|U|_1\ge R\int_{|U|_1\ge R}|A(U)|_1.$$

Now cutting the r.h.s. of (5.25) in two terms, corresponding to small and large values of U, we get

$$\begin{aligned}\int_\Omega|A(U)|_1|U|_1&\le 2I\|S\|_\infty\left(\int_{|U|_1\ge R}|A(U)|_1+\int_{|U|_1<R}|A(U)|_1\right)&(5.26)\\&\le\frac{2I\|S\|_\infty}{R}\int_\Omega|A(U)|_1|U|_1+2I\|S\|_\infty|\Omega|C_1(R).&(5.27)\end{aligned}$$

Taking $R=4I\|S\|_\infty$, we have

$$\int_\Omega|A(U)|_1|U|_1\le 4I\|S\|_\infty|\Omega|C_1(R).$$

Reusing computation (5.26), we eventually get

$$\begin{aligned}\int_\Omega|A(U)|_1&\le\int_{|U|_1\ge R}|A(U)|_1+\int_{|U|_1<R}|A(U)|_1\\&\le\frac{1}{R}\int_\Omega|A(U)|_1|U|_1+|\Omega|C_1(R)\\&\le\left(\frac{4I\|S\|_\infty}{R}+1\right)|\Omega|C_1(R),\end{aligned}$$

which gives the conclusion with $C(\Omega,I\|\mathrm{S}\|_\infty)=2\,|\Omega|\,C_1(4\,I\,\|\mathrm{S}\|_\infty)$. □

Corollary 5.1. (**H**) *There exists a constant $C(\Omega,I\|S\|_\infty)$ depending only on Ω and $I\|S\|_\infty$ such that for any $\tau>0$ with $\rho\tau<1/2$, for all $\sigma\in[0,1]$ and for all $U\in\mathrm{L}^\infty(\Omega)$,*

$$\Lambda(\sigma,u)=u\Longrightarrow\|U\|_\infty\le\frac{1}{\alpha\tau}C(\Omega,I\|S\|_\infty).$$

Proof. Thanks to the nonnegativity of U and the condition $\tau\rho < 1/2$, inequality (5.24) implies

$$-\Delta|A(U)|_1 \leq \frac{\sigma}{\tau}|S|_1 \leq \frac{1}{\tau}|S|_1, \qquad \text{a.e. on } \Omega.$$

Applying Lemma 5.6 to $w = |A(U)|_1 = \sum_{i=1}^{I} a_i(U)u_i \geq 0$, we get

$$0 \leq \sum_{i=1}^{I} a_i(U)u_i \leq C(\Omega)\left(\frac{1}{\tau}I\|S\|_\infty + \int_\Omega |A(U)|_1\right), \qquad \text{a.e. on } \Omega,$$

and the conclusion follows thanks to Lemma 5.2, the nonnegativity of U, and Assumption **H2** : a_i is lower bounded by $\alpha > 0$. □

End of the proof of Theorem 5.3.

End of the proof of Theorem 5.3. We just invoke Theorem 5.4, and we use Lemma 5.1 and Corollary 5.1 to check the assumptions on Λ. □

5.2.2 Estimates for the scheme

Applying iteratively Theorem 5.3 we get the existence of the family $(U^k)_k$ in Theorem 5.2. In particular, we already know that it satisfies for all $k \geq 1$,

$$U^0 \geq \eta > 0, \tag{5.28}$$

$$U^k \geq 0, \text{ and } U^k \in \mathrm{L}^\infty(\Omega)^I, \tag{5.29}$$

$$A(U^k) \in \mathrm{H}^2_\nu(\Omega)^I. \tag{5.30}$$

In this subsection, we prove that the family $(U^k)_k$ satisfies estimates (5.17)–(5.22).

Non uniform estimates (*i.e.* depending on τ)

Let us first give a few properties of regularity for the family $(U^k)_{1\leq k\leq N-1}$.

Proposition 5.1 (H). *For all $k \geq 1$ and $p \in [1, \infty[$,*

$$U^k \in \mathscr{C}^0(\overline{\Omega})^I,$$
$$U^k \geq \eta_{A,R,\tau} \text{ on } \overline{\Omega},$$
$$A(U^k) \in \mathrm{W}^{2,p}_\nu(\Omega)^I,$$

where $\eta_{A,R,\tau} > 0$ is a strictly positive constant depending on the maps A and R and τ.

Proof. Since R is continuous, for each $k \geq 0$, $R(U^k) \in \mathrm{L}^\infty(\Omega)^I$. We hence can write, for any positive constant $M > 0$ and any $k \geq 1$

$$MA(U^k) - \Delta[A(U^k)] = \frac{U^{k-1} - U^k}{\tau} + R(U^k) + MA(U^k) \in \mathrm{L}^\infty(\Omega)^I,$$

so that we can directly apply Lemma 5.5 of the Appendix to get $A(U^k) \in \mathrm{W}^{2,p}(\Omega)^I$ for all finite values of p, whence, by Sobolev embedding, $A(U^k) \in \mathscr{C}^0(\overline{\Omega})^I$, and $U^k \in \mathscr{C}^0(\overline{\Omega})^I$ thanks to Assumption **H3**. For the lower bound on U^k, we will proceed by induction and prove that if $U^{k-1} \geq \varepsilon$ for some constant $\varepsilon > 0$, then $U^k \geq \varepsilon'$ for another constant $\varepsilon' > 0$. The result will follow by taking the minimum of the constructed finite family. Assuming hence $U^{k-1} \geq \varepsilon > 0$ (which is true by assumption for $k = 1$), because of Assumption **H2**, if M is large enough, we get $MA(U^k) - \Delta[A(U^k)] \geq U^{k-1}/\tau \geq U^{k-1} \geq \varepsilon$. We infer hence, by the maximum principle, that $A(U^k) \geq \varepsilon/M$, whence $U^k \geq \varepsilon/C$, where $C = M \sup_i \|a_i(U^k)\|_\infty$ (not vanishing because of Assumption **H2**). □

(Uniform) L^1 estimate

We write down the standard L^1 estimate obtained by a direct integration of the equations :

Proposition 5.2 (**H**). *Assuming that $\rho\tau < 1/2$, the family $(U^k)_k$ satisfies*

$$\max_{0\leq k\leq N-1}\int_\Omega U^k \leq 2^{2\rho\tau N}\int_\Omega U^0, \tag{5.31}$$

$$\sum_{k=1}^{N-1}\tau\int_\Omega \left(\rho U^k - R(U^k)\right) \leq 2^{2\rho\tau N}\int_\Omega U^0. \tag{5.32}$$

Proof. For (5.31), we prove in fact the more precise estimate for $k\geq 1$:

$$\int_\Omega U^k \leq (1-\rho\tau)^{-k}\int_\Omega U^0. \tag{5.33}$$

Indeed, thanks to Assumption **H2**, (5.16) implies (almost everywhere on $\overline{\Omega}$)

$$\frac{U^k - U^{k-1}}{\tau} - \Delta A(U^k) \leq \rho U^k. \tag{5.34}$$

Integrating then (5.34) on Ω, we get

$$(1-\rho\tau)\int_\Omega U^k \leq \int_\Omega U^{k-1},$$

so that (5.33) follows by a straightforward induction. Since $\tau N = T$ and $\rho\tau < 1/2$, we have $(1-\rho\tau)^{-N}\leq 2^{2\rho\tau N}$, whence (5.31). Integrating the first equation in (5.16) on Ω, and summing for $1\leq k\leq N-1$, we get

$$-\sum_{k=1}^{N-1}\tau\int_\Omega R(U^k) \leq \int_\Omega U^0,$$

so that using (5.33),

$$\begin{aligned}\sum_{k=1}^{N-1}\tau\int_\Omega \left(\rho U^k - R(U^k)\right) &\leq \tau\rho\sum_{k=1}^{N-1}(1-\rho\tau)^{-k}\int_\Omega U^0 + \int_\Omega U^0\\ &= \left[\frac{\tau\rho}{1-\rho\tau}\frac{(1-\rho\tau)^{-(N-1)}-1}{(1-\rho\tau)^{-1}-1}+1\right]\int_\Omega U^0\\ &= (1-\rho\tau)^{-(N-1)}\int_\Omega U^0 \leq (1-\rho\tau)^{-N}\int_\Omega U^0\end{aligned}$$

and (5.32) follows. □

(Uniform) Duality estimate

We now focus on another uniform (in τ) estimate for this scheme, which is reminiscent of a duality lemma first introduced in [36], which writes :

Lemma 5.3. *Let $\rho > 0$. Let $\mu : [0,T]\times\Omega\to\mathbb{R}_+$ be a continuous function lower bounded by a positive constant. Smooth nonnegative solutions of the differential inequality*

$$\begin{aligned}\partial_t u - \Delta(\mu u) &\leq \rho u \text{ on } [0,T]\times\Omega,\\ \partial_n(\mu u) &= 0 \text{ on } [0,T]\times\partial\Omega,\end{aligned}$$

satisfy the bound

$$\int_{Q_T}\mu u^2 \leq \exp(2\rho T)\times\left(\mathrm{C}_\Omega^2\,\|u^0\|^2_{\mathrm{H}_m^{-1}(\Omega)} + \langle u^0\rangle^2\int_{Q_T}\mu\right),$$

where $u^0 := x\mapsto u(0,x)$, $\langle u^0\rangle$ denotes its mean value on Ω and C_Ω is the Poincaré-Wirtinger constant.

The proof of the previous lemma can be easily adapted from the proof of lemma A.1 in Appendix A of [4]. We are here concerned with the following discretized version :

Lemma 5.4. *Fix $\rho > 0$ and $\tau > 0$ such that $\rho\tau < 1$. Let $(\mu^k)_{0\le k\le N-1}$ be a family of nonnegative functions which are integrable on Ω. Consider a family $(u^k)_{0\le k\le N-1}$ of nonnegative bounded functions, such that for all k, $\mu^k u^k \in \mathrm{H}^2(\Omega)$, and which satisfies in the strong sense*

$$\frac{u^k - u^{k-1}}{\tau} - \Delta(\mu^k u^k) \le \rho u^k, \text{ on } \Omega,$$
$$\partial_n(\mu^k u^k) = 0, \text{ on } \partial\Omega.$$

Then, this family satisfies the bound

$$\sum_{k=1}^{N-1} \tau \int_\Omega \mu^k |u^k|^2 \le (1-\rho\tau)^{-2N} \left(\mathrm{C}_\Omega^2 \, \|u^0\|^2_{\mathrm{H}^{-1}_m} + \langle u^0 \rangle^2 \sum_{k=1}^{N-1} \tau \int_\Omega \mu^k \right).$$

Proof. Since $\rho\tau < 1$, the sequence of nonnegative functions $v^k := (1-\rho\tau)^k u^k$ satisfies

$$v^k - \frac{\tau}{1-\rho\tau} \Delta\mu^k v^k \le v^{k-1}, \text{ a.e. in } \Omega,$$
$$\partial_n v^k = 0, \text{ a.e. on } \partial\Omega.$$

Summing from $k=1$ to $k=n$ we get for all $1 \le n \le N-1$,

$$v^n - \frac{1}{1-\rho\tau} \Delta S^n \le v^0 \text{ a.e. in } \Omega,$$

where

$$S^n := \tau \sum_{k=1}^{n} \mu^k v^k \in \mathrm{H}^2(\Omega).$$

We multiply this last inequality by $\tau\mu^n v^n = S^n - S^{n-1}$ (with the convention $S^0 = 0$) and integrate over Ω. We get

$$\tau \int_\Omega \mu^n |v^n|^2 + \frac{1}{1-\rho\tau} \int_\Omega (\nabla S^n - \nabla S^{n-1}) \cdot \nabla S^n \le \int_\Omega v^0 (S^n - S^{n-1}),$$

and therefore,

$$\tau \int_\Omega \mu^n |v^n|^2 + \frac{1}{2(1-\rho\tau)} \int_\Omega |\nabla S^n|^2 - |\nabla S^{n-1}|^2 \le \int_\Omega v^0 (S^n - S^{n-1}).$$

We sum up over n again to obtain

$$\sum_{n=1}^{N-1} \tau \int_\Omega \mu^n |v^n|^2 + \frac{1}{2(1-\rho\tau)} \int_\Omega |\nabla S^{N-1}|^2 \le \int_\Omega v^0 S^{N-1}.$$

Using Poincaré-Wirtinger's and Young's inequalities, the right-hand side can be dominated by

$$\begin{aligned}
\int_\Omega v^0 S^{N-1} &= \int_\Omega v^0 (S^{N-1} - \langle S^{N-1} \rangle) + \langle v^0 \rangle \int_\Omega S^{N-1} \\
&\le \mathrm{C}_\Omega \|v^0\|_{\mathrm{H}^{-1}_m(\Omega)} \|\nabla S^{N-1}\|_2 + \langle v^0 \rangle \int_\Omega S^{N-1} \\
&\le \frac{\mathrm{C}_\Omega^2 \|v^0\|^2_{\mathrm{H}^{-1}_m}}{2} + \frac{\|\nabla S^{N-1}\|_2^2}{2} + \langle v^0 \rangle \int_\Omega S^{N-1},
\end{aligned}$$

from which we get, since $\rho\tau < 1$,

$$\sum_{n=1}^{N-1} \tau \int_\Omega \mu^n |v^n|^2 \le \frac{\mathrm{C}_\Omega^2 \|v^0\|^2_{\mathrm{H}^{-1}_m}}{2} + \langle v^0 \rangle \int_\Omega S^{N-1}.$$

Using Cauchy-Schwarz inequality one easily gets from the definition of S^{N-1}

$$\langle v^0\rangle \int_\Omega S^{N-1} \leq \sqrt{\sum_{n=1}^{N-1} \tau \int_\Omega \mu^n |v^n|^2} \sqrt{\langle v^0\rangle^2 \sum_{n=1}^{N-1} \tau \int_\Omega \mu^n},$$

so that using another time Young's inequality, one obtains

$$\sum_{n=1}^{N-1} \tau \int_\Omega \mu^n |v^n|^2 \leq \mathrm{C}_\Omega^2 \|v^0\|^2_{\mathrm{H}^{-1}_m} + \langle v^0\rangle^2 \sum_{n=1}^{N-1} \tau \int_\Omega \mu^n,$$

from which we may conclude using $v^n = (1-\rho\tau)^n u^n$. $\square$

We eventually apply the previous lemma to get the following estimate :

Corollary 5.2 (H). *Suppose $\rho\tau < 1/2$. Then there exists a constant $C(\Omega, U^0, A, \rho, N\tau)$ depending only on Ω, A, ρ, $N\tau$ and $\|U^0\|_{\mathrm{L}^1\cap \mathrm{H}^{-1}_m(\Omega)}$ such that the family $(U^k)_k$ satisfies*

$$\sum_{k=0}^{N-1} \tau \int_\Omega \left(\sum_{i=1}^I u_i^k\right)\left(\sum_{i=1}^I a_i(U^k) u_i^k\right) \leq C(\Omega, U^0, A, \rho, N\tau). \tag{5.35}$$

Proof. In order to apply Lemma 5.4 to inequality (5.34), we introduce two families of real-valued functions :

$$\begin{aligned} u^k &:= \sum_{i=1}^I u_i^k, \\ \mu^k &:= \frac{\sum_{i=1}^I a_i(U^k) u_i^k}{\sum_{i=1}^I u_i^k}. \end{aligned}$$

Notice that μ^k is a well-defined nonnegative function on Ω and $\mu^k u^k \in \mathrm{H}^2(\Omega)$ thanks to Proposition 5.1. Summing all coordinates of the vectorial inequality (5.34), we get (almost everywhere on Ω)

$$\frac{u^k - u^{k-1}}{\tau} - \Delta(\mu^k u^k) \leq \rho u^k.$$

Lemma 5.4 yields then the following inequality :

$$\sum_{k=0}^{N-1} \tau \int_\Omega \mu^k |u^k|^2 \leq 2^{4\rho N\tau} C(\Omega, u^0)\left(1 + \sum_{k=0}^{N-1} \tau \int_\Omega \mu^k\right).$$

From the definition of μ^k and u^k and the continuity of the mapping A, it is clear that (for any $L > 0$) $|u^k| \leq L$ implies $|\mu^k| \leq C(L)$, where $C(L) > 0$ is some constant depending on L and A, so that the integrals in the r.h.s. may be handled in the following way :

$$\begin{aligned} \int_\Omega \mu^k &\leq C(L)|\Omega| + \int_{|u^k|>L} \mu^k \\ &\leq C(L)|\Omega| + \frac{1}{L^2}\int_\Omega \mu^k |u^k|^2. \end{aligned}$$

Then, if L is large enough to satisfy $2^{4\rho N\tau} C(\Omega, u^0) < L^2/2$, we get

$$\sum_{k=0}^{N-1} \tau \int_\Omega \mu^k |u^k|^2 \leq 2 \times 2^{4\rho N\tau} C(\Omega, u^0)\left[1 + N\tau C(L)|\Omega|\right],$$

from which we easily conclude. $\square$

5.3 The entropy estimate for two species

This section is devoted to the elucidation of the hidden entropy structure for equations of the form (5.2). The results of this section are not really needed in the proof of Theorem 5.1, since the computations which are presented here as *a priori* estimates will be performed a second time at the level of the approximated system.

Let us first recall that in [15] was investigated a system that took the following general form :

$$\partial_t u_1 - \Delta\big[(d_{11}(u_1) + a_{12}(u_2))\, u_1\big] = u_1\big(\rho_1 - s_{11}(u_1) - s_{12}(u_2)\big), \tag{5.36}$$

$$\partial_t u_2 - \Delta\big[(d_{22}(u_2) + a_{21}(u_1))\, u_2\big] = u_2\big(\rho_2 - s_{22}(u_2) - s_{21}(u_1)\big), \tag{5.37}$$

under various conditions on the functions d_{ij}, a_{ij}, s_{ij}, for $i,j \in \{1,2\}$, One of these conditions was that both a_{12} and a_{21} had to be increasing and concave. We intend here to relax this assumption in order to include several convex/concave cases. Due to the large number of possibilities, the treatment of this system in its full generality (that is, all possible functions d_{ij}, a_{ij} and s_{ij}) leads to lengthy if not tedious statements and computations. To ease a little bit the understanding of this entropy structure, we will present first the specific case of power rates coefficients (subsection 5.3.1) and then treat a more general framework (subsection 5.3.2).

5.3.1 A simple specific example

Since self-diffusion (d_{ii} functions) usually tends to improve the estimates, we consider the case of constant self-diffusion rates. Similarly, since reaction terms have no real influence on the entropy structure, we will not consider them here. Consider hence the following system :

$$\partial_t u_1 - \Delta\Big[u_1(d_1 + u_2^{\gamma_2})\Big] = 0, \tag{5.38}$$

$$\partial_t u_2 - \Delta\Big[u_2(d_2 + u_1^{\gamma_1})\Big] = 0, \tag{5.39}$$

where $d_1, d_2, \gamma_1, \gamma_2 > 0$. The entropy exhibited in [15], corresponds to the limitation : $\gamma_1 \in]0,1[$, $\gamma_2 \in]0,1[$ (we speak only about the control of the entropy here). Let us explain how to control an entropy in cases when $\gamma_2 > 1$ under the condition $\gamma_1 < 1/\gamma_2$.

We present the following result :

Proposition 5.3. *Consider $d_1 > 0$, $d_2 > 0$ and $\gamma_2 > 1$, $0 < \gamma_1 < 1/\gamma_2$. Let (u_1, u_2) be a classical (that is, belonging to $\mathscr{C}^2([0,T] \times \overline{\Omega})$) positive (that is, both u_1 and u_2 are positive on Q_T) solution to* (5.38) – (5.39) *with homogeneous Neumann boundary conditions on $\partial\Omega$. Then the following* a priori *estimates hold for $i = 1, 2$ and all $t \in [0,T]$*

$$\int_\Omega u_i(t) = \int_\Omega u_i(0), \tag{5.40}$$

and

$$\sup_{t\in[0,T]} \int_\Omega u_2(t)^{\gamma_2} + C\int_0^T \int_\Omega \Big\{|\nabla u_1^{\gamma_1/2}|^2 + |\nabla u_2^{\gamma_2/2}|^2 + \Big|\nabla(u_1^{\gamma_1/2} u_2^{\gamma_2/2})\Big|^2\Big\} \leq C_{T,u_1(0),u_2(0)}. \tag{5.41}$$

Proof. Integrating on $[0,t[\times\Omega$ eq. (5.38) – (5.39), we obtain estimate (5.40).

Define

$$h_1(t) := t - \frac{t^{\gamma_1}}{\gamma_1}, \quad h_2(t) := \frac{t^{\gamma_2}}{\gamma_2} - t,$$

so that both functions reach their minimum for $t = 1$. Define the corresponding entropy

$$\mathrm{E}(u_1, u_2) := \frac{\gamma_1}{1-\gamma_1}\int_\Omega [h_1(u_1) - h_1(1)] + \frac{\gamma_2}{\gamma_2 - 1}\int_\Omega [h_2(u_2) - h_2(1)]\ .$$

Differentiating this functional and performing the adequate integrations by parts, we get the following identity :

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}(u_1,u_2)+\gamma_1 d_1\int_\Omega u_1^{\gamma_1-2}|\nabla u_1|^2+\gamma_2 d_2\int_\Omega u_2^{\gamma_2-2}|\nabla u_2|^2$$
$$+\int_\Omega u_1^{\gamma_1}\,u_2^{\gamma_2}\left[\gamma_1\left|\frac{\nabla u_1}{u_1}\right|^2+\gamma_2\left|\frac{\nabla u_2}{u_2}\right|^2+2\gamma_1\gamma_2\frac{\nabla u_1}{u_1}\cdot\frac{\nabla u_2}{u_2}\right]=0.$$

Since $0<\gamma_1\,\gamma_2<1$, the quadratic form Q associated to the matrix $\begin{pmatrix}\gamma_2 & \gamma_1\gamma_2\\ \gamma_1\gamma_2 & \gamma_1\end{pmatrix}$ is positive definite, whence the existence of a constant $C>0$ such as

$$Q(x,y)\geq C\left(x^2+y^2\right).$$

Using the previous inequality in the entropy identity, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}(u_1(t),u_2(t))+\gamma_1 d_1\int_\Omega u_1^{\gamma_1-2}|\nabla u_1|^2$$
$$+\gamma_2 d_2\int_\Omega u_2^{\gamma_2-2}|\nabla u_2|^2+C\int_\Omega u_1^{\gamma_1}\,u_2^{\gamma_2}\left[\left|\frac{\nabla u_1}{u_1}\right|^2+\left|\frac{\nabla u_2}{u_2}\right|^2\right]\leq 0,$$

from which we obtain, changing the constant C

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}(u_1(t),u_2(t))+C\int_\Omega|\nabla u_1^{\gamma_1/2}|^2+C\int_\Omega|\nabla u_2^{\gamma_2/2}|^2+C\int_\Omega\left|\nabla\sqrt{u_1^{\gamma_1}\,u_2^{\gamma_2}}\right|^2\leq 0. \tag{5.42}$$

Since h_1 reaches its minimum at point 1, we have $h_1(u_1)-h(1)\geq 0$, and integrating the previous inequality on $[0,t]$ leads to

$$\frac{1}{\gamma_2-1}\int_\Omega u_2(t)^{\gamma_2}+C\int_0^t\int_\Omega|\nabla u_1^{\gamma_1/2}|^2+C\int_0^t\int_\Omega|\nabla u_2^{\gamma_2/2}|^2$$
$$+C\int_0^t\int_\Omega\left|\nabla\sqrt{u_1^{\gamma_1}\,u_2^{\gamma_2}}\right|^2\leq\frac{\gamma_2}{\gamma_2-1}\int_\Omega u_2(t)+\mathrm{E}(u_1,u_2)(0),$$

and the conclusion follows using (5.40). □

5.3.2 The general entropy structure

Let us consider the general form (5.2) in the case of two species. As before, we assume that $R=0$ in order to simplify the presentation.

We will now perform rather formal (unjustified) computations, in order to bring out the entropy structure. In Section 5.4, all these computations will be rigorously justified (under the corresponding set of assumptions), at the (semi-)discrete level, in order to prove the existence of global weak solutions to eq. (5.7), (5.8) [Theorem 5.1].

We consider a function $\Phi:\mathbb{R}^2\to\mathbb{R}$. If U is solution of (5.2) with $R=0$, a straightforward computation (yet completely formal) leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega\Phi(U)-\int_\Omega\langle\nabla\Phi(U),\Delta[A(U)]\rangle=0,$$

where $\langle\cdot,\cdot\rangle$ is the inner-product on $\mathbb{R}^2$, whence after integration by parts, using the repeated index convention,

$$\begin{aligned}\int_\Omega\langle\nabla\Phi(U),\Delta[A(U)]\rangle&=\int_\Omega(\partial_i\Phi)(U)\partial_{jj}[A_i(U)]\\&=-\int_\Omega\partial_j[(\partial_i\Phi)(U)]\partial_j[A_i(U)]\\&=-\int_\Omega\partial_k\partial_i\Phi(U)\partial_j u_k\partial_\ell A_i(U)\partial_j u_\ell.\end{aligned}$$

Summing first in the i index, we recognize a matrix product and we can write

$$\int_\Omega \langle \nabla\Phi(U), \Delta[A(U)]\rangle = -\sum_{j=1}^d \int_\Omega \langle \partial_j U, \mathrm{D}^2\Phi(U)\mathrm{D}(A)(U)\partial_j U\rangle,$$

where $\mathrm{D}(A)$ is the Jacobian matrix of A, and $\mathrm{D}^2(\Phi)$ is the Hessian matrix of Φ. We eventually get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Phi(U) + \sum_{j=1}^d \int_\Omega \langle \partial_j U, \mathrm{D}^2\Phi(U)\mathrm{D}(A)(U)\partial_j U\rangle = 0. \tag{5.43}$$

This identity implies that $\Phi(U)$ becomes a Lyapunov functional of the system, as soon as $\mathrm{D}^2(\Phi)\mathrm{D}(A)$ is positive-semidefinite (in the sense of symmetric matrices, that is, its symmetric part is positive-semidefinite), i.e. as soon as Φ is an entropy for (5.2) in the sense of Definition 5.1.

Remark 5.5. *Because of the nonnegativity of Φ, one easily gets the estimate $\Phi(U) \in \mathrm{L}^\infty_t(\mathrm{L}^1_x)$ (depending on the initial data), but in fact* (5.43) *often implies much more than this simple estimate for the solutions of the system. Indeed, in many situations, the second term in the l.h.s. of* (5.43) *yields estimates on the gradients of the unknowns (as in Subsection 5.3.1). This will be of crucial importance in Section 5.4, since no other estimate on the gradients is known for the system considered in this application.*

Remark 5.6. *In Definition 5.1, the set D depends on the type of system that we consider. It is the set of expected values for the vector solution U. In our framework, we expect positive solutions, that is $D = \mathbb{R}_+^* \times \mathbb{R}_+^*$, but it is sometimes useful to consider bounded sets for D, this is for instance the case in [29].*

We end this section with a simple generic example, for two species, for which we do have an entropy on $\mathbb{R}_+^* \times \mathbb{R}_+^*$, and which will cover the specific example treated in Subsection 5.3.1. As explained before, self-diffusion generally eases the study of the system. To simplify the presentation, we hence assume here again that the diffusion terms are purely of cross-diffusion type, that is $A(U) = (u_i a_i(u_j))_{i=1,2}$ with $j \neq i$. The idea is then simple, if $\det \mathrm{D}(A)$ and $\mathrm{Tr}\,\mathrm{D}(A)$ are both nonnegative, then $\mathrm{D}(A)$ has two nonnegative eigenvalues and is hence not far from being positive-semidefinite, in the sense that it would indeed be positive-semidefinite if it were symmetric ; this last property may be satisfied after multiplication by a diagonal matrix, keeping the positiveness of the trace and the determinant : this will be done thanks to $\mathrm{D}^2(\Phi)$. More precisely, we present the following elementary proposition, which explains how to find a nontrivial entropy of a specific shape (a sum of functions of one variable) when the matrix A satisfies assumptions often satisfied in generalizations of the Shigesada-Kawasaki-Teramoto model :

Proposition 5.4. *Consider $a_1, a_2 : \mathbb{R}_+^* \to \mathbb{R}_+$ two $\mathscr{C}^1$ functions and for $X = (x_1, x_2) \in \mathbb{R}_+^* \times \mathbb{R}_+^*$ define*

$$\begin{aligned} A(X) &:= (x_i a_i(x_j))_i \quad (i \neq j), \\ \Phi(X) &:= \phi_1(x_1) + \phi_2(x_2), \end{aligned}$$

where ϕ_i is a nonnegative second primitive of $z \mapsto a_j'(z)/z$ $(i \neq j)$. If a_1, a_2 are increasing and $\det \mathrm{D}(A) \geq 0$*, then Φ is an entropy on $\mathbb{R}_+^* \times \mathbb{R}_+^*$ for the system* (5.2)*, in the sense of Definition 5.1.*

Proof. We compute

$$\mathrm{D}(A)(X) = \begin{pmatrix} a_1(x_2) & x_1 a_1'(x_2) \\ x_2 a_2'(x_1) & a_2(x_1) \end{pmatrix}, \quad \mathrm{D}^2(\Phi)(X) = \begin{pmatrix} \frac{a_2'(x_1)}{x_1} & 0 \\ 0 & \frac{a_1'(x_2)}{x_2} \end{pmatrix},$$

so that

$$M(X) := \mathrm{D}^2(\Phi)\mathrm{D}(A)(X) = \begin{pmatrix} \star & a_2'(x_1)a_1'(x_2) \\ a_1'(x_2)a_2'(x_1) & \star \end{pmatrix}$$

is obviously symmetric. If the functions a_i are increasing, all the coefficients of $M(X)$ are nonnegative, so that $\mathrm{Tr}\, M(X) \geq 0$; we also see that

$$\det M(X) = \det \mathrm{D}^2(\Phi)(X) \det \mathrm{D}(A)(X) \geq 0,$$

which allows to conclude. □

Remark 5.7. *Let us explain how the computations go if one considers self-diffusion. This amounts to add to the vector* $A(X)$ *a vector* $B(X) = (b_i(x_i))_i$*, and hence to add to the diffusion matrix* $\mathrm{D}(A)(X)$ *a diagonal matrix, namely* $\mathrm{D}(B)(X) = \mathrm{diag}(b_1'(x_1), b_2'(x_2))$*. In that case, if one replaces the assumption* $\det \mathrm{D}(A)(X) \geq 0$ *by* $\det \mathrm{D}(A+B)(X) \geq 0$ *(together with* b_i *increasing), then* Φ *is an entropy on* $\mathbb{R}_+^* \times \mathbb{R}_+^*$ *for the system* (5.2)*, in the sense of Definition 5.1. Indeed,*

$$M(X) := \mathrm{D}^2(\Phi)\mathrm{D}(A+B)(X) = \mathrm{D}^2(\Phi)\mathrm{D}(A)(X) + \mathrm{D}^2(\Phi)\mathrm{D}(B)(X),$$

is a sum of symmetric matrices whence still symmetric, and $\det M(X) \geq 0$ *and* $\mathrm{Tr}M(X) \geq 0$ *so that* Φ *is an entropy.*

5.4 Global weak solutions for two species

We plan in this section to prove Theorem 5.1. The proof is described in subsections 5.4.1 to 5.4.3.

5.4.1 Scheme

Proof of Theorem 5.1 : In this Section, we will just invoke the results stated in Theorem 5.2 of Section 5.2.1. Since in the approximation scheme, the sequence should be initialized with a bounded function, we will introduce a sequence $(U_N^0)_N$ of bounded functions, satisfying $U_N^0 \geq \eta_N > 0$, and approximating U^{in} in $\mathrm{L}^1 \cap \mathrm{H}_m^{-1}(\Omega) \times \mathrm{L}^{\gamma_2} \cap \mathrm{H}_m^{-1}(\Omega)$. In order to apply Theorem 5.3, we have to exhibit the vectorial functions A and R and check the assumptions **H**. We define here

$$\begin{aligned} R : \mathbb{R}_+^2 &\longrightarrow \mathbb{R}^2 \\ X := \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &\longmapsto \begin{pmatrix} x_1\,(\rho_1 - x_1^{s_{11}} - x_2^{s_{12}}) \\ x_2\,(\rho_2 - x_2^{s_{22}} - x_1^{s_{21}}) \end{pmatrix}; \end{aligned} \tag{5.44}$$

$$\begin{aligned} A : \mathbb{R}_+^2 &\longrightarrow \mathbb{R}^2 \\ X &\longmapsto \begin{pmatrix} x_1\,(d_1 + x_2^{\gamma_2}) \\ x_2\,(d_2 + x_1^{\gamma_1}) \end{pmatrix}. \end{aligned} \tag{5.45}$$

We easily check that **H1** is satisfied, and since for $X \geq 0$, $R(X) \leq \max(\rho_1, \rho_2)X$ and $A(X) \geq \min(d_1, d_2)X$, so is **H2**. As for **H3**, this falls within the scope of the particular case treated in the Appendix (see Proposition 5.6). Indeed,

$$\mathrm{D}(A)(X) = \begin{pmatrix} d_1 + x_2^{\gamma_2} & \gamma_2 x_1 x_2^{\gamma_2 - 1} \\ \gamma_1 x_2 x_1^{\gamma_1 - 1} & d_2 + x_1^{\gamma_1} \end{pmatrix},$$

and this matrix has a positive determinant for $x_1, x_2 > 0$, since $\gamma_1\gamma_2 < 1$. We therefore apply Theorem 5.2 (for $\tau = T/N$ small enough) in order to get the existence of a sequence $(U_N^k)_{0 \leq k \leq N-1}$, which is (for $k \geq 1$) a strong solution (in the sense of Definition (5.3)) of

$$\frac{U_N^k - U_N^{k-1}}{\tau} - \Delta[A(U_N^k)] = R(U_N^k) \text{ on } \Omega, \tag{5.46}$$

$$\partial_n A(U_N^k) = 0 \text{ on } \partial\Omega. \tag{5.47}$$

5.4.2 Uniform estimates

We aim at passing to the limit $\tau \to 0$ in identity (5.46). In order to do so, we need uniform (w.r.t. τ, N) estimates. We recall here that thanks to Theorem 5.2, we know that for all $p \in [1, \infty[$,

$$U^k \in \mathscr{C}^0(\overline{\Omega})^2, \tag{5.48}$$

$$U^k \geq \eta_{A,R,N} > 0, \tag{5.49}$$

$$A(U^k) \in \mathrm{W}_\nu^{2,p}(\Omega)^2, \tag{5.50}$$

and in fact, using Proposition 5.6, we see that A is a $\mathscr{C}^1$-diffeomorphism from $\mathbb{R}_+^* \times \mathbb{R}_+^*$ to itself whence, using (5.49) – (5.50), the following regularity estimate, for all $p \in [1, \infty[$,

$$U^k \in \mathrm{W}^{1,p}(\Omega)^2. \tag{5.51}$$

But as noticed in Remark 5.3, estimates (5.48) – (5.51) all depend on τ, and we cannot use them in the passage to the limit. They will however be of great help to justify several computations on the approximated system. For instance, (5.50) allows to see that the equation defining the scheme is meaningful (that is, all terms are defined almost everywhere).

Dual and L^1 estimates

Thanks to Section 5.2.2, we already have proven three (uniform w.r.t. τ) estimates : the dual estimate (5.22) and the L^1 estimates (5.20) and (5.21) given by Theorem 5.2.

Entropy estimate

The following estimate on the sequence $(U_N^k)_{0\leq k\leq N-1}$ holds (in this paragraph, we drop the index N to ease the presentation) :

Proposition 5.5 (H). *There exists a constant $K_T > 0$ depending only on T, Ω and the data of the equations (r_i, d_i, γ_i, s_{ij}) such that (for τ small enough), for all $N \in \mathbb{N}$, the corresponding sequence $(U^k)_{0\leq k\leq N-1}$ satisfying* (5.46)*, also satisfies the following bound :*

$$\max_{0\leq \ell\leq N-1}\int_\Omega (u_2^\ell)^{\gamma_2} + \sum_{k=0}^{N-1}\tau\int_\Omega (u_2^k)^{\gamma_2}\left\{(u_1^k)^{s_{21}} + (u_2^k)^{s_{22}}\right\} \tag{5.52}$$

$$+\sum_{k=0}^{N-1}\tau\int_\Omega \left\{|\nabla (u_1^k)^{\gamma_1/2}|^2 + |\nabla (u_2^k)^{\gamma_2/2}|^2 + \left|\nabla\sqrt{(u_1^k)^{\gamma_1}\,(u_2^k)^{\gamma_2}}\right|^2\right\} \tag{5.53}$$

$$\leq K_T\,(1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2}). \tag{5.54}$$

Proof. We introduce as in Subsection 5.3.1 the functions

$$\phi_i(z) := \frac{\gamma_i}{\gamma_i - 1}\left(\frac{t^{\gamma_i}}{\gamma_i} - t + 1 - \frac{1}{\gamma_i}\right).$$

Since $0 < \gamma_i \neq 1$, one easily checks that ϕ_i is a nonnegative continuous convex function defined on $\mathbb{R}_+$, and smooth on $\mathbb{R}_+^*$, so that for all $z, y > 0$,

$$\phi_i'(z)(z-y) \geq \phi_i(z) - \phi_i(y). \tag{5.55}$$

We define $\Phi : \mathbb{R}^2 \to \mathbb{R}$ by the formula

$$\Phi(x_1, x_2) := \phi_1(x_1) + \phi_2(x_2).$$

Using (5.48) – (5.51), we see that for all k, $\nabla\Phi(U^k)$ is well-defined and belongs to $\in \mathrm{W}^{1,p}(\Omega)^2$ for all $p \in [1,\infty[$. We take the inner product of $\tau\nabla\Phi(U^k)$ with the vectorial equation (5.46) (which has a meaning a.e.). Using (5.55), we get

$$\Phi(U^k) - \Phi(U^{k-1}) - \tau\langle\nabla\Phi(U^k), \Delta[A(U^k)]\rangle \leq \tau\langle\nabla\Phi(U^k), R(U^k)\rangle.$$

We now plan to reproduce (but this time at the rigorous level) the formal computation performed in Subsection 5.3.2. Since each term of the previous inequality is (at least) integrable, we can integrate it on Ω, and sum over $1 \leq k \leq \ell$ in order to get

$$\int_\Omega \Phi(U^\ell) - \sum_{k=1}^{\ell}\tau\int_\Omega\langle\nabla\Phi(U^k), \Delta[A(U^k)]\rangle \leq \sum_{k=1}^{\ell}\tau\int_\Omega\langle\nabla\Phi(U^k), R(U^k)\rangle + \int_\Omega\Phi(U^0). \tag{5.56}$$

Now since $\nabla\Phi(U^k) \in \mathrm{W}^{1,p}(\Omega)^2$ for all $p < \infty$ (see above), the following integration by parts rigorously holds (because $A(U^k)$ satisfies homogeneous Neumann boundary conditions)

$$\begin{aligned}-\int_\Omega\langle\nabla\Phi(U^k), \Delta A(U^k)\rangle &= \sum_{j=1}^{d}\int_\Omega\langle\partial_j U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\partial_j U^k\rangle\\ &= \int_\Omega\langle\nabla U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\nabla U^k\rangle,\end{aligned} \tag{5.57}$$

where $\mathrm{D}(A)$ is the Jacobian matrix of A, and $\mathrm{D}^2(\Phi)$ is the Hessian matrix of Φ (and the last line is a small abuse of notation). At this stage, we know, thanks to Proposition 5.4 and the very definition of Φ, that the r.h.s. of (5.57) is nonnegative. However, as noticed in Remark 5.5, the mere lower bound by 0 is most probably a bad estimate. Indeed, we will see that the r.h.s. of (5.57) will allow us to obtain estimates for the gradient of U^k (as it was the case in Subsection 5.3.1). We can first compute $\mathrm{D}(A)$ (recall the definition of A in (5.45)) and $\mathrm{D}^2(\Phi)$:

$$\mathrm{D}(A)(X) = \begin{pmatrix} d_1 + x_2^{\gamma_2} & \gamma_2 x_1 x_2^{\gamma_2-1} \\ \gamma_1 x_2 x_1^{\gamma_1-1} & d_2 + x_1^{\gamma_1} \end{pmatrix}, \quad \mathrm{D}^2(\Phi)(X) = \begin{pmatrix} \gamma_1 x_1^{\gamma_1-2} & 0 \\ 0 & \gamma_2 x_2^{\gamma_2-2} \end{pmatrix}.$$

Writing $\mathrm{D}(A)(X) = \mathrm{diag}(d_1, d_2) + M_A(X)$, we get

$$\begin{aligned} \int_\Omega \langle \nabla U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\nabla U^k\rangle &= \int_\Omega \langle \nabla U^k, \mathrm{D}^2(\Phi)\,\mathrm{diag}(d_1,d_2)(U^k)\nabla U^k\rangle \\ &\quad + \int_\Omega \langle \nabla U^k, \mathrm{D}^2(\Phi)(U^k) M_A(U^k)\nabla U^k\rangle, \end{aligned}$$

and since $\mathrm{D}^2(\Phi)$ is diagonal,

$$\begin{aligned} \int_\Omega \langle \nabla U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\nabla U^k\rangle &= d_1\gamma_1 \int_\Omega (u_1^k)^{\gamma_1-2}|\nabla u_1^k|^2 + d_2\gamma_2 \int_\Omega (u_2^k)^{\gamma_2-2}|\nabla u_2^k|^2 \\ &\quad + \int_\Omega \langle \nabla U^k, S(U^k)\nabla U^k\rangle, \end{aligned} \tag{5.58}$$

where $S(X) = \mathrm{D}^2(\Phi)(X) M_A(X)$. Let us now write

$$\begin{aligned} S(X) &= \begin{pmatrix} \gamma_1 x_1^{\gamma_1-2} & 0 \\ 0 & \gamma_2 x_2^{\gamma_2-2} \end{pmatrix} \begin{pmatrix} x_2^{\gamma_2} & \gamma_2 x_1 x_2^{\gamma_2-1} \\ \gamma_1 x_2 x_1^{\gamma_1-1} & x_1^{\gamma_1} \end{pmatrix} \\ &= \begin{pmatrix} \gamma_1 x_1^{\gamma_1-2} x_2^{\gamma_2} & \gamma_1\gamma_2 x_1^{\gamma_1-1} x_2^{\gamma_2-1} \\ \gamma_1\gamma_2 x_2^{\gamma_2-1} x_1^{\gamma_1-1} & \gamma_2 x_2^{\gamma_2-2} x_1^{\gamma_1} \end{pmatrix} \\ &= x_1^{\gamma_1} x_2^{\gamma_2} \begin{pmatrix} \gamma_1 x_1^{-2} & \gamma_1\gamma_2 x_1^{-1} x_2^{-1} \\ \gamma_1\gamma_2 x_2^{-1} x_1^{-1} & \gamma_2 x_2^{-2} \end{pmatrix}, \end{aligned}$$

so that eventually

$$S(X) = x_1^{\gamma_1} x_2^{\gamma_2} \begin{pmatrix} x_1^{-1} & 0 \\ 0 & x_2^{-1} \end{pmatrix} \overbrace{\begin{pmatrix} \gamma_1 & \gamma_1\gamma_2 \\ \gamma_1\gamma_2 & \gamma_2 \end{pmatrix}}^{:=L} \begin{pmatrix} x_1^{-1} & 0 \\ 0 & x_2^{-1} \end{pmatrix},$$

which means that (the quadratic form associated to) the matrix $S(X)$ acts on $W := (w_1, w_2)$ through

$$\langle W, S(X)W\rangle = x_1^{\gamma_1} x_2^{\gamma_2} \langle Z, LZ\rangle,$$

where $Z := (w_1/x_1, w_2/x_2)$. But since $\gamma_1\gamma_2 < 1$, the quadratic form associated to L is positive definite, whence the existence of a constant $C := C(\gamma_1, \gamma_2) > 0$ such as

$$\langle W, S(X)W\rangle \geq C\left(\frac{w_1^2}{x_1^2} + \frac{w_2^2}{x_2^2}\right) x_1^{\gamma_1} x_2^{\gamma_2}.$$

Going back to (5.58) and using the previous inequality, we get

$$\begin{aligned} \int_\Omega \langle \nabla U^k, \mathrm{D}^2(\Phi)(U^k)\mathrm{D}(A)(U^k)\nabla U^k\rangle &\geq d_1\gamma_1 \int_\Omega (u_1^k)^{\gamma_1-2}|\nabla u_1^k|^2 + d_2\gamma_2 \int_\Omega (u_2^k)^{\gamma_2-2}|\nabla u_2^k|^2 \\ &\quad + C\int_\Omega \left(\frac{|\nabla u_1^k|^2}{(u_1^k)^2} + \frac{|\nabla u_2^k|^2}{(u_2^k)^2}\right)(u_1^k)^{\gamma_1}(u_2^k)^{\gamma_2} \\ &\geq C\int_\Omega \left\{|\nabla (u_1^k)^{\gamma_1/2}|^2 + |\nabla (u_2^k)^{\gamma_2/2}|^2\right\} \\ &\quad + C\int_\Omega \left|\nabla\sqrt{(u_1^k)^{\gamma_1}\,(u_2^k)^{\gamma_2}}\right|^2, \end{aligned}$$

where we changed the constant C in the last line. If we call Γ_k the r.h.s. of the previous equality, we sum up the previous estimates (5.56) and write

$$\int_\Omega \Phi(U^\ell) + \sum_{k=1}^{\ell} \tau\Gamma_k \leq C\left(\sum_{k=1}^{\ell}\tau\int_\Omega \langle\nabla\Phi(U^k), R(U^k)\rangle + \int_\Omega \Phi(U^0)\right).$$

Since U^0 $(=U_N^0)$ approaches U^{in} in $\mathrm{L}^1(\Omega)\times\mathrm{L}^{\gamma_2}(\Omega)$ and $|\Phi(x_1,x_2)| \lesssim 1+|x_1|+|x_2|^{\gamma_2}$, it is easy to check that $\|\Phi(U_N^0)\|_1 \lesssim 1+\|u_1^{in}\|_1+\|u_2^{in}\|_{\gamma_2}^{\gamma_2}$ up to some irrelevant constant (independent of N of course). On the other hand, $\phi_1 \geq 0$ and $z^{\gamma_2} \lesssim \phi_2(z)+z$. Using the L^1 estimate (5.20) given by Theorem 5.2, we infer eventually

$$\int_\Omega (u_2^\ell)^{\gamma_2} + \sum_{k=1}^{\ell}\tau\Gamma_k \leq C\left(\sum_{k=1}^{\ell}\tau\int_\Omega\langle\nabla\Phi(U^k), R(U^k)\rangle + 1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2}\right).$$

Obtaining the desired estimate now reduces to handling the reaction terms. Notice that from the definition of R, $R(X) = (\rho_1 x_1, \rho_2 x_2) - R^-(X)$, with $R^-(X)\geq 0$ given by

$$R^-(X) = \begin{pmatrix} x_1(x_1^{s_{11}} + x_2^{s_{12}}) \\ x_2(x_2^{s_{22}} + x_1^{s_{21}})\end{pmatrix}.$$

Since $\rho = \max(\rho_1,\rho_2)$, estimate (5.21) of Theorem 5.2 implies

$$\sum_{k=1}^{N-1}\tau\int_\Omega R^-(U^k) \leq C(\|u_1^{in}\|_1 + \|u_2^{in}\|_1). \tag{5.59}$$

Using the definition of ϕ_i, one easily checks that for all $x_i > 0$, $x_i\phi_i'(x_i) \lesssim \phi_i(x_i)+1$, up to some irrelevant constant. We hence get

$$\begin{aligned}\int_\Omega (u_2^\ell)^{\gamma_2} + \sum_{k=1}^{\ell}\tau\Gamma_k \leq C\Big[&\sum_{k=1}^{\ell}\tau\int_\Omega\Phi(U^k) + 1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2}\Big]\\ &- C\sum_{k=1}^{\ell}\tau\int_\Omega\langle\nabla\Phi(U^k), R^-(U^k)\rangle,\end{aligned}$$

which, using $\phi_1(z)\lesssim 1+z$ and $\phi_2(z)\lesssim 1+z^{\gamma_2}$ together with estimate (5.20), may be written

$$\begin{aligned}\int_\Omega (u_2^\ell)^{\gamma_2} + \sum_{k=1}^{\ell}\tau\Gamma_k \leq C\Big[&\sum_{k=1}^{\ell}\tau\int_\Omega(u_2^k)^{\gamma_2} + 1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2}\Big]\\ &- C\sum_{k=1}^{\ell}\tau\int_\Omega\langle\nabla\Phi(U^k), R^-(U^k)\rangle.\end{aligned}$$

Expanding $\langle\nabla\Phi(X), R^-(X)\rangle$, we get

$$\langle\nabla\Phi(X), R^-(X)\rangle = \phi_1'(x_1)x_1(x_1^{s_{11}} + x_2^{s_{12}}) + \phi_2'(x_2)x_2(x_2^{s_{22}} + x_1^{s_{21}}).$$

Since $\gamma_2 > 1$, we can write $\phi_2'(x_2)x_2 = c_2(x_2^{\gamma_2} - x_2)$ with $c_2 > 0$. Furthermore, if $x_1 \geq 1$, one easily checks that $\phi_1'(x_1)\geq 0$, and on the other hand, $x_1 \mapsto x_1\phi_1'(x_1)$ continuously extends to $\mathbb{R}_+$ and is hence lower bounded for $x_1 \leq 1$ by some negative constant m_1. All in all, we get for $X\in\mathbb{R}_+^2$ the estimate

$$\langle\nabla\Phi(X), R^-(X)\rangle \geq m_1(x_1^{s_{11}} + x_2^{s_{12}}) + c_2(x_2^{\gamma_2} - x_2)(x_2^{s_{22}} + x_1^{s_{21}}),$$

whence

$$c_2 x_2^{\gamma_2}(x_2^{s_{22}} + x_1^{s_{21}}) - \langle\nabla\Phi(X), R^-(X)\rangle \leq |m_1|(x_1^{s_{11}} + x_2^{s_{12}}) + c_2 x_2(x_2^{s_{22}} + x_1^{s_{21}}).$$

Remember now that $s_{11} < 1$ and $s_{12} < \gamma_2 + s_{22}/2$. The last inequality implies in particular the existence of a constant $C > 0$ such as $|m_1|x_2^{s_{12}} \leq C + c_2 x^{\gamma_2+s_{22}}/2$, so that we have using $x_1^{s_{11}} \leq 1 + x_1$

$$\frac{c_2}{2}x_2^{\gamma_2}(x_2^{s_{22}} + x_1^{s_{21}}) - \langle\nabla\Phi(X), R^-(X)\rangle \leq |m_1|(1+x_1) + c_2 x_2(x_2^{s_{22}} + x_1^{s_{21}}),$$

and we may eventually write (changing the constant C again)

$$\int_\Omega (u_2^\ell)^{\gamma_2} + \sum_{k=1}^{\ell} \tau \int_\Omega (u_2^k)^{\gamma_2} \left\{(u_1^k)^{s_{21}} + (u_2^k)^{s_{22}}\right\} + \sum_{k=1}^{\ell} \tau \Gamma_k \tag{5.60}$$

$$\leq C \left(\sum_{k=1}^{\ell} \tau \int_\Omega (u_2^k)^{\gamma_2} + 1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2} \right), \tag{5.61}$$

where we used estimates (5.20) and (5.21) (with its consequence (5.59)) to get the estimate

$$\sum_{k=1}^{\ell} \tau \int_\Omega u_1^k + \sum_{k=1}^{\ell} \tau \int_\Omega u_2^k \{(u_2^k)^{s_{22}} + (u_1^k)^{s_{21}}\} \leq C(\|u_1^{in}\|_1 + \|u_2^{in}\|_1).$$

We may now conclude using a discrete Gronwall Lemma. Indeed, if we call w_ℓ the first integral in the l.h.s. of (5.60) and define $w_0 := C(1 + \|u_1^{in}\|_1 + \|u_2^{in}\|_{\gamma_2}^{\gamma_2})$, we have (since $\Gamma_k \geq 0$)

$$(1 - C\tau) w_\ell \leq C\tau \sum_{k=1}^{\ell-1} w_k + w_0,$$

whence, as soon as $C\tau < 1$,

$$(1 - C\tau)^\ell \, w_\ell \leq C\tau \sum_{k=1}^{\ell-1} (1 - C\tau)^{\ell-1} \, w_k + (1 - C\tau)^{\ell-1} \, w_0,$$

from which we get by a straightforward induction

$$w_\ell \leq \frac{w_0}{(1 - C\tau)^\ell} \,,$$

and the conclusion of the proof of Proposition 5.5 easily follows from this last estimate. □

5.4.3 Passage to the limit

We come back to the proof of Theorem 5.1. We introduce at this level the

Definition 5.4. *For a given family $h := (h^k)_{0 \leq k \leq N-1}$ of functions defined on Ω, we denote by $\underline{h}^N$ the step (in time) function defined on $\mathbb{R} \times \Omega$ by*

$$\underline{h}^N(t, x) := \sum_{k=0}^{N-1} h^k(x) \mathbf{1}_{]k\tau, (k+1)\tau]}(t).$$

We then have by definition, for all $p, q \in [1, \infty[$,

$$\|\underline{h}^N\|_{\mathrm{L}^q\left([0,T];\mathrm{L}^p(\Omega)\right)} = \left(\sum_{k=0}^{N-1} \tau \|h^k\|_{\mathrm{L}^p(\Omega)}^q \right)^{1/q},$$

and in particular

$$\|\underline{h}^N\|_{\mathrm{L}^p(Q_T)} = \left(\sum_{k=0}^{N-1} \tau \int_\Omega |h^k(x)|^p \, \mathrm{d}x \right)^{1/p}.$$

Using an analogous notation for the family of vectors $(U_N^k)_{0 \leq k \leq N-1}$, one easily checks that equation (5.46) can be rewritten as (since the functions are extended by 0 on $\mathbb{R}_-$)

$$\partial_t \underline{U}^N = \sum_{k=1}^{N-1} (U_N^k - U_N^{k-1}) \otimes \delta_{t^k} + U_N^0 \otimes \delta_0 \text{ in } \mathscr{D}'(] - \infty, T[\times \Omega)^2 \tag{5.62}$$

$$= \sum_{k=1}^{N-1} \tau ((\Delta[A(U^k)] + R(U^k)) \otimes \delta_{t^k} + U_N^0 \otimes \delta_0 \text{ in } \mathscr{D}'(] - \infty, T[\times \Omega)^2, \tag{5.63}$$

where $t^k = k\tau$ and δ_{t^k} is the Dirac mass centred on t^k. We intend to pass to the limit $N = 1/\tau \to \infty$ in eq. (5.63).

In order to do so, let us recall the bounds (all are uniform w.r.t. N) obtained so far :

$$\underline{u_1}^N + \underline{u_2}^N \in \mathrm{L}^\infty_t(\mathrm{L}^1_x), \tag{5.64}$$
$$(\underline{u}_1^N + \underline{u}_2^N)((d_1 + (\underline{u}_2^N)^{\gamma_2})\underline{u}_1^N + (d_2 + (\underline{u}_1^N)^{\gamma_1})\underline{u}_2^N) \in \mathrm{L}^1_{t,x}, \tag{5.65}$$
$$\underline{u_1}^N + \underline{u_2}^N \in \mathrm{L}^2_{t,x}, \tag{5.66}$$
$$\underline{u}_2^N \in \mathrm{L}^\infty_t(\mathrm{L}^{\gamma_2}_x), \tag{5.67}$$
$$(\underline{u}_2^N)^{\gamma_2}\left\{(\underline{u}_1^N)^{s_{21}} + (\underline{u}_2^N)^{s_{22}}\right\} \in \mathrm{L}^1_{t,x}, \tag{5.68}$$
$$\nabla(\underline{u}_1^N)^{\gamma_1/2} \in \mathrm{L}^2_{t,x}, \tag{5.69}$$
$$\nabla(\underline{u}_2^N)^{\gamma_2/2} \in \mathrm{L}^2_{t,x}, \tag{5.70}$$

where (5.64) is a consequence of estimate (5.20), (5.65) is a consequence of estimate (5.22) (both in Theorem 5.2), (5.66) is a consequence of (5.65) (each term is nonnegative) and (5.67) – (5.70) are all consequences of estimate (5.52) in Proposition 5.5. Then, thanks to (5.68) and (5.66), we have the uniform (w.r.t. N) bound

$$\underline{u}_i^N \in \mathrm{L}^{\gamma_i^+}_{t,x}, \text{ for } i = 1, 2. \tag{5.71}$$

This means that $(\underline{u}_i^N)^{\gamma_i/2}$ is bounded in $\mathrm{L}^{2^+}_{t,x}$, so that using (5.65) and writing for $i \neq j$

$$\underline{u}_j^N(\underline{u}_i^N)^{\gamma_i} = \overbrace{\underline{u}_j^N(\underline{u}_i^N)^{\gamma_i/2}}^{\in \mathrm{L}^2_{t,x}}\overbrace{(\underline{u}_i^N)^{\gamma_i/2}}^{\in \mathrm{L}^{2^+}_{t,x}},$$

we get the uniform (w.r.t. N) bound

$$A(\underline{U}^N) \in \mathrm{L}^{1^+}_{t,x} \times \mathrm{L}^{1^+}_{t,x}. \tag{5.72}$$

As for the reaction terms, the coefficients s_{ij} are precisely chosen in such a way that the correspon-ding nonlinearities may all be handled. Indeed, $s_{11} < 1$, so that $(\underline{u}_1^N)^{s_{11}+1} \in \mathrm{L}^{1^+}_{t,x}$ using (5.66). Then $(\underline{u}_2^N)^{s_{22}+1} \in \mathrm{L}^{1^+}_{t,x}$ using (5.68). Also, since $s_{21} < 2$, we see that

$$\underline{u}_2^N(\underline{u}_1^N)^{s_{21}} = \overbrace{\underline{u}_2^N(\underline{u}_1^N)^{s_{21}/\gamma_2}}^{\in \mathrm{L}^{\gamma_2}_{t,x}}\overbrace{(\underline{u}_1^N)^{s_{21}/\gamma_2'}}^{\in \mathrm{L}^{(\gamma_2')^+}_{t,x}} \in \mathrm{L}^{1^+}_{t,x},$$

where $1/\gamma_2 + 1/\gamma_2' = 1$. Now if $s_{12} \leq \gamma_2/2$, we know from (5.65) that $\underline{u}_1^N(\underline{u}_2^N)^{s_{12}} \in \mathrm{L}^{1^+}_{t,x}$. Otherwise, $\gamma_2/2 < s_{12} < \gamma_2 + s_{22}/2$, and we use (5.65) and (5.68) in order to get

$$\underline{u}_1^N(\underline{u}_2^N)^{s_{12}} = \overbrace{\underline{u}_1^N(\underline{u}_2^N)^{\gamma_2/2}}^{\in \mathrm{L}^2_{t,x}}\overbrace{(\underline{u}_2^N)^{s_{12}-\gamma_2/2}}^{\in \mathrm{L}^{2^+}_{t,x}} \in \mathrm{L}^{1^+}_{t,x}.$$

Finally, all previous bounds being uniform (w.r.t. N), we get the uniform (w.r.t. N) bound

$$R(\underline{U}^N) \in \mathrm{L}^{1^+}_{t,x} \times \mathrm{L}^{1^+}_{t,x}. \tag{5.73}$$

The previous bounds allow (at least) to obtain (up to extraction of some subsequence) $\mathrm{L}^1_{t,x}$ weak conver-gence (thanks to Dunford-Pettis Theorem) for $(\underline{U}^N)_N$, $(A(\underline{U}^N))_N$ and $(R(\underline{U}^N))_N$. The strategy is then classical : one has to commute the weak limits and non-linearities, possibly by proving some strong compactness. Estimates (5.69) – (5.70) are of course very helpful in this situation, since they show that oscillations w.r.t. the x variable cannot develop.

But since we kept in our assumptions the possibility that $\gamma_2 > 2$, estimate (5.70) degenerates. Indeed $\nabla f = \frac{2}{\gamma_2} f^{\frac{2-\gamma_2}{2}} \nabla f^{\gamma_2/2}$, and for small values of f, no information on ∇f can be recovered from $\nabla(f^{\gamma_2/2})$.

This type of situation is frequent in the study of degenerate parabolic equation (such as the porous medium equation for instance) and the usual Aubin-Lions Lemma cannot directly be applied. Notice that for $(\underline{u}_1^N)_N$, there is no such issue : (5.69) automatically yields an estimate on $\nabla \underline{u}_1^N$ (this is the strategy used to recover compactness in [8, 15] for instance) : $\nabla \underline{u}_1^N = \frac{2}{\gamma_1}(\underline{u}_1^N)^{\frac{2-\gamma_1}{2}} \nabla (\underline{u}_1^N)^{\gamma_1/2}$ is bounded (at least) in $\mathrm{L}^1_{t,x}$. Indeed, $(\underline{u}_1^N)^{\frac{2-\gamma_1}{2}}$ is bounded in $\mathrm{L}^{4/(2-\gamma_1)}_{t,x}$ thanks to (5.66) and $\nabla[(\underline{u}_1^N)^{\gamma_1/2}]$ is bounded in $\mathrm{L}^{4/(2+\gamma_1)}_{t,x}$ since it is bounded in $\mathrm{L}^2_{t,x}$ (because of (5.69)). Furthermore, let us write $S_\tau(\underline{U}^N) : (t,x) \mapsto \underline{U}^N(t-\tau,x)$. Using (5.72) and (5.73) to get the (uniform w.r.t. N) bound

$$\frac{\underline{U}^N - S_\tau \underline{U}^N}{\tau} = \Delta[A(\underline{U}^N)] + R(\underline{U}^N) \in \mathrm{L}^1_t(\mathrm{W}^{-2,1}_x) \times \mathrm{L}^1_t(\mathrm{W}^{-2,1}_x),$$

one can then apply a discrete version of Aubin-Lions lemma to $(\underline{u}_1^N)_N$ (see for instance [18]) to recover strong compactness for $(\underline{u}_1^N)_N$ in $\mathrm{L}^1_{t,x}$.

To prove that $(\underline{u}_2^N)_N$ is relatively compact in $\mathrm{L}^1_{t,x}$, we first evaluate (5.63) on some test function $\Psi \in \mathscr{D}(]-\infty,T[\times\Omega)^2$, to get

$$\begin{aligned}\langle \partial_t \underline{U}^N, \Psi\rangle_{\mathscr{D}',\mathscr{D}} &= \sum_{k=1}^{N-1} \tau \int_\Omega \langle \Delta[A(U_N^k)] + R(U_N^k), \Psi(t^k)\rangle + \int_\Omega \langle U_N^0, \Psi(0)\rangle \\ &= \sum_{k=1}^{N-1} \tau \int_\Omega \langle A(U_N^k), \Delta\Psi(t^k)\rangle + \tau\int_\Omega \langle R(U_N^k), \Psi(t^k)\rangle + \int_\Omega \langle U_N^0, \Psi(0)\rangle. \end{aligned} \tag{5.74}$$

Using estimates (5.72), (5.73) and (5.64), we hence have (using $N\tau = T$)

$$\left|\langle \partial_t \underline{U}^N, \Psi\rangle_{\mathscr{D}',\mathscr{D}}\right| \le C_T \|\Psi\|_{\mathrm{L}^\infty_t(\mathrm{H}^L_x)},$$

where L is a sufficiently large integer. Using this estimate together with (5.70), we may apply Corollary 5.3 of the Appendix to get that $(u_2^N)_N$ is relatively compact in $\mathrm{L}^2_{\mathrm{loc}}(]0,T[\times\Omega)$. Then, up to the extraction of a subsequence (using the L^1-equi-continuity of $(u_2^N)_N$)

$$\underline{U}^N \underset{N\to\infty}{\longrightarrow} U \qquad \text{in } \mathrm{L}^1([0,T]\times\Omega)\times \mathrm{L}^1([0,T]\times\Omega). \tag{5.75}$$

This strong convergence ensures that the weak limits of $(A(\underline{U}^N))_N$ and $(R(\underline{U}^N))_N$ are respectively $A(U)$ and $R(U)$.

We now can go back to (5.74), and write it as

$$-\int_0^T \int_\Omega \langle \underline{U}^N, \partial_t \Psi\rangle = \sum_{k=1}^{N-1} \tau \int_\Omega \langle \Delta[A(U_N^k)] + R(U_N^k), \Psi(t^k)\rangle + \int_\Omega \langle U_N^0, \Psi(0)\rangle,$$

so that a straightforward density argument allows to replace Ψ by some test function Ψ lying in $\mathscr{C}^1_c([0,T[;\mathscr{C}^2_\nu(\overline{\Omega}))^2$.

We get

$$-\int_0^T \int_\Omega \langle \underline{U}^N, \partial_t \Psi\rangle = \int_\tau^T \int_\Omega \langle A(\underline{U}^N), \Delta\widetilde{\Psi^N}\rangle + \int_\tau^T \int_\Omega \langle R(\underline{U}^N), \widetilde{\Psi^N}\rangle + \int_\Omega \langle U_N^0, \Psi(0)\rangle,$$

where

$$\widetilde{\Psi}^N(t,x) := \sum_{k=1}^{N-1} \Psi(t^k,x)\mathbf{1}_{]t^k,t^{k+1}]}(t) \underset{N\to\infty}{\overset{\mathrm{L}^\infty([0,T]\times\Omega)}{\longrightarrow}} \Psi,$$

and we have the same convergence for $\Delta\widetilde{\Psi}^N$ towards $\Delta\Psi$. We now know that the three sequences $(\underline{U}^N)_N$, $(A(\underline{U}^N))_N$ and $(R(\underline{U}^N))_N$ converge weakly (up to a subsequence) in $\mathrm{L}^1_{t,x}$, so that the three first integrals of the equality will converge to the expected quantities, that is,

$$-\int_0^T \int_\Omega \langle \underline{U}^N, \partial_t \Psi\rangle \underset{N\to\infty}{\longrightarrow} -\int_0^T \int_\Omega \langle U, \partial_t\Psi\rangle, \tag{5.76}$$

$$\int_\tau^T \int_\Omega \langle A(\underline{U}^N), \Delta\widetilde{\Psi^N}\rangle \underset{N\to\infty}{\longrightarrow} \int_0^T \int_\Omega \langle A(U), \Delta\Psi\rangle, \tag{5.77}$$

$$\int_\tau^T \int_\Omega \langle R(\underline{U}^N), \widetilde{\Psi^N}\rangle \underset{N\to\infty}{\longrightarrow} \int_0^T \int_\Omega \langle R(U), \Psi\rangle, \tag{5.78}$$

whereas for the initial datum,

$$\int_\Omega \langle U_N^0, \Psi(0)\rangle \underset{N\to\infty}{\longrightarrow} \int_\Omega \langle U^{in}, \Psi(0)\rangle, \tag{5.79}$$

thanks to the fact that $(U_N^0)_N$ approaches U^{in} in $\mathrm{L}^1(\Omega)\times\mathrm{L}^{\gamma_2}(\Omega)$. We have proved that U is a nonnegative *local* (in time) (very) weak solution to (5.7)–(5.9) on $[0,T]\times\Omega$ (that is, the weak formulation (5.11)–(5.12) is satisfied for all ψ_1, ψ_2 in $\mathscr{C}_c^1([0,T),\mathscr{C}_\nu^2(\overline{\Omega}))$).

Let us now show that we can extend U on $\mathbb{R}_+\times\Omega$ so that it gives a global (in time) solution. To do this, we make appear explicitly the dependency in τ (and then indirectly in $T=\tau N$) of our semi-discrete approximation : we write $\underline{h}_\tau^N$ the function $\underline{h}^N$ defined in Definition 5.4. Notice that it is then clear that given an infinite sequence $(h^k)_{k\in\mathbb{N}}$ of functions defined on Ω, for all $m\in\mathbb{N}-\{0\}$ the function $\underline{h}_\tau^{mN}$ is well defined on $\mathbb{R}\times\Omega$ and it coincides with $\underline{h}_\tau$ on $[0,mT]\times\Omega$, where $\underline{h}_\tau(t,\cdot) := \sum_{k=0}^\infty h^k \mathbf{1}_{]k\tau,(k+1)\tau]}(t)$. Applying iteratively Theorem 5.3, we get the existence of an infinite sequence $(U^k)_{k\in\mathbb{N}}$ solving (5.16) and satisfying (5.17)–(5.22) with N replaced by any $N'\geq N$. Then $\underline{U}_\tau^{mN}$ is defined for all $m\in\mathbb{N}-\{0\}$ and it furthermore coincides with $\underline{U}_\tau$ on $[0,mT]\times\Omega$. Extracting subsequences, we can perform the proof of convergence on $[0,2T]$, $[0,3T]$, ..., so that by Cantor's diagonal argument, we get that convergence (5.75) (together with the existence of the limit U) and convergences (5.76)–(5.79) hold true with T replaced by mT and $\underline{U}^N$ replaced by $\underline{U}_\tau^{mN}$ (or equivalently by $\underline{U}_\tau$), for any $m\in\mathbb{N}-\{0\}$ and for Ψ any test function in $\mathscr{C}_c^1([0,mT[;\mathscr{C}_\nu^2(\overline{\Omega}))^2$. At the end of the day, U is defined in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^1(\Omega))\times\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^2(\Omega))$ and is a global (in time) (very) weak solution to (5.7)–(5.9).

To conclude the proof, it suffices to show estimates (5.13), (5.14), (5.15) for any $s>0$. This is done by passing to the limit $N\to\infty$ in estimates (5.20), (5.22) and (5.52), with T and N replaced by some $mT>s$ and mN. We use the strong convergence of $\underline{U}_\tau^N$ in $\mathrm{L}^1([0,mT]\times\Omega)$ and Fatou's lemma to compute the limits in (5.22) and the two first integrals in (5.52). To compute the limits of the remaining terms in (5.52), we notice that $(\underline{u}_{\tau,1}^N)^{\gamma_1/2}$, $(\underline{u}_{\tau,2}^N)^{\gamma_2/2}$, $(\underline{u}_{\tau,1}^N)^{\gamma_1/2}(\underline{u}_{\tau,2}^N)^{\gamma_2/2}$ are bounded in $\mathrm{L}^{2+}([0,mT]\times\Omega)$ (thanks to estimates (5.65) and (5.68)), hence the weak convergence of these sequences in $\mathrm{L}^2([0,mT]\times\Omega)$, and use the weak lower semi-continuity of the norm in $\mathrm{L}^2([0,mT]\times\Omega)$ on the sequences of the gradients. To get (5.14), we first use again the strong convergence of $\underline{U}_\tau^N$ in $\mathrm{L}^1([0,mT]\times\Omega)$ and Fatou's lemma to compute the limit in (5.20), which gives that U is in $\mathrm{L}^\infty_{\mathrm{loc}}(\mathbb{R}_+,\mathrm{L}^1(\Omega))$. It does not give directly the very estimate (5.14), but it is sufficient to compute rigorously for $i\neq j$ and for almost every $s\in\mathbb{R}_+$ (by taking in identities (5.11)–(5.12) a sequence of functions ψ_i which are uniform in space, $\mathscr{C}_c^1$ in time, uniformly bounded in $\mathrm{L}^\infty(\mathbb{R}_+)$ and approximate the function $\mathbf{1}_{t\in[0,s]}$ in $\mathrm{BV}(\mathbb{R}_+)$, that is the sequence of ψ_i approximates $\mathbf{1}_{t\in[0,s]}$ in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+)$ and the sequence of the derivatives $\partial_t\psi_i$ approximate $\partial_t\mathbf{1}_{t\in[0,s]}=\delta_s-\delta_0$ weakly in the sense of Radon measures on $\mathbb{R}_+$)

$$\int_\Omega u_i(s,x)\,\mathrm{d}x = \int_0^s\int_\Omega u_i(t,x)\left(\rho_i - u_i(t,x)^{s_{ii}} - u_j(t,x)^{s_{ij}}\right)\mathrm{d}x\,\mathrm{d}t \leq \rho_i\int_0^s\int_\Omega u_i(t,x)\,\mathrm{d}x\,\mathrm{d}t,$$

and we conclude using a Gronwall's lemma.

5.5 More systems

In this section, we explain on two examples how our methods can be used to prove existence theorems for other systems.

5.5.1 Two-species with self-diffusion

As we stated in Remark 5.2, the proof of Theorem 5.1 applies to more general systems. It is possible indeed to replace the power laws by general increasing continuous functions (without changing the structure of the proof) or to include self-diffusion coefficients. We focus here on the second generalization. As a matter of fact, reproducing *mutatis mutandis* the arguments shown before, one is able to prove the existence of global weak solutions to some systems of the form

$$\partial_t u_1 - \Delta[u_1 a_1(u_1,u_2)] = 0, \tag{5.80}$$
$$\partial_t u_2 - \Delta[u_2 a_2(u_1,u_2)] = 0, \tag{5.81}$$

where a_1 and a_2 are defined by (5.5), with $d_{ii}>0$. Actually if we look closely at the proof above, apart from the usual conditions of positivity of the coefficients d_i (and nonnegativity of d_{ij}, δ_{ij}) the only constraint is that the diffusion matrix has a strictly positive determinant, which can be summarized in the algebraic condition, for all $x_1, x_2 > 0$,

$$\begin{vmatrix} d_1 + d_{11}(\delta_{11}+1)x_1^{\delta_{11}} + d_{12}x_2^{\delta_{12}} & d_{12}\delta_{12}x_2^{\delta_{12}-1}x_1 \\ d_{21}\delta_{21}x_1^{\delta_{21}-1}x_2 & d_2 + d_{22}(\delta_{22}+1)x_2^{\delta_{22}} + d_{21}x_1^{\delta_{21}} \end{vmatrix} > 0. \tag{5.82}$$

As it was noticed in Remark 5.7, the condition (5.82) ensures that the entropy defined in the self-diffusion-free case (that is, taking $d_{11} = d_{22} = 0$, as in Theorem 5.1) will also be an entropy for the system with $d_{11},\, d_{22} > 0$. But condition (5.82) also implies (see Proposition 5.6) that condition **H3** is fulfilled. The pattern of the proof of Theorem 5.1 is hence left intact : the same approximation procedure applies and similar estimates may be obtained (including the Duality estimate which forbids any concentration phenomenon). The only step for which one has to be a little bit cautious is the gradient estimates. Let us explain why, as far as gradient estimates are concerned, the self-diffusion term will in fact help us. As usual we rewrite system (5.80) – (5.81) as a vectorial equation

$$\partial_t U - \Delta[M(U)] = 0,$$

where $M(X)$ may be splitted in this way

$$M(X) = A(X) + B(X),$$

with $A(X)$ a vectorial mapping corresponding to the self-diffusion-free case ($d_{11} = d_{22} = 0$) and $B(X) = (d_{ii}x_i^{\delta_{ii}+1})_i$. This implies of course that $\mathrm{D}(M)(X) = \mathrm{D}(A)(X) + \mathrm{D}(B)(X)$ where $\mathrm{D}(B)(X)$ is the diagonal matrix

$$\mathrm{D}(B)(X) = \begin{pmatrix} d_{11}(\delta_{11}+1)x_1^{\delta_{11}} & 0 \\ 0 & d_{22}(\delta_{22}+1)x_2^{\delta_{22}} \end{pmatrix}.$$

Now, if we have a set of coefficients d_i, δ_{ij}, d_{ij} for $i \neq j$ satisfying the assumption of Theorem 5.1 for the corresponding self-diffusion-free system (vectorial mapping A), then we will be able to handle the more general case of the system including self-diffusion (vectorial mapping $M = A + B$) as soon as $d_{ii}, \delta_{ii} \geq 0$. Indeed, recall that in the previous section, we exhibited a convex entropy Φ such that $\mathrm{D}^2(\Phi)(X)\mathrm{D}(A)(X)$ is a positive symmetric matrix with (using the notation $\gamma_1 = \delta_{12},\, \gamma_2 = \delta_{21}$)

$$\mathrm{D}^2(\Phi)(X) = \begin{pmatrix} \gamma_1 x_1^{\gamma_1-2} & 0 \\ 0 & \gamma_2 x_2^{\gamma_2-2} \end{pmatrix},$$

so that

$$\mathrm{D}^2(\Phi)(X)\mathrm{D}(B)(X) = \begin{pmatrix} \omega_1 x_1^{\gamma_1+\delta_{11}-2} & 0 \\ 0 & \omega_2 x_2^{\gamma_2+\delta_{22}-2} \end{pmatrix},$$

where ω_i are nonnegative coefficients (strictly positive as soon as $d_{ii} > 0$). It is now clear that if we reproduce the entropy estimate, that is, we apply the quadratic form $\mathrm{D}^2(\Phi)(U)\mathrm{D}(M)(U)$ to the vector ∇U, we will have a positive part coming out of the term $\mathrm{D}^2(\Phi)(U)\mathrm{D}(A)(U)$ (which is in fact already lower bounded by gradients) plus the following term

$$\begin{aligned} \langle \nabla U, \mathrm{D}^2(\Phi)(U)\mathrm{D}(B)(U)\,\nabla U\rangle &= \omega_1|\nabla u_1|^2 u_1^{\gamma_1+\delta_{11}-2} + \omega_2|\nabla u_2|^2 u_2^{\gamma_2+\delta_{22}-2} \\ &= \frac{4\omega_1}{(\gamma_1+\delta_{11})^2}|\nabla u_1^{(\gamma_1+\delta_{11})/2}|^2 + \frac{4\omega_2}{(\gamma_2+\delta_{22})^2}|\nabla u_2^{(\gamma_2+\delta_{22})/2}|^2, \end{aligned}$$

so that we do manage to control more gradients.

Now that we have made sure that systems with self-diffusion can be treated with our method, let us discuss the use of these self-diffusion coefficients when one wishes to treat cases that fall outside of the scope of Theorem 5.1. The idea is the following : in our proof the core condition $\gamma_1\gamma_2 < 1$ was designed to ensure the positivity of $\det \mathrm{D}(A)$. If we consider more general cases in which $\gamma_1\gamma_2 > 1$, it could happen that $\det \mathrm{D}(A)$ takes negative values but that $\det \mathrm{D}(M)$ remains strictly positive (where $M = A + B$, that is, self-diffusion is added). In this way, on gets an entropy estimate thanks to the presence of self diffusion. This is for instance the strategy used in [29] in the proof of Theorem 4. This Theorem gives global weak solutions for the system

$$\partial_t u_1 - \Delta[u_1(d_1 + d_{11}u_1^s + d_{12}u_2^s)] = 0, \tag{5.83}$$

$$\partial_t u_2 - \Delta[u_2(d_2 + d_{22}u_2^s + d_{21}u_1^s)] = 0, \tag{5.84}$$

under the condition $1 < s < 4$ and $(1 - 1/s)d_{12}d_{21} \leq d_{11}d_{22}$ (plus assumptions on the initial data). As explained in [29], the condition $(1 - 1/s)d_{12}d_{21} \leq d_{11}d_{22}$ appears naturally when one looks for the systems having an entropy structure, whereas the second one ($1 < s < 4$) is only used in the regularization procedure.

Using our method of proof, we are able to prove the existence of global weak solutions of (5.83) – (5.84) under the less stringent condition $s > 1$ and

$$d_{11}d_{22} \geq \left(\frac{s-1}{s+1}\right)^2 d_{12}d_{21}, \tag{5.85}$$

without any upper bound on s (because in our approximation procedure, we do not regularize the diffusion matrix). Notice that this bound is indeed less restrictive that the one obtained in [29], since $\left(\frac{s-1}{s+1}\right)^2 < 1 - 1/s$.

Let us explain how condition (5.85) appears at the level of the entropy structure. As we did in Subsection 5.3.2, the following equality holds for any function $\Phi : \mathbb{R}^2 \to \mathbb{R}$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Phi(U) + \int_\Omega \langle \nabla U, \mathrm{D}^2\Phi(U)\mathrm{D}(M)(U)\nabla U\rangle = 0, \tag{5.86}$$

where as before $M = A + B$ (self-diffusion-free + self-diffusion). As explained above, we have to check condition (5.82) for the coefficients of the system (5.83)–(5.84). It amounts to find the coefficients such that

$$\begin{vmatrix} d_1 + d_{11}(s+1)x_1^s + d_{12}x_2^s & d_{12}sx_2^{s-1}x_1 \\ d_{21}sx_1^{s-1}x_2 & d_2 + d_{22}(s+1)x_2^s + d_{21}x_1^s \end{vmatrix} > 0, \tag{5.87}$$

that is

$$(d_1 + d_{11}(s+1)x_1^s + d_{12}x_2^s)(d_2 + d_{22}(s+1)x_2^s + d_{21}x_1^s) - d_{21}d_{12}s^2x_1^sx_2^s > 0,$$

that we can also write (since we need the inequality for all $z_1 = x_1^s$, $z_2 = x_2^s > 0$)

$$\forall (z_1, z_2) \in \mathbb{R}_+^2, \quad d_1d_2 + L(z_1, z_2) + Q(z_1, z_2) > 0,$$

where $L : \mathbb{R}^2 \to \mathbb{R}_+$ is linear and $Q : \mathbb{R}^2 \to \mathbb{R}$ is a quadratic form. The previous inequality is true if (and only if) the quadratic form Q takes nonnegative values on $\mathbb{R}_+^2$: if Q is negative at some vector (z_1, z_2), $Q(\lambda(z_1, z_2)) = \lambda^2 Q(z_1, z_2)$ will eventually dominate $d_1d_2 + \lambda L(z_1, z_2)$ for λ large enough. Now notice that if $a, b > 0$, the quadratic form $az_1^2 + bz_2^2 + cz_1z_2$ takes nonnegative values on $\mathbb{R}_+^2$ if and only if $c \geq -2\sqrt{ab}$ (this condition is much less restrictive than imposing Q nonnegative). For our quadratic form Q, it means that

$$d_{11}d_{22}(s+1)^2 - (s^2 - 1)d_{21}d_{12} \geq -2\sqrt{d_{11}d_{21}d_{22}d_{12}}(s+1),$$

that is (dividing first by $d_{12}d_{21}$), if (defining X by $(s+1)\sqrt{d_{11}d_{22}} = X\sqrt{d_{12}d_{21}}$),

$$X^2 + 2X - (s^2 - 1) = (X + s + 1)(X - (s-1)) \geq 0.$$

We recover therefore the condition $X \geq s - 1$, which is equivalent to (5.85). We notice that this condition implies in fact a stronger estimate than (5.87) : the same estimate holds taking $d_1 = d_2 = 0$ (the quadratic form depends neither on d_1 nor on d_2). This means that we can keep these pure diffusion terms to control the gradients as we did before. More precisely we have

$$\det\Big(\mathrm{D}(M) - \mathrm{diag}(d_1, d_2)\Big) > 0,$$

whence if Φ is the entropy function considered in the previous section, the matrix

$$\mathrm{D}^2(\Phi)\Big(\mathrm{D}(M) - \mathrm{diag}(d_1, d_2)\Big)$$

is symmetric, has strictly positive trace and determinant : it is (symmetric) positive-definite. Hence, going back to (5.86) we get :

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Phi(U) + \int_\Omega \langle \nabla U, \mathrm{D}^2\Phi(U)\mathrm{diag}(d_1, d_2)\nabla U\rangle < 0,$$

which, as we have done before, is enough to control $\nabla u_i^{s/2}$ in $\mathrm{L}^2_{t,x}$. Finally, our result enables to extend significantly the results of Theorem 4 of [29]. Note however that in comparison with Theorem 4 of [29], our global weak solutions will only satisfy $u_i^{s/2} \in \mathrm{L}^2_t(\mathrm{H}^1_x)$, whereas in [29] they also satisfy the stronger estimate $u_i^s \in \mathrm{L}^2_t(\mathrm{H}^1_x)$. This is not really surprising, since the condition (5.85) that we exhibited is less restrictive that the one in [29]. The philosophy behind this is the existence of two possible uses for the self-diffusion matrix $\mathrm{D}(B)(X)$: one can use it in order to obtain more gradients (as we did at the beginning of this Subsection) ; one can also use it to stiffen the underlying entropy structure. The less one uses $\mathrm{D}(B)(X)$ for one of these two tasks, the more one can exploit it for the other one. Note finally that thanks to our approximation procedure, we can remove the upper-bound $s < 4$ in [29].

5.5.2 An example with three species

Consider the system

$$\partial_t u_1 - \Delta[u_1\, a_1(u_2,u_3)] = 0, \tag{5.88}$$
$$\partial_t u_2 - \Delta[u_2\, a_2(u_1,u_3)] = 0, \tag{5.89}$$
$$\partial_t u_3 - \Delta[u_3\, a_3(u_1,u_2)] = 0, \tag{5.90}$$

with, for $0 < s < 1/\sqrt{3}$ and $d_1, d_2, d_3 > 0$,

$$a_1(u_2,u_3) = d_1 + u_2^s + u_3^s, \quad a_2(u_1,u_3) = d_2 + u_1^s + u_3^s, \quad a_3(u_1,u_2) = d_3 + u_1^s + u_2^s. \tag{5.91}$$

We claim that 1) this system has a convex entropy and 2) the system satisfies **(H)**. Then we explain briefly how we can use these two claims to obtain an existence theorem.

We first present a convex entropy for this system. Define

$$h(t) := t - \frac{t^s}{s}$$

Let us check that

$$\Phi(u_1,u_2,u_3) = \frac{1}{1-s}[h(u_1) + h(u_2) + h(u_3) - 3h(1)]$$

is a convex entropy on $(\mathbb{R}_+^*)^3$ for (5.88)–(5.90) in the sense of Definition 5.1. Since the function h reaches its minimum in 1, Φ is nonnegative and Φ is clearly convex. For all $U = (u_1,u_2,u_3) \in (\mathbb{R}_+^*)^3$,

$$\begin{aligned} \mathrm{D}^2\Phi(U) &= \begin{pmatrix} u_1^{s-2} & 0 & 0 \\ 0 & u_2^{s-2} & 0 \\ 0 & 0 & u_3^{s-2} \end{pmatrix} \\ \mathrm{D}A(U) &= \begin{pmatrix} d_1 + u_2^s + u_3^s & s\, u_1\, u_2^{s-1} & s\, u_1\, u_3^{s-1} \\ s\, u_2\, u_1^{s-1} & d_2 + u_1^s + u_3^s & s\, u_2\, u_3^{s-1} \\ s\, u_3\, u_1^{s-1} & s\, u_3\, u_2^{s-1} & d_3 + u_1^s + u_2^s \end{pmatrix}. \end{aligned} \tag{5.92}$$

Therefore, the matrix

$$\mathrm{D}^2\Phi(U)\,\mathrm{D}A(U) = \begin{pmatrix} (d_1 + u_2^s + u_3^s)\, u_1^{s-2} & s\, u_1^{s-1}\, u_2^{s-1} & s\, u_1^{s-1}\, u_3^{s-1} \\ s\, u_2^{s-1}\, u_1^{s-1} & (d_2 + u_1^s + u_3^s)\, u_2^{s-2} & s\, u_2^{s-1}\, u_3^{s-1} \\ s\, u_3^{s-1}\, u_1^{s-1} & s\, u_3^{s-1}\, u_2^{s-1} & (d_3 + u_1^s + u_2^s)\, u_3^{s-2} \end{pmatrix}$$

is symmetric. We use Sylvester's criteria to check that it is positive definite : that is, writing

$$\mathrm{D}A(U) = D_1 = \begin{pmatrix} \begin{matrix} D_2 \end{matrix} & & * \\ & & * \\ * & * & * \end{pmatrix} = \begin{pmatrix} D_3 & * & * \\ * & * & * \\ * & * & * \end{pmatrix}, \tag{5.93}$$

and

$$\mathrm{D}^2(\Phi)(U)\mathrm{D}(A)(U) = C_1 = \begin{pmatrix} \begin{matrix} C_2 \end{matrix} & & * \\ & & * \\ * & * & * \end{pmatrix} = \begin{pmatrix} C_3 & * & * \\ * & * & * \\ * & * & * \end{pmatrix},$$

with $C_i = \mathrm{diag}(u_1^{s-2}, \ldots, u_{4-i}^{s-2}) \times D_i$, it suffices to check that $\det(C_i) > 0$ for $i = 1,2,3$. Since $\det(C_i) = u_1^{s-2} \times \cdots \times u_{4-i}^{s-2} \times \det(D_i)$ for $i = 1,2,3$, it amounts to check that $\det(D_i) > 0$.

Clearly, $D_3 = d_1 + u_2^s + u_3^s > 0$. Furthermore,

$$\begin{aligned}\det(D_2) &= \begin{vmatrix} d_1 + u_2^s + u_3^s & s\, u_1\, u_2^{s-1} \\ s\, u_2\, u_1^{s-1} & d_2 + u_1^s + u_3^s \end{vmatrix} \\ &= (d_1 + u_2^s + u_3^s)\,(d_2 + u_1^s + u_3^s) - s^2\, u_1^s\, u_2^s \\ &= (d_1 + u_3^s)\,(d_2 + u_1^s + u_3^s) + u_2^s\,(d_2 + u_3^s) + (1 - s^2)\, u_1^s\, u_2^s > 0.\end{aligned}$$

Then, (directly, by Sarrus' rule)

$$\begin{aligned}\det(D_3) = \det(DA) = {} & (d_1 + u_2^s + u_3^s)\,(d_2 + u_1^s + u_3^s)\,(d_3 + u_1^s + u_2^s) + 2\, s^3\, u_2^s\, u_1^s\, u_3^s \\ & - (d_1 + u_2^s + u_3^s)\, s^2 u_3^s\, u_2^s - (d_2 + u_1^s + u_3^s) s^2\, u_3^s\, u_1^s - (d_3 + u_1^s + u_2^s) s^2\, u_1^s\, u_2^s.\end{aligned} \tag{5.94}$$

Since $s < 1/\sqrt{3}$,

$$(d_1 + u_2^s + u_3^s)\, s^2 u_3^s\, u_2^s < \frac{1}{3}(d_1 + u_2^s + u_3^s)\, u_3^s\, u_2^s < \frac{1}{3}(d_1 + u_2^s + u_3^s)\,(d_2 + u_1^s + u_3^s)\,(d_3 + u_1^s + u_2^s),$$

and similarly,

$$\begin{aligned}(d_2 + u_1^s + u_3^s) s^2\, u_3^s\, u_1^s &< \frac{1}{3}(d_1 + u_2^s + u_3^s)\,(d_2 + u_1^s + u_3^s)\,(d_3 + u_1^s + u_2^s), \\ (d_3 + u_1^s + u_2^s) s^2\, u_1^s\, u_2^s &< \frac{1}{3}(d_1 + u_2^s + u_3^s)\,(d_2 + u_1^s + u_3^s)\,(d_3 + u_1^s + u_2^s).\end{aligned}$$

Summing the last three inequalities and reinserting in (5.94), we get

$$\det(D_3) > 2\, s^3\, u_2^s\, u_1^s\, u_3^s > 0. \tag{5.95}$$

Finally, $\det(C_i) > 0$, so that Sylvester's criteria ensures that $\mathrm{D}^2(\Phi)(U)\mathrm{D}(A)(U)$ is positive definite. We have proven that Φ is an entropy on $(\mathbb{R}_+^*)^3$ for (5.88)–(5.90). Let us now explain how this entropy gives (at least, at the formal level) estimates for the gradients of the solutions of (5.88)–(5.90). First, notice that in this subsection, the only assumption used for the parameters d_i is nonnegativity. In particular, all computations above hold if we take $d_1 = d_2 = d_3 = 0$. Therefore, the matrix

$$\mathrm{D}^2(\Phi)\Big(\mathrm{D}(A) - \mathrm{diag}(d_1, d_2, d_3)\Big)$$

is (symmetric) positive-definite for all $U \in (\mathbb{R}_+^*)^3$. Then, consider a solution U of (5.88)–(5.90). A (formal) straightforward computation shows that (5.86) holds. Using the positivity of the matrix $\mathrm{D}^2(\Phi)(\mathrm{D}(A) - \mathrm{diag}(d_1, d_2, d_3))$ in (5.86), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Phi(U) + \int_\Omega \langle \nabla U, \mathrm{D}^2\Phi(U)\,\mathrm{diag}(d_1, d_2, d_3)\nabla U\rangle < 0.$$

Integrating on $[0, T]$ and using the computation of $\mathrm{D}^2\Phi$ in (5.92), this gives an estimate for $\nabla u_i^{s/2}$ in $\mathrm{L}^2_{t,x}$ ($i = 1, 2, 3$).

Let us now check that the system (5.88)–(5.90) satisfies assumption **(H)**. **H1** and **H2** are clearly satisfied (with $a_i \geq \alpha := \min(d_1, d_2, d_2) > 0$). Assumption **H3** is given by Proposition 5.7 and Remark 5.8. Indeed, recall the notations (5.93). Reusing computations (5.93)–(5.95), we can easily check that $\det(D_3) > 0$ on $(\mathbb{R}_+^*)^3$, $\det(D_2) > 0$ on $\mathbb{R}_+^* \times \mathbb{R}_+^* \times \{0\}$ and $\det(D_3) > 0$ on $\mathbb{R}_+^* \times \{0\} \times \{0\}$. By a symmetry argument, the assumptions of Remark 5.8 are verified, so that the conclusion of Proposition 5.7 holds, that is, **H3** is satisfied.

To conclude, assumption **(H)** allows to consider the semi-discrete approximation (5.16). More precisely, Theorem 5.2 gives the existence of a sequence of smooth solutions of the semi-discrete approximation, which furthermore satisfies (uniformly w. r. t. the time step) the estimates (5.20)–(5.22). By Remark 5.4 the sequence also satisfies (uniformly in the time step) some gradient estimates given by the entropy structure described in this subsection ($\nabla u_i^{s/2}$ in $\mathrm{L}^2_{t,x}$, $i = 1, 2, 3$). These estimates enable to get the strong compactness of the sequence in $\mathrm{L}^1_{t,x}$. After extraction of a converging subsequence, the limit gives a solution of (5.88)–(5.90).

5.6 Appendix

5.6.1 Examples of systems satisfying H3

In this section, we provide sufficient conditions on the functions $a_i : \mathbb{R}_+^I \to \mathbb{R}_+$, allowing to prove that

$$A : \mathbb{R}_+^I \longrightarrow \mathbb{R}_+^I$$
$$X := \begin{pmatrix} x_1 \\ \vdots \\ x_I \end{pmatrix} \longmapsto \begin{pmatrix} a_1(X)\, x_1 \\ \vdots \\ a_I(X)\, x_I \end{pmatrix}$$

is a homeomorphism from $\mathbb{R}_+^I$ to itself. More precisely, in our framework assumptions **H1** and **H2** are satisfied for the functions a_i (that is, continuity and positive lower bound) and we assume the existence of a convex entropy. This last property implies in particular that A is non-singular with $\det \mathrm{D}(A) > 0$. We investigate two cases where these assumptions allow to prove that A is a homeomorphism, that is, **H3** is satisfied.

Two species with increasing diffusions

We start here with the case when $I = 2$ (two species).

Proposition 5.6. *Assume that $a_1, a_2 : \mathbb{R}_+^2 \to \mathbb{R}_+$ are continuous functions, lower bounded by $\alpha > 0$. Assume that on $\mathbb{R}_+ \times \mathbb{R}_+$, A is strictly increasing (that is, each component is strictly increasing w.r.t. each of its variables) and that on $\mathbb{R}_+^* \times \mathbb{R}_+^*$, A is $\mathscr{C}^1$ and $\det \mathrm{D}(A)$ remains strictly positive. Then A is a homeomorphism from $\mathbb{R}_+^2$ to itself and a $\mathscr{C}^1$-diffeomorphism from $(\mathbb{R}_+^*)^2$ to itself.*

Proof. It suffices to prove that A is a bijection from $\mathbb{R}_+^2$ to itself. Then, the inverse function theorem ensures that A is a diffeomorphism on $(\mathbb{R}_+^*)^2$. Thanks to the positive lower bound for a_1 and a_2 and the continuity of A on $(\mathbb{R}_+)^2$, it is easy to check that A^{-1} is continuous on $(\mathbb{R}_+)^2$.

Let us fix $(f, g) \in \mathbb{R}_+^2$ and find $(u, v) \in \mathbb{R}_+^2$ such that $A(u, v) = (f, g)$, that is

$$\begin{pmatrix} A_1(u,v) \\ A_2(u,v) \end{pmatrix} = \begin{pmatrix} a_1(u,v)\, u \\ a_2(u,v)\, v \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}.$$

We first solve the first equation, considering u as the unknown : for any $v \geq 0$, the function $A_1(\cdot, v) : u \in \mathbb{R}_+ \mapsto a_1(u,v)\, u \in \mathbb{R}_+$ is strictly increasing (by assumption) and onto (due to the continuity and positivity of $a_1(\cdot, v)$). Therefore it is a bijection : we write $u = u_f(v)$ the only solution in $\mathbb{R}_+$ of $a_1(u,v)\, u = f$.

The monotonicity of A_1 (in u and v) implies that u_f is strictly decreasing on $\mathbb{R}_+$. This together with the continuity of A_1 on $\mathbb{R}_+^2$ implies that u_f belongs to the class $\mathscr{C}^0(\mathbb{R}_+)$: indeed, for any $v \geq 0$, if v_n is a decreasing (resp. increasing) sequence converging to v, then $u_f(v_n)$ is increasing (resp. decreasing) and upper (resp. lower) bounded by $u_f(v)$, therefore it converges to some limit l satisfying $A(l, v) = \lim A(u_f(v_n), v_n) = f$, that is, $l = u_f(v)$. Furthermore, we have on $(\mathbb{R}_+^*)^2$, $\det \mathrm{D}(A) = [\partial_u A_1][\partial_v A_2] - [\partial_1 A_2][\partial_2 A_1] > 0$. By the assumption of monotonicity of A, the four derivatives appearing here are nonnegative, hence $\partial_u A_1 > 0$. Therefore by the implicit function theorem, u_f belongs to the class $\mathscr{C}^1(\mathbb{R}_+^*)$, and for all $v > 0$, $u_f'(v) = -\{\partial_v A_1 / \partial_u A_1\}(u, u_f(v))$.

We then inject $u = u_f(v)$ in the second equation : we want to solve $a_2(u_f(v), v)v = g$. For $v > 0$, we compute the derivative

$$\begin{aligned} \partial_v \{A_2(u_f(v), v)\} &= [u_f'(v)\partial_u A_2 + \partial_v A_2](u_f(v), v) \\ &= \frac{1}{\partial_u A_1} \det \begin{pmatrix} \partial_u A_1 & \partial_v A_1 \\ \partial_u A_2 & \partial_v A_2 \end{pmatrix} (u_f(v), v) > 0. \end{aligned}$$

The function $v \in \mathbb{R}_+ \mapsto a_2(u_f(v), v)v \in \mathbb{R}_+$ is continuous, strictly increasing by the previous computation, and it is onto (by continuity and thanks to the lower bound for a_2). We write $v_{f,g}$ the only solution $v \geq 0$ of $a_2(u_f(v), v)\, v = g$. Then $(u, v) = (u_f(v_{f,g}), v_{f,g})$ is the only solution of $A(u, v) = (f, g)$. □

A nonsingular on the closed set $\mathbb{R}_+^I$

In the following, we prove the statement

Proposition 5.7. *Assume that the functions $a_i : \mathbb{R}_+^I \to \mathbb{R}_+$ are continuous and lower bounded by $\alpha > 0$. Assume that on $\mathbb{R}_+^I$, A is $\mathscr{C}^1$ and nonsingular with* $\det \mathrm{D}(A) > 0$. *Then A is a homeomorphism from $\mathbb{R}_+^I$ to itself and a $\mathscr{C}^1$ diffeomorphism from $(\mathbb{R}_+^*)^I$ to itself.*

Remark 5.8. *The restriction "A is $\mathscr{C}^1$ on the boundary" does not allow the use of every power $x_i^{\gamma_{ij}}$ in the cross dependencies (they typically need to be bigger than 1). However we can see in the proof (Step 3) that the assumption that A is $\mathscr{C}^1$ and nonsingular on the closed set $\mathbb{R}_+^I$ is not optimal : it could be replaced by the weaker assumption that the restriction of A on any half-(sub)space of the form $\prod_{i=1..I} \pi_i$, with $\pi_i = \{0\}$ or $\mathbb{R}_+^*$, is $\mathscr{C}^1$ and nonsingular.*

This stronger version of the proposition would include the case of small (less than 1) power $x_i^{\gamma_{ij}}$.

Proof. The proposition is essentially adapted from Hadamard global inverse mapping theorem and might be derived from [24]. We prove here the main points. For convenience we write $A_|$ the restriction/corestriction of A from $(\mathbb{R}_+^*)^I$ to itself, $A_| : (\mathbb{R}_+^*)^I \to (\mathbb{R}_+^*)^I, x \mapsto A(x)$. Note that indeed $A((\mathbb{R}_+^*)^I) \subset (\mathbb{R}_+^*)^I$ thanks to the positivity of the functions a_i, so that $A_|$ is well-defined.

Step 1. The functions A and $A_|$ are proper. We claim that :

Inverse images by A of compact set of $\mathbb{R}_+^I$ (resp. $(\mathbb{R}_+^*)^I$) are compact sets of $\mathbb{R}_+^I$ (resp. $(\mathbb{R}_+^*)^I$).

Let K be a compact set of $\mathbb{R}_+^I$, then it is included in $[m, M]^I$ where $m > 0$ if the compact is a subset of $(\mathbb{R}_+^*)^I$. Thanks to the positive lower bound α for the functions a_i,

$$A_i(x) \le M \Rightarrow x_i \le \alpha^{-1} M.$$

It follows, by continuity of the a_i, that

$$\|x\|_\infty \le \alpha^{-1} M \Rightarrow \max(a_i(x)) \le C(\alpha^{-1} M),$$

and finally

$$A(x) \in [m, M]^I \Rightarrow x \in [C(\alpha^{-1}M)^{-1} m, \alpha^{-1} M]^I = [m', M']^I.$$

We conclude using the continuity of A that $A^{-1}(K)$ is then a closed bounded set of $[m', M']^I$ (with $m' > 0$ for the case $(\mathbb{R}_+^*)^I$).

Step 2. The functions A and $A_|$ are surjective. We claim that

$$A(\mathbb{R}_+^I) = \mathbb{R}_+^I \text{ and } A((\mathbb{R}_+^*)^I) = (\mathbb{R}_+^*)^I.$$

We use the property that the image of an application which is proper and continuous is a closed set. Thanks to the previous step, this property applied to A and $A_|$ gives that $A((\mathbb{R}_+^*)^I)$ is a closed set of $(\mathbb{R}_+^*)^I$ (for the induced topology on $(\mathbb{R}_+^*)^I$) and $A(\mathbb{R}_+^I)$ is a closed set (of $\mathbb{R}_+^I$).

The assumption of nonsingularity of A implies by the implicit function theorem that $A((\mathbb{R}_+^*)^I)$ is also an open set of $(\mathbb{R}_+^*)^I$. By connectedness, we therefore have

$$A((\mathbb{R}_+^*)^I) = (\mathbb{R}_+^*)^I.$$

Then since $A(\mathbb{R}_+^I)$ is a closed set of $\mathbb{R}_+^I$ containing $(\mathbb{R}_+^*)^I = A((\mathbb{R}_+^*)^I)$, we get the conclusion

$$A(\mathbb{R}_+^I) = \mathbb{R}_+^I.$$

Step 3. The functions A and $A_|$ are one-to-one. Finally, knowing that $A_|$ is onto from $(\mathbb{R}_+^*)^I$ to itself we can use theorem B in [24] to conclude that $A_|$ is a bijection. To prove it is also the case for A on $\mathbb{R}_+^I$, we only need to prove the injectivity on the boundary.

We write $\partial\mathbb{R}_+^I = \cup_i \{x \in \mathbb{R}_+^I : x_i = 0\}$. Let us notice that thanks to the positivity of the functions a_i, it suffices to show the injectivity on each of the spaces $\{x \in \mathbb{R}_+^I : x_i = 0\}$. Without loss of generality, we consider the set $\{x \in \mathbb{R}_+^I : x_I = 0\}$ and we want to show that on this set $A = (A_1, \cdots, A_{I-1}, 0)$ is one-to-one. Therefore, the initial problem of size I reduces to the problem of size $I - 1$ which consists in showing that the function $\tilde{A} := (A_1, \cdots, A_{I-1})(\cdot, 0) : \mathbb{R}_+^{I-1} \to \mathbb{R}_+^{I-1}$ is one-to-one. The function $\tilde{A}$ is $\mathscr{C}^1$ and nonsingular since for all $\tilde{x} \in \mathbb{R}_+^{I-1}$,

$$0 < \det \mathrm{D}(A)(\tilde{x}, 0) = \det \begin{pmatrix} \mathrm{D}(\tilde{A})(\tilde{x}) & 0_{1,I-1} \\ * \cdots * & a_I(\tilde{x}, 0) \end{pmatrix} = a_I(\tilde{x}, 0) \det \mathrm{D}(\tilde{A})(\tilde{x}).$$

Therefore, it satisfies the assumptions of Proposition 5.7 with I replaced by $I-1$. We conclude by iteration on the integer I, noticing that in the case $I = 1$ we have $\partial\mathbb{R}_+^I = \{0\}$ and the injectivity on the unit set $\{0\}$ is obvious.

This ends the proof. □

5.6.2 Leray-Schauder fixed point Theorem

This fixed point Theorem may be stated in the following way (see for example Theorem 11.6 p.286 in [21]) :

Theorem 5.4. *[Leray-Schauder] Let $\mathfrak{B}$ be a Banach space and let Λ be a continuous and compact mapping of $[0,1] \times \mathfrak{B}$ into $\mathfrak{B}$ such that $\Lambda(0, x) = 0$ for all $x \in \mathfrak{B}$. Suppose that there exists a constant $L > 0$ such that for all $\sigma \in [0,1]$,*

$$\Lambda(\sigma, x) = x \implies \|x\|_{\mathfrak{B}} < L.$$

Then the mapping $\Lambda(1, \cdot)$ of $\mathfrak{B}$ into itself has at least one fixed point.

5.6.3 Elliptic estimates

We start by recalling the following standard elliptic estimate (see for instance Theorem 2.3.3.6 in [25])

Lemma 5.5. *For any $p \in (1, \infty)$ and any regular open set Ω, there exists positive constants $M_{p,\Omega}$ and $C_{p,\Omega}$ such that for all $M > M_{p,\Omega}$,*

$$\left.\begin{array}{l} Mw - \Delta w = f \in \mathrm{L}^p(\Omega), \\ w \in \mathrm{W}_\nu^{2,1}(\Omega). \end{array}\right\} \Longrightarrow \|w\|_{\mathrm{W}^{2,p}(\Omega)} \le C_{p,\Omega} \|f\|_p \,.$$

Using this result we get the following useful Lemma :

Lemma 5.6. *Let $f \in \mathrm{L}^\infty(\Omega)$, and let w satisfy*

$$w \in \mathrm{H}_\nu^2(\Omega), \; w \ge 0, \quad -\Delta w \le f \; \text{ in } \Omega.$$

Then there exists $C := C(\Omega)$ such that

$$\|w\|_\infty \le C \left(\|f\|_\infty + \|w\|_1 \right). \tag{5.96}$$

Proof. First, we fix $p \in (d/2, \infty)$ and $M > M_{p,\Omega}$ (see Lemma 5.5) and rewrite the equation as $Mw - \Delta w \le f + Mw$. Using $w \ge 0$, the comparison principle, the elliptic estimate of Lemma 5.5 and the Sobolev embedding $\mathrm{W}^{2,p}(\Omega) \hookrightarrow \mathrm{L}^\infty(\Omega)$, we get

$$\begin{aligned} \|w\|_\infty &\le C \left(\|f + Mw\|_p \right) \le C \left(\|f\|_p + M\|w\|_p \right) \\ &\le C \left(\|f\|_p + M \|w\|_\infty^{(p-1)/p} \|w\|_1^{1/p} \right) \\ &\le C \left(\|f\|_p + \varepsilon \|w\|_\infty + c(\varepsilon) \|w\|_1 \right) \; \text{(Young's inequality)}, \end{aligned}$$

and we conclude by choosing ε small enough. □

Remark 5.9. Obviously, the conclusion of Lemma 5.6 would be the same when one only assumes that $f \in \mathrm{L}^p(\Omega)$, for some $p > d/2$.

5.6.4 An Aubin-Lions Lemma for degenerate estimates

Here $\alpha < \beta$ are two real numbers and $\Omega \subset \mathbb{R}^d$ a smooth and bounded open set. We consider a function $\Theta \in \mathscr{C}^1(\mathbb{R},\mathbb{R})$ such that $\{z \in \mathbb{R} : \Theta'(z) = 0\}$ is finite, with $|\Theta'|$ lower bounded by a positive value near $\pm\infty$. The following result deals with the strong compactness of a sequence of functions $(t,x) \mapsto a_n(t,x)$ defined on $[\alpha,\beta] \times \Omega$ and satisfying some nonlinear estimate described by the function Θ. For the proof we refer to Theorem 1. of [39].

Lemma 5.7. *Consider a sequence of* $\mathrm{W}^{1,1}_{\mathrm{loc}}(]\alpha,\beta[\times\Omega)$ *functions* $(a_n)_n$ *such that both sequences* $(a_n)_n$ *and* $(\nabla_x\Theta(a_n))_n$ *are bounded in* $\mathrm{L}^2(]\alpha,\beta[\times\Omega)$*. If furthermore there exists* $\mathrm{C} > 0$ *such that for all test functions* $\varphi \in \mathscr{C}^0([\alpha,\beta];\mathscr{D}(\Omega))$

$$|\langle \partial_t a_n, \varphi\rangle| \leq \mathrm{C}\, \|\varphi\|_{\mathrm{L}^\infty(]\alpha,\beta[;\mathrm{H}^m(\Omega))}, \tag{5.97}$$

then $(a_n)_n$ *is relatively compact in* $\mathrm{L}^2(]\alpha,\beta[\times\Omega)$*.*

Corollary 5.3. *In estimate* (5.97) *of the previous Lemma, if one replaces the space of test functions by the smaller one* $\mathscr{D}(]\alpha,\beta[\times\Omega)$*, we then have* $(a_n)_n$ *is relatively compact in* $\mathrm{L}^2_{\mathrm{loc}}(]\alpha,\beta[\times\Omega)$*.*

Proof of the Corollary. A straightfoward density argument shows that estimate (5.97) holds for tests functions in $\mathscr{C}^0([\alpha+1/k,\beta-1/k];\mathscr{D}(\Omega))$ for all $k \geq 1$, so that the result follows by a diagonal extraction along the spaces $\mathrm{L}^2(]\alpha+1/k,\beta-1/k[\times\Omega)$, for which we have compactness thanks to Lemma 5.7. $\square$

Chapitre 6

Self- and cross-diffusion in the triangular cross-diffusion system

Abstract

This Chapter is taken from the paper [48]. We present new results of existence of global solutions for a class of reaction cross-diffusion systems of two equations presenting a cross-diffusion term in the first equation, and possibly presenting a self-diffusion term in any (or both) of the two equations. This class of systems arises in Population dynamics, and notably includes the triangular SKT system. In particular, we recover and extend existing results for the triangular SKT system. Our proof relies on entropy and duality methods.

Sommaire

6.1 Introduction

The purpose of this paper is to investigate existence and some properties of the solutions of the system

$$\partial_t u - \Delta_x[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u] = u\,(r_u - r_a\, u^a - r_b\, v^b) \qquad \text{in } \mathbb{R}_+ \times \Omega, \tag{6.1}$$

$$\partial_t v - \Delta_x[(d_v + d_\gamma v^\gamma)\, v] = v\,(r_v - r_c\, v^c - r_d\, u^d) \qquad \text{in } \mathbb{R}_+ \times \Omega, \tag{6.2}$$

$$\nabla_x u \cdot n = \nabla_x v \cdot n = 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega, \tag{6.3}$$

$$u(0,\cdot) = u_{in}, \qquad v(0,\cdot) = v_{in} \qquad \text{in } \Omega, \tag{6.4}$$

where $u = u(t,x) \geq 0$, $v = v(t,x) \geq 0$ are the unknowns, the variables (t,x) browse $\mathbb{R}_+ \times \Omega$ with Ω a bounded domain of $\mathbb{R}^m$ $(m \geq 1)$, $n = n(x)$ stands for the outward normal at point x of the boundary $\partial\Omega$, u_{in} and v_{in} are nonnegative initial data, and the remaining terms are nonnegative constant parameters satisfying

$$\begin{gathered} \mathrm{D} := \{d_u, d_v, d_\alpha, d_\beta, d_\gamma, r_u, r_v, r_a, r_b, r_c, r_d, a, b, c, d, \alpha, \beta, \gamma\} \in (\mathbb{R}_+^*)^{15} \times \mathbb{R}_+ \times \mathbb{R}_+^* \times \mathbb{R}_+, \\ (\alpha > 0,\ d < 2 + \alpha,\ a < 1 + \alpha) \text{ or } (\alpha = 0,\ d \leq 2,\ a \leq 1). \end{gathered} \tag{6.5}$$

The origin of this system is to be found in a well-studied system arising in Population Dynamics, known in the literature as the SKT system. The SKT system was introduced in [45] to model spatial segregation in two competing species of (let us say) animals (see also [41]). It has since then attracted the interest of many mathematicians, leading to a rich literature on the question of the existence of solutions (see for example [8] and references therein) and on the analysis of equilibria and stability (patterns are shown to appear; see for example [27]). Writing u and v the respective densities of the two different species, it takes the following form

$$\begin{aligned} \partial_t u - \Delta_x[(d_u + d_\alpha u + d_\beta v)\, u] &= u\,(r_u - r_a\, u - r_b\, v) \qquad \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t v - \Delta_x[(d_v + d_\gamma v + d_\delta u)\, v] &= v\,(r_v - r_c\, v - r_d\, u) \qquad \text{in } \mathbb{R}_+ \times \Omega, \\ \nabla_x u \cdot n = \nabla_x v \cdot n &= 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega. \end{aligned} \tag{6.6}$$

When $d_u = d_v = d_\alpha = d_\beta = d_\gamma = d_\delta = 0$, the system (6.6) reduces to the standard Lotka-Volterra competition ODS. The terms r_u, r_v are the intrinsic growth of the species, while r_b and r_d measure the demographic effect of the interspecific competition, and r_a, r_c indicate the demographic effect of the intraspecific competition. When non-zero, the terms $\Delta_x[(d_u + d_\alpha u + d_\beta v)\, u]$ and $\Delta_x[(d_v + d_\gamma v + d_\delta u)\, v]$ model the spatial movements of the individuals in the domain Ω. The positive constants d_u, d_v are standard diffusion rates, which indicate the frequency of the random walk of the individuals inside each species. The nonnegative constants d_β and d_δ are usually referred to as "cross-diffusion" coefficients, and ecologically measure the repulsive effect, on the individuals of one species, of the presence of the individuals of the other species (as a result of the interspecific competitive pressure). The nonnegative constants d_α and d_γ, referred to as "self-diffusion" coefficients, measure the repulsive effect on the individuals of the presence of the individuals of the same species (as a result of the intraspecific competitive pressure).

The system (6.6) is often called "triangular" when $d_\delta = 0$. From the point of view of modeling, this means that only the individuals of the first species tend to avoid the individuals of the other species. It therefore takes the form

$$\begin{aligned} \partial_t u - \Delta_x[(d_u + d_\alpha u + d_\beta v)\, u] &= u\,(r_u - r_a\, u - r_b\, v) \qquad \text{in } \mathbb{R}_+ \times \Omega, \\ \partial_t v - \Delta_x[(d_v + d_\gamma v)\, v] &= v\,(r_v - r_c\, v - r_d\, u) \qquad \text{in } \mathbb{R}_+ \times \Omega, \\ \nabla_x u \cdot n = \nabla_x v \cdot n &= 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega. \end{aligned} \tag{6.7}$$

In this case, the second equation is coupled to the first one only through zeroth-order terms (reaction), while in the full system (6.6) with $d_\delta > 0$ both equations are coupled to the other one through both zeroth-order (reaction) and second-order terms (cross-diffusion). The full system (6.6) has a completely different structure from the triangular case (in particular it is possible to exhibit an entropy structure when $d_\delta > 0$, see [8] and [16], but this entropy structure degenerates when $d_\delta = 0$).

In our study, we consider the class of systems (6.1)–(6.3). That is, we focus on a triangular type of cross-diffusion ($d_\delta = 0$) as in the system (6.7), but in contrast to the system (6.7) where the diffusion rates ($d_u + d_\alpha u + d_\beta v$, $d_v + d_\gamma v + d_\delta u$) and the growth rates ($r_u - r_a\, u - r_b\, v$, $r_v - r_c\, v - r_d\, u$) are required to be linear functions of u and v, in (6.1)–(6.3) we allow these functions to be more general power laws (with suitably chosen powers, (6.5)). Note that the class of systems we consider includes (6.7) (when $\alpha = \beta = \gamma = a = b = c = d = 1$).

We now present our main mathematical result for this class of systems.

6.1.1 Main Theorem

We clarify the notion of weak solution we will use in the

Definition 6.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^m$ ($m \in \mathbb{N}^*$) and let $\mathrm{D} \in (\mathbb{R}_+^*)^{15} \times \mathbb{R}_+ \times \mathbb{R}_+^* \times \mathbb{R}_+$. Let $u_{in} := u_{in}(x) \geq 0$ and $v_{in} := v_{in}(x) \geq 0$ be two functions lying in $L^1(\Omega)$.*

A couple of functions (u, v) such that $u := u(t, x) \geq 0$ and $v := v(t, x) \geq 0$, and lying in $L^{\max(1+a,d)}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ is a (global) **weak solution** *of* (6.1)-(6.4) *if*

$$\nabla_x \left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u \right],\ \nabla_x \left[(d_v + d_\gamma v^\gamma)\, v \right] \ \in\ L^1_{loc}(\mathbb{R}_+ \times \overline{\Omega})$$

and, for all test functions ψ_1, $\psi_2 \in C^1_c(\mathbb{R}_+ \times \overline{\Omega})$, we have the identities

$$\begin{aligned} -\int_0^\infty \int_\Omega (\partial_t \psi_1)\, u - \int_\Omega \psi_1(0, \cdot)\, u_{in} + \int_0^\infty \int_\Omega \nabla_x \psi_1 \cdot \nabla_x \left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u \right] \\ = \int_0^\infty \int_\Omega \psi_1\, u\, (r_u - r_a\, u^a - r_b\, v^b), \end{aligned} \tag{6.8}$$

$$\begin{aligned} -\int_0^\infty \int_\Omega (\partial_t \psi_2)\, v - \int_\Omega \psi_2(0, \cdot)\, v_{in} + \int_0^\infty \int_\Omega \nabla_x \psi_2 \cdot \nabla_x \left[(d_v + d_\gamma v^\gamma)\, v \right] \\ = \int_0^\infty \int_\Omega \psi_2\, v\, (r_v - r_c\, v^c - r_d\, u^d). \end{aligned}$$

Note that the assumptions on u_{in}, v_{in}, u, v, ψ_1, ψ_2 ensure that all integrals in the two identities above are finite.

Our main result is contained in the

Theorem 6.1. *Let Ω be a smooth bounded domain of $\mathbb{R}^m$ ($m \in \mathbb{N}^*$). Let the coefficients of system (6.1) – (6.2) satisfy condition* (6.5)*. Consider initial data $u_{in} \geq 0$, $v_{in} \geq 0$ such that $u_{in} \in \mathrm{L}^2(\Omega)$, $v_{in} \in \mathrm{L}^\infty(\Omega)$.*

Then,
i) *there exists $u = u(t, x) \geq 0$, $v = v(t, x) \geq 0$ such that $(u, v) \in L^{2+\alpha}_{loc}(\mathbb{R}_+ \times \overline{\Omega}) \times L^\infty_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ and (u, v) is a (global) weak solution of system (6.1) – (6.4) in the sense of Definition 6.1.*

Furthermore, this solution (u, v) satisfies for all $T > 0$

$$\sup_{[0,T]\times\Omega} v \leq \max \left\{ \sup_\Omega v_{in}, \left(\frac{r_v}{r_c} \right)^{1/c} \right\}, \tag{6.9}$$

$$\int_0^T \int_\Omega u^{2+\alpha} \leq C(\Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.10}$$

$$\int_0^T \int_\Omega \left| \nabla_x [v^{p/2}] \right|^2 \leq C(p, \Omega, T, u_{in}, v_{in}, \mathrm{D}) \qquad (\textit{for all } 0 < p < \infty), \tag{6.11}$$

$$\int_\Omega u(T) + \int_0^T \int_\Omega \left| \nabla_x [(1 + u)^{\alpha/2}] \right|^2 \leq C(\Omega, T, u_{in}, v_{in}, \mathrm{D}) \qquad (\textit{if } \alpha > 0), \tag{6.12}$$

$$\int_\Omega u(T) + \int_0^T \int_\Omega |\nabla_x [\log(1 + u)]|^2 \leq C(\Omega, T, u_{in}, v_{in}, \mathrm{D}) \qquad (\textit{if } \alpha = 0), \tag{6.13}$$

where the constant $C(\Omega, T, u_{in}, v_{in}, \mathrm{D})$ only depends on the domain Ω (and the dimension m), the time T, the norms of the initial data $\|u_{in}\|_{\mathrm{L}^2(\Omega)}$ and $\|v_{in}\|_{\mathrm{L}^\infty(\Omega)}$ and the choice of parameters D*, and the constant $C(p, \Omega, T, u_{in}, v_{in}, \mathrm{D})$ only depends on the same quantities and the parameter p.*

If u_{in} furthermore satisfies $u_{in}(x) > 0$ a.e. on Ω and $\log u_{in} \in \mathrm{L}^1(\Omega)$, resp., if v_{in} furthermore satisfies $v_{in}(x) > 0$ a.e. on Ω and $\log v_{in} \in \mathrm{L}^1(\Omega)$, then for all $T > 0$

$$\int_\Omega |\log u|(T) + d_u \int_0^T \int_\Omega |\nabla_x[\log u]|^2 \leq \int_\Omega |\log u_{in}| + C(\Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.14}$$

$$\textit{resp.,} \qquad \int_\Omega |\log v|(T) + d_v \int_0^T \int_\Omega |\nabla_x[\log v]|^2 \leq \int_\Omega |\log v_{in}| + C(\Omega, T, u_{in}, v_{in}, \mathrm{D}). \tag{6.15}$$

ii) *If $\alpha = 0$, we have the additional estimate, for some $\nu = \nu(\Omega, v_{in}, \mathrm{D}) > 0$ depending only on the domain Ω (and m), the norm $\|v_{in}\|_{\mathrm{L}^\infty(\Omega)}$ and the parameters D, for all $T > 0$, and for some $C_1(\Omega, T, u_{in}, v_{in}, \mathrm{D}) > 0$ depending only on the domain Ω (and m), the time T, the norms $\|u_{in}\|_{\mathrm{L}^2(\Omega)}$, and $\|v_{in}\|_{\mathrm{L}^\infty(\Omega)}$ and the parameters D,*

$$\int_0^T \int_\Omega u^{2+\nu} \leq C_1(\Omega, T, u_{in}, v_{in}, \mathrm{D}). \tag{6.16}$$

iii) *If $\gamma = 0$, assuming furthermore that $v_{in} \in \mathrm{W}^{2,q}(\Omega)$ for some $q > 1$ satisfying*

$$1 < q \leq (2+\alpha)/d \quad \textit{if } \alpha > 0, \qquad 1 < q \leq (2+\nu)/d \quad \textit{if } \alpha = 0,$$

(and assuming furthermore the compatibility condition $\nabla_x v_{in} \cdot n = 0$ on $\partial\Omega$ if $q \geq 3$), we have the additional estimate, for all $T > 0$,

$$\int_0^T \int_\Omega |\partial_t v|^q + \int_0^T \int_\Omega |\nabla_x^2 v|^q + \int_0^T \int_\Omega |\nabla_x v|^{2q} \leq C_2(q, \Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.17}$$

where the constant $C_2(q, \Omega, T, u_{in}, v_{in}, \mathrm{D})$ only depends on the parameter q, the domain Ω (and the dimension m), the time T, the norms of the initial data $\|u_{in}\|_{\mathrm{L}^2(\Omega)}$ and $\|v_{in}\|_{\mathrm{L}^\infty \cap \mathrm{W}^{2,q}(\Omega)}$ and the parameters D.

We list in the remark below some possible extensions of the results mentioned in Theorem 6.1.

Remark 6.1. *Thanks to the bound (6.9) given by a maximum principle for equation (6.2), the power laws "$v \mapsto v^\beta$" and "$v \mapsto v^b$" in (6.1) can be replaced by any continuous function of v on $\mathbb{R}_+$ which is smooth ($C^1(\mathbb{R}_+^*)$) and positive-valued on $\mathbb{R}_+^*$. The power law "$v \mapsto v^\gamma$" in (6.2) can be replaced by any continuous function on $\mathbb{R}_+$ which is non-decreasing, smooth, and positive-valued on $\mathbb{R}_+^*$. Following the same idea, but furthermore ensuring that the maximum principle remains valid for (6.2), the power law "$v \mapsto v^c$" can be replaced by any continuous function on $\mathbb{R}_+$ which is smooth, positive-valued on $\mathbb{R}_+^*$ and which furthermore tends to $+\infty$ in $+\infty$. With these replacements, all results of Theorem 6.1 hold, with the bound (6.9) adapted when necessary, and with the condition $\gamma = 0$ in iii) replaced by the condition that the function replacing "$v \mapsto v^\gamma$" is constant.*
The power laws "$u \mapsto u^a$" and "$u \mapsto u^d$" can be replaced by any continuous function of u on $\mathbb{R}_+$, smooth and positive-valued on $\mathbb{R}_+^*$, and dominated by (or having the same behaviour as) "$u \mapsto u^a$", resp. "$u \mapsto u^d$" in $+\infty$. The power law "$u \mapsto u^\alpha$" can be replaced by any non-decreasing continuous function of u on $\mathbb{R}_+$ which is smooth and positive-valued on $\mathbb{R}_+^*$ and have the same behaviour as "$u \mapsto u^\alpha$" in $+\infty$. With these replacements, all results of Theorem 6.1 hold.

Assume $\alpha = 0$. In this case, an estimate of type (6.10) ensures enough integrability (to get compactness) for the terms $r_a u^{1+a}$ in (6.1) and $r_d v u^d$ in (6.2) only when $a < 1$ and $d < 2$. The slightly better estimate (6.16) is therefore crucial to estimate these terms in the two cases ($a = 1$, $d \leq 2$) and ($a < 1$, $d = 2$). It even treats these terms when $a < 1 + \nu$ and $d < 2 + \nu$. As a consequence, we expect the results of Theorem 6.1 to hold when the condition ($\alpha = 0$, $a \leq 1$, $d \leq 2$) is replaced by the wider condition ($\alpha = 0$, $a < 1+\nu$, $d < 2+\nu$). Note that ν can indeed be chosen independent of a and d (see Section 6.5.1).

Assume $\alpha \geq 0$ and $1 + a$, $d < 2 + \alpha$. As seen in Sections 6.2–6.4, in this case the proof of existence entirely relies on estimates of the type (6.9)–(6.13) (in particular we do not use estimate (6.16)). As shown in the sequel, the proof of estimates of the type (6.9)–(6.13) only requires u_{in} to be in $\mathrm{L}^1 \cap \mathrm{H}_m^{-1}(\Omega)$, where the space $\mathrm{H}_m^{-1}(\Omega)$ is defined in Section 6.1.3. Therefore in the case $\alpha \geq 0$ and $1 + a$, $d < 2 + \alpha$, the results i) and iii) for any $1 < q \leq (2+\alpha)/d$ hold with the assumption $u_{in} \in \mathrm{L}^2(\Omega)$ replaced by the weaker assumption $u_{in} \in \mathrm{L}^1 \cap \mathrm{H}_m^{-1}(\Omega)$ (and with the constants C and C_2 depending on $\|u_{in}\|_{\mathrm{L}^1 \cap \mathrm{H}_m^{-1}(\Omega)}$

instead of $\|u_{in}\|_{\mathrm{L}^2(\Omega)}$*).*

Assume $\alpha = 0$*. In ii), estimate* (6.16) *is a consequence of a Lemma relying on duality techniques (namely, Lemma 6.5), which is adapted from a similar result from [7]. This Lemma can be somewhat improved. Indeed, following Remark 2.3 in [7], the constraint* $u_{in} \in \mathrm{L}^2(\Omega)$ *can be replaced by the weaker constraint* $u_{in} \in \mathrm{L}^{2-\nu_1}(\Omega)$ *where* ν_1 *is a small positive constant. Therefore, all results of Theorem 6.1 hold when* u_{in} *only belongs to the space* $\mathrm{L}^{2-\nu_1}(\Omega)$ *(where* ν_1 *only depends on* Ω*,* m*,* $\|v_{in}\|_{\mathrm{L}^\infty(\Omega)}$ *and* D*), with the constants* C_1 *and* C_2 *depending on* $\|u_{in}\|_{\mathrm{L}^{2-\nu_1}(\Omega)}$ *instead of* $\|u_{in}\|_{\mathrm{L}^{2-\nu_1}(\Omega)}$*.*

Assume $\gamma = 0$*. Estimate* (6.17) *being a direct consequence of the properties of the heat kernel (see Section 6.5.2), we can replace the set* $\mathrm{W}^{2,q}(\Omega)$ *in iii) by the optimal set to apply the properties of the heat kernel, that is, the fractional Sobolev space* $\mathrm{W}^{2-2/q,q}(\Omega)$*. Furthermore, the compatibility condition required for the case* $q = 3$ *is actually slightly weaker than "*$\nabla_x v_{in} \cdot n = 0$ *on* $\partial\Omega$*" (see for example [33]).*

6.1.2 In the literature

In the last decades, mathematicians dedicated a considerable effort to the question of the existence of solutions for systems of the form (6.1)–(6.3), and particularly for the original system (6.7).

The local (in time) existence of classical solutions was established by Amann in 1990 in the two papers [2], [3]. His theorem also provides a criterium to show that these solutions are global : it suffices to prove that the solutions do not blow up in finite time in suitable Sobolev spaces.

The global existence for the original system (6.7) has been investigated under various restrictive assumptions. Most results rely on Amann's theory, therefore the problem is to prove bounds in appropriate Sobolev spaces. One of the main difficulties lies in the use of Sobolev embedding theorems in the parabolic estimates, which provide satisfactory results only in low dimension. Therefore, many existing results require strong restrictions on the dimension and/or on the parameters of the system (typically, one assumes that the cross-diffusion is weak, in the sense that the cross-diffusion term d_β is small compared to some other parameters), see [10], [11], [35], [37], [38], [46], [49], [50], [53]. See [17] for a more detailed bibliography.

So far, three groups managed to remove this type of assumptions on the dimension and/or parameters, in particular cases : Choi, Lui and Yamada in [11] (in the presence of self-diffusion in the first equation and in the absence of self-diffusion in the second equation, i.e. $d_\alpha > 0$ and $d_\gamma = 0$) and, very recently, Desvillettes and Trescases in [17] (in the absence of self-diffusion in both equations, i.e. $d_\alpha = d_\gamma = 0$), and Hoang, Nguyen and Phan in [26] (in the presence of self-diffusion in the first equation, i.e. $d_\alpha > 0$). For the original system (6.7), our result is the first to treat the case ($d_\alpha = 0, d_\gamma > 0$). Furthermore, it provides a unifying proof for the cases with and without self-diffusion (in one or both equations).

We now mention some results of existence of global solutions for systems of form (6.1)–(6.3). Wang obtained it in [52] in the presence of self-diffusion in the first equation ($d_\alpha > 0$) and in the absence of self diffusion in the second equation ($d_\gamma = 0$), under a condition (depending on the dimension) of smallness of the parameter d w.r.t. the parameter a. The case without self-diffusion ($d_\alpha = d_\gamma = 0$) was solved by Pozio and Tesei in [44] under some strong assumption on the reaction coefficients, and by Yamada in [54] under the assumption $a > d$. We also mention the work of Murakawa [40] in which the reaction terms considered are Lipschitz continuous functions of u, v (and no self-diffusion appears). The results in the case without self-diffusion were extended by Desvillettes and Trescases in [17]. More precisely, in [17], the authors obtain global weak solutions for systems of the form (6.1)–(6.3) in the absence of self-diffusion ($d_\alpha = d_\gamma = 0$) with the following constraint on the parameters : ($\beta \geq 1$, $a \leq 1$, $d \leq 2$) or ($\beta \geq 1$, $a < d$). (Note that this indeed includes the original system (6.7) when $d_\alpha = d_\gamma = 0$.) The main ingredients of the proof are entropy and duality methods.

In the continuation of [17], the present paper deals with weak forms of solutions and exploits entropy and duality methods. These methods give rise to L^p estimates for the solution which are quite explicit. Furthermore, considering weak forms of solutions allows us to consider initial data of low regularity (in comparison with most of previous works which rely on Amann's theory). In comparison with [17], our Theorem includes the cases with self-diffusion terms ($d_\alpha > 0$ and/or $d_\gamma > 0$). Another improvement is the possibility, for the first time, to consider cross-diffusion terms v^β which are quite singular functions of v in zero, since we remove the assumption $\beta \geq 1$ and replace it by the assumption $\beta > 0$.

Finally, we refer to [16] for systems of the form (6.1)–(6.3) presenting in addition a cross-diffusion term in the second equation (non-triangular case).

6.1.3 Notations

When $T > 0$ is fixed, we write $\mathrm{L}^p = \mathrm{L}^p(]0,T[\times\Omega)$ for any $p \in [1,\infty]$. For $p \in [1,\infty[$, we denote by $\mathrm{L}^{p+} = \mathrm{L}^{p+}(]0,T[\times\Omega)$ the union of all spaces $\mathrm{L}^q(]0,T[\times\Omega)$ for $q > p$. We write $\mathrm{H}^1_m(\Omega)$ the space of functions of $\mathrm{H}^1(\Omega)$ with zero-mean value on Ω, and we write $\mathrm{H}^{-1}_m(\Omega)$ its dual space.

We recall that D is the set of parameters, defined in (6.5). In the sequel, $C(...)$ always denotes a positive constant, which only depends on its explicitly written arguments and may change from line to line. For example, $C(\Omega, \mathrm{D})$ is a positive constant that only depends on Ω and D. Furthermore, when it depends on D, the constant $C(..., \mathrm{D})$ can be chosen continuous in D on the set $\{\mathrm{D} \in (\mathbb{R}^*_+)^{15} \times \mathbb{R}_+ \times \mathbb{R}^*_+ \times \mathbb{R}_+ : a \leq 1+\alpha,\, d \leq 2+\alpha\}$.

6.1.4 Plan of the paper

We will first prove our result of existence under the following condition, which is slightly more restrictive than (6.5),

$$\alpha \geq 0,\ d < 2+\alpha,\ a < 1+\alpha. \tag{6.18}$$

More precisely, we will assume condition (6.18) in Section 6.4.

In Section 6.2, we perform formal computations to establish *a priori* estimates on the solutions of system (6.1)–(6.4). In Section 6.3, we define a semi-discrete (in time) scheme designed to be a smooth approximation of system (6.1)–(6.4), and we prove (rigorously) estimates on the solution of this scheme that are independent of the time step. We use these estimates in Section 6.4 to pass to the limit in the approximating scheme under condition (6.18). This proves the existence of solution and the estimates required in i) when condition (6.18) is satisfied. Finally, we come to the end of the proof of Theorem 6.1 in Section 6.5.

6.2 *A priori* estimates

This section only contains formal computations. They will not be used in the proof of Theorem 6.1, but we believe that these computations are useful to clarify the main tools at the origin of our result of existence. Similar computations will be performed rigorously in Section 6.3 at the level of an approximating scheme.

Therefore, suppose that (u, v) is a classical solution of system (6.1)–(6.4) for some smooth positive-valued initial data $u_{in} = u_{in}(x) > 0$ and $v_{in} = v_{in}(x) > 0$, and such that u and v are positive-valued and sufficiently smooth to perform all following computations (for example, in $C^2_c(\mathbb{R}_+ \times \overline{\Omega})$). Fix $T > 0$. Assume condition (6.5). In the following Sections 6.2.1–6.2.3, we compute estimates for the solution (u, v) on $[0,T] \times \Omega$.

6.2.1 Basic estimates

Maximum principle for v

A direct application of the maximum principle to equation (6.2) gives

$$\boxed{\sup_{[0,T]} v(t) \leq \max\{\sup_\Omega v_{in}, \left(\tfrac{r_v}{r_c}\right)^{1/c}\}.} \tag{6.19}$$

Mass conservation for u

We integrate the equation for u on $[0,T] \times \Omega$:

$$\int_\Omega u(T) = \int_\Omega u_{in} + \int_0^T \int_\Omega u\,(r_u - r_a\, u^a - r_b\, v^b).$$

Since (for all $u \geq 0$) $r_u u \leq C(a, r_u, r_a) + \frac{r_a}{2} u^{1+a}$, we have

$$\boxed{\textstyle\int_\Omega u(T) + \frac{r_a}{2} \int_0^T \int_\Omega u^{1+a} \leq \int_\Omega u_{in} + |\Omega|\, T\, C(a, r_u, r_a).} \tag{6.20}$$

6.2.2 Duality estimate

We now present an *a priori* estimate obtained thanks to a recent lemma relying on duality methods. This type of lemma was introduced in [43] and has since then showed to be very useful in the context of cross-diffusion (see [4], [5], [14], [15]). We cite here a version coming from [16].

Lemma 6.1. *Let $r_u > 0$. Let $M : [0,T] \times \Omega \to \mathbb{R}_+$ be a positive continuous function lower bounded by a positive constant. Smooth nonnegative solutions of the differential inequality*

$$\partial_t u - \Delta(Mu) \leq r_u u \text{ on } \Omega,$$
$$\partial_n(Mu) = 0, \text{ on } \partial\Omega,$$

satisfy the bound

$$\int_0^T \int_\Omega M u^2 \leq \exp(2r_u T) \times \left(C_\Omega^2 \, \|u_{in}\|^2_{\mathrm{H}_m^{-1}(\Omega)} + \langle u_{in} \rangle^2 \int_{\Omega_T} M \right),$$

where $\langle u_{in} \rangle$ denote the mean value of $x \mapsto u(0,x)$ on Ω and C_Ω is the Poincaré-Wirtinger constant.

We check that $M := d_u + d_\alpha u^\alpha + d_\beta v^\beta$ is lower bounded by $d_u > 0$. We therefore can apply the lemma to equation (6.1) to get

$$\int_0^T \int_\Omega [d_u + d_\alpha u^\alpha + d_\beta v^\beta] u^2 \leq C(\Omega, T, u_{in}, r_u) \times \left(1 + \int_0^T \int_\Omega [d_u + d_\alpha u^\alpha + d_\beta v^\beta] \right).$$

In particular, since all terms in the LHS are nonnegative,

$$\begin{aligned} \int_0^T \int_\Omega d_\alpha u^{\alpha+2} \quad &\leq C(\Omega, T, u_{in}, r_u) \times \left(1 + \textstyle\int_0^T \int_\Omega [d_u + d_\alpha u^\alpha + d_\beta v^\beta] \right) \\ &\leq C(\Omega, T, u_{in}, v_{in}, \mathrm{D}) \times \left(1 + \textstyle\int_0^T \int_\Omega [1 + d_\alpha u^\alpha] \right), \end{aligned}$$

where we used the L^∞ bound (6.19) in the last line. As a consequence, using furthermore the inequality (for $\epsilon > 0$ small enough, and for all $z \geq 0$) $z^\alpha \leq C_\epsilon + \epsilon z^{2+\alpha}$, we have

$$\boxed{\textstyle\int_0^T \int_\Omega u^{2+\alpha} \leq C(\Omega, T, u_{in}, v_{in}, \mathrm{D}).} \tag{6.21}$$

6.2.3 Entropy estimates

We now present two new estimates which are crucial to obtain weak compactness on the solutions (as they yield a bound for the gradients of the solutions). These estimates are obtained thanks to the introduction of two functionals whose evolution along the flow of the solutions can be controlled. When decreasing, such functionals are called Lyapunov functionals and sometimes "entropies". By a small abuse, we will refer to the resulting estimates as "entropy estimates".

Entropy estimate for v

For any $p \neq 1$, define

$$E_v(t) := \int_\Omega \frac{v^p}{p}(t).$$

We compute the derivative

$$\mathrm{d}_t E_v(t) = \int_\Omega \partial_t v \, v^{p-1}(t)$$
$$= \int_\Omega v^p (r_v - r_c \, v^c - r_d \, u^d) + \int_\Omega v^{p-1} \Delta_x [(d_v + d_\gamma v^\gamma) \, v],$$

where the last term writes

$$\begin{aligned} \int_\Omega v^{p-1} \Delta_x [(d_v + d_\gamma v^\gamma) \, v] &= - \int_\Omega \nabla_x [v^{p-1}] \cdot \nabla_x [(d_v + d_\gamma v^\gamma) \, v] \\ &= -4 \frac{p-1}{p^2} \int_\Omega |\nabla_x v^{p/2}|^2 \, [(d_v + d_\gamma (\gamma + 1) \, v^\gamma)]. \end{aligned}$$

We integrate on $t \in [0, T]$:

$$\int_\Omega \frac{v^p}{p}(T) \; + \; 4\frac{p-1}{p^2}\int_0^T \int_\Omega \left|\nabla_x[v^{p/2}]\right|^2 [(d_v + d_\gamma(\gamma+1)\, v^\gamma)]$$
$$= \int_\Omega \frac{v^p}{p}(0) \; + \; \int_0^T \int_\Omega v^p(r_v - r_c\, v^c - r_d\, u^d).$$

Now taking $0 < p < 1$, we get

$$\int_0^T \int_\Omega \left|\nabla_x[v^{p/2}]\right|^2 \leq C(p, \mathrm{D}) \left(\int_\Omega v^p(T) \; + \int_0^T \int_\Omega v^p(v^c + u^d) \right)$$

and using the L^∞ bound (6.19) and the dual estimate (6.21) with $d \leq 2 + \alpha$ (given by condition (6.5)),

$$\int_0^T \int_\Omega \left|\nabla_x[v^{p/2}]\right|^2 \leq C(p, \Omega, T, u_{in}, v_{in}, \mathrm{D}) \qquad \text{(for all } 0 < p < 1). \tag{6.22}$$

Now, let $q \geq 1$. Let us pick some $p \in]0, 1[$. We can write $\nabla_x v^{q/2} = (q/p)\, v^{(q-p)/2} \times \nabla_x v^{p/2} \in L^\infty \times L^2$ by (6.19) and (6.22). Therefore

$$\boxed{\int_0^T \int_\Omega \left|\nabla_x[v^{p/2}]\right|^2 \leq C(p, \Omega, T, u_{in}, v_{in}, \mathrm{D}) \qquad \text{(for all } 0 < p < \infty).} \tag{6.23}$$

Entropy estimate for u

Define

$$E_u(t) := \int_\Omega \log(1+u)(t).$$

We compute the derivative

$$\mathrm{d}_t E_u(t) = \int_\Omega \frac{\partial_t u}{1+u}(t)$$
$$= \int_\Omega \frac{u}{1+u}(r_u - r_a\, u^a - r_b\, v^b) + \int_\Omega \frac{1}{1+u}\Delta_x[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u],$$

where the last term writes

$$\int_\Omega \frac{1}{1+u}\Delta_x[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u] = -\int_\Omega \nabla_x[\frac{1}{1+u}] \cdot \nabla_x[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\, u]$$
$$= \int_\Omega |\nabla_x[\log(1+u)]|^2 \, (d_u + d_\alpha(1+\alpha)u^\alpha + d_\beta v^\beta) + \int_\Omega d_\beta \frac{u}{1+u}\nabla_x[\log(1+u)] \cdot \nabla_x v^\beta.$$

We integrate on $t \in [0, T]$:

$$\begin{aligned} \int_\Omega \log(1+u)(0) \; + \; \int_0^T \int_\Omega |\nabla_x[\log(1+u)]|^2 \, (d_u + d_\alpha(1+\alpha)u^\alpha + d_\beta v^\beta) \\ = \int_\Omega \log(1+u)(T) \; - \; \int_0^T \int_\Omega \frac{u}{1+u}(r_u - r_a\, u^a - r_b\, v^b) \\ - \int_0^T \int_\Omega d_\beta \frac{u}{1+u}\nabla_x[\log(1+u)] \cdot \nabla_x v^\beta. \end{aligned} \tag{6.24}$$

Using the elementary inequality $2xy \leq x^2 + y^2$,

$$\left| \int_0^T \int_\Omega \frac{u}{1+u}\nabla_x[\log(1+u)] \cdot \nabla_x v^\beta \right| = 2 \left| \int_0^T \int_\Omega \frac{u}{1+u}\nabla_x[\log(1+u)]\, v^{\beta/2} \cdot \nabla_x v^{\beta/2} \right|$$
$$\leq \frac{1}{2}\int_0^T \int_\Omega |\nabla_x[\log(1+u)]|^2 \; v^\beta + 2\int_0^T \int_\Omega \left(\frac{u}{1+u}\right)^2 \left|\nabla_x v^{\beta/2}\right|^2.$$

Reinserting in (6.24) (and using $u/(1+u) \le 1$), we get

$$\begin{aligned}\int_\Omega \log(1+u)(0) \; + \; \int_0^T \int_\Omega |\nabla_x[\log(1+u)]|^2\,(d_u + d_\alpha(1+\alpha)u^\alpha + \frac{d_\beta}{2} v^\beta)\\ \le \int_\Omega \log(1+u)(T) \; + \; \int_0^T \int_\Omega (r_u + r_a\, u^a + r_b\, v^b) \; + \; 2d_\beta \int_0^T \int_\Omega \left|\nabla_x v^{\beta/2}\right|^2.\end{aligned}$$

In the RHS, the first integral and the second term of the second integral are controlled thanks to the L^1 estimate (6.20) and the last term of the second integral is controlled thanks to the L^∞ bound (6.19) :

$$\begin{aligned}\int_\Omega \log(1+u)(0) \; + \; \int_0^T \int_\Omega |\nabla_x[\log(1+u)]|^2\,(d_u + d_\alpha(1+\alpha)u^\alpha + \frac{d_\beta}{2} v^\beta)\\ \le C(\Omega, T, u_{in}, a, b, r_u, r_a, r_b) \; + \; 2d_\beta \int_0^T \int_\Omega \left|\nabla_x v^{\beta/2}\right|^2.\end{aligned}$$

Finally, the last term is controlled thanks to (6.23), so that

$$\boxed{\int_0^T \int_\Omega |\nabla_x[\log(1+u)]|^2\,(1+u^\alpha) \le C(\Omega, T, u_{in}, \mathrm{D}).} \tag{6.25}$$

6.3 Approximating scheme

In this section we define a semi-discrete (in time) scheme intended to approximate system (6.1)–(6.4), and establish rigorously uniform estimates (w.r.t the time step) for the solution of this scheme. Thanks to these uniform estimates, we will be able to pass to the limit in the approximating scheme in the following Section (under condition (6.18)).

6.3.1 Definition of the scheme

The scheme takes the following form : (u_0, v_0) are given and for $1 \le k \le N$ ($N = T/\tau$, $T > 0$)

$$\frac{u_k - u_{k-1}}{\tau} - \Delta_x[(d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta)u_k] \;=\; u_k\,(r_u - r_a\, u_k^a - r_b\, v_k^b), \text{ on } \Omega, \tag{6.26}$$

$$\frac{v_k - v_{k-1}}{\tau} - \Delta_x[(d_v + d_\gamma v_k^\gamma)v_k] \;=\; v_k\,(r_v - r_c\, v_k^c - r_d\, u_k^d), \text{ on } \Omega, \tag{6.27}$$

$$\partial_n u_k = \partial_n v_k \;=\; 0, \text{ on } \partial\Omega. \tag{6.28}$$

This scheme was introduced in [16] in a more general setting. More precisely, in [16] systems of the following form are studied :

$$\begin{aligned}\frac{U_k - U_{k-1}}{\tau} - \Delta_x[A(U_k)] = R(U_k), \text{ on } \Omega,\\ \partial_n A(U_k) = 0, \text{ on } \partial\Omega,\end{aligned} \tag{6.29}$$

where

$$A: \begin{array}{ccc} \mathbb{R}_+^I & \to & \mathbb{R}_+^I \\ U = \begin{pmatrix} u_1 \\ \vdots \\ u_I \end{pmatrix} & \mapsto & \begin{pmatrix} a_1(U)u_1 \\ \vdots \\ a_I(U)u_I \end{pmatrix} \end{array} \quad \text{and} \quad R: \begin{array}{ccc} \mathbb{R}_+^I & \to & \mathbb{R}^I \\ U = \begin{pmatrix} u_1 \\ \vdots \\ u_I \end{pmatrix} & \mapsto & \begin{pmatrix} r_1(U)u_1 \\ \vdots \\ r_I(U)u_I \end{pmatrix} \end{array} \tag{6.30}$$

satisfy the following assumptions :

H1 For all i, the functions a_i and r_i are continuous from $\mathbb{R}_+^I$ to $\mathbb{R}$.

H2 For all i, a_i is lower bounded by some positive constant $\underline{a} > 0$, and r_i is upper bounded by a positive constant $\overline{r} > 0$. That is $a_i(U) \ge \underline{a} > 0$, $r_i(U) \le \overline{r}$ for all $U \in \mathbb{R}_+^I$.

H3 A is a homeomorphism from $\mathbb{R}_+^I$ to itself.

Following [16], we introduce the

Definition 6.2 (Strong solution)**.** *Assume **H1**, **H2**, **H3**. Let $\tau > 0$ and let U_{k-1} be a nonnegative vector-valued function in* $\mathrm{L}^\infty(\Omega)^I$. *A nonnegative vector-valued function U_k is a strong solution of* (6.29) *if U_k lies in* $\mathrm{L}^\infty(\Omega)^I$, *$A(U_k)$ lies in* $\mathrm{H}^2(\Omega)^I$ *and* (6.29) *is satisfied almost everywhere on Ω, resp. $\partial\Omega$.*

The general theorem from [16] writes

Theorem 6.2. *Assume **H1**, **H2**, **H3**. Let Ω be a bounded open set of $\mathbb{R}^m$ with smooth boundary. Fix $T > 0$ and an integer N large enough such that $\overline{r}\tau < 1/2$, where $\tau := T/N$ and $\overline{r}$ is the positive number defined in* **H2**. *Fix $\eta > 0$ and a vector-valued function $\mathrm{L}^\infty(\Omega)^I \ni U_0 \geq \eta$. Then there exists a sequence of positive vector-valued functions $(U_k)_{1\leq k\leq N}$ in $\mathrm{L}^\infty(\Omega)^I$ which solve (6.29) (in the sense of Definition 6.2). Furthermore, it satisfies the following estimates : for all $k \geq 1$ and $p \in [1,\infty[$,*

$$U_k \in \mathscr{C}^0(\overline{\Omega})^I, \tag{6.31}$$

$$U_k \geq \eta_{A,R,\tau} \text{ on } \overline{\Omega}, \tag{6.32}$$

$$A(U_k) \in \mathrm{W}^{2,p}(\Omega)^I, \tag{6.33}$$

where $\eta_{A,R,\tau} > 0$ is a positive constant depending on the maps A and R and τ, and

$$\sum_{k=1}^{N} \tau \int_\Omega \left(\sum_{i=1}^{I} U_{k,i}\right)\left(\sum_{i=1}^{I} A_i(U_k)\right) \leq C(\Omega, U_0, A, \overline{r}, N\tau), \tag{6.34}$$

where $C(\Omega, U_0, A, \overline{r}, N\tau)$ is a positive constant depending only on Ω, A, $\overline{r}$, $N\tau$ and $\|U_0\|_{\mathrm{L}^1\cap\mathrm{H}_m^{-1}(\Omega)}$.

Let us go back to system (6.26)–(6.28). It can be written in the form (6.29)–(6.30) with $I = 2$ and

$$\begin{aligned} a_1(u,v) &= d_u + d_\alpha u^\alpha + d_\beta v^\beta, \qquad & r_1(u,v) &= r_u - r_a\, u^a - r_b\, v^b,\\ a_2(u,v) &= d_v + d_\gamma v^\gamma, \qquad & r_2(u,v) &= r_v - r_c\, v^c - r_d\, u^d. \end{aligned} \tag{6.35}$$

Applying Theorem 6.2 directly gives rise to the following existence theorem

Corollary 6.1. *Let Ω be a bounded open set of $\mathbb{R}^m$ with smooth boundary. Let the parameters of system* (6.26)–(6.27) $\mathrm{D} \in (\mathbb{R}_+^*)^{15} \times \mathbb{R}_+ \times \mathbb{R}_+^* \times \mathbb{R}_+$. *Fix $T > 0$ and an integer N large enough such that* $\max(r_u, r_v)\tau < 1/2$, *where $\tau := T/N$. Fix $\eta > 0$ and a couple of functions $\mathrm{L}^\infty(\Omega)^2 \ni (u_0, v_0) \geq \eta$. Then there exists a sequence of couples of positive functions $(u_k, v_k)_{1\leq k\leq N}$ in $\mathrm{L}^\infty(\Omega)^2$ which solve* (6.26)–(6.28) *(in the sense of Definition 6.2). Furthermore, it satisfies the following estimates : for all $k \geq 1$ and $p \in [1,\infty[$,*

$$(u_k, v_k) \in \mathscr{C}^0(\overline{\Omega})^2, \tag{6.36}$$

$$u_k \geq \eta_{\mathrm{D},\tau},\ v_k \geq \eta_{\mathrm{D},\tau} \text{ on } \overline{\Omega}, \tag{6.37}$$

$$([d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta,]u_k,\ [d_v + d_\gamma v_k^\gamma]v_k) \in \mathrm{W}^{2,p}(\Omega)^2, \tag{6.38}$$

where $\eta_{\mathrm{D},\tau} > 0$ is a positive constant depending on D *and τ, and*

$$\sum_{k=1}^{N} \tau \int_\Omega (1 + u_k^\alpha)\, u_k^2 \leq C(\Omega, u_0, v_0, \mathrm{D}, N\tau), \tag{6.39}$$

where $C(\Omega, u_0, v_0, \mathrm{D}, N\tau)$ is a positive constant depending only on Ω, D, *$N\tau$ and $\|(u_0, v_0)\|_{\mathrm{L}^1\cap\mathrm{H}_m^{-1}(\Omega)}$.*

Proof of Corollary 6.1. It suffices to check assumptions **H1**–**H3** for A and R defined by (6.35). Assumptions **H1** and **H2** are clearly satisfied with $\underline{a} = \min(d_u, d_v) > 0$ and $\overline{r} = \max(r_u, r_v) > 0$. It remains to prove that the map A is a homeomorphism from $\mathbb{R}_+^2$ to itself. By a monotonicity argument, it is easy to see that the map A is a continuous bijection from $\mathbb{R}_+^2$ to itself. Since the map A is furthermore proper (thanks to the inequality $|A(u,v)| \geq \min(d_u, d_v)|(u,v)|$ for all $u, v \geq 0$), it is a homeomorphism. □

6.3.2 Uniform estimates

Let $\mu > 0$ and let $U_0 = (u_0, v_0)$ be a couple of positive functions in $\mathrm{L}^\infty(\Omega)^2$ such that $u_0, v_0 \geq \mu > 0$ a. e. on Ω. Let $U_k = (u_k, v_k)$ be a solution of (6.26)–(6.28) (in the sense of Definition 6.2). We now establish uniform (w. r. t. N) estimates for U_k that will allow us to pass in the limit in the approximating scheme (in Section 6.4). Note that some of these estimates (namely, (6.40), (6.41), (6.54)) can be seen as the "discretized" (in time) version of the *a priori* estimates (6.19), (6.23), (6.25), while (6.39) can be seen as the "discretized" (in time) version of the *a priori* estimate (6.21). To establish rigorously these uniform estimates, we will use all the time the smoothness of $U_k = (u_k, v_k)$ (for any fixed N) specified by estimates (6.36)–(6.38).

Maximum principle

Lemma 6.2. *We have*

$$\max_{k=1..N}\sup_{\Omega} v_k \le \max\{\sup_{\Omega} v_0, \left(\frac{r_v}{r_c}\right)^{1/c}\}. \tag{6.40}$$

Proof of Lemma 6.2. Recall equation (6.27). By the maximum principle, for all $1 \le k \le N$, we have $\sup_{\Omega} v_k \le \max\{\sup_{\Omega} v_{k-1}, \left(\frac{r_v}{r_c}\right)^{1/c}\}$, so that (6.40) follows by iteration on $k = 1..N$. □

Entropy estimate for v

Lemma 6.3. *Assume condition* (6.5)*. For all $p \in \mathbb{R}_+^*$, we have*

$$\sum_{k=1}^{N} \tau \int_{\Omega} \left|\nabla_x v_k^{p/2}\right|^2 \le C(p, \Omega, N\tau, u_0, v_0, \mathrm{D}), \tag{6.41}$$

$$\sup_{0\le k\le N} \int_{\Omega} |\log v_k| \,+\, d_v \sum_{k=1}^{N} \tau \int_{\Omega} |\nabla_x \log v_k|^2 \le \int_{\Omega} |\log v_0| \,+\, C(\Omega, N\tau, u_0, v_0, \mathrm{D}), \tag{6.42}$$

where the first constant only depends on $p, \Omega, N\tau, \|u_0\|_{\mathrm{L}^1\cap \mathrm{H}_m^{-1}(\Omega)}, \sup_{\Omega} v_0, \mathrm{D}$ and the second constant only depends on $\Omega, N\tau, \|u_0\|_{\mathrm{L}^1\cap \mathrm{H}_m^{-1}(\Omega)}, \sup_{\Omega} v_0, \mathrm{D}$.

Proof of Lemma 6.3. Define for all $p \in]0,1[$ and all $z > 0$

$$\phi_p(z) = z - \frac{z^p}{p} - 1 + \frac{1}{p} \ge 0, \qquad \phi_0(z) = z - \log z > 0. \tag{6.43}$$

We have (for all $p \in]0,1[$ and all $z > 0$)

$$\phi_p'(z) = 1 - z^{p-1}, \qquad \phi_0'(z) = 1 - \frac{1}{z}, \qquad \phi_p''(z) = (1-p)z^{p-2} > 0, \qquad \phi_0''(z) = \frac{1}{z^2} > 0. \tag{6.44}$$

For any $p \in [0,1[$, by convexity of ϕ_p, for all $y > 0$, $z > 0$ we have $\phi_p'(z)(z-y) \ge \phi_p(z) - \phi_p(y)$. Multiplying equation (6.27) by $\phi_p'(v_k)$ and integrating over Ω, we therefore get

$$\int_{\Omega} [\phi_p(v_k) - \phi_p(v_{k-1})] - \tau \int_{\Omega} \phi_p'(v_k)\Delta_x[(d_v + d_\gamma v_k^\gamma)v_k] \le \tau \int_{\Omega} \phi_p'(v_k) v_k \,(r_v - r_c\, v_k^c - r_d\, u_k^d). \tag{6.45}$$

Since (u_k, v_k) satisfy the homogeneous Neumann boundary conditions (6.28), we can rewrite the second term as

$$-\tau \int_{\Omega} \phi_p'(v_k)\Delta_x[(d_v + d_\gamma v_k^\gamma)v_k] = \tau \int_{\Omega} \nabla_x[\phi_p'(v_k)] \cdot \nabla_x[(d_v + d_\gamma v_k^\gamma)v_k] \tag{6.46}$$

$$= \tau \int_{\Omega} \phi_p''(v_k) d_v |\nabla_x v_k|^2 + \tau \int_{\Omega} \phi_p''(v_k) d_\gamma(\gamma+1) v_k^\gamma |\nabla_x v_k|^2. \tag{6.47}$$

The last term being nonnegative, we have

$$-\tau \int_{\Omega} \phi_p'(v_k)\Delta_x[(d_v + d_\gamma v_k^\gamma)v_k] \ge \tau \int_{\Omega} \phi_p''(v_k) d_v |\nabla_x v_k|^2, \tag{6.48}$$

so that reinserting in (6.45) and summing for $k = 1..N$

$$\int_{\Omega} \phi_p(v_N) + \sum_{k=1}^{N} \tau \int_{\Omega} \phi_p''(v_k) d_v |\nabla_x v_k|^2 \le \int_{\Omega} \phi_p(v_0) + \sum_{k=1}^{N} \tau \int_{\Omega} \phi_p'(v_k) v_k \,(r_v - r_c\, v_k^c - r_d\, u_k^d). \tag{6.49}$$

Thanks to estimate (6.39) and the assumption $d \le 2+\alpha$ (consequence of condition (6.5)), we can control u_k^d in L^1, so that, using furthermore the L^∞ bound (6.40) and the continuity of $v \mapsto v\phi_p'(v)$ on $\mathbb{R}_+$, we get

$$\int_{\Omega} \phi_p(v_N) + \sum_{k=1}^{N} \tau \int_{\Omega} \phi_p''(v_k) d_v |\nabla_x v_k|^2 \le \int_{\Omega} \phi_p(v_0) + C(p, \Omega, N\tau, u_0, v_0, \mathrm{D}). \tag{6.50}$$

Using the definition of ϕ_0 and ϕ_p for $0 < p < 1$, we have

$$\int_\Omega \phi_p''(v_k) d_v |\nabla_x v_k|^2 = \int_\Omega (1-p) v_k^{p-2} d_v |\nabla_x v_k|^2 = \int_\Omega (1-p) d_v \frac{4}{p^2} |\nabla_x v_k^{p/2}|^2, \tag{6.51}$$

$$\int_\Omega \phi_0''(v_k) d_v |\nabla_x v_k|^2 = \int_\Omega v_k^{-2} d_v |\nabla_x v_k|^2 = \int_\Omega d_v |\nabla_x [\log v_k]|^2, \tag{6.52}$$

so that (6.50) with $0 < p < 1$ gives (6.41) for $p < 1$ and, using furthermore the elementary inequality (for all $z > 0$) $|\log z| \le z - \log z$, (6.50) with $p = 0$ gives (6.42).

It remains to show (6.41) for $p \ge 1$. Let $p \ge 1$, and let us fix $\tilde p \in]0, 1[$. Combining (6.40) and (6.41) with p replaced by $\tilde p$, we have

$$\sum_{k=1}^N \tau \int_\Omega \left|\nabla_x v_k^{p/2}\right|^2 = \sum_{k=1}^N \tau \frac{p^2}{\tilde p^2} \int_\Omega v_k^{p-\tilde p} \left|\nabla_x v_k^{\tilde p/2}\right|^2 \le C(p, \Omega, N\tau, u_0, v_0, \mathrm{D}). \tag{6.53}$$

$\square$

Entropy estimate for u

Lemma 6.4. *We have*

$$\sup_{0\le k\le N} \int_\Omega u_k \; + \sum_{k=1}^N \tau \int_\Omega \left|\frac{\nabla_x u_k}{1+u_k}\right|^2 (1 + u_k^\alpha) \le C(\Omega, N\tau, u_0, v_0, \mathrm{D}), \tag{6.54}$$

$$\sup_{0\le k\le N} \int_\Omega |\log u_k| \; + \; d_u \sum_{k=1}^N \tau \int_\Omega |\nabla_x \log u_k|^2 \le \int_\Omega |\log u_0| \; + \; C(\Omega, N\tau, u_0, v_0, \mathrm{D}), \tag{6.55}$$

where the constant $C(\Omega, N\tau, u_0, v_0, \mathrm{D})$ only depends on $\Omega, N\tau, \|u_0\|_{\mathrm{L}^1\cap \mathrm{H}_m^{-1}(\Omega)}, \sup_\Omega v_0, \mathrm{D}$.

Proof of Lemma 6.4. Let $\phi(z) = 2z - \log(\mu + z)$ for all $z > 0$, with $\mu = 0$ or $\mu = 1$. It is useful to compute

$$\phi(z) = 2z - \log(\mu + z), \qquad \phi'(z) = 2 - \frac{1}{\mu + z}, \qquad \phi''(z) = \frac{1}{(\mu+z)^2} > 0. \tag{6.56}$$

By convexity of ϕ, for all $y \ge 0$, $z \ge 0$ we have $\phi'(z)(z-y) \ge \phi(z) - \phi(y)$. Multiplying equation (6.26) by $\phi'(u_k)$ and integrating over Ω, we therefore get

$$\int_\Omega [\phi(u_k) - \phi(u_{k-1})] - \tau \int_\Omega \phi'(u_k) \Delta_x [(d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta) u_k] \le \tau \int_\Omega \phi'(u_k) u_k \, (r_u - r_a\, u_k^a - r_b\, v_k^b). \tag{6.57}$$

Thanks to the homogeneous Neumann boundary conditions (6.28), we can rewrite the second term as

$$-\tau \int_\Omega \phi'(u_k) \Delta_x [(d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta) u_k] = \tau \int_\Omega \nabla_x \phi'(u_k) \cdot \nabla_x [(d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta) u_k] \tag{6.58}$$

$$= \tau \int_\Omega \nabla_x \phi'(u_k) \cdot [(d_u + d_\alpha (1+\alpha) u_k^\alpha + d_\beta v_k^\beta) \nabla_x u_k] + \tau \int_\Omega \nabla_x \phi'(u_k) \cdot [u_k \nabla_x d_\beta v_k^\beta] \tag{6.59}$$

$$= \tau \int_\Omega \phi''(u_k) (d_u + d_\alpha (1+\alpha) u_k^\alpha + d_\beta v_k^\beta) |\nabla_x u_k|^2 + \tau \int_\Omega \phi''(u_k) u_k \nabla_x u_k \cdot \nabla_x d_\beta v_k^\beta. \tag{6.60}$$

Therefore

$$\int_\Omega [\phi(u_k) - \phi(u_{k-1})] + \tau \int_\Omega \phi''(u_k) (d_u + d_\alpha (1+\alpha) u_k^\alpha + d_\beta v_k^\beta) |\nabla_x u_k|^2 \tag{6.61}$$

$$\le -\tau \int_\Omega \phi''(u_k) u_k \nabla_x u_k \cdot \nabla_x d_\beta v_k^\beta + \tau \int_\Omega \phi'(u_k) u_k \, (r_u - r_a\, u_k^a - r_b\, v_k^b). \tag{6.62}$$

The first term of the RHS can be rewritten

$$\begin{aligned} -\tau \int_\Omega \phi''(u_k) u_k \nabla_x u_k \cdot \nabla_x d_\beta v_k^\beta \quad &= \quad -\tau \int_\Omega \phi''(u_k) u_k \nabla_x u_k \cdot d_\beta \, 2\, v_k^{\beta/2} \nabla_x v_k^{\beta/2} &(6.63)\\ &\le \quad \frac{\tau}{2} \int_\Omega \phi''(u_k)^2 u_k^2 |\nabla_x u_k|^2 d_\beta \, v_k^\beta + 2\tau \int_\Omega d_\beta \, |\nabla_x v_k^{\beta/2}|^2 &(6.64)\\ &\le \quad \frac{\tau}{2} \int_\Omega \phi''(u_k) |\nabla_x u_k|^2 d_\beta \, v_k^\beta + 2\tau \int_\Omega d_\beta \, |\nabla_x v_k^{\beta/2}|^2, &(6.65) \end{aligned}$$

where we used the elementary inequality $2ab \leq a^2 + b^2$ (for all $a, b \in \mathbb{R}$) and the bound $\phi''(z)\, z^2 = [z/(\mu + z)]^2 \leq 1$ (for all $z > 0$). Reinserting in (6.61), we get

$$\int_\Omega [\phi(u_k) - \phi(u_{k-1})] + \tau \int_\Omega \phi''(u_k)(d_u + d_\alpha(1+\alpha)u_k^\alpha + \frac{d_\beta}{2} v_k^\beta)|\nabla_x u_k|^2 \tag{6.66}$$

$$\leq 2\tau \int_\Omega d_\beta\, |\nabla_x v_k^{\beta/2}|^2 + \tau \int_\Omega \phi'(u_k) u_k\, (r_u - r_a\, u_k^a - r_b\, v_k^b). \tag{6.67}$$

Now using that (for all $z > 0$) $\phi'(z) z (r_u - r_a\, z^a) = (2 - 1/(\mu + z)) z (r_u - r_a\, z^a) \leq C(r_u, r_a, a)$, we have

$$\int_\Omega [\phi(u_k) - \phi(u_{k-1})] + \tau \int_\Omega \phi''(u_k)(d_u + d_\alpha(1+\alpha)u_k^\alpha + \frac{d_\beta}{2} v_k^\beta)|\nabla_x u_k|^2 \tag{6.68}$$

$$\leq 2\tau \int_\Omega d_\beta\, |\nabla_x v_k^{\beta/2}|^2 + \tau |\Omega| C(r_u, r_a, a). \tag{6.69}$$

Summing for $k = 1..N$ we get

$$\int_\Omega \phi(u_N) + \sum_{k=1}^N \tau \int_\Omega \phi''(u_k)(d_u + d_\alpha(1+\alpha)u_k^\alpha + \frac{d_\beta}{2} v_k^\beta)|\nabla_x u_k|^2 \tag{6.70}$$

$$\leq \int_\Omega \phi(u_0) + 2 \sum_{k=1}^N \tau \int_\Omega d_\beta\, |\nabla_x v_k^{\beta/2}|^2 + N\tau |\Omega| C(r_u, r_a, a), \tag{6.71}$$

and using furthermore estimate (6.41) with $p = \beta$ and $\phi''(z) \geq 0$ (for all $z > 0$),

$$\int_\Omega \phi(u_N) + \sum_{k=1}^N \tau \int_\Omega \phi''(u_k)(d_u + d_\alpha(1+\alpha)u_k^\alpha)|\nabla_x u_k|^2 \leq \int_\Omega \phi(u_0) + C(\Omega, N\tau, u_0, v_0, \mathrm{D}). \tag{6.72}$$

We conclude (6.54) by taking $\mu = 1$ and using the inequality $2z \geq \phi(z) = 2z - \log(1+z) \geq z$ (for all $z \geq 0$), and we conclude (6.55) by taking $\mu = 0$ and using the inequality $\phi(z) = 2z - \log z \geq |\log z|$ (for all $z > 0$). □

6.4 Proof of Existence

We are now ready to pass to the limit in the approximating scheme (6.26)–(6.28) in order to obtain a solution of system (6.1)–(6.4), at least when the condition (6.18) is fulfilled.

Proof of i) under condition (6.18). Fix $T > 0$. Define the sequence

$$(u_0, v_0) = (u_0^N, v_0^N) := (\min(u_{in}, N) + 1/N, v_{in} + 1/N),$$

so that (u_0, v_0) approximates (u_{in}, v_{in}) in $(\mathrm{L}^1(\Omega) \cap \mathrm{H}_m^{-1}(\Omega)) \times \mathrm{L}^\infty(\Omega)$ (when $N \longrightarrow \infty$), and for all N, $(u_0, v_0) \in \mathrm{L}^\infty(\Omega)^2$ and $(u_0, v_0) \geq 1/N > 0$. For any N large enough ($N > 2T \max(r_u, r_v)$), use Corollary 6.1 to define the family of couple of functions $(u_k, v_k)_{1 \leq k \leq N}$ solving (6.26)–(6.28) with initial value (u_0^N, v_0^N).

Note that (6.39), (6.40), (6.41), (6.54), (6.55), (6.42) are therefore valid with u_0 (resp. v_0) replaced by u_{in} (resp. v_{in}) in the constant C in the RHS. If $\log u_{in}$ is in $\mathrm{L}^1(\Omega)$, we furthermore have that $\log u_0$ approximates $\log u_{in}$ in $\mathrm{L}^1(\Omega)$, so that (6.55) actually yields a uniform bound (w. r. t. N). For the same reason, if $\log v_{in}$ is in $\mathrm{L}^1(\Omega)$, then (6.42) actually yields a uniform bound (w. r. t. N).

Definition 6.3. *For $h := (h_k)_{0 \leq k \leq N}$ a given family of functions defined on Ω, we denote by $\underline{h}^N$ the step in time function defined on $\mathbb{R} \times \Omega$ by*

$$\underline{h}^N(t, x) := h_0(x) \mathbf{1}_{]-\tau, 0]}(t) + \sum_{k=1}^N h_k(x) \mathbf{1}_{](k-1)\tau, k\tau]}(t) + h_N(x) \mathbf{1}_{]N\tau, +\infty[}(t).$$

Note that by definition, for all $p \in [1, \infty[$, we have

$$\|\underline{h}^N\|_{\mathrm{L}^p(]0,T[\times\Omega)} = \left(\sum_{k=1}^N \tau \int_\Omega |h_k(x)|^p \, \mathrm{d}x \right)^{1/p}.$$

With this notation, for any family $h := (h_k)_{0\le k\le N}$ of distributions on Ω, we have

$$\partial_t \underline{h}^N = h_0(x) \otimes \delta_{-\tau}(t) + \sum_{k=0}^{N-1} \{h_{k+1}(x) - h_k(x)\} \otimes \delta_{k\tau}(t) \quad \text{in } \mathscr{D}'(\mathbb{R}\times\Omega)/ \tag{6.73}$$

In particular, we can rewrite equations (6.26)–(6.27) as

$$\begin{aligned} \partial_t \underline{u}^N &= u_0(x) \otimes \delta_{-\tau}(t) + \sum_{k=1}^{N} \tau \Big(\Delta_x[(d_u + d_\alpha u_k^\alpha + d_\beta v_k^\beta)u_k] + (r_u - r_a u_k^a - r_b v_k^b)u_k\Big) \otimes \delta_{k\tau}(t), \\ \partial_t \underline{v}^N &= v_0(x) \otimes \delta_{-\tau}(t) + \sum_{k=1}^{N} \tau \Big(\Delta_x[(d_v + d_\gamma v_k^\gamma)v_k] + (r_v - r_c v_k^c - r_d u_k^d)v_k\Big) \otimes \delta_{k\tau}(t). \end{aligned} \tag{6.74}$$

We want to pass to the limit when $N = T/\tau \to \infty$ in the two equations above. Estimates (6.39), (6.40), (6.41), (6.54) and (6.55), (6.42) can be respectively rewritten as

$$\int_0^T \int_\Omega (\underline{u}^N)^2\,(1 + (\underline{u}^N)^\alpha) \le C(\Omega, u_{in}, v_{in}, \mathrm{D}, T), \tag{6.75}$$

$$\sup_{[0,T]} \sup_\Omega \underline{v}^N \le \max\{\sup_\Omega v_{in}, \left(\frac{r_v}{r_c}\right)^{1/c}\}, \tag{6.76}$$

$$\text{for all } 0 < p < \infty, \quad \int_0^T \int_\Omega \left|\nabla_x (\underline{v}^N)^{p/2}\right|^2 \le C(p, \Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.77}$$

$$\sup_{[0,T]} \int_\Omega \underline{u}^N + \int_0^T \int_\Omega \left|\frac{\nabla_x \underline{u}^N}{1 + \underline{u}^N}\right|^2 (1 + (\underline{u}^N)^\alpha) \le C(\Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.78}$$

$$\sup_{[0,T]} \int_\Omega |\log \underline{u}^N| + d_u \int_0^T \int_\Omega \left|\nabla_x \log \underline{u}^N\right|^2 \le \int_\Omega |\log u_0^N| + C(\Omega, T, u_{in}, v_{in}, \mathrm{D}), \tag{6.79}$$

$$\sup_{[0,T]} \int_\Omega |\log \underline{v}^N| + d_v \int_0^T \int_\Omega \left|\nabla_x \log \underline{v}^N\right|^2 \le \int_\Omega |\log v_0^N| + C(\Omega, T, u_{in}, v_{in}, \mathrm{D}). \tag{6.80}$$

Note that all bounds give rise to estimates which are uniform with respect to N (with the additional assumption that $\log u_{in}$, resp. $\log v_{in}$, lies in $\mathrm{L}^1(\Omega)$ for (6.79), resp. (6.80)). As a consequence of (6.75)–(6.78), we have uniformly w.r.t. N

$$\underline{u}^N \in \mathrm{L}^{2+\alpha}, \qquad \underline{v}^N \in \mathrm{L}^\infty, \qquad \nabla_x \underline{u}^N \in \mathrm{L}^1, \qquad \nabla_x \underline{v}^N \in \mathrm{L}^2. \tag{6.81}$$

The first bound is a direct consequence of (6.75), while the third bound is obtained by writing $\nabla_x \underline{u}^N = (1 + \underline{u}^N) \times (\nabla_x \underline{u}^N/(1 + \underline{u}^N)) \in \mathrm{L}^{2+\alpha} \times \mathrm{L}^2$ thanks to estimates (6.75) and (6.78). The second and last bounds are a direct consequence of (6.76) and (6.77) with $p = 2$. Using furthermore condition (6.18), (6.81) leads to

$$(r_u - r_a(\underline{u}^N)^a - r_b(\underline{v}^N)^b)\underline{u}^N \in \mathrm{L}^{1+\mu}, \qquad (r_v - r_c(\underline{v}^N)^c - r_d(\underline{u}^N)^d)\underline{v}^N \in \mathrm{L}^{1+\mu}, \tag{6.82}$$

$$(d_u + d_\alpha(\underline{u}^N)^\alpha + d_\beta(\underline{v}^N)^\beta)\underline{u}^N \in \mathrm{L}^{1+1/(1+\alpha)}, \qquad (d_v + d_\gamma(\underline{v}^N)^\gamma)\underline{v}^N \in \mathrm{L}^\infty, \tag{6.83}$$

where $1 + \mu = (2 + \alpha)/\max(1 + a, d) > 1$.

Rewriting system (6.26)–(6.27) as the following equalities (which hold in $\mathscr{D}'(]0, T[\times\Omega)$)

$$\frac{1}{\tau}\{\underline{u}^N - S_\tau \underline{u}^N\} = \Delta_x[(d_u + d_\alpha(\underline{u}^N)^\alpha + d_\beta(\underline{v}^N)^\beta)\underline{u}^N] + (r_u - r_a(\underline{u}^N)^a - r_b(\underline{u}^N)^b)\underline{u}^N, \tag{6.84}$$

$$\frac{1}{\tau}\{\underline{v}^N - S_\tau \underline{v}^N\} = \Delta_x[(d_v + d_\gamma(\underline{v}^N)^\gamma)\underline{v}^N] + (r_v - r_c(\underline{u}^N)^c - r_d(\underline{u}^N)^d)\underline{v}^N, \tag{6.85}$$

where $S_\tau : u(t, x) \mapsto u(t - \tau, x)$, we finally get

$$\frac{1}{\tau}\{\underline{u}^N - S_\tau \underline{u}^N\} \in \mathrm{L}^1(]0, T[, \mathrm{W}^{-2,1}(\Omega)), \qquad \frac{1}{\tau}\{\underline{v}^N - S_\tau \underline{v}^N\} \in \mathrm{L}^1(]0, T[, \mathrm{W}^{-2,1}(\Omega)). \tag{6.86}$$

The uniform (w.r.t. N) bounds (6.81), (6.86) are sufficient to apply a discrete version of Aubin-Lions lemma (see for example [18]) to get the strong convergences (up to a subsequence) when $N \longrightarrow \infty$

$$\underline{u}^N \longrightarrow u \ge 0 \text{ in } \mathrm{L}^1, \qquad \underline{v}^N \longrightarrow v \ge 0 \text{ in } \mathrm{L}^1. \tag{6.87}$$

Let us first check that these strong convergences allow us to pass to the limit in the uniform estimates (6.75)–(6.80) to get estimates (6.9)–(6.15). We can directly pass to the limit in estimate (6.76), and we use Fatou's lemma to pass to the limit in estimate (6.75) and in the first terms in estimates (6.78), (6.79) and (6.80). To pass to the limit in (6.77), we first notice that $(\underline{v}^N)^{p/2}$ is uniformly bounded in L^{2+} thanks to estimate (6.76), so that it converges weakly in L^2. We conclude by using the weak lower semi-continuity of the $\mathrm{L}^2(]0,T[,\mathrm{W}^{1,2}(\Omega))$ norm.

To compute the remaining limit in (6.78), it is convenient to notice that $(1+u^\alpha)\sim(1+u)^\alpha$ (in the sense that there exist c_α, $C_\alpha>0$ such that for $u\geq 0$, we have $c_\alpha(1+u)^\alpha\leq(1+u^\alpha)\leq C_\alpha(1+u)^\alpha$), so that (6.78) actually yields a uniform bound in L^1 for $|\nabla_x\underline{u}^N|^2\,(1+\underline{u}^N)^{\alpha-2}=4/\alpha^2\,|\nabla_x(1+\underline{u}^N)^{\alpha/2}|^2$ if $\alpha>0$ (resp. for $|\nabla_x\underline{u}^N|^2\,(1+\underline{u}^N)^{\alpha-2}=|\nabla_x\log(1+\underline{u}^N)|^2$ if $\alpha=0$). Since $(1+\underline{u}^N)^{\alpha/2}$ (resp. $\log(1+\underline{u}^N)$) is uniformly bounded in L^{2+} thanks to estimate (6.75), it converges weakly in L^2. Using the weak lower semi-continuity of the $\mathrm{L}^2(]0,T[,\mathrm{W}^{1,2}(\Omega))$ norm, we get the desired bound.

To compute the remaining limit in (6.79), we first observe that, thanks to Poincaré-Wirtinger's inequality,

$$\begin{aligned}\int_0^T\int_\Omega\left|\log\underline{u}^N\right|^2&=\int_0^T\int_\Omega\left||\Omega|^{-1}\int_\Omega\log\underline{u}^N\;+\;\log\underline{u}^N\;-\;|\Omega|^{-1}\int_\Omega\log\underline{u}^N\right|^2\\&\leq 2\int_0^T\int_\Omega|\Omega|^{-2}\left|\int_\Omega\log\underline{u}^N\right|^2\;+\;2\int_0^T\int_\Omega\left|\log\underline{u}^N-|\Omega|^{-1}\int_\Omega\log\underline{u}^N\right|^2\\&\leq 2T|\Omega|^{-1}\left(\sup_{[0,T]}\int_\Omega\left|\log\underline{u}^N\right|\right)^2\;+\;2C(\Omega)^2\int_0^T\int_\Omega\left|\nabla_x\log\underline{u}^N\right|^2,\end{aligned}$$

so that (6.79) yields a uniform bound for $\log\underline{u}^N$ in L^2. Together with the strong convergence (6.87), this implies that $\log\underline{u}^N$ converges towards $\log u$ weakly in L^1, which allows us to pass to the limit in the second term of (6.79) thanks to the weak lower semi-continuity of the L^2 norm. The same arguments allow us to pass to the limit in (6.80).

It remains to check that (u,v) is a solution of (6.1)–(6.4) in the sense of Definition 6.1. Clearly (u,v) lies in $L^{\max(1+a,d)}\times L^\infty$ thanks to estimates (6.9), (6.10) and condition (6.18). Furthermore, using estimates (6.9)–(6.13), it is classical to validate the following computations (thanks to regularized approximations of $(1+u)^{\alpha/2}$ and v^β) when $\alpha>0$

$$\nabla_x[d_\alpha\,u^{1+\alpha}]=d_\alpha\left(2+\frac{2}{\alpha}\right)\overbrace{\nabla_x(1+u)^{\alpha/2}}^{\in\mathrm{L}^2}\overbrace{u^\alpha/(1+u)^{\alpha/2-1}}^{\in\mathrm{L}^2}\in\mathrm{L}^1,$$

$$\nabla_x[(d_u+d_\beta v^\beta)u]=\frac{2}{\alpha}\overbrace{(d_u+d_\beta v^\beta)}^{\in\mathrm{L}^\infty}\overbrace{(1+u)^{1-\alpha/2}}^{\in\mathrm{L}^2}\overbrace{\nabla_x(1+u)^{\alpha/2}}^{\in\mathrm{L}^2}+d_\beta\overbrace{\nabla_x v^\beta}^{\in\mathrm{L}^2}\overbrace{u}^{\in\mathrm{L}^2}\in\mathrm{L}^1,$$

and, (thanks to regularized approximations of $\log(1+u)$ and v^β) when $\alpha=0$,

$$\nabla_x[(d_u+d_\alpha+d_\beta v^\beta)u]=\frac{2}{\alpha}\overbrace{(d_u+d_\alpha+d_\beta v^\beta)}^{\in\mathrm{L}^\infty}\overbrace{(1+u)}^{\in\mathrm{L}^2}\overbrace{\nabla_x\log(1+u)}^{\in\mathrm{L}^2}+d_\beta\overbrace{\nabla_x v^\beta}^{\in\mathrm{L}^2}\overbrace{u}^{\in\mathrm{L}^2}\in\mathrm{L}^1.$$

Therefore, we also have that $\nabla_x\left[(d_u+d_\alpha u^\alpha+d_\beta v^\beta)\,u\right]$, $\nabla_x\left[(d_v+d_\gamma v^\gamma)\,v\right]$ lie in L^1. Let ψ_1, ψ_2 be two test functions in $C_c^2([0,T[\times\overline{\Omega})$. Let us first extend ψ_1, ψ_2 on $\mathbb{R}_+\times\overline{\Omega}$ by zero; then we extend ψ_1, ψ_2 on $\mathbb{R}\times\overline{\Omega}$ in such a way that ψ_1, ψ_2 lie in $C_c^2(\mathbb{R}\times\overline{\Omega})$. Testing the first equation of (6.74) with ψ_1 gives

$$\begin{aligned}&-\int_{-\infty}^\infty\int_\Omega(\partial_t\psi_1)\,\underline{u}^N-\int_\Omega\psi_1(-\tau,\cdot)\,u_0\\&=\sum_{k=1}^N\tau\int_\Omega\Delta_x\psi_1(k\tau)\left[(d_u+d_\alpha u_k^\alpha+d_\beta v_k^\beta)\,u_k\right]+\sum_{k=1}^N\tau\int_\Omega\psi_1(k\tau)\,u_k\,(r_u-r_a\,u_k^a-r_b\,v_k^b),\end{aligned}$$

where all terms are well defined (all integrands are integrable on their respective domains of integration).

We rewrite this equation as

$$-\int_{-\infty}^{\infty}\int_\Omega (\partial_t\psi_1)\,\underline{u}^N - \int_\Omega \psi_1(-\tau,\cdot)\,u_0 \tag{6.88}$$

$$= \int_{-\infty}^{\infty}\int_\Omega \Delta_x\tilde{\psi}_1^N\left[(d_u + d_\alpha(\underline{u}^N)^\alpha + d_\beta(\underline{v}^N)^\beta)\,\underline{u}^N\right] \tag{6.89}$$

$$+\int_{-\infty}^{\infty}\int_\Omega \tilde{\psi}_1^N\,\underline{u}^N\,(r_u - r_a\,(\underline{u}^N)^a - r_b\,(\underline{v}^N)^b), \tag{6.90}$$

where

$$\tilde{\psi}_1^N(t,x) := \sum_{k=1}^N \psi_1(k\tau,x)\mathbf{1}_{](k-1)\tau,k\tau]}(t) \longrightarrow \psi_1(t,x)\mathbf{1}_{]0,T]}(t) \quad \text{in } \mathrm{L}^\infty(\mathbb{R}\times\Omega). \tag{6.91}$$

Note that we also have

$$\Delta_x\tilde{\psi}_1^N(t,x) = \sum_{k=1}^N \Delta_x\psi_1(k\tau,x)\mathbf{1}_{](k-1)\tau,k\tau]}(t) \longrightarrow \Delta_x\psi_1(t,x)\mathbf{1}_{]0,T]}(t) \quad \text{in } \mathrm{L}^\infty(\mathbb{R}\times\Omega). \tag{6.92}$$

Therefore, thanks to the uniform integrability (given by (6.77)–(6.78)) and the strong convergences (6.87), we have the convergences when $N \longrightarrow \infty$

$$-\int_{-\infty}^{\infty}\int_\Omega (\partial_t\psi_1)\,\underline{u}^N \longrightarrow -\int_0^T\int_\Omega (\partial_t\psi_1)\,u,$$

$$\int_{-\infty}^{\infty}\int_\Omega \tilde{\psi}_1^N\,\underline{u}^N\,(r_u - r_a\,(\underline{u}^N)^a - r_b\,(\underline{v}^N)^b) \longrightarrow \int_0^T\int_\Omega \psi_1\,u\,(r_u - r_a\,u^a - r_b\,v^b),$$

$$\int_{-\infty}^{\infty}\int_\Omega \Delta_x\tilde{\psi}_1^N\left[(d_u + d_\alpha(\underline{u}^N)^\alpha + d_\beta(\underline{v}^N)^\beta)\,\underline{u}^N\right] \longrightarrow \int_0^T\int_\Omega \Delta_x\psi_1\left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\,u\right],$$

where the last term can be rewritten (since $\nabla_x\left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\,u\right]$ lies in L^1)

$$\int_0^T\int_\Omega \Delta_x\psi_1\left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\,u\right] = -\int_0^T\int_\Omega \nabla_x\psi_1\cdot\nabla_x\left[(d_u + d_\alpha u^\alpha + d_\beta v^\beta)\,u\right]. \tag{6.93}$$

It remains to treat the term coming from the initial data in (6.88). By the dominated convergence theorem and the definition of u_0,

$$-\int_\Omega \psi_1(-\tau,\cdot)\,u_0 \longrightarrow -\int_\Omega \psi_1(0,\cdot)\,u_{in}. \tag{6.94}$$

Replacing these four convergences in (6.88), we get that (6.8) is satisfied. A straightforward density argument allows us to replace ψ_1 in (6.8) by any test function in $C_c^1([0,T[\times\overline{\Omega})$. Performing very similar computations for the second equation of (6.74) with the test function ψ_2, we can finally show that (u,v) is a local (in time) weak solution solution of (6.1)–(6.4) on $[0,T]$.

Performing iteratively this proof on $[0,2T]$, $[0,3T]$, ..., we can define (u,v) on $\mathbb{R}_+\times\Omega$ in such a way that (u,v) is a (global) weak solution of (6.1)–(6.4) and it satisfies estimates (6.9)–(6.13) for any $T>0$. □

6.5 Special cases

This section is devoted to the end of the proof of Theorem 6.1, that is, the proof of i) when condition (6.18) is not fulfilled and the proof of ii) and iii).

Recall condition (6.5). "Condition (6.18) is not fulfilled" exactly means that

$$\alpha = 0 \text{ and } \{(a=1,\, d\le 2) \text{ or } (a<1,\, d=2)\}. \tag{6.95}$$

In the subsection below, we will prove together i) and ii) under the wider condition

$$\alpha = 0 \text{ and } (a\le 1,\, d\le 2), \tag{6.96}$$

which is the condition required in ii) in our Theorem. Note that we therefore freely have a second proof of i) in the case $\alpha=0$ and $a<1$, $d<2$.

The last subsection is devoted to the proof of iii).

6.5.1 The case $\alpha = 0$

The following Lemma is crucial to establish estimate (6.16). It is adapted from a similar result in [17] (one main difference being that the version stated below tackles weaker forms of solutions), which is itself adapted from an original result in [7].

Lemma 6.5. *We consider $T > 0$, Ω a bounded regular open set of $\mathbb{R}^m$ ($m \in \mathbb{N}^*$), $q > 1$, a function R in $L^q(]0,T[\times\Omega)$, and a function M in $L^\infty(]0,T[\times\Omega)$ satisfying*

$$R(t,x) \le K \qquad \text{and} \qquad 0 < m_0 \le M(t,x) \le m_1 \qquad \text{for } t \in]0,T[\text{ and } x \in \Omega, \tag{6.97}$$

for some constants $K > 0$, $m_0, m_1 > 0$. Then, one can find $\nu \in]0,1[$ depending only on Ω and the constants m_0, m_1, such that for any initial datum u_{in} in $L^2(\Omega)$, any nonnegative ***very weak*** *solution $u \in L^{2-\nu}(]0,T[\times\Omega)$ of the system*

$$\begin{cases} \partial_t u - \Delta_x(Mu) = R \le K \text{ in }]0,T[\times\Omega, \\ u(0,x) = u_{in}(x) \text{ in } \Omega, \\ \nabla_x(Mu)(t,x)\cdot n(x) = 0 \text{ on }]0,T[\times\partial\Omega, \end{cases} \tag{6.98}$$

(in the sense that for all test functions $\psi \in C_c^2([0,T[\times\overline{\Omega})$ satisfying $\nabla_x\psi\cdot n = 0$ on $[0,T]\times\partial\Omega$, the equality

$$\int_0^T\int_\Omega u\partial_t\psi + \int_\Omega u_{in}\psi(0,\cdot) + \int_0^T\int_\Omega Mu\Delta_x\psi + \int_0^T\int_\Omega \psi R = 0 \tag{6.99}$$

is verified), satisfies

$$\|u\|_{L^{2+\nu}(]0,T[\times\Omega)} \le C_T\left(\|u_{in}\|_{L^2(\Omega)} + K\right), \tag{6.100}$$

where the constant $C_T > 0$ depends only on Ω, T and the constants m_0, m_1.

Proof of Lemma 6.5. The proof relies on the study of the dual problem. More precisely since here we consider very weak types of solutions for (6.98), the analysis can be done rigorously only through (the dual problem of) a "regularized" version of (6.98) (that is, a family of systems with smooth data and from which we can recover asymptotically the original system (6.98) in some sense). The first step of the proof is to define a "regularized" version of (6.98) and study its dual problem (6.107). The second step is to ensure that any solution u (of the original problem) considered is the very limit (in some sense specified later) of the solutions of the "regularized" problem (note that this is a result of uniqueness for the original problem). Finally, the third step is to establish an estimate of the type (6.100) for the solution of the "regularized" system, so that (6.100) follows after passage to the limit.

First step : regularization and dual problem. Let $(\rho^\epsilon)_{0<\epsilon<1}$ be a family of mollifiers on $\mathbb{R}^{m+1}$ such that for all $0 < \epsilon < 1$,

$$\rho^\epsilon \ge 0, \qquad \rho^\epsilon \in C_c^\infty(\mathbb{R}^{m+1}), \qquad \operatorname{supp}\rho^\epsilon \subset B_{m+1}(0,\epsilon), \qquad \int_\mathbb{R}\int_{\mathbb{R}^m}\rho^\epsilon = 1. \tag{6.101}$$

We extend M by $(m_0+m_1)/2$ on a layer of width 1 around $]0,T[\times\Omega$, then extend it by 0 on $\mathbb{R}^{m+1}$, that is,

$$M(t,x) = (m_0+m_1)/2 \quad \text{if} \quad 0 < \operatorname{dist}((t,x),]0,T[\times\Omega) < 1, \tag{6.102}$$

$$M(t,x) = 0 \quad \text{if} \quad 1 < \operatorname{dist}((t,x),]0,T[\times\Omega), \tag{6.103}$$

and we define the family $M^\epsilon := [\rho^\epsilon * M]_{|[0,T]\times\overline{\Omega}}$ (convolution in $\mathbb{R}^{m+1}$ then restriction on $[0,T]\times\overline{\Omega}$). Therefore

$$\text{for all } \epsilon \in]0,1[, \qquad M^\epsilon \in C^\infty([0,T]\times\overline{\Omega}), \qquad m_0 \le M^\epsilon \le m_1, \tag{6.104}$$

$$\text{for all } p \in [1,\infty[, \qquad M^\epsilon \longrightarrow M \text{ in } L^p(]0,T[\times\Omega) \quad \text{when} \quad \epsilon \longrightarrow 0. \tag{6.105}$$

We also define a family $(u_{in}^\epsilon)_\epsilon$ of smooth functions on $\overline{\Omega}$, which are identically zero on a (ϵ-dependent) neighborhood of $\partial\Omega$, and which approximates u_{in} in $\mathrm{L}^2(\Omega)$.

We are now ready to consider the following problem (which can be seen as a "regularized" version of (6.98))

$$\begin{cases} \partial_t u^\epsilon - \Delta_x(M^\epsilon u^\epsilon) = R \text{ in }]0,T[\times\Omega, \\ u^\epsilon(0,x) = u^\epsilon_{in}(x) \text{ in } \Omega, \\ \nabla_x(M^\epsilon u^\epsilon)(t,x)\cdot n(x) = 0 \text{ on }]0,T[\times\partial\Omega, \end{cases} \tag{6.106}$$

Note that since M^ϵ is C^∞, we can always write $\Delta_x[M^\epsilon u^\epsilon] = \Delta_x M^\epsilon\, u^\epsilon + 2\nabla_x M^\epsilon \cdot \nabla_x u^\epsilon + M^\epsilon\, \Delta_x u^\epsilon$ in the sense of distributions (for u^ϵ a distribution). By classical results of the Theory of Linear Parabolic Equations (see for example Theorem 9.1, together with the final sentence in paragraph 9, in Chapter IV in [33]), there exists a unique u^ϵ satisfying $\partial_t u^\epsilon$, $\nabla^2_x u^\epsilon \in \mathrm{L}^q(]0,T[\times\Omega)$ which solves the problem (6.106) in the strong sense.
We now introduce the dual problem

$$\begin{cases} \partial_t v^\epsilon + M^\epsilon \Delta_x v^\epsilon = f \text{ in } [0,T]\times\overline{\Omega}, \\ v^\epsilon(T,x) = 0 \text{ in } \overline{\Omega}, \\ \nabla_x v^\epsilon(t,x)\cdot n(x) = 0 \text{ on } [0,T]\times\partial\Omega, \end{cases} \tag{6.107}$$

where f is any smooth function on $[0,T]\times\overline{\Omega}$. Since M^ϵ and f are smooth, this problem has a unique classical solution $v^\epsilon \in C^\infty([0,T]\times\overline{\Omega})$ (see for example Theorem 5.3, Chapter IV in [33]). We claim that there exists $\nu_1 \in]0,1[$ depending only on Ω, m_0, m_1 such that for all $r \in [2-\nu_1, 2+\nu_1]$ and all $\epsilon \in]0,1[$,

$$\begin{aligned} \|\Delta_x v^\epsilon\|_{\mathrm{L}^r(]0,T[\times\Omega)} &\le C(\Omega, m_0, m_1, p)\|f\|_{\mathrm{L}^r(]0,T[\times\Omega)}, \\ \|v^\epsilon(0,\cdot)\|_{\mathrm{L}^2(\Omega)} &\le C(\Omega, m_0, m_1, p, T)\|f\|_{\mathrm{L}^r(]0,T[\times\Omega)}. \end{aligned} \tag{6.108}$$

Lemma 2.2 (together with Remark 2.3) in [7] states that for any $r \in]1,2[$, if (with the notations of [7])

$$C_{\frac{m_0+m_1}{2},r}\frac{m_1-m_0}{2} < 1, \tag{6.109}$$

then (6.108) is true. The proof of Lemma 2.2 (and Remark 2.3) never uses the fact $r<2$, so we can use that (6.109) $\Longrightarrow$ (6.108) for any $r>1$. It therefore suffices to check (6.109) for $|r-2|$ small. This is done in the case $r<2$ in the proof of Lemma 3.2 in [7]. For $r>2$, following the ideas of the proof of Lemma 3.2, an appropriate interpolation leads to the bound for all $m>0$, $4>r>2$

$$C_{m,r} \le m^{-\theta} C_{m,4}^{1-\theta}, \qquad \text{where} \qquad \frac{\theta}{2} + \frac{1-\theta}{4} = \frac{1}{r}, \tag{6.110}$$

that is, for all $m>0$, $4>r>2$,

$$C_{m,p} \le m^{1-4/r} C_{m,4}^{2-4/r}. \tag{6.111}$$

Therefore for all $2<r<4$,

$$C_{\frac{m_0+m_1}{2},r}\frac{m_1-m_0}{2} \le \left(\frac{m_0+m_1}{2}\right)^{1-4/r} C^{2-4/r}_{\frac{m_0+m_1}{2},4}\frac{m_1-m_0}{2}. \tag{6.112}$$

The RHS is a numerical function depending only on Ω, m_0, m_1 and r, and it tends to $\frac{m_1-m_0}{m_0+m_1} < 1$ when $r>2$ tends to 2. Therefore there exists a small $\nu_1>0$ depending only on Ω, m_0, m_1 such that the RHS is <1 for all $2<r\le 2+\nu_1$. This implies (6.109) for all $2<r\le 2+\nu_1$.

Second step : uniqueness. Let $p \in [2, 2+\nu_1[$ and let u be a very weak solution of (6.98) such that $u \in \mathrm{L}^{p'}$ (where $1/p+1/p'=1$). We claim that u is the (unique) strong limit in $\mathrm{L}^{(2+\nu_1)'}$ of the family $(u^\epsilon)_\epsilon$ defined in (6.106).

Since v^ϵ is a smooth function satisfying the homogeneous Neumann boundary condition, we can use it as a test function in (6.99) and against (6.106). Subtracting the two equalities thus obtained, we get

$$\int_0^T\int_\Omega (u^\epsilon - u)\partial_t v^\epsilon + \int_\Omega (u^\epsilon_{in} - u_{in})v^\epsilon(0,\cdot) + \int_0^T\int_\Omega (M^\epsilon u^\epsilon - Mu)\Delta_x v^\epsilon = 0. \tag{6.113}$$

Using the smoothness of v^ϵ, f and using $u^\epsilon, u \in \mathrm{L}^1$, we can perform rigorously the following computations : we use the definition of v^ϵ in (6.107)

$$\int_0^T\int_\Omega (u^\epsilon - u)\partial_t v^\epsilon = -\int_0^T\int_\Omega M^\epsilon(u^\epsilon-u)\Delta_x v^\epsilon + \int_0^T\int_\Omega (u^\epsilon - u)f,$$

and replace in (6.113) to get

$$\int_0^T \int_\Omega (u^\epsilon - u) f + \int_\Omega (u_{in}^\epsilon - u_{in}) v^\epsilon(0,\cdot) + \int_0^T \int_\Omega (M^\epsilon - M) u \Delta_x v^\epsilon = 0.$$

Using (6.108) with $r = 2 + \nu_1$ and Hölder's inequality, it yields

$$\begin{aligned} &\left| \int_0^T \int_\Omega (u^\epsilon - u) f \right| \\ \leq \quad & \left| \int_\Omega (u_{in}^\epsilon - u_{in}) v^\epsilon(0,\cdot) \right| + \left| \int_0^T \int_\Omega (M^\epsilon - M) u \Delta_x v^\epsilon \right| \\ \leq \quad & C(\Omega, m_0, m_1, T) \left(\|u_{in}^\epsilon - u_{in}\|_{\mathrm{L}^2(\Omega)} + \|(M^\epsilon - M) u\|_{\mathrm{L}^{(2+\nu_1)'}(]0,T[\times\Omega)} \right) \|f\|_{\mathrm{L}^{2+\nu_1}(]0,T[\times\Omega)}. \end{aligned}$$

By duality, we obtain

$$\|u^\epsilon - u\|_{\mathrm{L}^{(2+\nu_1)'}(]0,T[\times\Omega)} \leq C(\Omega, m_0, m_1, T) \left(\|u_{in}^\epsilon - u_{in}\|_{\mathrm{L}^2(\Omega)} + \|(M^\epsilon - M) u\|_{\mathrm{L}^{(2+\nu_1)'}(]0,T[\times\Omega)} \right).$$

Using again Hölder's inequality, we end up with

$$\begin{aligned} &\|u^\epsilon - u\|_{\mathrm{L}^{(2+\nu_1)'}(]0,T[\times\Omega)} \\ &\leq C(\Omega, m_0, m_1, T) \left(\|u_{in}^\epsilon - u_{in}\|_{\mathrm{L}^2(\Omega)} + \|M^\epsilon - M\|_{\mathrm{L}^s(]0,T[\times\Omega)} \|u\|_{\mathrm{L}^{p'}(]0,T[\times\Omega)} \right), \end{aligned}$$

where $1/(2+\nu_1) + 1/s = 1/p$. Letting ϵ tend to zero, we get that $\|u^\epsilon - u\|_{\mathrm{L}^{(2+\nu_1)'}(]0,T[\times\Omega)} \to 0$.

Third step : uniform bound for the regularized problem. Let us choose $f \leq 0$ in (6.107). By the maximum principle, we have $v^\epsilon \geq 0$. Since v^ϵ is a smooth function, we can use it as a test function against (6.106). We get

$$\int_0^T \int_\Omega u^\epsilon \partial_t v^\epsilon + \int_\Omega u_{in}^\epsilon v^\epsilon(0,\cdot) + \int_0^T \int_\Omega M^\epsilon u^\epsilon \Delta_x v^\epsilon + \int_0^T \int_\Omega R v^\epsilon = 0. \tag{6.114}$$

As before, using the smoothness of v^ϵ, f and using $u^\epsilon \in \mathrm{L}^1$, we can rigorously compute

$$\int_0^T \int_\Omega u^\epsilon \partial_t v^\epsilon = -\int_0^T \int_\Omega M^\epsilon u^\epsilon \Delta_x v^\epsilon + \int_0^T \int_\Omega u^\epsilon f, \tag{6.115}$$

and replace in (6.114) to get

$$-\int_0^T \int_\Omega u^\epsilon f = \int_\Omega u_{in}^\epsilon v^\epsilon(0,\cdot) + \int_0^T \int_\Omega R v^\epsilon \leq \int_\Omega u_{in}^\epsilon v^\epsilon(0,\cdot) + K \int_0^T \int_\Omega v^\epsilon, \tag{6.116}$$

where we have used the bound $R \leq K$ and the nonnegativity of v^ϵ. The last term can be rewritten

$$K \int_0^T \int_\Omega v^\epsilon = K \int_0^T \int_0^t \int_\Omega \partial_t v^\epsilon = K \int_0^T \int_0^t \int_\Omega [-M^\epsilon \Delta_x v^\epsilon + f]. \tag{6.117}$$

Replacing in (6.116) and using (6.108) with $r = 2 - \nu_1$ and Hölder's inequality, it gives

$$\int_0^T \int_\Omega u^\epsilon(-f) \leq C(\Omega, m_0, m_1, T) \left(\|u_{in}^\epsilon\|_{\mathrm{L}^2(\Omega)} + K \right) \|f\|_{\mathrm{L}^{2-\nu_1}(]0,T[\times\Omega)}. \tag{6.118}$$

Using the strong convergence of u^ϵ in L^1 and the smoothness of f to pass to the limit in the LHS, we get

$$\int_0^T \int_\Omega u(-f) \leq C(\Omega, m_0, m_1, T) \left(\|u_{in}\|_{\mathrm{L}^2(\Omega)} + K \right) \|f\|_{\mathrm{L}^{2-\nu_1}(]0,T[\times\Omega)}. \tag{6.119}$$

Since $u \geq 0$ by assumption, this yields by duality

$$\|u\|_{\mathrm{L}^{(2-\nu_1)'}(]0,T[\times\Omega)} \leq C(\Omega, m_0, m_1, T) \left(\|u_{in}\|_{\mathrm{L}^2(\Omega)} + K \right). \tag{6.120}$$

This concludes the proof for some $0 < \nu < \min\{(2-\nu_1)' - 2, 2 - (2+\nu_1)'\}$. □

We are now ready to perform the

End of proof of i) and proof of ii). Let $\alpha = 0$ and a, d satisfy condition (6.96). Let $(a_\epsilon)_\epsilon \subset [a/2, a]$ and $(d_\epsilon)_\epsilon \subset [d/2, d]$ be two (strictly) increasing families of real numbers such that $a_\epsilon \to a$ and $d_\epsilon \to d$ when $\epsilon \to 0$. This implies that for all $\epsilon > 0$, $a_\epsilon < 1 = 1 + \alpha$ and $d_\epsilon < 2 = 2 + \alpha$, so that condition (6.18) is satisfied with (a, d) replaced by (a_ϵ, d_ϵ). Therefore, we can apply the results of Section 6.4 with this choice of parameters. For all $\epsilon > 0$, there exists a weak solution $(u_\epsilon \geq 0, v_\epsilon \geq 0)$ of (6.1)–(6.4) with (a, d) replaced by (a_ϵ, d_ϵ). Furthermore, for any fixed $T > 0$, this solution satisfies estimates (6.9)–(6.13) (and (6.14), resp. (6.15) when $\log u_{in}$, resp. $\log v_{in}$, is in $\mathrm{L}^1(\Omega)$) with (u, v) replaced by (u_ϵ, v_ϵ). Since the constant $C(..., \mathrm{D})$ is chosen to be continuous in D on the set $\{\mathrm{D} : a \leq 1 + \alpha,\ d \leq 2 + \alpha\}$, the estimates actually give uniform bounds w.r.t. ϵ. As a consequence, we have the following uniform (w.r.t. ϵ) bounds (for all $p > 0$)

$$u_\epsilon \in \mathrm{L}^2, \qquad v_\epsilon \in \mathrm{L}^\infty, \qquad \nabla_x \log(1 + u_\epsilon) \in \mathrm{L}^2, \qquad \nabla_x v_\epsilon^p \in \mathrm{L}^2. \tag{6.121}$$

Let us check that we can apply Lemma 6.5 to u_ϵ. We define $R_\epsilon := (r_u - r_a u_\epsilon^{a_\epsilon} - r_b v_\epsilon^b) u_\epsilon$ and $M_\epsilon := d_u + d_\alpha + d_\beta v_\epsilon^\beta$. For all $\epsilon > 0$, $R_\epsilon \in \mathrm{L}^{q_\epsilon}$ where $q_\epsilon := 2/(1 + a_\epsilon) > 1$, and

$$R_\epsilon \leq \sup_{u \geq 0} (r_u - r_a u^{a_\epsilon}) u = r_u \frac{a_\epsilon}{a_\epsilon + 1} \left(\frac{r_u}{r_a (a_\epsilon + 1)} \right)^{1/a_\epsilon} \leq r_u \left(\frac{r_u}{r_a} \right)^{1/a_\epsilon} \leq K,$$

where $K := r_u \left(\frac{r_u}{r_a} \right)^{2/a}$ if $r_u > r_a$, $K := r_u \left(\frac{r_u}{r_a} \right)^{1/a}$ if $r_u < r_a$. Thanks to the bound (6.9) for v_ϵ, we also have for all $\epsilon > 0$, $M_\epsilon \in L^\infty$ and

$$0 < m_0 := d_u + d_\alpha \leq M_\epsilon \leq d_u + d_\alpha + d_\beta \max \left\{ \sup_\Omega v_{in}^\beta, \left(\frac{r_v}{r_c} \right)^{\beta/c} \right\} =: m_1 < \infty.$$

We can therefore apply Lemma 6.5, which yields the bound for all $\epsilon > 0$

$$\|u_\epsilon\|_{L^{2+\nu}} \leq C(T, \Omega, m_0, m_1) \left(\|u_{in}\|_{L^2(\Omega)} + K \right), \tag{6.122}$$

where $\nu = \nu(\Omega, m_0, m_1) > 0$. Note that the constants K, m_0 and m_1 being independent of ϵ, this bound is also independent of ϵ.

From (6.121), (6.122), we have the uniform (w. r. t. ϵ) bounds

$$\nabla_x u_\epsilon \in \mathrm{L}^{1+\nu/(4+\nu)}, \qquad \nabla_x v^\epsilon \in \mathrm{L}^2, \tag{6.123}$$

$$(r_u - r_a u_\epsilon^{a_\epsilon} - r_b v_\epsilon^b) u_\epsilon \in \mathrm{L}^{1+\nu/2}, \qquad (r_v - r_c v_\epsilon^c - r_d u_\epsilon^{d_\epsilon}) v_\epsilon \in \mathrm{L}^{1+\nu/2}, \tag{6.124}$$

$$(d_u + d_\alpha + d_\beta v_\epsilon^\beta) u_\epsilon \in \mathrm{L}^{2+\nu}, \qquad (d_v + d_\gamma v_\epsilon^\gamma) v_\epsilon \in \mathrm{L}^\infty, \tag{6.125}$$

where we used the computation $\nabla_x u_\epsilon = (1 + u_\epsilon) \nabla_x \log(1 + u_\epsilon) \in \mathrm{L}^{2+\nu} \times \mathrm{L}^2$ for (6.123) and the assumptions on the parameters $a_\epsilon < a \leq 1$ and $d_\epsilon < d \leq 2$ for (6.124). Using the equations of (u_ϵ, v_ϵ), estimates (6.124)–(6.125) yield a uniform (w. r. t. ϵ) bound for $\partial_t u_\epsilon$, $\partial_t v_\epsilon$ in $\mathrm{L}^{1+\nu/2}(]0, T[, \mathrm{W}^{-2,1+\nu/2}(\Omega))$. Combined with the gradient estimates (6.123), this allows us to apply Aubin-Lions Lemma, so that, up to a subsequence, when $\epsilon \longrightarrow 0$,

$$u_\epsilon \longrightarrow u \geq 0 \text{ in } \mathrm{L}^1, \qquad v_\epsilon \longrightarrow v \geq 0 \text{ in } \mathrm{L}^1. \tag{6.126}$$

We obtain estimates (6.9)–(6.15) for (u, v) with the same arguments as in the passage to the limit in estimates (6.75)–(6.80) in Section 6.4, and we obtain (6.16) thanks to (6.122) and Fatou's lemma. As in Section 6.4, estimates (6.9)–(6.13) enable us to check that $(u, v) \in \mathrm{L}^{\max(1+a,d)} \times \mathrm{L}^\infty$ with $\nabla_x[(d_u + d_\alpha + d_\beta v^\beta) u]$ and $\nabla_x[(d_v + d_\gamma v^\gamma) v]$ in L^1. Using furthermore estimates (6.124) and (6.125), it is classical to check that (u, v) is a global weak solution of (6.1)–(6.4). □

6.5.2 The case $\gamma = 0$

Proof of iii). When $\gamma = 0$, the system satisfied (in the weak sense) by v can be rewritten as

$$\partial_t v - d_v' \Delta_x v = f \qquad \text{in } \mathbb{R}_+ \times \Omega, \tag{6.127}$$

$$\nabla_x v \cdot n = 0 \qquad \text{on } \mathbb{R}_+ \times \partial\Omega, \tag{6.128}$$

$$v(0, \cdot) = v_{in} \qquad \text{in } \Omega, \tag{6.129}$$

where $d'_v = d_v + d_\gamma > 0$, $f = v\,(r_v - r_c\, v^c - r_d\, u^d) \in \mathrm{L}^q_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ (thanks to the estimates (6.9), (6.10) and (6.16)) and $v_{in} \in W^{2,q}(\Omega)$ (by assumption). Using the properties of the heat kernel, we get the $\mathrm{L}^q_{loc}(\mathbb{R}_+ \times \overline{\Omega})$ bounds for $\partial_t v$ and $\nabla^2_x v$ stated in (6.17). The bound for $\nabla_x v$ is obtained by interpolating (6.9) and the bound for $\nabla^2_x v$. $\square$

Troisième partie

Régularité de l'équation de Boltzmann en domaine borné

Chapitre 7

Regularity of the Boltzmann equation in convex domains

Abstract

This Chapter is an extract from the paper [77] in collaboration with Y. Guo, C. Kim and D. Tonon. The basic question of the regularity of the solution of the Boltzmann equation in the presence of physical boundary conditions has long been open due to two effects in competition : on the one hand, the characteristic nature of the boundary; on the other hand, the non-local mixing of the collision operator. We consider the Boltzmann equation in a strictly convex domain with the diffuse boundary condition. We first construct weighted $W^{1,p}$ solutions for $1 < p < 2$. With the aid of a distance function towards the grazing set, we construct weighted $W^{1,p}$ solutions for $2 \leq p \leq \infty$, then we construct classical C^1 solutions away from the grazing boundary. To complete the results, we show that second derivatives do not exist up to the boundary in general by constructing counterexamples.

Sommaire

7.1 Introduction

Boundary effects play an important role in the dynamics of the solutions of the Boltzmann equation

$$\partial_t F + v \cdot \nabla_x F = Q(F, F), \tag{7.1}$$

where $F(t, x, v)$ denotes the particle distribution at time t, position $x \in \Omega$ and velocity $v \in \mathbb{R}^3$. Throughout this paper the collision operator takes the form

$$\begin{aligned} Q(F_1, F_2) &:= Q_{\text{gain}}(F_1, F_2) - Q_{\text{loss}}(F_1, F_2) \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} |v-u|^\kappa q_0(\theta)\Big[F_1(u')F_2(v') - F_1(u)F_2(v)\Big]\mathrm{d}\omega\mathrm{d}u, \end{aligned} \tag{7.2}$$

where $u' = u + [(v-u)\cdot\omega]\omega$, $v' = v - [(v-u)\cdot\omega]\omega$ and $0 \le \kappa \le 1$ (hard potential) and $0 \le q_0(\theta) \le C|\cos\theta|$ (angular cutoff) with $\cos\theta = \frac{v-u}{|v-u|}\cdot\omega$.

Despite extensive developments in the study of the Boltzmann equation, many basic questions regarding solutions in a physical bounded domain, such as their regularity, have remained largely open. This is partly due to the characteristic nature of boundary conditions in the kinetic theory. In [75], it is shown that in convex domains, Boltzmann solutions are continuous away from the grazing set. On the other hand, in [81], it is shown that singularity (discontinuity) does occur for Boltzmann solutions in a non-convex domain, and such singularity propagates precisely along the characteristics emanating from the grazing set. The boundary of the phase space is

$$\gamma := \{(x, v) \in \partial\Omega \times \mathbb{R}^3\},$$

where $n = n(x)$ is the outward normal direction at $x \in \partial\Omega$. We decompose γ as

$$\begin{aligned} \gamma_- &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x)\cdot v < 0\}, && (\textit{the incoming set}), \\ \gamma_+ &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x)\cdot v > 0\}, && (\textit{the outcoming set}), \\ \gamma_0 &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x)\cdot v = 0\}, && (\textit{the grazing set}). \end{aligned}$$

In general the boundary condition is imposed only for the incoming set γ_- for general kinetic PDEs [63, 65, 73, 75].

Throughout this paper we assume that Ω is a bounded open subset of $\mathbb{R}^3$ and that there exists $\xi : \mathbb{R}^3 \to \mathbb{R}$ such that $\Omega = \{x \in \mathbb{R}^3 : \xi(x) < 0\}$, and $\partial\Omega = \{x \in \mathbb{R}^3 : \xi(x) = 0\}$. Moreover we assume that the domain is smooth ($\xi \in C^3$) and *strictly convex*, that is, for all $x \in \bar{\Omega} = \Omega \cup \partial\Omega$ (therefore $\xi(x) \le 0$),

$$\sum_{i,j} \partial_{ij}\xi(x)\zeta_i\zeta_j \ge C_\xi|\zeta|^2 \quad \text{for all} \quad \zeta \in \mathbb{R}^3. \tag{7.3}$$

We assume that $\nabla\xi(x) \neq 0$ when $|\xi(x)| \ll 1$ and we define the *outward normal* as $n(x) \equiv \frac{\nabla\xi(x)}{|\nabla\xi(x)|}$.

We consider the diffuse boundary condition : for $(x, v) \in \gamma_-$

$$F(t, x, v) = c_\mu \mu(v)\int_{n(x)\cdot u > 0} F(t, x, u)\{n(x)\cdot u\}\mathrm{d}u,$$

where $c_\mu \int_{n(x)\cdot u>0} \mu(u)\{n(x)\cdot u\}\mathrm{d}u = 1$.

For $(x, v) \in \bar{\Omega} \times \mathbb{R}^3$ we define the *backward exit time* $t_{\mathbf{b}}(x, v)$ by

$$t_{\mathbf{b}}(x, v) := \inf\{\tau > 0 : x - \tau v \notin \Omega\}, \tag{7.4}$$

and, for $v \neq 0$, $x_{\mathbf{b}}(x, v) := x - t_{\mathbf{b}} v \in \partial\Omega$.

The characteristics ODE of the Boltzmann equation (7.1) is

$$\frac{\mathrm{d}X(s)}{\mathrm{d}s} = V(s), \quad \frac{\mathrm{d}V(s)}{\mathrm{d}s} = 0.$$

Before the trajectory hits the boundary, $t - s < t_{\mathbf{b}}(x, v)$, we have $[X(s; t, x, v), V(s; t, x, v)] = [x - (t-s)v, v]$ with the initial condition $[X(t; t, x, v), V(t; t, x, v)] = [x, v]$. On the other hand, when the trajectory hits the boundary we define the generalized characteristics as follows :

Definition 7.1 ([75]). *Let $(x, v) \notin \gamma_0$, $v \neq 0$.*
We define recursively the stochastic (diffuse) cycles by $(t^0, x^0, v^0) := (t, x, v)$ and for $\ell \geq 0$,

$$\begin{aligned} &\text{pick up some } v^{\ell+1} \text{ such that } n(x_{\mathbf{b}}(x^\ell, v^\ell)) \cdot v^{\ell+1} > 0 \quad \text{and define} \\ &(t^{\ell+1}, x^{\ell+1}, v^{\ell+1}) := (t^\ell - t_{\mathbf{b}}(x^\ell, v^\ell), x_{\mathbf{b}}(x^\ell, v^\ell), v^{\ell+1}). \end{aligned} \tag{7.5}$$

We define the backward trajectory as

$$X_{\mathbf{cl}}(s; t, x, v) \;:=\; \sum_\ell \mathbf{1}_{[t^{\ell+1}, t^\ell)}(s)\big\{x^\ell - (t^\ell - s)v^\ell\big\}, \quad V_{\mathbf{cl}}(s; t, x, v) \;:=\; \sum_\ell \mathbf{1}_{[t^{\ell+1}, t^\ell)}(s) v^\ell.$$

Note that if $G(t, x, v)$ solves $\partial_t G + v \cdot \nabla_x G = 0$ with the diffuse boundary condition then

$$G(t, x, v) = G(s, X_{\mathbf{cl}}(s; t, x, v), V_{\mathbf{cl}}(s; t, x, v)).$$

In this paper we establish the first Sobolev regularity away from the grazing set γ_0 for Boltzmann solutions in convex domains. One of the crucial ingredient is the construction of a distance function towards the grazing set γ_0 to achieve this goal.

Definition 7.2 (Kinetic Distance). *For $(x, v) \in \bar{\Omega} \times \mathbb{R}^3$,*

$$\alpha(x, v) := |v \cdot \nabla \xi(x)|^2 - 2\{v \cdot \nabla^2 \xi(x) \cdot v\}\xi(x).$$

Due to (7.3), the kinetic distance $\alpha(x, v)$ vanishes if and only if $(x, v) \in \gamma_0$. The important technique to treat α along the trajectory is based on the geometric lemma :

Lemma 7.1 (Velocity lemma, Lemma 1 of [75]). *Along the backward trajectory we define*

$$\alpha(s; t, x, v) := \alpha(X_{\mathbf{cl}}(s; t, x, v), V_{\mathbf{cl}}(s; t, x, v)).$$

Then there exists $\mathcal{C} = \mathcal{C}(\xi) > 0$ such that, for all $0 \leq s_1, s_2 \leq t$,

$$e^{-\mathcal{C}|v||s_1 - s_2|}\alpha(s_1; t, x, v) \;\leq\; \alpha(s_2; t, x, v) \;\leq\; e^{\mathcal{C}|v||s_1 - s_2|}\alpha(s_1; t, x, v).$$

Proof. The proof is basically the same as the proof of Lemma 1 of [75] but the definition of α is slightly different. By explicit computation, we have

$$\begin{aligned} v \cdot \nabla_x \alpha &= 2v \cdot \nabla \xi(x)[v \cdot \nabla^2 \xi \cdot v] - 2v \cdot \nabla \xi(x)[v \cdot \nabla^2 \xi \cdot v] - 2v\{v \cdot \nabla^3 \xi(x) \cdot v\}\xi(x) \\ &= -2v\{v \cdot \nabla^3 \xi(x) \cdot v\}\xi(x) = O_\xi(1)|v|^3|\xi(x)| \\ &= O_\xi(1)|v|\alpha(x, v), \end{aligned} \tag{7.6}$$

where we used $\{v \cdot \nabla^2 \xi(x) \cdot v\} \backsim |v|^2$ from (7.3). Therefore there exists $\mathcal{C} = \mathcal{C}_\xi > 0$ such that

$$-\mathcal{C}|v|\alpha(x, v) \;\leq\; v \cdot \nabla_x \alpha(x, v) \;\leq\; \mathcal{C}|v|\alpha(x, v).$$

Since $\frac{d}{ds}\alpha(X_{\mathbf{cl}}(s; t, x, v), V_{\mathbf{cl}}(s; t, x, v)) = v \cdot \nabla_x \alpha(X_{\mathbf{cl}}(s; t, x, v), V_{\mathbf{cl}}(s; t, x, v))$, we conclude the lemma. $\square$

This crucial invariant property of α under operator $v \cdot \nabla_x$ is the key for our analysis. On the other hand, unless $\nabla^3 \xi \equiv 0$ (which is the case for example when the domain is a ball or an ellipsoid), a growth factor $|v|$ creates a geometric effect which is out of control for our analysis. We introduce a strong decay factor $e^{-\varpi \langle v \rangle t}$ with sufficiently large $\varpi > 0$ to overcome such a geometric effect : consider

$$e^{-\varpi \langle v \rangle t}\alpha(x, v). \tag{7.7}$$

A direct computation yields

$$\begin{aligned} \{\partial_t + v \cdot \nabla_x\}[e^{-\varpi \langle v \rangle t}\alpha(x, v)] &= -\varpi \langle v \rangle e^{-\varpi \langle v \rangle t}\alpha(x, v) - e^{-\varpi \langle v \rangle t} 2v\{v \cdot \nabla^3 \xi(x) \cdot v\} \\ &\lesssim (-\varpi + O_\xi(1))\langle v \rangle e^{-\varpi \langle v \rangle t}\alpha(x, v), \end{aligned}$$

with the geometric contribution $O_\xi(1) = \frac{2v\{v \cdot \nabla^3 \xi(x) \cdot v\}\xi}{\alpha \langle v \rangle}$ where we used the convexity of ξ in (7.3). Throughout this paper we assume

$$\varpi > \max \frac{2v\{v \cdot \nabla^3 \xi(x) \cdot v\}\xi}{\alpha \langle v \rangle}. \tag{7.8}$$

Remark that if ξ is quadratic (for example if the domain is a ball or an ellipsoid) then we are able to set $\varpi = 0$ and $\{\partial_t + v\cdot\nabla_x\}\alpha \equiv 0$.

We denote $F = \sqrt{\mu} f$ (but we do not assume that f is small) where $\mu = e^{-\frac{|v|^2}{2}}$ is a global normalized Maxwellian. Then f satisfies

$$\partial_t f + v\cdot\nabla_x f = \Gamma_{\text{gain}}\,(f,f) - \nu(\sqrt{\mu} f) f. \tag{7.9}$$

Here

$$\begin{aligned}\nu(\sqrt{\mu}f)(v) = \nu(F)(v) &:= \frac{1}{\sqrt{\mu(v)}} Q_{\text{loss}}(\sqrt{\mu}f,\sqrt{\mu}f)(v)\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-u,\omega)\sqrt{\mu(u)} f(u)\mathrm{d}\omega\mathrm{d}u,\end{aligned} \tag{7.10}$$

and the gain term of the nonlinear Boltzmann operator is given by

$$\begin{aligned}\Gamma_{\text{gain}}(f_1,f_2)(v) &:= \frac{1}{\sqrt{\mu}} Q_{\text{gain}}(\sqrt{\mu}f_1,\sqrt{\mu}f_2)(v)\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-u,\omega)\sqrt{\mu(u)} f_1(u') f_2(v')\mathrm{d}\omega\mathrm{d}u.\end{aligned} \tag{7.11}$$

The diffuse boundary condition, once rewritten for f, is :

$$f(t,x,v) = c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \quad \text{on } \gamma_-. \tag{7.12}$$

Notation We write $X \lesssim Y$ when there exists a constant $C > 0$ (independant of X and Y) such that $X \leq CY$. We write $X \lesssim_\alpha Y$ in the same situation when we want to emphasize that the constant $C = C(\alpha)$ depends on some quantity α.

7.1.1 Main results : propagation of Sobolev regularity

We denote $||\cdot||_p$ the $L^p(\Omega\times\mathbb{R}^3)$ norm, while $|\cdot|_{\gamma,p}$ is the $L^p(\partial\Omega\times\mathbb{R}^3;\mathrm{d}\gamma)$ norm and $|\cdot|_{\gamma_\pm,p} = |\cdot\mathbf{1}_{\gamma_\pm}|_{\gamma,p}$ where $\mathrm{d}\gamma = |n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v$ with the surface measure $\mathrm{d}S_x$ on $\partial\Omega$. Denote $\langle v\rangle = \sqrt{1+|v|^2}$. We define

$$\partial_t f(0) = \partial_t f_0 \equiv -v\cdot\nabla_x f_0 + \Gamma_{\text{gain}}(f_0,f_0) - \nu(\sqrt{\mu}f_0)f_0. \tag{7.13}$$

Throughout this paper we always assume

$$F_0 = \sqrt{\mu} f_0 \geq 0.$$

Theorem 7.1. *Let $0\leq\kappa\leq 1$ in (7.2), $1<p<2$, and $0<\theta<\frac{1}{4}$. Assume $f_0\in W^{1,p}(\Omega\times\mathbb{R}^3)$ and $||\nabla_x f_0||_p + ||\nabla_v f_0||_p + ||e^{\theta|v|^2} f_0||_\infty < +\infty$ and the compatibility condition on $(x,v)\in\gamma_-$,*

$$f_0(x,v) = c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f_0(x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \tag{7.14}$$

then there exists $T_* = T_*(||e^{\theta|v|^2} f_0||_\infty) > 0$ such that $f\in L^\infty_{loc}([0,T_*);W^{1,p}(\Omega\times\mathbb{R}^3))$ solves the Boltzmann equation (7.9) with diffuse boundary condition (7.12), and for all $0\leq t<T_*$

$$\begin{aligned}&||\nabla_x f(t)||_p^p + ||\nabla_v f(t)||_p^p + \int_0^t \left[\,|\nabla_x f(s)|_{\gamma,p}^p + |\nabla_v f(s)|_{\gamma,p}^p\right]\mathrm{d}s\\ &\lesssim_t\ ||\nabla_x f_0||_p^p + ||\nabla_v f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty),\end{aligned} \tag{7.15}$$

where P is some polynomial.

Furthermore, if $F_0 = \mu + \sqrt{\mu} g_0$ with $||e^{\theta|v|^2} g_0||_\infty \ll 1$, then $T_* = \infty$, that is, the estimate above holds for all $t\geq 0$.

There is no size restriction on the initial data $F_0 = \sqrt{\mu} f_0$. On the other hand, we also remark that from [75, 67], the assumption $||e^{\theta|v|^2} g_0||_\infty \ll 1$ for $F_0 = \mu + \sqrt{\mu} g_0$ ensures a uniform-in-time bound : $\sup_{0\leq t<\infty} ||e^{\theta|v|^2} g(t)||_\infty \lesssim ||e^{\theta|v|^2} g_0||_\infty$ (but not a decay, which requires the supplementary constraint on the mass $\iint_{\Omega\times\mathbb{R}^3} g_0\sqrt{\mu}\mathrm{d}v\mathrm{d}x = 0$). In this case, the estimate (7.15) is a global-in-x estimate which includes the grazing set γ_0 and the constant grows exponentially in time.

Moreover, we show that the estimate (7.15) in Theorem 7.1 for $p < 2$ is indeed optimal even for the free transport equation $\partial_t f + v \cdot \nabla_x f = 0$ with the diffuse boundary condition (Lemma 7.8). In fact, the boundary integral blows up at $p = 2$.

We now illustrate the main ideas of the proof of Theorem 7.1. Clearly, both t and v derivatives behave nicely for the diffuse boundary condition as for $(x, v) \in \gamma_-$,

$$\partial_t f(t,x,v) = c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u>0} \partial_t f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \tag{7.16}$$

$$\nabla_v f(t,x,v) = c_\mu \nabla_v \sqrt{\mu(v)} \int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u. \tag{7.17}$$

Let $\tau_1(x)$ and $\tau_2(x)$ be two unit tangential vectors to $\partial\Omega$ satisfying $\tau_1(x)\cdot n(x) = 0 = \tau_2(x)\cdot n(x)$ and $\tau_1(x)\times\tau_2(x) = n(x)$. Define $\mathcal{T}$ to be the orthonormal transformation from $\{n, \tau_1, \tau_2\}$ to the standard bases $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, i.e. $\mathcal{T}(x)n(x) = \mathbf{e}_1,\ \mathcal{T}(x)\tau_1(x) = \mathbf{e}_2,\ \mathcal{T}(x)\tau_2(x) = \mathbf{e}_3$, and $\mathcal{T}^{-1} = \mathcal{T}^t$. Upon a change of variable : $u' = \mathcal{T}(x)u$, we have

$$n(x)\cdot u = n(x)\cdot\mathcal{T}^t(x)u' = n(x)^t\mathcal{T}^t(x)u' = [\mathcal{T}(x)n(x)]^t u' = \mathbf{e}_1\cdot u' = u_1',$$

then

$$\begin{aligned} &c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\ &= c_\mu\sqrt{\mu(v)}\int_{u_1'>0} f(t,x,\mathcal{T}^t(x)u')\sqrt{\mu(u')}\{u_1'\}\mathrm{d}u', \end{aligned}$$

so that we can further take tangential derivatives ∂_{τ_i} as, for $(x, v) \in \gamma_-$,

$$\begin{aligned} &\partial_{\tau_i} f(t,x,v) \\ &= c_\mu\sqrt{\mu(v)}\int_{u_1'>0}\Big\{\partial_{\tau_i} f(t,x,\mathcal{T}^t(x)u') + \nabla_v f(t,x,\mathcal{T}^t(x)u')\frac{\partial\mathcal{T}^t(x)}{\partial\tau_i}u'\Big\}\sqrt{\mu(u')}\{u_1'\}\mathrm{d}u' \\ &= c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0}\partial_{\tau_i} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\ &\quad + c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0}\nabla_v f(t,x,u)\frac{\partial\mathcal{T}^t(x)}{\partial\tau_i}\mathcal{T}(x)u\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u. \end{aligned} \tag{7.18}$$

The difficulty is always the control of the normal spatial derivative $\partial_n f$. From the general method of proving regularity in PDE with boundary conditions, it is natural to use the Boltzmann equation to solve the normal derivative $\partial_n f$ inside the region, in terms of $\partial_t f$, $\nabla_v f$, and $\partial_\tau f$ as :

$$\partial_n f(t,x,v) = -\frac{1}{n(x)\cdot v}\Big\{\partial_t f + \sum_{i=1}^{2}(v\cdot\tau_i)\partial_{\tau_i} f - \Gamma_{\text{gain}}(f,f) + \nu(\sqrt{\mu}f)f\Big\}, \tag{7.19}$$

at least near $\partial\Omega$. Unfortunately, this standard approach encounters a severe difficulty : $\frac{1}{n(x)\cdot v} \notin L^1_{loc}(\mathbb{R}^3)$ in the velocity space.

The first new ingredient of our approach is to use (7.19) *not* inside the domain, but at the boundary $\partial\Omega$. Using the special feature of the diffuse boundary condition and (7.16), (7.17) and (7.18), we can express $\partial_n f$ at $(x,v) \in \gamma_-$ as

$$
\begin{aligned}
&\partial_n f(t,x,v) \\
&= -\frac{1}{n(x)\cdot v}\Big\{ \sqrt{\mu(v)}\int_{n(x)\cdot u>0} \partial_t f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\
&\qquad + \sum_{i=1}^{2}(v\cdot\tau_i)\sqrt{\mu(v)}\int_{n(x)\cdot u>0} \partial_{\tau_i} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\
&\qquad + \sum_{i=1}^{2}(v\cdot\tau_i)\sqrt{\mu(v)}\int_{n(x)\cdot u>0} \nabla_v f(t,x,u)\frac{\partial \mathcal{T}^t(x)}{\partial \tau_i}\mathcal{T}(x)u\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\
&\qquad - \Gamma_{\mathrm{gain}}(f,f) + \nu(\sqrt{\mu}f)f \Big\}.
\end{aligned}
\tag{7.20}
$$

Due to the additional u integral in (7.20) and the crucial factor $|n(x)\cdot u|$ in the measure $\mathrm{d}\gamma$ on the boundary γ, it is clear that the singularity of $|\partial_n f|^p|n\cdot v|$ in (7.20) is roughly of the order

$$\frac{1}{\{n\cdot v\}^{p-1}},$$

so that its $v-$integration is precisely finite if $1 \le p < 2$.

However, in order to control $\partial_t f, \nabla_v f$ and $\partial_\tau f$ for $p<2$, a new difficulty arises. It is well-known from [75, 67] that a crucial boundary estimate for diffuse boundary takes the form of a L^2-contraction :

$$\int_{\gamma_-} h^2 \mathrm{d}\gamma \le \int_{\gamma_+} h^2\mathrm{d}\gamma.$$

Unfortunately, this is not expected to be valid for $p \neq 2$, so it is impossible to absorb the incoming part γ_- solely by the outgoing part γ_+.

Our second new ingredient is to split the γ_+ integral into the near grazing set γ_+^ε and the remaining part in our boundary representation for the derivatives (7.16), (7.17), (7.18), and (7.20). For small $\varepsilon > 0$ we define γ_+^ε, the set of almost grazing or large (outgoing) velocities at the boundary

$$\gamma_+^\varepsilon = \{(x,v)\in\gamma_+ : v\cdot n(x) < \varepsilon \text{ or } |v| > 1/\varepsilon\}. \tag{7.21}$$

Denote $\partial = [\partial_t, \nabla_x, \nabla_v]$. We can roughly obtain

$$
\begin{aligned}
\int_{\gamma_-}|\partial f|^p &\lesssim \int_{\partial\Omega}\left(\int_{n\cdot v>0}|\partial f|\mu^{1/4}\{n\cdot v\}\mathrm{d}v\right)^p + \text{good terms}, \\
&\lesssim \int_{\partial\Omega}\left(\int_{\{v:(x,v)\in\gamma_+^\varepsilon\}}|\partial f|\mu^{1/4}\{n\cdot v\}\right)^p + \int_{\partial\Omega}\left(\int_{\{v:(x,v)\in\gamma_+\setminus\gamma_+^\varepsilon\}}|\partial f|\mu^{1/4}\{n\cdot v\}\right)^p \\
&\quad + \text{good terms}, \\
&\lesssim \sup_x\left(\int_{\{v:(x,v)\in\gamma_+^\varepsilon\}}\mu^{q/4}\{n\cdot v\}\mathrm{d}v\right)^{p/q}\int_{\gamma_+^\varepsilon}|\partial f|^p\mathrm{d}\gamma + \int_{\gamma_+\setminus\gamma_+^\varepsilon}|\partial f|^p\mathrm{d}\gamma + \text{good terms}.
\end{aligned}
$$

It is important to realize that $\sup_x\left(\int_{\{v:(x,v)\in\gamma_+^\varepsilon\}}\mu^{q/4}\{n\cdot v\}\mathrm{d}v\right)^{p/q}$ has a small measure of order ε, for $p>1$, so that it can be absorbed by the outgoing part $\int_{\gamma_+}$. Fortunately, the outgoing boundary integral $\int_{\gamma_+\setminus\gamma_+^\varepsilon}$ can be further bounded by the integration in the bulk and initial data (Lemma 7.6) thanks to a crucial time integration. On the other hand, such a process produces a large constant in the Gronwall estimates and leads to a growth in time. Of course, such approach breaks down at $p=1$.

Theorem 7.2. *Assume the compatibility condition (7.14) and $0<\kappa\le 1$ and recall (7.13).*

For any fixed $2 \le p < \infty$ and $\frac{p-2}{2p} < \beta < \frac{p-1}{2p}$, if $||\alpha^\beta\nabla_{x,v}f_0||_p + ||e^{\theta|v|^2}f_0||_\infty < \infty$ for some $0<\theta<\frac{1}{4}$, then there exists $T_* = T_*(||e^{\theta|v|^2}f_0||_\infty) > 0$ such that $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f$, $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_v f \in L^\infty_{loc}([0,T_*); L^p(\Omega\times\mathbb{R}^3))$ and for all $0\le t<T_*$,

$$
\begin{aligned}
&||e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_{x,v}f(t)||_p^p + \int_0^t |e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_{x,v}f(s)|_{\gamma,p}^p\mathrm{d}s \\
&\lesssim_t \ ||\alpha^\beta\nabla_{x,v}f_0||_p^p + P(||e^{\theta|v|^2}f_0||_\infty),
\end{aligned}
$$

where P is some polynomial.

If $||\alpha^{1/2}\nabla_{x,v}f_0||_\infty + ||e^{\theta|v|^2}f_0||_\infty < +\infty$ for some $0<\theta<\frac{1}{4}$, then $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v}f \in L^\infty([0,T_*);L^\infty(\Omega\times\mathbb{R}^3))$ such that for all $0\le t<T_*$,

$$||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v}f(t)||_\infty \ \lesssim_t \ ||\alpha^{1/2}\nabla_{x,v}f_0||_\infty + P(||e^{\theta|v|^2}f_0||_\infty).$$

If $\alpha^{1/2}\nabla f_0 \in C^0(\bar{\Omega}\times\mathbb{R}^3)$ and

$$v\cdot\nabla_x f_0 - \Gamma(f_0,f_0) = c_\mu\sqrt{\mu}\int_{n\cdot u>0}\{u\cdot\nabla_x f_0 - \Gamma(f_0,f_0)\}\sqrt{\mu}\{n\cdot u\}\mathrm{d}u, \tag{7.22}$$

is valid for $\gamma_-\cup\gamma_0$, then $f\in C^1$ away from the grazing set γ_0.

Furthermore, if $F_0=\mu+\sqrt{\mu}g_0$ with $||e^{\theta|v|^2}g_0||_\infty \ll 1$, then $T_*=\infty$, that is, the estimates above hold for all $t\ge 0$.

Again, there is no size restriction on the initial data $F_0=\sqrt{\mu}f_0$. On the other hand, we also remark that from [75, 67], the assumption $||e^{\theta|v|^2}g_0||_\infty \ll 1$ for $F_0=\mu+\sqrt{\mu}g_0$ ensures a uniform-in-time bound : $\sup_{0\le t\le\infty}||e^{\theta|v|^2}g(t)||_\infty \lesssim ||e^{\theta|v|^2}g_0||_\infty$ (but not a decay, which requires the supplementary constraint on the mass $\iint_{\Omega\times\mathbb{R}^3} g_0\sqrt{\mu}\mathrm{d}v\mathrm{d}x=0$).

We remark for $\varpi\neq 0$, $\partial f(t)\sim e^{\varpi\langle v\rangle t}$ so that in terms of solution $f(t)$, such an estimate not only creates an exponential growth in time, but also creates less integrability in velocity. Furthermore, when $\varpi\neq 0$, we crucially need a strong weight function $e^{\theta|v|^2}$ to balance such a factor $e^{-\varpi\langle v\rangle t}$, which produces a super exponential growth e^{t^2} in time. We suspect that it is impossible to obtain a uniform in time estimate especially when $\varpi\neq 0$. The distance function α plays an important role in the study of regularity in convex domains for Vlasov equations ([73, 79]), which can be controlled along the characteristics via the geometric Velocity lemma (Lemma 7.1). However, such an approach has not been successful in the study of Boltzmann equation due to the non-local nature of the Boltzmann collision operator, which mixes up different velocities so that their distance towards γ_0 can not be controlled. In addition to the key boundary representation, we establish a delicate estimate for interaction of $e^{-\varpi\langle v\rangle t}\alpha(x,v)$ and the collision kernel $e^{-\varpi\langle v\rangle t}\alpha(x,v)^\beta\Gamma_{\text{gain}}(\frac{\partial f}{e^{-\varpi\langle v\rangle t}\alpha^\beta},f)$ in (7.87) for $\beta<\frac{p-1}{2p}$. An additional requirement $\beta>\frac{p-2}{2p}$ is needed to control the boundary singularity in (7.90). These estimates are sufficient to treat the case for $\beta<1/2$, but unfortunately these fail for the case $\beta=1/2$, which accounts for the important C^1 estimate. In order to establish the C^1 estimate, we employ the Lagrangian view point, estimating along the stochastic cycles [75, 67] in Definition 7.1.

Our fourth new ingredient is the dynamical non-local to local estimates (Lemma 7.2). Even though $e^{-\varpi\langle v\rangle t}\sqrt{\alpha}\Gamma_{\text{gain}}(\frac{\partial f}{e^{-\varpi\langle v\rangle t}\sqrt{\alpha}},f)$ is impossible to estimate directly due to severe singularity of $\frac{1}{e^{-\varpi\langle v\rangle t}\sqrt{\alpha(x,v)}}$ in the velocity space, along the characteristics, $\frac{1}{e^{-\varpi\langle v\rangle(t-s)}\sqrt{\alpha(x-(t-s)v,v)}}$ is integrable in time for a convex domain. Therefore the integral

$$\int_{t-t_{\mathbf{b}}(x,v)}^t e^{-\varpi\langle v\rangle(t-s)}\sqrt{\alpha(x,v)}\Gamma_{\text{gain}}(\frac{\partial f}{e^{-\varpi\langle v\rangle(t-s)}\sqrt{\alpha(x-(t-s)v,v)}},f)\mathrm{d}s$$

can be controlled by first integrating over time, and we can close the desired estimate.

7.1.2 Dynamical non-local to local estimates

Lemma 7.2. *Let $(t,x,v)\in[0,\infty)\times\bar{\Omega}\times\mathbb{R}^3$ and $\frac{1}{2}<\beta<\frac{3}{2}$ and $0<\kappa\le 1$ and $r\in\mathbb{R}$ and $Z(s,x,v)\ge 0$. Let $X_{\mathbf{cl}}(s;t,x,v)=x-(t-s)v$ on $s\in[t-t_{\mathbf{b}}(x,v),t]$.*

For any $\varepsilon>0$, there exist $l\gg_\xi 1$ such that

$$\begin{aligned}
&\int_{t-t_{\mathbf{b}}(x,v)}^t\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)]^\beta}\frac{\langle u\rangle^r}{\langle v\rangle^r}Z(s,x,v)\mathrm{d}u\mathrm{d}s\\
&\lesssim \ \min\left\{\frac{\varepsilon^{\frac{3}{2}-\beta}}{|v|^2\{\alpha(x,v)\}^{\beta-1}},\frac{\{\alpha(x,v)\}^{\frac{1}{4}-\frac{\beta}{2}}|t_Z|^{\frac{3}{2}-\beta}}{|v|^{2\beta-1}}\right\}\sup_{s\in[t-t_{\mathbf{b}}(x,v),t]}\{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\}\\
&\quad+\frac{C_\varepsilon}{\{\alpha(x,v)\}^{\beta-1/2}}\int_{t-t_{\mathbf{b}}(x,v)}^t e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s,
\end{aligned}\tag{7.23}$$

where $t_Z=\sup\{s:Z(s,x,v)\neq 0\}$.

The control of $\int_u \frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}} \frac{1}{\alpha(u)^\beta}$ is addressed throughout such so-called dynamical non-local to local estimates. We discover that the non-local u integration does not destroy the local property, upon a crucial time integration along the characteristics. The proof of such non-local to local estimates are a combination of analytical and geometrical arguments. The first part is a precise estimate of u integration which is bounded via $\frac{1}{|v|^{2\beta-1}|\xi(x-(t-s)v)|^{\beta-1/2}}$. In this part of the proof we make use of a series of change of variables to obtain the precise power. The second part is to relate $\frac{1}{|\xi(x-(t-s)v)|^{\beta-1/2}}$ back to $\frac{1}{\alpha}$. Clearly,

$$\frac{1}{|\xi(x-(t-s)v)|^2} \backsim \frac{1}{\alpha} \backsim \frac{1}{|v\cdot\nabla\xi(x-(t-s)v|^2+|\xi(x-(t-s)v)||v|^2}.$$

for $|\xi(X_{\mathbf{cl}}(s))||v|^2$ larger than $|v\cdot\nabla\xi(X_{\mathbf{cl}}(s))|$. On the other hand, when $|v\cdot\nabla\xi(X_{\mathbf{cl}}(s))|$ dominates, this can only be achieved through a crucial use of time integration and geometric Velocity lemma (Lemma 7.1), by connecting

$$\mathrm{d}t \backsim \frac{\mathrm{d}\xi}{|v\cdot\nabla\xi|},$$

and recover α as in the bound of $\xi-$integration through the geometric Velocity Lemma (Lemma 7.1).

The more striking feature is that not only our estimates retain the local structure for α, but they *gain* $\sqrt{\alpha}$ order of regularity. In order to squeeze out a small constant for $|v|\gg 1$, we need to use the decay of $e^{-l\langle v\rangle(t-s)}$. This requires a precise regrouping of the cycles according to the time scale of

$$t|v|\sim 1.$$

Within such an important time scale, $V_{\mathbf{cl}}(s;t,x,v)$ stays almost *invariant* due to the Velocity Lemma (Lemma 7.1). We then are able to obtain precise estimate for the number of bounces within $t|v|\backsim 1$ and extract smallness from $e^{-l\langle v\rangle(t-s)}$ for $t-s\geq\frac{1}{|v|}$. On the other hand, for $t-s\leq\frac{1}{|v|}$, the smallness comes from Lemma 7.2.

7.1.3 Non-existence of $\nabla^2 f$ up to the boundary

In the appendix, we demonstrate that, our estimates can not be valid for higher order derivatives. Otherwise, if $\partial^2 f$ exists up to the boundary, we observe that from taking second derivatives of the Boltzmann equation :

$$v_n\partial_n^2 f = -\partial_{tn}f-(\partial_n v_n)\partial_n f-\sum_{i=1}^2\partial_n(v_{\tau_i})\partial_{\tau_i}f-\sum_{i=1}^2 v_{\tau_i}\partial_{n\tau_i}f-\nu(F)\partial_n f+\partial_n K(f)+\partial_n\Gamma_{\text{gain}}(f,f).$$

If $|\partial_n f|\geq\frac{1}{\sqrt{\alpha}}$ and $\partial_n K(f)\sim K(\partial_n f)$ then at the boundary we have

$$|\partial_n f|\geq\frac{1}{|v_n|}\notin L^1_{loc}(\mathbb{R}^1),$$

so that $\partial_n K(f)$ is not defined. Since $|\partial_n f|$ is expected to behave at least as bad as $\frac{1}{\sqrt{\alpha}}$, we are able to identify initial conditions such that $|\partial_n f|\geq\frac{1}{|v_n|}$ for some future time.

7.2 Preliminary

7.2.1 Collisional operator estimates

Recall Γ_{gain} and ν in (7.10), (7.11). Thanks to Grad's change of variable [70], we can write

$$\begin{aligned}&\nu(\sqrt{\mu}g)=\int_{\mathbb{R}^3}\mathbf{k}_1(v,u)g(u)\mathrm{d}u,\\&\Gamma_{\text{gain}}(\sqrt{\mu},g)+\Gamma_{\text{gain}}(g,\sqrt{\mu})=\int_{\mathbb{R}^3}\mathbf{k}_2(v,u)g(u)\mathrm{d}u,\end{aligned}\tag{7.24}$$

with

$$\begin{aligned}\mathbf{k}_1(u,v) &= |u-v|^{\kappa} e^{-\frac{|v|^2+|u|^2}{2}} \int_{\mathbb{S}^2} q_0\Big(\frac{v-u}{|v-u|}\cdot\omega\Big)\mathrm{d}\omega,\\ \mathbf{k}_2(u,v) &= \frac{2}{|u-v|^2} e^{-\frac{1}{8}|u-v|^2-\frac{1}{8}\frac{(|u|^2-|v|^2)^2}{|u-v|^2}}\\ &\quad\times\int_{w\cdot(u-v)=0} q_0\Big(\frac{u-v}{\sqrt{|u-v|^2+|w|^2}}\cdot\frac{u-v}{|u-v|}\Big)e^{-|w+\varsigma|^2}(|w|^2+|u-v|^2)^{\frac{\kappa}{2}}\mathrm{d}w,\end{aligned} \tag{7.25}$$

where $\varsigma := \big(\frac{v+u}{2}\cdot\frac{w}{|w|}\big)\frac{w}{|w|}$. See page 315 of [74] for details.

Lemma 7.3. *Let $0\le\kappa\le 1$. Recall Grad's estimate from [70], for all $u,v\in\mathbb{R}^3$,*

$$\begin{aligned}|\mathbf{k}_1(u,v)|+|\mathbf{k}_2(u,v)| &\lesssim \{|v-u|^{\kappa}+|v-u|^{-2+\kappa}\}e^{-\frac{1}{8}|v-u|^2-\frac{1}{8}\frac{(|v|^2-|u|^2)^2}{|v-u|^2}}\\ &\lesssim \frac{e^{-\frac{1}{10}|v-u|^2-\frac{1}{10}\frac{(|v|^2-|u|^2)^2}{|v-u|^2}}}{|v-u|^{2-\kappa}}.\end{aligned}$$

Let $0<\kappa\le 1$, $\varrho>0$, $-2\varrho<\theta<2\varrho$ and $\zeta\in\mathbb{R}$. We have the estimate, for all $v\in\mathbb{R}^3$,

$$\int_{\mathbb{R}^3}\{|v-u|^{\kappa}+|v-u|^{-2+\kappa}\}e^{-\varrho|v-u|^2-\varrho\frac{(|v|^2-|u|^2)^2}{|v-u|^2}}\frac{\langle v\rangle^{\zeta}e^{\theta|v|^2}}{\langle u\rangle^{\zeta}e^{\theta|u|^2}}\mathrm{d}u \lesssim \langle v\rangle^{-1}.$$

Proof. The proof is based on [75]. First note that

$$\frac{\langle v\rangle^{\zeta}e^{\theta|v|^2}}{\langle u\rangle^{\zeta}e^{\theta|u|^2}} \lesssim [1+|v-u|^2]^{\frac{\zeta}{2}}e^{-\theta(|u|^2-|v|^2)},$$

so that it suffices to prove the desired estimate for

$$\int_{\mathbb{R}^3}\{|v-u|^{\kappa}+|v-u|^{-2+\kappa}\}e^{-\varrho|v-u|^2-\varrho\frac{(|v|^2-|u|^2)^2}{|v-u|^2}}[1+|v-u|^2]^{\frac{\zeta}{2}}e^{-\theta(|u|^2-|v|^2)}\mathrm{d}u.$$

Set $v-u=\eta$ in the integral. Now we compute the total exponent of e in the integrand as

$$\begin{aligned}&-\varrho|\eta|^2-\varrho\frac{||\eta|^2-2v\cdot\eta|^2}{|\eta|^2}-\theta\{|v-\eta|^2-|v|^2\}\\ &=-2\varrho|\eta|^2+4\varrho\{v\cdot\eta\}-4\varrho\frac{|v\cdot\eta|^2}{|\eta|^2}-\theta\{|\eta|^2-2v\cdot\eta\}\\ &=(-\theta-2\varrho)\,|\eta|^2+(4\varrho+2\theta)\,v\cdot\eta-4\varrho\frac{|v\cdot\eta|^2}{|\eta|^2}.\end{aligned}$$

Since $-2\varrho<\theta<2\varrho$, the discriminant of the above quadratic form of $|\eta|$ and $\frac{v\cdot\eta}{|\eta|}$ is negative : $(4\varrho+2\theta)^2+16\varrho(-\theta-2\varrho)=4\theta^2-16\varrho^2<0$. We thus have

$$-\varrho|\eta|^2-\varrho\frac{||\eta|^2-2v\cdot\eta|^2}{|\eta|^2}-\theta\{|v-\eta|^2-|v|^2\} \lesssim_{\varrho,\theta} -\Big\{\frac{|\eta|^2}{2}+|v\cdot\eta|\Big\}.$$

Hence, for $0\le\kappa\le 1$ the integral is bounded by

$$\int_{\mathbb{R}^3}\Big\{|\eta|^{\kappa}+|\eta|^{-2+\kappa}\Big\}\langle\eta\rangle^{\zeta}e^{-C_{\varrho,\theta}|\eta|^2}\mathrm{d}\eta \lesssim_{\varrho,\theta,\kappa,\zeta} 1,$$

so that the desired estimate is proved for $|v|\le 1$. Therefore, to conclude Lemma 7.3 it suffices to consider the case $|v|\ge 1$. We make another change of variables $\eta_{\|}=\Big\{\eta\cdot\frac{v}{|v|}\Big\}\frac{v}{|v|}$ and $\eta_{\perp}=\eta-\eta_{\|}$, so that $|v\cdot\eta|=|v||\eta_{\|}|$ and $|v-u|\ge|\eta_{\perp}|$. We can absorb $\langle\eta\rangle^{\zeta}$, $|\eta|\langle\eta\rangle^{\zeta}$ by $e^{-C_{\varrho,\theta}|\eta|^2}$, and bound the integral by

$$\begin{aligned}
&\int_{\mathbb{R}^3}\{1+|\eta|^{-2+\kappa}\}e^{-C_{\varrho,\theta}\left\{\frac{|\eta|^2}{2}+|v\cdot\eta|\right\}}\mathrm{d}\eta\\
&=\int_{\mathbb{R}^3}\{1+|\eta|^{-2+\kappa}\}e^{-\frac{C_{\varrho,\theta}}{2}|\eta|^2}e^{-C_{\varrho,\theta}|v\cdot\eta|}\mathrm{d}\eta\\
&\le\int_{\mathbb{R}^2}\{1+|\eta_\perp|^{-2+\kappa}\}e^{-\frac{C_{\varrho,\theta}}{2}|\eta_\perp|^2}\left\{\int_{\mathbb{R}}e^{-C_{\varrho,\theta}|v|\times|\eta_\parallel|}\mathrm{d}|\eta_\parallel|\right\}\mathrm{d}\eta_\perp\\
&\lesssim\int_{\mathbb{R}^2}\{1+|\eta_\perp|^{-2+\kappa}\}e^{-\frac{C_{\varrho,\theta}}{2}|\eta_\perp|^2}\mathrm{d}\eta_\perp\left\{\langle v\rangle^{-1}\int_0^\infty e^{-C_{\varrho,\theta}y}\mathrm{d}y\right\},\\
&\lesssim_{\varrho,\theta,\kappa}\langle v\rangle^{-1},
\end{aligned}$$

where we used $|v|\ge 1$ to get the third line and we used $0<\kappa\le 1$ to check that the first integral in the fourth line is finite. □

We define

$$\Gamma_{\mathrm{gain},v}(g_1,g_2)(v):=\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}B(v-u,\omega)\nabla_v(\sqrt{\mu})(u)g_1(u')g_2(v')\mathrm{d}\omega\mathrm{d}u, \tag{7.26}$$

where $u'=u-[(u-v)\cdot\omega]\omega$ and $v'=v+[(u-v)\cdot\omega]\omega$.

Lemma 7.4. *Let $0<\theta<\frac14$ and $0\le\kappa\le 1$. Then we have :*
(i) For $(i,j)=(1,2)$ or $(2,1)$,

$$|\Gamma_{\mathrm{gain}}(g_1,g_2)(v)|\ \lesssim_\theta\ ||e^{\theta|v|^2}g_i||_\infty\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_j(u)|\mathrm{d}u, \tag{7.27}$$

and

$$\begin{aligned}
\big|\Gamma_{\mathrm{gain}}(g_1,g_2)(v)\big|&\lesssim_\theta\ \langle v\rangle^\kappa e^{-\theta|v|^2}||e^{\theta|v|^2}g_1||_\infty||e^{\theta|v|^2}g_2||_\infty,\\
|\Gamma_{\mathrm{gain},v}(g_1,g_2)(v)|&\lesssim_\theta\ \langle v\rangle^\kappa e^{-\theta|v|^2}||e^{\theta|v|^2}g_1||_\infty||e^{\theta|v|^2}g_2||_\infty,\\
|\nu(\sqrt{\mu}g_1)|&\lesssim_\theta\ e^{\theta|v|^2}\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_1(u)|\mathrm{d}u.
\end{aligned}$$

(ii) For all $p\in[1,\infty)$ and for $(i,j)=(1,2)$ or $(i,j)=(2,1)$,

$$\begin{aligned}
\|\Gamma_{\mathrm{gain}}(g_1,g_2)\|_p&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_i||_\infty\|g_j\|_p,\\
\|\nu(\sqrt{\mu}g_1)g_2\|_p&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_2||_\infty\|g_1\|_p,\\
\Big|\iint_{\Omega\times\mathbb{R}^3}\Gamma_{\mathrm{gain}}(g_1,g_2)g_3\mathrm{d}v\mathrm{d}x\Big|&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_i||_\infty\|g_j\|_p\|g_3\|_q,\\
\Big|\iint_{\Omega\times\mathbb{R}^3}\nu(\sqrt{\mu}g_1)g_2g_3\mathrm{d}v\mathrm{d}x\Big|&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_2||_\infty\|g_1\|_p\|g_3\|_q.
\end{aligned}$$

(iii) For $p\in[1,\infty)$ and for $(i,j)=(1,2)$ or $(i,j)=(2,1)$,

$$\begin{aligned}
\|\nabla_v[\Gamma_{\mathrm{gain}}(g_1,g_2)]\|_p&\lesssim_{\theta,p}\ \sum_{(i,j)}||e^{\theta|v|^2}g_i||_\infty\|\nabla_vg_j\|_p,\\
\|\nu(\sqrt{\mu}\nabla_vg_1)g_2\|_p&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_2||_\infty\|\nabla_vg_1\|_p,\\
\Big|\iint_{\Omega\times\mathbb{R}^3}\nabla_v\Gamma_{\mathrm{gain}}(g_1,g_2)g_3\mathrm{d}v\mathrm{d}x\Big|&\lesssim_{\theta,p}\ \sum_{(i,j)}||e^{\theta|v|^2}g_i||_\infty||\nabla_vg_j||_p||g_3||_q,\\
\Big|\iint_{\Omega\times\mathbb{R}^3}\nu(\sqrt{\mu}\nabla_vg_1)g_2g_3\mathrm{d}v\mathrm{d}x\Big|&\lesssim_{\theta,p}\ ||e^{\theta|v|^2}g_2||_\infty||\nabla_vg_1||_p||g_3||_q.
\end{aligned}$$

(iv) Let $[Y,W]=[Y(x,v),W(x,v)]\in\Omega\times\mathbb{R}^3$. For $\partial_{\mathbf{e}}$ with $\mathbf{e}\in\{x,v\}$,

$$\begin{aligned}
&|\partial_{\mathbf{e}}\Gamma_{\mathrm{gain}}(g,g)(Y,W)|\\
&\lesssim|\partial_{\mathbf{e}}Y|||e^{\theta|v|^2}g||_\infty\int_{\mathbb{R}^3}\frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}}|\nabla_xg(Y,u)|\mathrm{d}u\\
&\quad+\ |\partial_{\mathbf{e}}W|||e^{\theta|v|^2}g||_\infty\int_{\mathbb{R}^3}\frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}}|\nabla_vg(Y,u)|\mathrm{d}u+\langle v\rangle^\kappa e^{-\theta|v|^2}|\partial_{\mathbf{e}}W|||e^{\theta|v|^2}g||_\infty^2.
\end{aligned}$$

Proof. *(i)* First we show (7.27) for $(i,j)=(1,2)$. Clearly

$$|\Gamma_{\text{gain}}(g_1,g_2)| \ \lesssim \ |\Gamma_{\text{gain}}(e^{-\theta|v|^2},|g_2|)| \times ||e^{\theta|v|^2}g_1||_\infty.$$

Then we follow the Grad estimate, page 315 of [74], to bound $|\Gamma_{\text{gain}}(e^{-\theta|v|^2},|g_2|)|$ by the integral $\int_{\mathbb{R}^2}\mathbf{k}_2(v,u)|g_2(u)|\mathrm{d}u$ with different exponent of $\mathbf{k}_2(v,u)$. We use Lemma 7.3 to conclude (7.27).

For the second estimate we use (7.11)

$$\begin{aligned}|\Gamma_{\text{gain}}(g_1,g_2)(v)| &\lesssim \Gamma_{\text{gain}}(e^{-\theta|v|^2},e^{-\theta|v|^2}) \times ||e^{\theta|v|^2}g_1||_\infty||e^{\theta|v|^2}g_2||_\infty\\ &= e^{-\theta|v|^2}\iint B(v-u,\omega)\sqrt{\mu(u)}e^{-\theta|u|^2}\mathrm{d}\omega\mathrm{d}u \times ||e^{\theta|v|^2}g_1||_\infty||e^{\theta|v|^2}g_2||_\infty\\ &\lesssim \langle v\rangle^\kappa e^{-\theta|v|^2}||e^{\theta|v|^2}g_1||_\infty||e^{\theta|v|^2}g_2||_\infty,\end{aligned}$$

where we have used $|u'|^2+|v'|^2=|u|^2+|v|^2$. The third estimate follows similarly with $\nabla_u(\sqrt{\mu})(u)\lesssim \mu(u)^{1/2-\delta}$ for any $\delta>0$. The forth estimate follows from

$$e^{-\theta|v|^2}\nu(\sqrt{\mu}g_1)(v)\lesssim \int_{\mathbb{R}^3}|v-u|^\kappa e^{-\theta|v|^2}\sqrt{\mu(u)}|g_1(u)|\mathrm{d}u \lesssim \int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_1(u)|\mathrm{d}u,$$

and $e^{-\theta|v|^2}|v-u|^\kappa\sqrt{\mu(u)}\lesssim \frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}$.

(ii) First two estimates are a direct consequence of *(i)* :

$$\begin{aligned}||\Gamma_{\text{gain}}(g_1,g_2)||_p &\lesssim ||e^{\theta|v|^2}g_i||_\infty\Big|\Big|\Big(\int_u\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\Big)^{1/q}\Big(\int_u\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_j(u)|^p\Big)^{1/p}\Big|\Big|_{L^p_v}\\ &\lesssim ||e^{\theta|v|^2}g_i||_\infty\Big(\int_u\frac{e^{-C_\theta|u|^2}}{|u|^{2-\kappa}}\Big)^{1/q}\Big(\int_u|g_j(u)|^p\int_v\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\Big)^{1/p}\\ &\lesssim ||e^{\theta|v|^2}g_i||_\infty\Big(\int_u\frac{e^{-C_\theta|u|^2}}{|u|^{2-\kappa}}\Big)||g_j||_p\\ &\lesssim ||e^{\theta|v|^2}g_i||_\infty||g_j||_p.\end{aligned}$$

Using the forth estimate of *(i)*, the same proof holds for $||\nu(\sqrt{\mu}g_1)g_2||_p\lesssim_{\theta,p}||e^{\theta|v|^2}g_2||_\infty||g_1||_p$.

For the third estimate we use (7.27) to bound as

$$\begin{aligned}&||e^{\theta|v|^2}g_i||_\infty\iiint_{\Omega\times\mathbb{R}^3\times\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_j(x,u)||g_3(x,v)|\mathrm{d}u\mathrm{d}v\mathrm{d}x\\ &\lesssim \Big(\iiint\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_j(x,u)|^p\Big)^{1/p}\Big(\iiint\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|g_3(x,u)|^q\Big)^{1/q}\\ &\lesssim ||g_j||_p||g_3||_q.\end{aligned}$$

The same proof holds with exchanging i and j. Using the forth estimate of *(i)*, the same proof holds for the forth estimate.

(iii) We compute the velocity derivative of Γ_{gain} after the change of variable $u:=v-u$:

$$\begin{aligned}\nabla_v\Gamma_{\text{gain}}(g_1,g_2) &= \nabla_v\Big[\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}B(u,\omega)\sqrt{\mu(u)}g_1(u-(u\cdot\omega)\omega)g_2(v+(u\cdot\omega)\omega)\mathrm{d}\omega\mathrm{d}u\Big]\\ &= \Gamma_{\text{gain}}(g_1,\nabla_vg_2)+\Gamma_{\text{gain}}(\nabla_vg_1,g_2)+\Gamma_{\text{gain},v}(g_1,g_2).\end{aligned}$$

The two first terms are estimated directly by *(ii)*. For the $\Gamma_{\text{gain},v}$ we use the fact $|\nabla_v(\sqrt{\mu})(v-u)|\le C\mu(v-u)^{1/4}$ and then apply *(ii)*. The other estimates are direct consequence of the previous estimates.

(iv) It suffices to show the following computation : For $0 < \theta < \frac{1}{4}$,

$$
\begin{aligned}
&|\partial_{\mathbf{e}}\Gamma_{\text{gain}}(g,g)(Y,W)| \\
&= \Big|\partial_{\mathbf{e}}\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}|u|^\kappa q_0\Big(\frac{u}{|u|}\cdot\omega\Big)e^{-\frac{|u+W|^2}{4}}g(Y,W+[u\cdot\omega]\omega)g(Y,W+u-(u\cdot\omega)\omega)\mathrm{d}\omega\mathrm{d}u\Big| \\
&= |\Gamma_{\text{gain}}(\partial_{\mathbf{e}}Y\cdot\nabla_x g,g)(Y,W)| + |\Gamma_{\text{gain}}(g,\partial_{\mathbf{e}}Y\cdot\nabla_x g)(Y,W)| \\
&\quad + |\Gamma_{\text{gain}}(\partial_{\mathbf{e}}W\cdot\nabla_v g,g)(Y,W)| + |\Gamma_{\text{gain}}(g,\partial_{\mathbf{e}}W\cdot\nabla_v g)(Y,W)| \\
&\quad + \Big|\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}|u|^\kappa q_0\Big(\frac{u}{|u|}\cdot\omega\Big)(\frac{-1}{2})(u+W)\cdot\partial_{\mathbf{e}}W\sqrt{\mu(u+W)} \\
&\qquad\qquad\qquad \times g(Y,W+[u\cdot\omega]\omega)g(Y,W+u-(u\cdot\omega)\omega)\mathrm{d}\omega\mathrm{d}u\Big| \\
&\lesssim |\partial_{\mathbf{e}}Y|||e^{\theta|v|^2}g||_\infty\int_{\mathbb{R}^3}\frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}}|\partial_x g(Y,u)|\mathrm{d}u \\
&\quad + |\partial_{\mathbf{e}}W|||e^{\theta|v|^2}g||_\infty\int_{\mathbb{R}^3}\frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}}|\partial_v g(Y,u)|\mathrm{d}u + |\partial_{\mathbf{e}}W|\langle v\rangle^\kappa e^{-\theta|v|^2}||e^{\theta|v|^2}g||_\infty^2,
\end{aligned}
\tag{7.28}
$$

where we have used the change of variables $u - V \mapsto u$.

□

7.2.2 Local existence

Lemma 7.5 (Local Existence)**.** *Let $0 < \theta' < \theta < 1/4$ and $f_0 \geq 0$ such that $||e^{\theta|v|^2}f_0||_\infty < +\infty$. Then there exists $T_* = T_*(||e^{\theta|v|^2}f_0||_\infty) > 0$ such that there exists a unique $F = \sqrt{\mu}f \geq 0$ which solves the Boltzmann equation (7.1) in $[0,T_*) \times \Omega \times \mathbb{R}^3$ with initial datum f_0 and boundary condition (7.12) and such that for all $t < T_*$,*

$$||e^{\theta'|v|^2}f(t)||_\infty \lesssim_{\theta',t} P(||e^{\theta|v|^2}f_0||_\infty), \tag{7.29}$$

for some polynomial P. Furthermore if f_0 is continuous and satisfies the compatibility condition (7.14) then f is continuous away from the grazing set γ_0.

Moreover, let $0 \leq \bar\theta < \frac{1}{4}$. If $||e^{\bar\theta|v|^2}\partial_t f_0||_\infty \equiv \big|\big|e^{\bar\theta|v|^2}\frac{-v\cdot\nabla_x F_0 + Q(F_0,F_0)}{\sqrt{\mu}}\big|\big|_\infty < +\infty$ and if compatibility condition (7.14) is verified then for all $t < T_*$,

$$||e^{\bar\theta|v|^2}\partial_t f(t)||_\infty \lesssim_t P(||e^{\bar\theta|v|^2}\partial_t f_0||_\infty) + P(||e^{\theta|v|^2}f_0||_\infty), \tag{7.30}$$

for some polynomial P.

Finally, if $||e^{\theta|v|^2}(f_0 - \sqrt{\mu})||_\infty \ll 1$ then $T_* = +\infty$, that is, the results hold for all $t \geq 0$.

Proof. We use the positive preserving iteration of [75, 81]

$$\partial_t F^{m+1} + v\cdot\nabla_x F^{m+1} + \nu(F^m)F^{m+1} = Q_{\text{gain}}(F^m,F^m), \quad F^{m+1}|_{t=0} = F_0 \geq 0, \tag{7.31}$$

which is equivalent to, with $F^m := \sqrt{\mu}f^m$,

$$\partial_t f^{m+1} + v\cdot\nabla_x f^{m+1} + \nu(F^m)f^{m+1} = \Gamma_{\text{gain}}(f^m,f^m), \quad f^{m+1}|_{t=0} = f_0. \tag{7.32}$$

The starting of this iteration is $F^0 \equiv F_0 \geq 0$, $f^0 \equiv f_0$ and let $F^{-m} \equiv F^0$, $f^{-m} \equiv f^0$ for all $m \in \mathbb{N}$.

Along the trajectory we have the Duhamel formula (ignoring the boundary condition) :

$$
\begin{aligned}
f^{m+1}(t,x,v) &= e^{-\int_0^t \nu(\sqrt{\mu}f^m)(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))\mathrm{d}s}f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0)) \\
&\quad + \int_0^t e^{-\int_s^t \nu(\sqrt{\mu}f^m)(\tau,X_{\mathbf{cl}}(\tau),V_{\mathbf{cl}}(\tau))}\Gamma_{\text{gain}}(f^m,f^m)(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))\mathrm{d}s.
\end{aligned}
$$

The local existence theorem without boundary is standard :

$$
\begin{aligned}
&|e^{(\theta-t)|v|^2} f^{m+1}(t,x,v)| \\
&\lesssim |e^{(\theta-t)|v|^2} f_0| + \int_0^t |\Gamma_{\text{gain}}(f^m,f^m)(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))| \mathrm{d}s \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty \\
&\quad + e^{(\theta-t)|v|^2} \int_0^t \iint_{\mathbb{R}^3\times\mathbb{S}^2} B(V_{\mathbf{cl}}(s)-u,\omega)\sqrt{\mu(u)} |f^m(s,X_{\mathbf{cl}}(s),u')||f^m(s,X_{\mathbf{cl}}(s),v')| \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty \\
&\quad + \big(\sup_{0\le s\le t} ||e^{(\theta-s)|v|^2} f^m(s)||_\infty\big)^2 \int_0^t \iint B(v-u,\omega)\sqrt{\mu(u)} e^{(\theta-t)|v|^2} e^{-(\theta-s)|u'|^2} e^{-(\theta-s)|v'|^2} \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty + \big(\sup_{0\le s\le t} ||e^{(\theta-s)|v|^2} f^m(s)||_\infty\big)^2 \int_0^t e^{-(t-s)|v|^2} \int_u |v-u|^\kappa \sqrt{\mu(u)} \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty + \big(\sup_{0\le s\le t} ||e^{(\theta-s)|v|^2} f^m(s)||_\infty\big)^2 \int_0^t e^{-(t-s)|v|^2} \langle v\rangle \{\mathbf{1}_{|v|>N} + \mathbf{1}_{|v|\le N}\} \mathrm{d}s \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty + \big(\sup_{0\le s\le t} ||e^{(\theta-s)|v|^2} f^m(s)||_\infty\big)^2 \Big\{\frac{1}{N^2} + Nt\Big\}.
\end{aligned}
$$

Now we choose sufficiently large $N \gg 1$ and then small $0 < T \ll \theta$ to obtain the uniform-in-m estimate

$$\sup_{0\le t\le T} ||e^{\theta'|v|^2} f^{m+1}(t)||_\infty \lesssim ||e^{\theta|v|^2} f_0||_\infty. \tag{7.33}$$

With the diffuse boundary condition the Duhamel form is evolved with the condition, on $(x,v)\in\gamma_-$,

$$f^{m+1}(t,x,v) \;=\; c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u>0} f^m(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u. \tag{7.34}$$

We follow the proof of [75, 81] to obtain the same estimate (7.33). □

7.3 Traces and the In-flow Problems

Recall the almost grazing set γ_+^ε defined in (7.21). We first estimate the outgoing trace on $\gamma_+\setminus\gamma_+^\varepsilon$. We remark that for the outgoing part, our estimate is global in time without cut-off, in contrast to the general trace theorem.

Lemma 7.6. *Assume that $\varphi=\varphi(v)$ is $L^\infty_{loc}(\mathbb{R}^3)$. For any small parameter $\varepsilon>0$, there exists a constant $C_{\varepsilon,T,\Omega}>0$ such that for any h in $L^1([0,T],L^1(\Omega\times\mathbb{R}^3))$ with $\partial_t h + v\cdot\nabla_x h + \varphi h$ in $L^1([0,T],L^1(\Omega\times\mathbb{R}^3))$, we have for all $0\le t\le T$,*

$$\int_0^t \int_{\gamma_+\setminus\gamma_+^\varepsilon} |h| \mathrm{d}\gamma \mathrm{d}s \le C_{\varepsilon,T,\Omega}\left[\, ||h_0||_1 + \int_0^t \big\{\|h(s)\|_1 + \big\|[\partial_t + v\cdot\nabla_x + \varphi]h(s)\big\|_1\big\}\mathrm{d}s \,\right].$$

Furthermore, for any (s,x,v) in $[0,T]\times\Omega\times\mathbb{R}^3$ the function $h(s+s',x+s'v,v)$ is absolutely continuous in s' in the interval $[-\min\{t_{\mathbf{b}}(x,v),s\},\min\{t_{\mathbf{b}}(x,-v),T-s\}]$.

Proof. With a proper change of variables (e.g. Page 247 in [63]) we have

$$
\begin{aligned}
&\int_0^T \iint_{\Omega\times\mathbb{R}^3} h(t,x,v\mathrm{d})\mathrm{d}v\mathrm{d}x\mathrm{d}t \\
&= \int_{-\min\{T,t_{\mathbf{b}}(x,v)\}}^{0} \iint_{\Omega\times\mathbb{R}^3} h(T+s,x+sv,v)\mathrm{d}v\mathrm{d}x\mathrm{d}s \\
&+ \int_0^{\min\{T,t_{\mathbf{b}}(x,-v)\}} \iint_{\Omega\times\mathbb{R}^3} h(0+s,x+sv,v)\mathrm{d}v\mathrm{d}x\mathrm{d}s \\
&+ \int_0^T \int_{\gamma_+} \int_{-\min\{t,t_{\mathbf{b}}(x,v)\}}^{0} h(t+s,x+sv,v)\mathrm{d}s\mathrm{d}\gamma\mathrm{d}t \\
&+ \int_0^T \int_{\gamma_-} \int_0^{\min\{T-t,t_{\mathbf{b}}(x,-v)\}} h(t+s,x+sv,v)\mathrm{d}s\mathrm{d}\gamma\mathrm{d}t.
\end{aligned} \tag{7.35}
$$

For $(t,x,v)\in[0,T]\times\gamma_+$ and $0\le s\le \min\{t,t_{\mathbf{b}}(x,v)\}$,

$$h(t,x,v) = h(t-s,x-sv,v)e^{-\varphi(v)s} + \int_{-s}^{0} e^{\varphi(v)\tau}[\partial_t h + v\cdot\nabla_x h + \varphi(v)h](t+\tau,x+\tau v,v)\mathrm{d}\tau.$$

Now for $(t,x,v)\in[\varepsilon_1,T]\times\gamma_+\setminus\gamma_+^\varepsilon$, we integrate over $\int_{\varepsilon_1}^T\int_{\gamma_+\setminus\gamma_+^\varepsilon}\int_{\min\{t,t_{\mathbf{b}}(x,v)\}}^0$ to get

$$
\begin{aligned}
&\min\{\varepsilon_1,\varepsilon^3\}\times \int_{\varepsilon_1}^T \int_{\gamma_+\setminus\gamma_+^\varepsilon} |h(t,x,v)|\mathrm{d}\gamma\mathrm{d}t \\
&\lesssim \min_{[\varepsilon_1,T]\times[\gamma_+\setminus\gamma_+^\varepsilon]}\{t,t_{\mathbf{b}}(x,v)\}\times \int_{\varepsilon_1}^T \int_{\gamma_+\setminus\gamma_+^\varepsilon} |h(t,x,v)|\mathrm{d}\gamma\mathrm{d}t \\
&\lesssim \int_0^T \int_{\gamma_+} \int_{-\min\{t,t_{\mathbf{b}}(x,v)\}}^{0} |h(t+s,x+sv,v)|\mathrm{d}s\mathrm{d}\gamma\mathrm{d}t \\
&\quad + T\int_0^T \int_{\gamma_+} \int_{-\min\{t,t_{\mathbf{b}}(x,v)\}}^{0} |\partial_t h + v\cdot\nabla_x h + \varphi h|(t+\tau,x+\tau v,v)\mathrm{d}\tau\mathrm{d}\gamma\mathrm{d}t \\
&\lesssim \int_0^T ||h(t)||_1\mathrm{d}t + \int_0^T ||[\partial_t + v\cdot\nabla_x+\varphi]h(t)||_1\mathrm{d}t,
\end{aligned}
$$

where we have used the integration identity (7.35), and (40) of [75] to obtain $t_{\mathbf{b}}(x,v)\ge C_\Omega|n(x)\cdot v|/|v|^2\ge C_\Omega\varepsilon^3$ for $(x,v)\in\gamma_+\setminus\gamma_+^\varepsilon$. Now we choose $\varepsilon_1=\varepsilon_1(\Omega,\varepsilon)$ as

$$\varepsilon_1\le C_\Omega\varepsilon^3\le \inf_{(x,v)\in\gamma_+\setminus\gamma_+^\varepsilon} t_{\mathbf{b}}(x,v).$$

We only need to show, for $\varepsilon_1\le C_\Omega\varepsilon^3$,

$$\int_0^{\varepsilon_1}\int_{\gamma_+\setminus\gamma_+^\varepsilon}|h(t,x,v)|\mathrm{d}\gamma\mathrm{d}t \lesssim_{\Omega,\varepsilon,\varepsilon_1} ||h_0||_1 + \int_0^{\varepsilon_1}||[\partial_t+v\cdot\nabla_x+\varphi]h(t)||_1\mathrm{d}t.$$

Because of our choice ε and ε_1, $t_{\mathbf{b}}(x,v)>t$ for all $(t,x,v)\in[0,\varepsilon_1]\times\gamma_+\setminus\gamma_+^\varepsilon$. Then

$$|h(t,x,v)|\lesssim |h_0(x-tv,v)| + \int_0^t \Big|[\partial_t+v\cdot\nabla_x+\varphi(v)]h(s,x-(t-s)v,v)\Big|\mathrm{d}s,$$

where the second contribution is bounded, from (7.35), by

$$
\begin{aligned}
&\int_0^{\varepsilon_1}\int_{\gamma_+\setminus\gamma_+^\varepsilon}\int_0^t \Big|[\partial_t+v\cdot\nabla_x+\varphi(v)]h(s,x-(t-s)v,v)\Big|\mathrm{d}s\mathrm{d}\gamma\mathrm{d}t \\
&\lesssim \int_0^{\varepsilon_1}||[\partial_t+v\cdot\nabla_x+\varphi(v)]h(t)||_1\mathrm{d}t.
\end{aligned}
$$

Consider the initial datum contribution of $|h_0(x-tv,v)|$: We may assume $\partial_{x_3}\xi(x_0)\neq 0$. By the implicit function theorem $\partial\Omega$ can be represented locally by the graph $\eta=\eta(x_1,x_2)$ satisfying

$\xi(x_1,x_2,\eta(x_1,x_2))=0$ and $(\partial_{x_1}\eta(x_1,x_2),\partial_{x_2}\eta(x_1,x_2))=(-\partial_{x_1}\xi/\partial_{x_3}\xi,-\partial_{x_2}\xi/\partial_{x_3}\xi)$ at $(x_1,x_2,\eta(x_1,x_2))$. We define the change of variables

$$(x,t)\in\partial\Omega\cap\{x\sim x_0\}\times[0,\varepsilon_1]\mapsto y=x-tv\in\bar{\Omega},$$

where $\left|\frac{\partial y}{\partial(x,t)}\right|=-v_1\frac{\partial_{x_1}\xi}{\partial_{x_3}\xi}-v_2\frac{\partial_{x_2}\xi}{\partial_{x_3}\xi}-v_3$.

Therefore

$$\begin{aligned}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}t&=(n(x)\cdot v)\Big[1+(\frac{\partial_{x_1}\xi}{\partial_{x_3}\xi})^2+(\frac{\partial_{x_2}\xi}{\partial_{x_3}\xi})^2\Big]^{1/2}\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}t\\&=\Big[-v_1\frac{\partial_{x_1}\xi}{\partial_{x_3}\xi}-v_2\frac{\partial_{x_2}\xi}{\partial_{x_3}\xi}-v_3\Big]\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}t=\mathrm{d}y,\end{aligned}$$

and $\int_0^{\varepsilon_1}\int_{\gamma_+\backslash\gamma_+^\varepsilon\cap\{x\sim x_0\}}|h_0(x-tv,v)|\mathrm{d}\gamma\mathrm{d}t\ \lesssim_{\varepsilon,\varepsilon_1,x_0}\ \iint_{\Omega\times\mathbb{R}^3}|h_0(y,v)|\mathrm{d}y\mathrm{d}v$. Since $\partial\Omega$ is compact we can choose a finite covers of $\partial\Omega$ and repeat the same argument for each piece to conclude

$$\int_0^{\varepsilon_1}\int_{\gamma_+\backslash\gamma_+^\varepsilon}|h_0(x-tv,v)|\mathrm{d}\gamma\mathrm{d}t\ \lesssim_{\Omega,\varepsilon,\varepsilon_1}\ \iint_{\Omega\times\mathbb{R}^3}|h_0(y,v)|\mathrm{d}y\mathrm{d}v.$$

□

Lemma 7.7 (Green's Identity)**.** *For $p\in[1,\infty)$ assume that $f,\partial_t f+v\cdot\nabla_x f\in L^p([0,T];L^p(\Omega\times\mathbb{R}^3))$ and $f_{\gamma_-}\in L^p([0,T];L^p(\gamma))$. Then $f\in C^0([0,T];L^p(\Omega\times\mathbb{R}^3))$ and $f_{\gamma_+}\in L^p([0,T];L^p(\gamma))$ and for almost every $t\in[0,T]$:*

$$||f(t)||_p^p+\int_0^t|f|_{\gamma_+,p}^p=||f(0)||_p^p+\int_0^t|f|_{\gamma_-,p}^p+p\int_0^t\iint_{\Omega\times\mathbb{R}^3}\{\partial_t f+v\cdot\nabla_x f\}|f|^{p-2}f.$$

See [75] for the proof. Now we state and prove following propositions for the in-flow problems :

$$\{\partial_t+v\cdot\nabla_x+\nu\}f=H,\quad f(0,x,v)=f_0(x,v),\quad f(t,x,v)|_{\gamma_-}=g(t,x,v),\tag{7.36}$$

where $\nu(t,x,v)\geq 0$. For notational simplicity, we define

$$\partial_t f_0\ \equiv\ -v\cdot\nabla_x f_0-\nu(0,\cdot,\cdot)f_0+H(0,\cdot,\cdot),\tag{7.37}$$

$$\nabla_x g\ \equiv\ \frac{n}{n\cdot v}\Big\{-\partial_t g-\sum_{i=1}^2(v\cdot\tau_i)\partial_{\tau_i}g-\nu g+H\Big\}+\sum_{i=1}^2\tau_i\partial_{\tau_i}g.\tag{7.38}$$

We remark that $\partial_t f_0$ is obtained from formally solving (7.36), and (7.38) leads to the usual tangential derivatives of $\partial_{\tau_i}g$, while it defines the 'normal derivative' $\partial_n g$ from formally solving (7.36).

Proposition 7.1. *Assume the compatibility condition*

$$f_0(x,v)=g(0,x,v)\quad\textit{for}\quad(x,v)\in\gamma_-.\tag{7.39}$$

Let $p\in[1,\infty)$ and $0<\theta<1/4$. Assume

$$\begin{aligned}\nabla_x f_0,\nabla_v f_0,-v\cdot\nabla_x f_0-\nu(0,\cdot,\cdot)f_0+H(0,\cdot,\cdot)\ &\in\ L^p(\Omega\times\mathbb{R}^3),\\ \partial_t g,\nabla_v g,\partial_{\tau_i}g,\frac{1}{n(x)\cdot v}\{-\partial_t g-\sum_i(v\cdot\tau_i)\partial_{\tau_i}g-\nu g+H\}\ &\in\ L^p([0,T]\times\gamma_-),\\ \partial_t H,\ \nabla_x H,\ \nabla_v H,\ &\in\ L^p([0,T]\times\Omega\times\mathbb{R}^3),\\ e^{-\theta|v|^2}\partial_t\nu,\ e^{-\theta|v|^2}\nabla_x\nu,\ e^{-\theta|v|^2}\nabla_v\nu\ &\in\ L^p([0,T]\times\Omega\times\mathbb{R}^3),\end{aligned}$$

$$e^{\theta|v|^2}f_0\in L^\infty(\Omega\times\mathbb{R}^3),\qquad e^{\theta|v|^2}g\in L^\infty([0,T]\times\gamma_-),\qquad e^{\theta|v|^2}H\ \in L^\infty([0,T]\times\Omega\times\mathbb{R}^3),\tag{7.40}$$

Then there exists a unique solution f to (7.36) such that $f,\partial_t f,\nabla_x f,\nabla_v f\in C^0([0,T];L^p(\Omega\times\mathbb{R}^3))$ and the traces satisfy

$$\begin{aligned}\partial_t f|_{\gamma_-}=\partial_t g,\ \nabla_v f|_{\gamma_-}=\nabla_v g,\ \nabla_x f|_{\gamma_-}=\nabla_x g,\quad\textit{on}\ \ \gamma_-,\\ \nabla_x f(0,x,v)=\nabla_x f_0,\ \nabla_v f(0,x,v)=\nabla_v f_0,\ \partial_t f(0,x,v)=\partial_t f_0,\quad\textit{in}\ \ \Omega\times\mathbb{R}^3,\end{aligned}\tag{7.41}$$

where $\partial_t f_0$ and $\nabla_x g$ are given by (7.37) and (7.38). Moreover for $\partial_{\mathbf{e}} \in \{\partial_t, \partial_x, \partial_v\}$

$$\begin{aligned} ||\partial_{\mathbf{e}} f(t)||_p^p + \int_0^t |\partial_{\mathbf{e}} f|_{\gamma_+,p}^p &= ||\partial_{\mathbf{e}} f_0||_p^p + \int_0^t |\partial_{\mathbf{e}} g|_{\gamma_-,p}^p \\ &+p \int_0^t \iint_{\Omega\times\mathbb{R}^3} \{\partial_{\mathbf{e}} H - [\partial_{\mathbf{e}} v]\nabla_x f - [\partial_{\mathbf{e}}\nu] f\}|\partial_{\mathbf{e}} f|^{p-2}\partial_{\mathbf{e}} f. \end{aligned} \tag{7.42}$$

Proof. The idea of the proof is to apply the trace theorem to the derivatives of f by explicit computation of the derivatives. Let us integrate the equation (7.36) along the backward trajectories. If the initial condition is reached before hitting the boundary (case $t < t_{\mathbf{b}}$), we have

$$f(t,x,v) = e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} f_0(x-tv,v) + \int_0^t e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} H(t-s,x-vs,v)\mathrm{d}s.$$

If the boundary is first reached (case $t > t_{\mathbf{b}}$), we have

$$f(t,x,v) = e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} g(t-t_{\mathbf{b}},x_{\mathbf{b}},v) + \int_0^{t_{\mathbf{b}}} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} H(t-s,x-vs,v)\mathrm{d}s.$$

To sum up,

$$\begin{aligned} f(t,x,v) =& \mathbf{1}_{\{t\le t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} f_0(x-tv,v) + \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} g(t-t_{\mathbf{b}},x_{\mathbf{b}},v) \\ &+ \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} H(t-s,x-vs,v)\mathrm{d}s. \end{aligned} \tag{7.43}$$

First notice that thanks to our assumptions on f_0, g and H,

$$\sup_{t\in[0,T]} \|e^{\theta|v|^2} f(t)\|_\infty \le \|e^{\theta|v|^2} f_0\|_\infty + \sup_{t\in[0,T]} |e^{\theta|v|^2} g(t)|_{\gamma_-,\infty} + \int_0^t \|e^{\theta|v|^2} H(t)\|_\infty \mathrm{d}s < \infty.$$

We now want to take derivative of f with respect to time, space and velocity for $t \neq t_{\mathbf{b}}$. Recall the following derivatives of $x_{\mathbf{b}}$ and $t_{\mathbf{b}}$ (from Lemma 2 in [75]) :

$$\begin{aligned} &\nabla_x t_{\mathbf{b}} = \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}, \quad \nabla_v t_{\mathbf{b}} = -\frac{t_{\mathbf{b}} n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}, \\ &\nabla_x x_{\mathbf{b}} = I - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})} \otimes v, \quad \nabla_v x_{\mathbf{b}} = -t_{\mathbf{b}} I + \frac{t_{\mathbf{b}} n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})} \otimes v. \end{aligned} \tag{7.44}$$

Since g is defined on a surface, we cannot define its space ($\mathbb{R}^3$) gradient. We then use directly the space gradient of $g(x_{\mathbf{b}})$. Regarding $g(t-t_{\mathbf{b}}, x_{\mathbf{b}}(x,v), v)$ as a function on $[0,T]\times\bar{\Omega}\times\mathbb{R}^3$ we obtain from (7.44)

$$\begin{aligned} \nabla_x[g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)] &= -\nabla_x t_{\mathbf{b}} \partial_t g + \nabla_x x_{\mathbf{b}} \nabla_\tau g = -\frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\partial_t g + \left(I - \frac{n\otimes v}{n\cdot v}\right)\nabla_\tau g \\ &= \tau_1 \partial_{\tau_1} g + \tau_2 \partial_{\tau_2} g - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\left\{\partial_t g + v\cdot\tau_1\partial_{\tau_1} g + v\cdot\tau_2\partial_{\tau_2} g\right\}, \\ \nabla_v[g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)] &= -t_{\mathbf{b}}\nabla_x[g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)] + \nabla_v g, \end{aligned}$$

where $\tau_1(x)$ and $\tau_2(x)$ are unit vectors satisfying $\tau_1(x)\cdot n(x) = 0 = \tau_2(x)\cdot n(x)$ and $\tau_1(x)\times\tau_2(x) = n(x)$.

Therefore by direct computation for $t \neq t_{\mathbf{b}}$, we deduce

$$\begin{aligned} &\partial_t f(t,x,v)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}} \\ &= -\mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} [\nu_{|t=0} f_0 + v\cdot\nabla_x f_0 - H_{|t=0}](x-tv,v) \\ &-\mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^t \partial_t\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau\right) f_0(x-tv,v) \\ &+\mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\partial_t g - \left(\int_0^{t_{\mathbf{b}}} \partial_t\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau\right) g\right\}(t-t_{\mathbf{b}},x_{\mathbf{b}},v) \\ &+ \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \partial_t H(t-s,x-vs,v)\,\mathrm{d}s \\ &- \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^s \partial_t\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau\right) H(t-s,x-vs,v)\,\mathrm{d}s, \end{aligned} \tag{7.45}$$

$$\begin{aligned}
&\nabla_x f(t,x,v)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\\
&= \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\nabla_x f_0(x-tv,v) - \left(\int_0^t \nabla_x \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau\right) f_0(x-tv,v)\right\}\\
&+ \mathbf{1}_{\{t>t_B\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\tau_i\partial_{\tau_i} g - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_B)}\big\{\partial_t g + (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H\big\}\right\}(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&- \mathbf{1}_{\{t>t_B\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^{t_{\mathbf{b}}} \nabla_x \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau\right) g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&+ \int_0^{\min(t,t_B)} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \nabla_x H(t-s,x-vs,v)\mathrm{d}s\\
&- \int_0^{\min(t,t_B)} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^s \nabla_x \nu(s-\tau,x-\tau v,v)\mathrm{d}\tau\right) H(t-s,x-vs,v)\,\mathrm{d}s,
\end{aligned} \tag{7.46}$$

$$\begin{aligned}
&\nabla_v f(t,x,v)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\\
&= \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} [-t\nabla_x f_0 + \nabla_v f_0](x-tv,v)\\
&- \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \int_0^t \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau f_0(x-tv,v)\\
&- \mathbf{1}_{\{t>t_{\mathbf{b}}\}} t_{\mathbf{b}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\tau_i\partial_{\tau_i} g - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\big\{\partial_t g + (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H\big\}\right\}(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&+ \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\nabla_v g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\right\}\\
&- \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{\int_0^{t_{\mathbf{b}}} \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau\right\} g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&+ \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \{\nabla_v H - s\nabla_x H\}(t-s,x-vs,v)\,\mathrm{d}s\\
&- \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \{\int_0^s \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau\} H(t-s,x-vs,v)\,\mathrm{d}s.
\end{aligned} \tag{7.47}$$

First we show that $\partial f\mathbf{1}_{\{t>t_{\mathbf{b}}\}} \in L^p$ and $\partial f\mathbf{1}_{\{t<t_{\mathbf{b}}\}} \in L^p$ separately. To compute the L^p norms above we use the changes of variables in Lemma 2.1 of [73] (and Jensen's inequality in $[0,t]$). More precisely, for $\phi \in L^1(\Omega\times\mathbb{R}^3)$ and $\phi_b \in L^1([0,t]\times\gamma)$ with $\phi,\phi_b \geq 0$,

$$\begin{aligned}
&\iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\{x-tv\in\Omega\}}\phi(x-tv,v)\\
&= \int_{\mathbb{R}^3}\left[\int_\Omega \mathbf{1}_{\{x-tv\in\Omega\}}\phi(x-tv,v)\mathrm{d}x\right]\mathrm{d}v \leq \iint_{\Omega\times\mathbb{R}^3}\phi(x,v),\\
&\iint_{\{\Omega\times\mathbb{R}^3\}\cap B((x_0,v_0);\delta)} \mathbf{1}_{\{t\geq t_{\mathbf{b}}\}}\phi_b(t-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v)\\
&\leq \int_0^t\int_{\partial\Omega\times\mathbb{R}^3}\phi_b(s,x,v)|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s = \int_0^t\int_\gamma \phi_b(s,x,v)\,\mathrm{d}\gamma\,\mathrm{d}s,
\end{aligned} \tag{7.48}$$

where for the second inequality we have used the change of variables for fixed t, v,

$$x \mapsto (t-t_{\mathbf{b}}(x,v), x_{\mathbf{b}}(x,v)). \tag{7.49}$$

In fact, without the loss of generality we may assume $\partial_{x_3}\xi(x_{\mathbf{b}}(x,v)) \neq 0$ for $(x,v)\in B((x_0,v_0);\delta)$ so that $x_{\mathbf{b}}(x,v) = (x_{\mathbf{b},1},x_{\mathbf{b},2},\eta(x_{\mathbf{b},1},x_{\mathbf{b},2}))$. Using (7.44), we compute the Jacobian

$$\det\begin{pmatrix} -\nabla_x t_{\mathbf{b}}\\ -\nabla_x x_{\mathbf{b},1}\\ -\nabla_x x_{\mathbf{b},2}\end{pmatrix} = \det\begin{pmatrix} -(v\cdot n)^{-1}n\\ -\nabla_x x_{\mathbf{b},1}\\ -\nabla_x x_{\mathbf{b},2}\end{pmatrix} = \left|-v_1\frac{\partial_{x_1}\xi}{\partial_{x_3}\xi} - v_2\frac{\partial_{x_2}\xi}{\partial_{x_3}\xi} + v_3\right|^{-1}.$$

Therefore

$$\mathrm{d}x\mathrm{d}v = \left|-v_1\frac{\partial_{x_1}\xi}{\partial_{x_3}\xi} - v_2\frac{\partial_{x_2}\xi}{\partial_{x_3}\xi} + v_3\right|\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}v\mathrm{d}t = |n\cdot v|\mathrm{d}S_x\mathrm{d}v\mathrm{d}t = \mathrm{d}\gamma\mathrm{d}t.$$

Using these changes of variables, we obtain

$$\|f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_p \leq \|f_0\|_p + \left[\int_0^t |g|^p_{\gamma_-,p}\mathrm{d}s\right]^{1/p} + t^{(p-1)/p}\left[\int_0^t \|H\|_p^p\mathrm{d}s\right]^{1/p},$$

$$\begin{aligned}\|\partial_t f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_p &\leq \|v\cdot\nabla_x f_0 + \nu(0,\cdot,\cdot)f_0 - H(0,\cdot,\cdot)\|_p + \left[\int_0^t |\partial_t g|^p_{\gamma_-,p}\mathrm{d}s\right]^{1/p}\\ &\quad + t^{(p-1)/p}\left[\int_0^t \|\partial_t H\|_p^p\mathrm{d}s\right]^{1/p} + K_t^\infty\left[\int_0^t \|e^{-\theta|v|^2}\partial_t\nu\|_p^p\mathrm{d}s\right]^{1/p},\end{aligned}$$

$$\begin{aligned}&\|\nabla_x f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_p\\ &\leq \|\nabla_x f_0\|_p + t^{(p-1)/p}\left[\int_0^t \|\nabla_x H(s)\|_p^p\mathrm{d}s\right]^{1/p} + K_t^\infty\left[\int_0^t \|e^{-\theta|v|^2}\nabla_x\nu\|_p^p\mathrm{d}s\right]^{1/p}\\ &\quad + \left[\int_0^t \Big|\sum_{i=1}^2 \tau_i\partial_{\tau_i}g - \frac{n}{v\cdot n}\big\{\partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i}g + \nu g - H\big\}\Big|^p_{\gamma_-,p}\mathrm{d}s\right]^{1/p},\end{aligned}$$

$$\begin{aligned}\|\nabla_v f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_p &\leq t\|\nabla_x f_0\|_p + \|\nabla_v f_0\|_p + \left[\int_0^t |\nabla_v g|^p_{\gamma_-,p}\mathrm{d}s\right]^{1/p}\\ &+ t\left[\int_0^t \Big|\sum_{i=1}^2 \tau_i\partial_{\tau_i}g - \frac{n}{v\cdot n}\big\{\partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i}g + \nu g - H\big\}\Big|^p_{\gamma_-,p}\mathrm{d}\gamma\mathrm{d}s\right]^{1/p}\\ &+ t^{(p-1)/p}\left[\int_0^t \|t|\nabla_x H| + |\nabla_v H|\|_p^p\mathrm{d}s\right]^{1/p} + K_t^\infty\left[\int_0^t \|e^{-\theta|v|^2}(t|\nabla_x\nu| + |\nabla_v\nu|)\|_p^p\mathrm{d}s\right]^{1/p},\end{aligned}$$

where we have written

$$K_t^\infty := t^{(p-1)/p}\left\{\|e^{\theta|v|^2}f_0\|_\infty + \sup_{[0,T]}|e^{\theta|v|^2}g|_{\gamma_-,\infty} + \int_0^t \|e^{\theta|v|^2}H(s)\|_\infty\,\mathrm{d}s\right\} < \infty.$$

From our assumptions on f_0, g, H and ν, all terms in the right-hand-sides above are finite. Therefore

$$\partial f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}} \equiv \left[\partial_t f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}, \nabla_x f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}, \nabla_v f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\right] \in L^\infty([0,T];L^p(\Omega\times\mathbb{R}^3)).$$

On the other hand, thanks to the compatibility condition, we can show that f has the same trace on the set

$$\mathcal{M} \equiv \{t = t_{\mathbf{b}}(x,v)\} \equiv \{(t_{\mathbf{b}}(x,v),x,v) \text{ for } (x,v)\in\Omega\times\mathbb{R}^3\} \subset [0,T]\times\Omega\times\mathbb{R}^3. \tag{7.50}$$

We claim the following fact : *For any $\phi(t,x,v)\in C_c^\infty((0,T)\times\Omega\times\mathbb{R}^3)$, we have*

$$\int_0^T\iint_{\Omega\times\mathbb{R}^3} f\partial\phi = -\int_0^T\iint_{\Omega\times\mathbb{R}^3}\partial f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\phi, \tag{7.51}$$

so that $f\in W^{1,p}$ with weak derivatives given by $\partial f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}$.

Proof of claim. We fix some test function $\phi\not\equiv 0$. There exists $\delta = \delta_\phi > 0$ such that $\phi(t,x,v)\neq 0$ for $t\geq\frac{1}{\delta}$, or $\mathrm{dist}(x,\partial\Omega)<\delta$, or $|v|\geq\frac{1}{\delta}$. Let $(t,x,v)\in\mathcal{M}$ with $\phi(t,x,v)\neq 0$. By (7.50) and (7.4), $t = t_{\mathbf{b}}(x,v), x_{\mathbf{b}} = x - t_{\mathbf{b}}v\in\partial\Omega$, and $|x-x_{\mathbf{b}}| = t_{\mathbf{b}}|v|$, and

$$\mathrm{dist}(x,\Omega)\leq |x-x_{\mathbf{b}}| = t_{\mathbf{b}}|v|.$$

Since $t_{\mathbf{b}}\leq\frac{1}{\delta}$, this implies that

$$|v|\geq\frac{\delta}{t_{\mathbf{b}}}\geq\delta^2.$$

Otherwise $\mathrm{dist}(x,\partial\Omega)\leq\delta$ so that $\phi(t,x,v)=0$. Furthermore, by the Velocity lemma and this lower bound of $|v|$, we conclude that there exists $\delta'(\delta,\Omega)>0$ such that

$$\begin{aligned}|v\cdot n(x_{\mathbf{b}})|^2 &\gtrsim_\Omega |v\cdot\nabla_x\xi(x_{\mathbf{b}})|^2 = \alpha(t-t_{\mathbf{b}};t,x,v)\\ &\geq e^{-C_\Omega\langle v\rangle t_{\mathbf{b}}}\alpha(t;t,x,v)\geq e^{-C_\Omega\langle v\rangle t_{\mathbf{b}}}C_\xi|v|^2|\xi(x)|\\ &\geq e^{-C_\Omega\delta^{-2}}C_\xi\delta^4\min_{\mathrm{dist}(x,\partial\Omega)\geq\delta}|\xi(x)|\\ &= 2\delta'(\delta,\Omega)>0.\end{aligned}$$

In particular, this lower bound and a direct computation of (7.44) imply that $\{\phi \neq 0\} \cap \mathcal{M}$ is a smooth 6D hypersurface.

We next take C^1 approximation of f_0^l, H^l, and g^l (by partition of unity and localization) such that

$$||f_0^l - f_0||_{W^{1,p}} \to 0, \quad ||g^l - g||_{W^{1,p}([0,T]\times\gamma_-\backslash\gamma_-^{\delta'})} \to 0, \quad ||H^l - H||_{W^{1,p}([0,T]\times\Omega\times\mathbb{R}^3)} \to 0.$$

This implies, from the trace theorem, that

$$f_0^l(x,v) \to f_0(x,v) \quad \text{and} \quad g^l(0,x,v) \to g(0,x,v) \quad \text{in} \quad L^1(\gamma_-\backslash\gamma_-^{\delta'}).$$

We define accordingly, for $(t,x,v) \in [0,T] \times \Omega \times \mathbb{R}^3$,

$$\begin{aligned} f^l(t,x,v) &= \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu} f_0^l(x-tv,v) + \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu} g^l(t-t_{\mathbf{b}}, x_{\mathbf{b}}, v) \\ &\quad + \int_0^{\min\{t,t_{\mathbf{b}}\}} e^{-\int_0^s \nu} H^l(t-s, x-sv, v)\mathrm{d}s, \end{aligned} \tag{7.52}$$

and $f_{\pm}^l(t,x,v) \equiv \mathbf{1}_{\{t \gtrless t_{\mathbf{b}}\}} f^l$. Therefore for all $(x,v) \in \gamma_-$,

$$f_+^l(s, x+sv, v) - f_-^l(s, x+sv, v) = e^{-\int_0^s \nu} g^l(0,x,v) - e^{-\int_0^s \nu} f_0^l(x,v).$$

Since $\{\phi \neq 0\} \cap \mathcal{M}$ is a smooth hypersurface, we apply the Gauss theorem to f^l to obtain

$$\begin{aligned} \iiint \partial_{\mathbf{e}} \phi f^l \mathrm{d}x\mathrm{d}v\mathrm{d}t &= \iint [f_+^l - f_-^l]\phi \, \mathbf{e} \cdot \mathbf{n}_{\mathcal{M}} \mathrm{d}\mathcal{M} \\ &\quad - \left\{ \iiint_{t>t_{\mathbf{b}}} \phi \, \partial_{\mathbf{e}} f_+^l \mathrm{d}x\mathrm{d}v\mathrm{d}t + \iiint_{t<t_{\mathbf{b}}} \phi \, \partial_{\mathbf{e}} f_-^l \mathrm{d}x\mathrm{d}v\mathrm{d}t \right\}, \end{aligned} \tag{7.53}$$

where $\partial_{\mathbf{e}} = [\partial_t, \nabla_x, \nabla_v] = [\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}, \partial_{v_1}, \partial_{v_2}, \partial_{v_3}]$ and

$$\mathbf{n}_{\mathcal{M}} = \frac{1}{\sqrt{1 + |\nabla_x t_{\mathbf{b}}|^2 + |\nabla_v t_{\mathbf{b}}|}} (1, -\nabla_x t_{\mathbf{b}}, -\nabla_v t_{\mathbf{b}}) \in \mathbb{R}^7.$$

We have used $(s, x+sv, v)$ and $(x,v) \in \gamma_-$ as our parametrization for the manifold $\mathcal{M} \cap \{\phi \neq 0\}$, so that $n(x_{\mathbf{b}}(x,v)) \cdot v \geq 2\delta'$ is equivalent to $n(x) \cdot v \geq 2\delta'$. Therefore the above hypersurface integration over $\{t \neq t_{\mathbf{b}}\}$ is bounded by

$$\begin{aligned} &\lesssim_{\phi,\delta} \int_0^{\frac{1}{\delta}} \int_{n(x)\cdot v \geq 2\delta'} |f_+^l(s,x+sv,v) - f_-^l(s,x+sv,v)| \mathrm{d}S_x \mathrm{d}v \mathrm{d}s \\ &\lesssim_{\phi,\delta} \int_{n(x)\cdot v \geq 2\delta'} |g^l(0,x,v) - f_0^l(s,v)| \mathrm{d}S_x \mathrm{d}v \to 0, \quad \text{as } l \to \infty, \end{aligned}$$

since the compatibility condition $f_0(x,v) = g(0,x,v)$ for $(x,v) \in \gamma_-$. Clearly, taking difference of (7.52) and (7.43), we deduce $f^l \to f$ strongly in $L^p(\{\phi \neq 0\})$ due to the first estimate of (7.50). Furthermore, due to (7.50), we have a uniform-in-l bound of $f_{\pm}^l$ in $W^{1,p}(\{t \gtrless t_{\mathbf{b}},\ \phi \neq 0\})$ such that, up to subsequence,

$$\partial_{\mathbf{e}} f_+^l \rightharpoonup \partial_{\mathbf{e}} f \mathbf{1}_{\{t>t_{\mathbf{b}}\}}, \quad \partial_{\mathbf{e}} f_-^l \rightharpoonup \partial_{\mathbf{e}} f \mathbf{1}_{\{t<t_{\mathbf{b}}\}}, \quad \text{weakly in } L^p(\{\phi \neq 0\}).$$

Finally we conclude the claim (7.51) by letting $l \to \infty$ in (7.53).

Now recall $\partial = [\partial_t, \nabla_x, \nabla_v]$. From our assumptions on H, ν and from the L^p-L^∞ bounds above, we have

$$\{\partial_t + v \cdot \nabla_x + \nu\}\partial f = \partial H - \partial v \cdot \nabla_x f - \partial \nu f \in L^p. \tag{7.54}$$

By the trace theorem (Lemma 7.6), traces of $\partial_t f, \nabla_x f, \nabla_v f$ exist. To evaluate these traces, we take derivatives along characteristics. Letting $t \to t_{\mathbf{b}}$ and $t \to 0$, we deduce (7.41). From the Green's identity, Lemma 7.7, we have (7.42), and $\partial f \in C^0([0,T]; L^p)$.

□

We now study the weighted $W^{1,p}$ estimate. Recall (7.7). We first define an effective collision frequency :

$$\nu_{\varpi,\beta}(t,x,v) = \nu(v) + \varpi\langle v\rangle - \beta\alpha^{-1}[v \cdot \nabla_x \alpha], \tag{7.55}$$

and

$$[\partial_t + v \cdot \nabla_x + \nu_{\varpi,\beta}](e^{-\varpi\langle v\rangle t}\alpha^\beta f) = e^{-\varpi\langle v\rangle t}\alpha^\beta[\partial_t f + v \cdot \nabla_x f + \nu f]. \tag{7.56}$$

Due to (7.6) and $\varpi \gg 1$, $\nu_{\varpi,\beta}(t,x,v) \sim \beta\langle v\rangle$.

Proposition 7.2. *Let f be a solution of (7.36). Assume (7.39) and $\langle v\rangle g \in L^\infty([0,T]\times\gamma_-)$, and $\nu, \langle v\rangle H \in L^\infty([0,T]\times\Omega\times\mathbb{R}^3)$. For any fixed $p\in[2,\infty]$, assume*

$$\begin{array}{rcl} e^{-\varpi\langle v\rangle t}\alpha^\beta\partial_t g,\ e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_\tau g & \in & L^\infty([0,T];L^p(\gamma_-)),\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\big\{|\nabla_\tau g| + \dfrac{1}{n(x)\cdot v}\big(|\partial_t g| + \langle v\rangle|\nabla_\tau g| + |H|\big)\big\} & \in & L^\infty([0,T];L^p(\gamma_-)),\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\big| - v\cdot\nabla_x f_0 - \nu f_0 + H_0\big| & \in & L^p(\Omega\times\mathbb{R}^3), \end{array}$$

and assume $1/p+1/q=1$ there exist $TC_T = O(T)$ and $\varepsilon \ll 1$ such that for all $t\in[0,T]$

$$\Big|\iint_{\Omega\times\mathbb{R}^3} e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H(t)h(t)\Big| \le C_T\big\{||h(t)||_q + \varepsilon||\nu_{l,\beta}^{1/q}h(t)||_q\big\}.$$

Then $f(t,x,v)$ satisfies

$$||f(t)||_\infty \le ||f_0||_\infty + \sup_{0\le s\le t}||g(s)||_\infty + \Big|\Big|\int_0^t H(s)ds\Big|\Big|_\infty.$$

Recall $\partial = [\partial_t, \nabla_x, \nabla_v]$, then

$$\begin{array}{rcl} \{\partial_t + v\cdot\nabla_x + \nu_{\varpi,\beta}\}[e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f] & = & e^{-\varpi\langle v\rangle t}\alpha^\beta\big[-\partial v\cdot\nabla_x f - \partial\nu f + \partial H\big],\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|_{t=0} & = & e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0, \quad e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|_{\gamma_-} \ = \ e^{-\varpi\langle v\rangle t}\alpha^\beta[\partial g|_{\gamma_-}], \end{array}$$

where $[\partial g|_{\gamma_-}]$ is given in (7.41). Moreover, recalling (7.37) and (7.38), we have for $2\le p<\infty$,

$$\begin{aligned} &\int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f(t)|^p + \int_0^t\int_{\Omega\times\mathbb{R}^3}\nu_{\varpi,\beta}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^p + \int_0^t\int_{\gamma_+}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^p\\ &\lesssim \int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0|^p + \int_0^t\int_{\gamma_-}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial g|^p\\ &\quad + \int_0^t\int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H - e^{-\varpi\langle v\rangle t}\alpha^\beta\partial v\cdot\nabla_x f - \partial\nu e^{-\varpi\langle v\rangle t}\alpha^\beta f||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^{p-1}, \qquad (7.57)\\ &||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f(t)||_\infty\\ &\lesssim ||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0||_\infty + ||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial g||_\infty\\ &\quad + \int_0^t ||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H - \partial v\cdot e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f - \partial\nu e^{-\varpi\langle v\rangle t}\alpha^\beta f||_\infty, \qquad \text{for } p=\infty. \end{aligned}$$

Proof. First we assume f_0, g and H have compact supports in $\{v\in\mathbb{R}^3 : |v|<m\}$. We estimate ∂f in the bulk. From the velocity lemma (Lemma 7.1), we have

$$\begin{aligned} &\sup_{t\le t_{\mathbf{b}}}\frac{e^{-\varpi\langle v\rangle t}\alpha^\beta(x,v)}{\alpha^\beta(x-tv,v)} \le e^{C_{m,\beta}t}, \quad \sup_{t\ge t_{\mathbf{b}}}\frac{e^{-\varpi\langle v\rangle t}\alpha^\beta}{e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta(x_{\mathbf{b}},v)} \le e^{C_{m,\beta}t_{\mathbf{b}}},\\ &\sup_{\max\{t-t_{\mathbf{b}},0\}\le s\le t}\frac{e^{-\varpi\langle v\rangle t}\alpha^\beta}{e^{-\varpi\langle v\rangle(t-s)}\alpha(x-sv,v)^\beta} \le e^{C_{m,\beta}s}. \end{aligned}$$

Multiply $e^{-\varpi\langle v\rangle t}\alpha^\beta$ by the above direct computations and use the above inequalities to get

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}\alpha^\beta|\partial_t f(t,x,v)|\\
&\lesssim\ e^{C_{m,\beta}t}e^{-\int_0^t\nu}\alpha^\beta\big|[\nu f_0+v\cdot\nabla_x f_0-H|_{t=0}](x-tv,v)\big|\mathbf{1}_{\{t<t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta\partial_t\big|g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\big|\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+\int_0^{\min(t,t_{\mathbf{b}})}e^{C_{m,\beta}s}e^{-\int_0^s\nu}e^{-\varpi\langle v\rangle(t-s)}\alpha^\beta\big|\partial_t H(t-s,x-vs,v)\big|\mathrm{d}s,\\
&e^{-\varpi\langle v\rangle t}\alpha^\beta|\nabla_x f(t,x,v)|\\
&\lesssim\ e^{C_{m,\beta}t}e^{-\int_0^t\nu}\alpha^\beta\big|\nabla_x f_0(x-tv,v)\big|\mathbf{1}_{\{t<t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}\tau_i e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta|\partial_{\tau_i}g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)|\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}n(x_{\mathbf{b}})\frac{e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta(x_{\mathbf{b}},v)}{|v\cdot n(x_{\mathbf{b}})|}\Big|\Big\{\partial_t g+(v\cdot\tau_i)\partial_{\tau_i}g+\nu g-H\Big\}(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\Big|\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+\int_0^{\min(t,t_{\mathbf{b}})}e^{C_{m,\beta}s}e^{-\int_0^s\nu}e^{-\varpi\langle v\rangle(t-s)}\alpha^\beta\big|\nabla_x H(t-s,x-vs,v)\big|\mathrm{d}s,\\
&e^{-\varpi\langle v\rangle t}\alpha^\beta|\nabla_v f(t,x,v)|\\
&\lesssim\ e^{C_{m,\beta}t}e^{-\int_0^t\nu}\alpha^\beta\big|[-t\nabla_x f_0+\nabla_v f_0-t\nabla_v\nu(v)f_0](x-tv,v)\big|\mathbf{1}_{\{t<t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}\tau_i e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta|\partial_{\tau_i}g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)|\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}n(x_{\mathbf{b}})\frac{e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta}{|v\cdot n(x_{\mathbf{b}})|}\Big|\Big\{\partial_t g+(v\cdot\tau_i)\partial_{\tau_i}g+\nu g-H\Big\}(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\Big|\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+e^{C_{m,\beta}t_{\mathbf{b}}}e^{-\int_0^{t_{\mathbf{b}}}\nu}e^{-\varpi\langle v\rangle(t-t_{\mathbf{b}})}\alpha^\beta\big\{|\nabla_v g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)|+|t_{\mathbf{b}}\nabla_v\nu(v)||g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)|\big\}\mathbf{1}_{\{t>t_{\mathbf{b}}\}}\\
&\quad+\int_0^{\min(t,t_{\mathbf{b}})}e^{C_{m,\beta}s}e^{-\int_0^s\nu}e^{-\varpi\langle v\rangle(t-s)}\alpha^\beta\big|\{\nabla_v H-s\nabla_x H-s\nabla\nu H\}(t-s,x-vs,v)\big|\mathrm{d}s.
\end{aligned}\tag{7.58}$$

Following (7.48) and (7.49) of Proposition 7.1 and using the condition of Proposition 7.2, we deduce

$$\begin{aligned}
||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial_t f(t)||_p&\lesssim_{t,m,\beta}||\alpha^\beta[v\cdot\nabla_x f_0+\nu f_0-H(0,\cdot,\cdot)]||_p\\
&\quad+\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial_t g(s)||_{\gamma,p}^p\mathrm{d}s\right]^{1/p}+\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial_t H(s)||_p^p\mathrm{d}s\right]^{1/p},\\
||e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f(t)||_p&\lesssim_{t,m,\beta}||\alpha^\beta\nabla_x f_0||_p+\sum_{i=1}^2\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial_{\tau_i}g(s)||_{\gamma,p}^p\mathrm{d}s\right]^{1/p}\\
&\quad+\left[\int_0^t\Big|\Big|\frac{e^{-\varpi\langle v\rangle t}\alpha^\beta}{v\cdot n}\{\partial_t g+\sum(v\cdot\tau_i)\partial_{\tau_i}g+\nu g-H\}\Big|\Big|_{\gamma,p}^p\mathrm{d}s\right]^{1/p}\\
&\quad+\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\nabla_x H(s)||_p^p\mathrm{d}s\right]^{1/p},
\end{aligned}$$

$$\begin{aligned}
&||e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_v f(t)||_p\\
&\qquad\lesssim_{t,m,\beta}||\alpha^\beta\nabla_v f_0||_p+\sum_{i=1}^2\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial_{\tau_i}g(s)||_{\gamma,p}^p\mathrm{d}s\right]^{1/p}+\sup_{0\le s\le t}||\langle v\rangle g(s)||_\infty\\
&\quad+\left[\int_0^t\Big|\Big|\frac{e^{-\varpi\langle v\rangle t}\alpha^\beta}{v\cdot n}\{\partial_t g+\sum(v\cdot\tau_i)\partial_{\tau_i}g+\nu g-H\}\Big|\Big|_{\gamma,p}^p\mathrm{d}s\right]^{1/p}\\
&\quad+\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\nabla_v g(s)||_p^p\mathrm{d}s\right]^{1/p}\\
&\quad+\left[\int_0^t||e^{-\varpi\langle v\rangle s}\alpha^\beta\nabla_v H(s)||_p^p+||e^{-\varpi\langle v\rangle s}\alpha^\beta\nabla_x H(s)||_p^p\mathrm{d}s\right]^{1/p}+\sup_{0\le s\le t}||\langle v\rangle H(s)||_\infty.
\end{aligned}$$

By the hypothesis of Proposition 7.2 and assumption on f_0, g and H to have compact support, the right hand sides are bounded and hence $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial_t f, e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f$, and $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_v f$ are in $L^\infty([0,T];L^p(\Omega\times\mathbb{R}^3))$.

Since f_0, g and H are compactly supported on $\{v\in\mathbb{R}^3 : |v|\le m\}$, the derivatives $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial_t f$, $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f$ and $e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_v f$ are compactly supported on $\{v\in\mathbb{R}^3 : |v|\le m\}$ and hence from (7.56) and (7.54)

$$\{\partial_t + v\cdot\nabla_x + \nu_{\varpi,\beta}\}[e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f] = e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H - \partial v\cdot e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f - \partial\nu(v)e^{-\varpi\langle v\rangle t}\alpha^\beta f.$$

Moreover, from the general definition of traces, by choosing a test function multiplied by $e^{-\varpi\langle v\rangle t}\alpha^\beta$, we deduce $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f$ has the same trace as $e^{-\varpi\langle v\rangle t}\alpha^\beta[\partial f|_\gamma]$.

Now we can apply Lemma 7.7 to have (7.57) which does not depend on the velocity cut-off. In order to remove the compact support assumption we employ the cut-off function χ used in (7.7). Define $f^m = \chi(|v|/m)f$ then f^m satisfies

$$\begin{aligned}\{\partial_t + v\cdot\nabla_x + \chi(|v|/m)\nu\}f^m &= \chi(|v|/m)H, \\ f^m(0,x,v) = \chi(|v|/m)f_0,\quad f^m|_{\gamma_-} &= \chi(|v|/m)g.\end{aligned} \tag{7.59}$$

Note that for $(x,v)\in\gamma_-$, we have $\nabla_v[\chi(|v|/m)g] = \chi(|v|/m)\nabla_v g + g\nabla_v\chi(|v|/m)$ and $\chi(|v|/m)f_0(x,v) = \chi(|v|/m)g(0,x,v)$. Apply previous result to compute the traces of the derivatives of f^m. It is standard (using Green's identity) to show that $\partial_t f^m, \nabla_x f^m$ and $\nabla_v f^m$ are Cauchy and we can pass a limit. $\square$

7.4 Dynamical Non-local to Local Estimate

The main purpose of this section is to prove Lemma 7.2.

Proof of (1) of Lemma 7.2. Since $\frac{\langle u\rangle^r}{\langle v\rangle^r}\lesssim\{1+|v-u|^2\}^{\frac{r}{2}}$ and $\langle V_{\mathbf{cl}}(s)-u\rangle^r e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}\lesssim e^{-C_{\theta,r}|V_{\mathbf{cl}}(s)-u|^2}$, it suffices to consider $r=0$ case. We prove (7.23).

Step 1. We show that

$$\int_{\mathbb{R}^3}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)]^\beta}\mathrm{d}u \lesssim \frac{1}{|v|^{2\beta-1}|\xi(X_{\mathbf{cl}}(s;t,x,v))|^{\beta-\frac12}}. \tag{7.60}$$

For fixed $s\in[0,t_{\mathbf{b}}(x,v))$ and therefore fixed $X_{\mathbf{cl}}(s) = x-(t_{\mathbf{b}}(x,v)-s)v\in\bar\Omega$.

Firstly, we consider the case of $|\xi(x)|\le\delta_\Omega\ll 1$. From the assumption, we have $\nabla\xi(x)\neq 0$ and therefore there is uniquely determined unit vector $n(X_{\mathbf{cl}}(s)) = \frac{\nabla\xi(X_{\mathbf{cl}}(s))}{|\nabla\xi(X_{\mathbf{cl}}(s))|}$. We choose two unit vector τ_1 and τ_2 so that $\{\tau_1,\tau_2,n(X_{\mathbf{cl}}(s))\}$ is an orthonormal basis of $\mathbb{R}^3$.

We decompose the velocity variables $u\in\mathbb{R}^3$ as

$$u = u_n n(X_{\mathbf{cl}}(s)) + u_\tau\cdot\tau = u_n n(X_{\mathbf{cl}}(s)) + \sum_{i=1}^2 u_{\tau,i}\tau_i.$$

We note that $u_\tau\in\mathbb{R}^2$ and $u_n\in\mathbb{R}$ are completely free coordinates. Therefore using the Fubini's theorem we can rearrange the order of integration freely. Now we split, for $0\le s\le t_{\mathbf{b}}(x,v)$,

$$\begin{aligned}&\int_{\mathbb{R}^3}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{1}{[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)]^\beta}\mathrm{d}u \\ &\lesssim\int_{\mathbb{R}^2}\int_{\mathbb{R}}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}\left[|u_n|^2+|\xi(X_{\mathbf{cl}}(s))||u|^2\right]^\beta}\mathrm{d}u_n\mathrm{d}u_\tau \\ &= \int_{|u|\ge5|v|} + \int_{|u|\le\frac{|v|}{2}} + \int_{\frac{|v|}{2}\le|u|\le5|v|} = (\mathbf{I})+(\mathbf{II})+(\mathbf{III}).\end{aligned}$$

For the first term $(\mathbf{I})$ we use, for $|u|\ge5|v|$ (therefore $|v|\le\frac{|u|}{5}$),

$$|u-v|^2 = \frac{|u-v|^2}{2}+\frac{|u-v|^2}{2}\ge\frac{\frac{|u|^2}{2}-|v|^2}{2}+\frac{\frac{|u|^2}{2}-|v|^2}{2}\ge\frac{23}{4}|v|^2+\frac{23}{100}|u|^2\gtrsim|v|^2+|u|^2,$$

and we use $\left[|u_n|^2+|\xi||u|^2\right]^\beta \geq \left[|u_n|^2+25|\xi||v|^2\right]^\beta \gtrsim \left[|u_n|^2+|\xi||v|^2\right]^\beta$ for $|u|\geq 5|v|$ to have

$$(\mathbf{I}) \lesssim e^{-C|v|^2}\int_{\mathbb{R}^2} \mathrm{d}u_\tau \frac{e^{-C|u_\tau|^2}}{|v_\tau-u_\tau|^{2-\kappa}}\int_{\mathbb{R}}\mathrm{d}u_n \frac{e^{-C|u_n|^2}}{\left[|u_n|^2+|\xi||v|^2\right]^\beta}.$$

Since $\frac{1}{|v_\tau-u_\tau|^{2-\kappa}} \in L^1_{\mathrm{loc}}(\{u_\tau\in\mathbb{R}^2\})$ for $\kappa>0$ we first integrate over u_τ is finite. Then

$$\begin{aligned}
(\mathbf{I}) &\lesssim e^{-C|v|^2}\int_{\mathbb{R}} \frac{e^{-C|u_n|^2}}{\left[|u_n|^2+|\xi||v|^2\right]^\beta}\mathrm{d}u_n \\
&\lesssim e^{-C|v|^2}\Big\{\int_{10}^{\infty}\frac{e^{-C|u_n|^2}}{|u_n|^{2\beta}\mathbf{1}_{\{|u_n|\geq 10\}}}\mathrm{d}|u_n| + \int_0^{10}\frac{\mathrm{d}|u_n|}{\left[|u_n|^2+|\xi||v|^2\right]^\beta}\Big\} \\
&\lesssim (1+\int_0^{10}\frac{\mathrm{d}|u_n|}{\left[|u_n|^2+|\xi||v|^2\right]^\beta})e^{-C|v|^2} \lesssim\ e^{-C|v|^2}(1+\int_0^{10}\frac{\mathrm{d}[|\xi|^{\frac12}|v|\tan\theta]}{|\xi|^\beta|v|^{2\beta}(1+\tan^2\theta)^\beta}) \\
&\lesssim e^{-C|v|^2}\Big(1+\frac{1}{|v|^{2\beta-1}}\frac{1}{|\xi|^{\beta-1/2}}\int_0^{\pi/2}(\cos\theta)^{2\beta-2}\mathrm{d}\theta\Big) \lesssim e^{-C|v|^2}\Big(1+\frac{1}{|v|^{2\beta-1}}\frac{1}{|\xi|^{\beta-1/2}}\Big) \\
&\lesssim \frac{e^{-C_\theta|v|^2}}{|v|^{2\beta-1}}\frac{1}{|\xi(X_{\mathbf{cl}}(s;t,x,v))|^{\beta-1/2}},
\end{aligned}$$

where we have used a change of variables : $|u_n|=|\xi|^{\frac12}|v|\tan\theta$ and $\mathrm{d}|u_n|=|\xi|^{\frac12}|v|\sec^2\theta\mathrm{d}\theta$ and $(\cos\theta)^{2\beta-2}\in L^1_{\mathrm{loc}}(\{\theta\in[0,\frac{\pi}{2}]\})$ for $\beta>\frac12$.

For the second term $(\mathbf{II})$, we use $|v-u|\geq|v|-|u|\geq|v|-\frac{|v|}{2}\geq\frac{|v|}{2}$ from $|u|\leq\frac{|v|}{2}$, and apply the change of variables $u\mapsto|v|u$ to have

$$\begin{aligned}
(\mathbf{II}) &\lesssim \frac{1}{|v|^{2-\kappa}}\int_{|u_n|+|u_\tau|\leq\frac{|v|}{2}}\frac{e^{-C|v|^2}\mathrm{d}u_n\mathrm{d}u_\tau}{\left[|u_n|^2+|\xi||u_\tau|^2\right]^\beta} \\
&= \frac{1}{|v|^{2-\kappa}}\int_{|v|(|u_n|+|u_\tau|)\leq\frac{|v|}{2}}\frac{e^{-C|v|^2}|v|\mathrm{d}u_n|v|^2\mathrm{d}u_\tau}{\left[|v|^2|u_n|^2+|\xi||v|^2|u_\tau|^2\right]^\beta} \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-\kappa-1}}\int_{|u_\tau|\leq\frac12}\int_{|u_n|\leq\frac12}\frac{1}{\left[|u_n|^2+|\xi||u_\tau|^2\right]^\beta}\mathrm{d}u_n\mathrm{d}u_\tau.
\end{aligned}$$

Now we apply the change of variables $|u_n|=|\xi|^{\frac12}|u_\tau|\tan\theta$ for $\theta\in[0,\frac{\pi}{2}]$ with $\mathrm{d}u_n=|\xi|^{\frac12}|u_\tau|\sec^2\theta\mathrm{d}\theta$ to have

$$\begin{aligned}
(\mathbf{II}) &\lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-\kappa-1}}\int_{|u_\tau|\leq\frac12}\mathrm{d}u_\tau\int_0^{\frac{\pi}{2}}\frac{|\xi|^{\frac12}|u_\tau|\sec^2\theta\mathrm{d}\theta}{\left[|\xi||u_\tau|^2\tan^2\theta+|\xi||u_\tau|^2\right]^\beta} \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-\kappa-1}|\xi|^{\beta-1/2}}\int_{|u_\tau|\leq\frac12}\frac{\mathrm{d}u_\tau}{|u_\tau|^{2\beta-1}}\int_0^{\pi/2}(\cos\theta)^{2\beta-2}\mathrm{d}\theta \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-\kappa-1}|\xi|^{\beta-1/2}},
\end{aligned}$$

where we have used $\frac{1}{|u_\tau|^{2\beta-1}}\in L^1_{\mathrm{loc}}(\{u_\tau\in\mathbb{R}^2\})$ for $\beta<\frac32$ and $(\cos\theta)^{2\beta-2}\in L^1_{\mathrm{loc}}(\{\theta\in[0,\frac{\pi}{2}]\})$ for $\beta>\frac12$.

For the last term $(\mathbf{III})$, we use the lower bound of $|u|$ ($|u|\geq\frac{|v|}{2}$) to have $\left[|u_n|^2+|\xi||u|^2\right]^\beta \geq \left[|u_n|^2+|\xi|\frac{|v|^2}{4}\right]^\beta \gtrsim \left[|u_n|^2+|\xi||v|^2\right]^\beta$ and

$$\begin{aligned}
\int_{\frac{|v|}{2}\leq|u|\leq5|v|} &\lesssim \int_{0\leq|u_\tau|\leq5|v|}\frac{e^{-\frac{C}{2}|v_\tau-u_\tau|^2}}{|v_\tau-u_\tau|^{2-\kappa}}\mathrm{d}u_\tau\int_0^{5|v|}\frac{1}{\left[|u_n|^2+|\xi||v|^2\right]^\beta}\mathrm{d}u_n \\
&\lesssim \int_0^{5|v|}\frac{1}{\left[|u_n|^2+|\xi||v|^2\right]^\beta}\mathrm{d}u_n,
\end{aligned}$$

where we have used $\frac{1}{|u_\tau|^{2-\kappa}} \in L^1_{\mathrm{loc}}(\mathbb{R}^2)$ for $\kappa > 0$. We apply a change of variables : $|u_n| = |\xi|^{1/2}|v|\tan\theta$ for $\theta \in [0, \pi/2]$ with $\mathrm{d}|u_n| = |\xi|^{\frac{1}{2}}|v|\sec^2\theta \mathrm{d}\theta$. Hence

$$(\mathbf{III}) \lesssim \int_0^{5|v|} \frac{1}{\left[|u_n|^2 + |\xi||v|^2\right]^\beta} \mathrm{d}u_n = \int_0^{\frac{\pi}{2}} \frac{(\cos\theta)^{2\beta-2}}{|\xi|^{\beta-\frac{1}{2}}|v|^{2\beta-1}} \mathrm{d}\theta \lesssim \frac{1}{|v|^{2\beta-1}} \frac{1}{|v|^{2\beta-1}},$$

where we used $(\cos\theta)^{2\beta-2} \in L^1_{\mathrm{loc}}(\{\theta \in [0, \frac{\pi}{2}]\})$ for $\beta > \frac{1}{2}$. Overall, we combine the estimates of $(\mathbf{I}), (\mathbf{II})$ and $(\mathbf{III})$ to conclude (7.60).

Secondly, we consider the case of $|\xi(x)| > \delta_\Omega$. Then we can choose any orthonormal basis, for example standard basis $\{\tau_1, \tau_2, n\} = (e_1, e_2, e_3)$, to decompose the velocity variables $u \in \mathbb{R}^3$ as $u = u_1 e_1 + u_2 e_2 + u_3 e_3 := u_{\tau,1} e_1 + u_{\tau,2} e_2 + u_n e_3$. Then

$$\begin{aligned}
\alpha(X_{\mathbf{cl}}(s), u) &= |u \cdot \nabla\xi(X_{\mathbf{cl}}(s))|^2 - 2\xi(X_{\mathbf{cl}}(s))\{u \cdot \nabla^2\xi(X_{\mathbf{cl}}(s)) \cdot u\} \\
&\geq 2|\xi(X_{\mathbf{cl}}(s))|\{u \cdot \nabla^2\xi(X_{\mathbf{cl}}(s)) \cdot u\} \\
&= \delta_\Omega C_\xi |u|^2 + |\xi(X_{\mathbf{cl}}(s))|\{u \cdot \nabla^2\xi(X_{\mathbf{cl}}(s)) \cdot u\} \\
&\gtrsim |u_n|^2 + |\xi(X_{\mathbf{cl}}(s; t, x, v))||u|^2.
\end{aligned}$$

Then we follow all the proof with the same decomposition for $v := v_{\tau,1} e_1 + v_{\tau,2} e_2 + v_n e_3$ as well to conclude (7.60) for $|\xi(x)| > \delta_\Omega$.

Step 2. In this step we establish (7.61) and (7.62).

We first assume $v \cdot \nabla\xi(x) \geq 0$ and $x \in \partial\Omega$. There exist $\sigma_1, \sigma_2 > 0$ such that

$$\begin{aligned}
|v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)| &\gtrsim \sqrt{\alpha(x - (t_{\mathbf{b}}(x,v) - s)v, v)} \\
&\qquad \text{for all } s \in [0, \sigma_1] \cup [t_{\mathbf{b}}(x,v) - \sigma_2, t_{\mathbf{b}}(x,v)],
\end{aligned} \tag{7.61}$$

and $|v|\sqrt{-\xi(x - (t_{\mathbf{b}}(x,v) - s)v)} \gtrsim \sqrt{\alpha(x - (t_{\mathbf{b}}(x,v) - s)v, v)}$ for all $s \in [\sigma_1, t_{\mathbf{b}}(x,v) - \sigma_2]$. The mapping $s \mapsto \xi(x - (t_{\mathbf{b}}(x,v) - s)v)$ is one-to-one and onto on $s \in [0, \sigma_1]$ or on $s \in [t_{\mathbf{b}}(x,v) - \sigma_2, t_{\mathbf{b}}(x,v)]$. Moreover this mapping $s \mapsto \xi(x - (t_{\mathbf{b}}(x,v) - s)v)$ is diffeomorphism and we have a change of variables on $s \in [0, \sigma_1]$ or $s \in [t_{\mathbf{b}}(x,v) - \sigma_2, t_{\mathbf{b}}(x,v)]$.

$$\mathrm{d}s = \frac{\mathrm{d}|\xi|}{|\nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \cdot v|} \lesssim \frac{\mathrm{d}|\xi|}{\sqrt{\alpha(x - (t_{\mathbf{b}}(x,v) - s)v)}}. \tag{7.62}$$

Firstly we prove (7.61). Recall the definition of α in Definition 7.2. It suffices to show when $s \in [0, \sigma_1] \cup [t_{\mathbf{b}}(x,v) - \sigma_2, t_{\mathbf{b}}(x,v)]$,

$$|v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)| \geq |v|\sqrt{-\xi(x - (t_{\mathbf{b}}(x,v) - s)v)},$$

and when $s \in [\sigma_1, t_{\mathbf{b}}(x,v) - \sigma_2]$

$$|v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)| \leq |v|\sqrt{-\xi(x - (t_{\mathbf{b}}(x,v) - s)v)}.$$

If $v = 0$ or $v \cdot \nabla\xi(x) = 0$ then (7.61) holds clearly. Therefore we may assume $v \neq 0$ and $v \cdot \nabla\xi(x) > 0$. Due to the Velocity lemma, $v \cdot \frac{\nabla\xi(x)}{|\nabla\xi(x)|} > 0$ and $v \cdot \frac{\nabla\xi(x_{\mathbf{b}}(x,v))}{|\nabla\xi(x_{\mathbf{b}}(x,v))|} < 0$. By the mean value theorem we choose $t^* \in (0, t_{\mathbf{b}}(x,v))$ solving $v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - t^*)v) = 0$. Moreover due to the convexity of ξ we have

$$\frac{d}{ds}\Big(v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)\Big) = v \cdot \nabla^2\xi(X_{\mathbf{cl}}(s)) \cdot v \geq C_\xi|v|^2,$$

and therefore $t^* \in (0, t_{\mathbf{b}}(x,v))$ is uniquely determined. Clearly we have $v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \geq 0$ for $s \in [t^*, t_{\mathbf{b}}(x,v)]$ and $v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \leq 0$ for $s \in [0, t^*]$.

Define $\Phi(s) = \big\{|v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)|^2 + |v|^2\xi(x - (t_{\mathbf{b}}(x,v) - s)v)\big\}$. Since $2\big(v \cdot \nabla^2\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \cdot v\big) + |v|^2 > 0$ we have

$$\frac{d}{ds}\Phi(s) = \big(v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)\big)\Big\{2\big(v \cdot \nabla^2\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \cdot v\big) + |v|^2\Big\},$$

is strictly negative for $s \in [0, t^*]$ and is strictly positive for $s \in [t^*, t_{\mathbf{b}}(x,v)]$. Note that $\Phi(0) > 0$ and $\Phi(t_{\mathbf{b}}(x,v)) > 0$ from $v \cdot \frac{\nabla\xi(x)}{|\nabla\xi(x)|} > 0$ and $v \cdot \frac{\nabla\xi(x_{\mathbf{b}}(x,v))}{|\nabla\xi(x_{\mathbf{b}}(x,v))|} < 0$. Note that Φ is continuous function on the interval $[0, t_{\mathbf{b}}(x,v)]$ so that it has a minimum. If $\min_{[0,t_{\mathbf{b}}(x,v)]} \Phi(s) \leq 0$, there exist $\sigma_1, \sigma_2 > 0$ satisfying

$$\Phi(t_{\mathbf{b}}(x,v) + \sigma_1) = \Phi(t_{\mathbf{b}}(x,v)) + \int_0^{\sigma_1} \frac{d}{ds}\Phi(s)\mathrm{d}s = 0,$$
$$\Phi(t_{\mathbf{b}}(x,v) - \sigma_2) = \Phi(t_{\mathbf{b}}(x,v)) - \int_{t_{\mathbf{b}}(x,v)-\sigma_2}^{t_{\mathbf{b}}(x,v)} \frac{d}{ds}\Phi(s)\mathrm{d}s = 0,$$

then $\sigma_1 \leq t^*$ and $t_{\mathbf{b}}(x,v) - \sigma_2 \geq t^*$ and there is no other $s \in [0, t_{\mathbf{b}}(x,v)]$ satisfying $\Phi(s) = 0$. Moreover we have $\Phi(s) \leq 0$ for $s \in [\sigma_1, t_{\mathbf{b}}(x,v) - \sigma_2]$. If $\min_{[0,t_{\mathbf{b}}(x,v)]} \Phi(s) > 0$, there does not exist such σ_1 and σ_2 then we let $\sigma_1 = t^*$ and $\sigma_2 = t_{\mathbf{b}}(x,v) - t^*$. This proves (7.61).

Secondly we prove (7.62). By the proof of (7.61) and the fact

$$\frac{d|\xi|}{ds} = -\frac{d}{ds}\xi(x - (t_{\mathbf{b}}(x,v) - s)v) = -v \cdot \nabla_x \xi(x - (t_{\mathbf{b}}(x,v) - s)v),$$

and the inverse function theorem we prove (7.62).

Step 3. For small $0 < \tilde{\delta} \ll 1$, we define

$$\tilde{\sigma}_1 := \min\Big\{\sigma_1, \tilde{\delta}\frac{\sqrt{\alpha(x,v)}}{|v|^2}\Big\}, \quad \tilde{\sigma}_2 := \min\Big\{\sigma_2, \tilde{\delta}\frac{\sqrt{\alpha(x,v)}}{|v|^2}\Big\}. \tag{7.63}$$

Then both of (7.61) and (7.62) hold on $s \in [0, \tilde{\sigma}_1] \cup [t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2, t_{\mathbf{b}}(x,v)]$ without constant changing. Moreover, if $s \in [0, \tilde{\sigma}_1] \cup [t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2, t_{\mathbf{b}}(x,v)]$ then by the Velocity lemma

$$\max\{|\xi|\} := \max_{s \in [0,\tilde{\sigma}_1] \cup [t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2, t_{\mathbf{b}}(x,v)]} |\xi(X_{\mathbf{cl}}(s))| \lesssim \tilde{\delta}\frac{\alpha(x,v)}{|v|^2}. \tag{7.64}$$

On $s \in [\tilde{\sigma}_1, t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2]$ we have the following estimate with $\tilde{\delta}-$dependent constant :

$$|v|\sqrt{-\xi(x - (t_{\mathbf{b}}(x,v) - s)v)} \gtrsim_{\xi,\tilde{\delta}} \sqrt{\alpha(x - (t_{\mathbf{b}}(x,v) - s)v, v)}. \tag{7.65}$$

The proof of (7.64) is due to, for $s \in [0, \tilde{\sigma}_1]$,

$$\begin{aligned} |\xi(x - (t_{\mathbf{b}}(x,v) - s)v)| &\leq \int_0^s |v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - \tau)v)|\mathrm{d}\tau \\ &\lesssim \sqrt{\alpha(x,v)}|s| \lesssim \min\left\{\sqrt{\alpha}t_Z, \frac{\tilde{\delta}\alpha}{|v|^2}\right\} \equiv B, \end{aligned} \tag{7.66}$$

where we have used $\alpha(X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau)) \lesssim_\xi \alpha(x,v)$ from the Velocity lemma (Lemma 7.1). The proof for $s \in [t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2, t_{\mathbf{b}}(x,v)]$ is exactly same.

Now we prove (7.65). Recall that $t^* \in [0, t_{\mathbf{b}}(x,v)]$ in the previous step : $v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - t^*)v) = 0$. Clearly $|\xi(X_{\mathbf{cl}}(s))|$ is an increasing function on $s \in [0, t^*]$ and a decreasing function on $s \in [t^*, t_{\mathbf{b}}(x,v)]$. This is due to the convexity of ξ :

$$\frac{d^2}{ds^2}[-\xi(s - (t_{\mathbf{b}}(x,v) - s)v)] = v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v) \cdot v \gtrsim_\xi |v|^2,$$

and $v \cdot \nabla\xi(x) > 0$ and $v \cdot \nabla\xi(x_{\mathbf{b}}(x,v)) < 0$.

Therefore

$$\begin{aligned} -\xi(x - (t_{\mathbf{b}}(x,v) - s)v) &= -\xi(x) - \int_{t_{\mathbf{b}}(x,v)}^s v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - \tau)v)\mathrm{d}\tau \\ &= \int_s^{t_{\mathbf{b}}(x,v)} v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - \tau)v)\mathrm{d}\tau \\ &\geq (t_{\mathbf{b}}(x,v) - s)(v \cdot \nabla\xi(x - (t_{\mathbf{b}}(x,v) - s)v)) \\ &\geq \tilde{\sigma}_2|v \cdot \nabla\xi(x - \tilde{\sigma}_2 v)| \quad \text{for } \ s \in [t^*, t_{\mathbf{b}}(x,v) - \tilde{\sigma}_2], \end{aligned}$$

$$\begin{aligned}-\xi(x-(t_{\mathbf{b}}(x,v)-s)v) &= -\xi(x_{\mathbf{b}}(x,v)) - \int_0^s v\cdot\nabla\xi(x-(t_{\mathbf{b}}(x,v)-\tau)v)\mathrm{d}\tau \\ &\geq s|v\cdot\nabla\xi(x-(t_{\mathbf{b}}-s)v)| \\ &\geq \tilde{\sigma}_1|v\cdot\nabla\xi(x_{\mathbf{b}}(x,v)+\tilde{\sigma}_1 v)| \quad \text{for} \quad s\in[0,t^*].\end{aligned}$$

Hence, for $s\in[\tilde{\sigma}_1, t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2]$,

$$\begin{aligned}|\xi(x-(t_{\mathbf{b}}-s)v)| &\geq \min\Big\{|\xi(x-\tilde{\sigma}_2 v)|, |\xi(x_{\mathbf{b}}(x,v)+\tilde{\sigma}_1 v)|\Big\} \\ &\geq \min\Big\{\tilde{\sigma}_2|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)|, \tilde{\sigma}_1|v\cdot\nabla\xi(x_{\mathbf{b}}(x,v)+\tilde{\sigma}_1 v)|\Big\}.\end{aligned}$$

From the definition of $\tilde{\sigma}_1$ and $\tilde{\sigma}_2$ in (7.63) we have

$$|v|^2|\xi(x-(t_{\mathbf{b}}(x,v)-s)v)| \geq \tilde{\delta}\sqrt{\alpha(x,v)}\min\Big\{|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)|, |v\cdot\nabla\xi(x_{\mathbf{b}}(x,v)+\tilde{\sigma}_1 v)|\Big\}.$$

Without loss of generality we may assume $|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)| = \min\big\{|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)|, |v\cdot\nabla\xi(x_{\mathbf{b}}(x,v)+\tilde{\sigma}_1 v)|\big\}$. Then by the Velocity lemma we have $\sqrt{\alpha(x,v)} \gtrsim_\xi |v||\xi(x-\tilde{\sigma}_2 v)|^{1/2}$. Then we choose $s = t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2$ to have $|v|^2|\xi(x-\tilde{\sigma}_2 v)| \geq \tilde{\delta}|v||\xi(x-\tilde{\sigma}_2 v)|^{1/2}\times|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)|$ and

$$|v||\xi(x-\tilde{\sigma}_2 v)|^{1/2} \gtrsim \tilde{\delta}\times|v\cdot\nabla\xi(x-\tilde{\sigma}_2 v)|.$$

The left hand side is the lower bound of $|v|^2|\xi(x-(t_{\mathbf{b}}(x,v)-s)v)|$ for $s\in[\tilde{\sigma}_1, t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2]$ and the right hand side is bounded below by the Velocity lemma : $e^{-\mathcal{C}|v|t_{\mathbf{b}}(x,v)}\alpha(x,v) \gtrsim_\xi \alpha(x,v)$. Therefore we conclude (7.65).

Step 4. We prove (7.23). From (7.60)

$$\begin{aligned}&\int_0^{t_{\mathbf{b}}(x,v)}\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|v-u|^2}}{|v-u|^\kappa\alpha(x-(t_{\mathbf{b}}(x,v)-s)v,u)}Z(s,v)\mathrm{d}u\mathrm{d}s \\ &\lesssim \int_0^{t_{\mathbf{b}}(x,v)} e^{-l\langle v\rangle(t-s)}\frac{1}{|v|^{2\beta-1}|\xi|^{\beta-\frac12}}Z(s,v)\mathrm{d}s.\end{aligned}$$

According to (7.63) we split the time integration as

$$\int_0^{t_{\mathbf{b}}(x,v)} e^{-l\langle v\rangle(t-s)}\frac{1}{|v|^{2\beta-1}|\xi|^{\beta-\frac12}}Z(s,v)\mathrm{d}s = \underbrace{\int_0^{\tilde{\sigma}_1} + \int_{t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2}^{t_{\mathbf{b}}(x,v)}}_{(\mathbf{IV})} + \underbrace{\int_{\tilde{\sigma}_1}^{t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2}}_{(\mathbf{V})}.$$

For the first two terms $(\mathbf{IV})$, we use the mapping of (7.62)

$$s\in[0,\tilde{\sigma}_1]\cup[t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2, t_{\mathbf{b}}(x,v)] \mapsto |\xi(x-(t_{\mathbf{b}}(x,v)-s)v)| \in \big[0,B\big),$$

where the range of $|\xi|$ has been bounded in (7.64), and B is given by (7.66). By the change of variables of (7.62)

$$\begin{aligned}(\mathbf{IV}) &\lesssim \sup_{0\leq s\leq t_{\mathbf{b}}(x,v)}\{e^{-l\langle v\rangle(t-s)}Z(s,v)\}\frac{1}{|v|^{2\beta-1}}\int_0^{C\tilde{\delta}\frac{\alpha(x,v)}{|v|^2}}\frac{1}{|\xi|^{\beta-1/2}}\frac{\mathrm{d}|\xi|}{\sqrt{\alpha(x,v)}} \\ &\lesssim \sup_{0\leq s\leq t_{\mathbf{b}}(x,v)}\{e^{-l\langle v\rangle(t-s)}Z(s,v)\}\frac{1}{|v|^{2\beta-1}}\frac{1}{\sqrt{\alpha(x,v)}}\Big[|\xi|^{-\beta+\frac32}\Big]_{|\xi|=0}^{|\xi|=B},\end{aligned}$$

where we have used $\beta<\frac32$. The lemma follows with B given by (7.66).

For $(\mathbf{V})$ we use $\sqrt{\alpha(X_{\mathbf{cl}}(s))} \lesssim_{\xi,\tilde{\delta}} |v|\sqrt{-\xi(X_{\mathbf{cl}}(s))}$ for $s\in[\tilde{\sigma}_1, t_{\mathbf{b}}(x,v)-\tilde{\sigma}_2]$, from (7.61), to have

$$\frac{1}{|v|^{2\beta-1}|\xi|^{\beta-\frac12}} = \frac{1}{\big(|v|\sqrt{-\xi}\,\big)^{2(\beta-\frac12)}} \lesssim \frac{1}{[\alpha(x,v)]^{\beta-\frac12}}.$$

Finally

$$\begin{aligned}(\mathbf{V}) &\lesssim \frac{1}{[\alpha(x,v)]^{\beta-1/2}}\int_0^{t_{\mathbf{b}}(x,v)} e^{-l\langle v\rangle(t-s)}Z(s,v)\mathrm{d}s \\ &\lesssim \frac{O(l^{-1})}{\langle v\rangle[\alpha(x,v)]^{\beta-1/2}}\sup_{0\leq s\leq t}\{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\}.\end{aligned}$$

Now we assume $x \notin \partial\Omega$. We find $\bar{x} \in \partial\Omega$ and $\bar{t}_{\mathbf{b}}$ so that

$$x - (t_{\mathbf{b}}(x,v) - s)v = \bar{x} - (\bar{t}_{\mathbf{b}} - s)v.$$

Therefore, by the *Step 1* and the fact $\bar{x} \in \partial\Omega$, we have

$$\begin{aligned}
&\int_0^{\bar{t}_{\mathbf{b}}} \int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)} \frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}\big[\alpha(\bar{x} - (\bar{t}_{\mathbf{b}} - s)v, u)\big]^{\beta}} Z(s,v)\mathrm{d}u\mathrm{d}s \\
\lesssim &\int_0^{\bar{t}_{\mathbf{b}}} e^{-l\langle v\rangle(t-s)} \frac{e^{-C|v-u|^2}}{|v|^{2\beta-1}|\xi|^{\beta-\frac{1}{2}}} Z(s,v)\mathrm{d}s.
\end{aligned}$$

We then deduce our lemma since $\alpha(\bar{x}, v) \backsim \alpha(x,v)$ via the Velocity Lemma with the fact that $\bar{t}_{\mathbf{b}}|v| \lesssim_\Omega 1$. $\square$

7.5 Diffuse Reflection BC

7.5.1 $W^{1,p}(1 < p < 2)$ Estimate

Proof of Theorem 7.1. Consider the iteration (7.31) with (7.34) and with $f^0 \equiv f_0$, and with the compatibility condition for the initial datum (7.14). From the proof of Lemma 7.5, we have the uniform L^∞ bound (7.33) for $0 < T \ll 1$. The proof of the theorem relies on the iterative application of Proposition 7.1 for $m = 0, 1, \ldots$ with

$$\nu = \nu(\sqrt{\mu} f^m) \geq 0, \quad H = \Gamma_{\text{gain}}(f^m, f^m), \quad g = c_\mu \sqrt{\mu(v)} \int_{n\cdot u>0} f^m(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u.$$

Let $m \in \mathbb{N}$. Suppose that the conclusion of Proposition 7.1 is true at ranks $0, 1, \ldots, m-1$ and let us show that we can apply it at rank m. The initial datum f_0 satisfies the assumptions of Proposition 7.1 by the hypothesis of Theorem 7.1. The assumption (7.40) can be checked as in the proof of Lemma 7.5 (with θ replaced by some $0 < \theta' < \theta$ and for $0 < T \ll 1$). Then H and ν are estimated thanks to the collisional operator estimates of Lemma 7.4 and (7.29) of Lemma 7.5 by

$$\begin{aligned}
|\partial\nu| &= |\partial[\nu(\sqrt{\mu} f^m)]| \\
&\lesssim \langle v\rangle^\kappa e^{-\theta'|v|^2} ||e^{\theta'|v|^2} f^m||_\infty + e^{\theta'|v|^2} \int_{\mathbb{R}^3} \frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}} |\partial f^m(u)|\mathrm{d}u \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty + e^{\theta'|v|^2} \left(\int_{\mathbb{R}^3} \frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}} |\partial f^m(u)|^p \mathrm{d}u\right)^{1/p},
\end{aligned} \tag{7.67}$$

$$\begin{aligned}
|\partial H| &= |\partial[\Gamma_{\text{gain}}(f^m, f^m)]| \\
&\lesssim ||e^{\theta'|v|^2} f^m||_\infty \int_{\mathbb{R}^3} \frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}} |\partial f^m(u)|\mathrm{d}u + \langle v\rangle^\kappa e^{-\theta'|v|^2} ||e^{\theta'|v|^2} f^m||_\infty^2 \\
&\lesssim ||e^{\theta|v|^2} f_0||_\infty \left(\int_{\mathbb{R}^3} \frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}} |\partial f^m(u)|^p \mathrm{d}u\right)^{1/p} + e^{-\frac{\theta'}{2}|v|^2} ||e^{\theta|v|^2} f_0||_\infty^2,
\end{aligned} \tag{7.68}$$

so that $e^{\theta'|v|^2}\partial\nu$ and ∂H lie in $L^p([0,T] \times \Omega \times \mathbb{R}^3)$.

It remains to estimate the boundary condition. Recall computation (7.18) and notation (7.38). For $(x,v) \in \gamma_-$, the boundary condition is bounded by

$$\begin{aligned}
|\partial g(t,x,v)| &= \left|\partial\left[c_\mu \sqrt{\mu(v)} \int_{n\cdot u>0} f^m(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u\right]\right| \\
&\lesssim |v|\sqrt{\mu(v)} \int_{n(x)\cdot u>0} |f^m(t,x,u)|\langle u\rangle\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\
&+ \sqrt{\mu(v)}\left(1 + \frac{\langle v\rangle}{|n(x)\cdot v|}\right) \int_{n(x)\cdot u>0} |\partial f^m(t,x,u)|\langle u\rangle\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u \\
&+ \frac{1}{|n(x)\cdot v|}\Big\{\nu(\sqrt{\mu} f^m)|f^{m+1}| + |\Gamma_{\text{gain}}(f^m, f^m)|\Big\}.
\end{aligned} \tag{7.69}$$

Using furthermore the uniform L^∞ bound (7.33), we have for $(x,v)\in\gamma_-$

$$\begin{aligned}|\partial g(t,x,v)| \lesssim \sqrt{\mu(v)}\left(1+\frac{\langle v\rangle}{|n(x)\cdot v|}\right)\int_{n(x)\cdot u>0}|\partial f^m(t,x,u)|\mu^{1/4}\{n(x)\cdot u\}\mathrm{d}u\\ + e^{-\frac{\theta}{2}|v|^2}\left(1+\frac{1}{|n(x)\cdot v|}\right)P(||e^{\theta|v|^2}f_0||_\infty),\end{aligned} \tag{7.70}$$

for some polynomial P. We compute the L^p integral $(1<p<2)$ on the outgoing boundary with

$$\begin{aligned}&\int_0^t\int_{\gamma_-}|\partial g(s)|^p\,\mathrm{d}\gamma\,\mathrm{d}s\\ &\lesssim_p \sup_{x\in\partial\Omega}\left(\int_{\mathbb{R}^3}\sqrt{\mu(v)}^p\left(|n\cdot v|+\frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\right)\mathrm{d}v\right.\\ &\quad\times\int_0^t\int_{\partial\Omega}\left[\int_{u\cdot n(x)>0}|\partial f^m|\mu^{1/4}\{n\cdot u\}\mathrm{d}u\right]^p\mathrm{d}S_x\mathrm{d}s\\ &\quad+\sup_{x\in\partial\Omega}\left(\int_{\mathbb{R}^3}\langle v\rangle^{-p\beta}|n\cdot v|^{1-p}\mathrm{d}v\right)\times tP(||e^{\theta|v|^2}f_0||_\infty)\\ &\lesssim_p\int_0^t\int_{\partial\Omega}\left[\int_{u\cdot n(x)>0}|\partial f^m(s,x,u)|\mu^{1/4}(u)\{n\cdot u\}\mathrm{d}u\right]^p\mathrm{d}S_x\mathrm{d}s+tP(||e^{\theta|v|^2}f_0||_\infty).\end{aligned} \tag{7.71}$$

Now we focus on $\int_0^t\int_{\partial\Omega}\left[\int_{u\cdot n(x)>0}|\partial f^m(s,x,u)|\mu^{1/4}(u)\{n\cdot u\}\mathrm{d}u\right]^p\mathrm{d}S_x\mathrm{d}s$. Recall the definition of γ_+^ε in (7.21). We split the $\{u\in\mathbb{R}^3 : n(x)\cdot u>0\}$ as

$$\int_0^t\int_{\partial\Omega}\left[\int_{n\cdot u>0}|\partial f^m|\mu^{1/4}\{n\cdot u\}\mathrm{d}u\right]^p\lesssim_p\int_0^t\int_{\partial\Omega}\left[\int_{(x,u)\in\gamma_+\setminus\gamma_+^\varepsilon}\mathrm{d}u\right]^p+\int_0^t\int_{\partial\Omega}\left[\int_{(x,u)\in\gamma_+^\varepsilon}\mathrm{d}u\right]^p. \tag{7.72}$$

We use Hölder's inequality

$$\left[\int_{(x,u)\in\gamma_+^\varepsilon}\mathrm{d}u\right]^p\leq\left[\int_{(x,u)\in\gamma_+^\varepsilon}\mu^{\frac{p}{4(p-1)}}\{n\cdot u\}\mathrm{d}u\right]^{p-1}\left[\int_{(x,u)\in\gamma_+^\varepsilon}|\partial f^m(s,x,u)|^p\{n(x)\cdot u\}\mathrm{d}u\right],$$

so that we can bound the second term of (7.72) as

$$\int_0^t\int_{\partial\Omega}\left[\int_{(x,u)\in\gamma_+^\varepsilon}\mathrm{d}u\right]^p\lesssim_p\lambda(\varepsilon)\int_0^t|\partial f^m(s)|^p_{\gamma_+,p}\mathrm{d}s, \tag{7.73}$$

where $\lambda(\varepsilon)\longrightarrow 0$ when $\varepsilon\longrightarrow 0$. For the first term (non-grazing part) of (7.72) we use Lemma 7.6 and Hölder's inequality to compute

$$\begin{aligned}&\int_0^t\int_{\partial\Omega}\left[\int_{(x,u)\in\gamma_+\setminus\gamma_+^\varepsilon}\mathrm{d}u\right]^p\\ &\lesssim_\varepsilon ||\partial f_0||_p^p+\int_0^t||\partial f^m(s)||_p^p\mathrm{d}s+\int_0^t\iint_{\Omega\times\mathbb{R}^3}\left|[\partial_t+v\cdot\nabla_x+\nu]\partial(f^m)^p\right|\\ &\lesssim_\varepsilon ||\partial f_0||_p^p+\int_0^t||\partial f^m(s)||_p^p\mathrm{d}s+\int_0^t\left\{\left\|\partial f^m\right\|_p^p+\left\|[\partial_t+v\cdot\nabla_x+\nu]\partial f^m\right\|_p^p\right\}.\end{aligned} \tag{7.74}$$

When $m\geq 1$, the last term is computed thanks to (7.67) and (7.68) (at rank $m-1$), and using again the uniform bound (7.33),

$$\begin{aligned}&\int_0^t\left\|[\partial_t+v\cdot\nabla_x+\nu]\partial f^m\right\|_p^p\\ &\qquad=\int_0^t\left\|-[\partial v]\cdot\nabla_x f^m-\partial[\nu(\sqrt{\mu}f^{m-1})]f^m+\partial[\Gamma_{\mathrm{gain}}(f^{m-1},f^{m-1})]\right\|_p^p\\ &\qquad\lesssim\int_0^t||\partial f^m(s)||_p^p+P(||e^{\theta|v|^2}f_0||_\infty)\left(t+\int_0^t||\partial f^{m-1}(s)||_p^p\right).\end{aligned}$$

When $m=0$, we compute $[\partial_t + v\cdot\nabla_x + \nu]\partial f_0 = [v\cdot\nabla_x + \nu]\partial f_0 = \Gamma(f_0,f_0) - \partial_t f_0$ by definition of $\partial_t f_0$, so that $\int_0^t \left\|[\partial_t + v\cdot\nabla_x + \nu]\partial f^0\right\|_p^p \lesssim t||\partial_t f^0(s)||_p^p + tP(||e^{\theta|v|^2} f_0||_\infty)$, therefore the previous estimate is true with the convention $f^{-1}=0$. Reinserting in (7.74), we obtain

$$\int_0^t \int_{\partial\Omega} \left[\int_{(x,u)\in\gamma_+\setminus\gamma_+^\varepsilon} \mathrm{d}u\right]^p \lesssim_\varepsilon ||\partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty)\left(t + \sum_{i=m-1,m} \int_0^t ||\partial f^i(s)||_p^p\right). \tag{7.75}$$

Thanks to our assumptions on f_0 and our assumption that the conclusion of Propostion 7.1 is true at ranks $0,1,...,m-1$, all integrals above are finite. We have proved that ∂g lies in $L^p([0,T]\times\gamma_-)$, therefore Proposition 7.1 can be applied at rank m.

We now claim that for $1<p<2$, if $0<T'_*\ll 1$, then we have the uniform-in-m estimate for all $0\le t<T'_*$,

$$||\partial f^m||_p^p(t) + \int_0^t |\partial f^m|_{\gamma,p}^p \lesssim_t ||\partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty), \tag{7.76}$$

for some polynomial P.

Recall that the sequence (7.31) is the one used in Lemma 7.5 and shown to be Cauchy in L^∞. Therefore the limit function f is a solution of the Boltzmann equation on $[0,T_*)\times\Omega\times\mathbb{R}^3$ with the diffuse boundary condition. On the other hand, due to the weak lower semi-continuity for L^p with $p>1$, once we have (7.76) then we can pass to the limit $\partial f^m \rightharpoonup \partial f$ weakly in $\sup_{t\in[0,T'_*)} ||\cdot||_p^p$ and $\partial f^m|_\gamma \rightharpoonup \partial f|_\gamma$ in $\int_0^{T'_*} |\cdot|_{\gamma,p}^p$ to conclude that ∂f satisfies the same estimate as ∂f^m in (7.76). Repeat the same procedure on $[T'_*, 2T'_*], [2T'_*, 3T'_*], \cdots$, to conclude Theorem 7.1.

We prove the claim (7.76) by induction. From Proposition 7.1, ∂f^1 exists. Because of our choice ∂f^0 the estimate (7.76) is valid for $m=1$. Now assume that ∂f^i exists and (7.76) is valid for all $i=1,2,\cdots,m$. By Proposition 7.1, ∂f^{m+1} exists and from (7.42), we have

$$\begin{aligned}
&\sup_{0\le s\le t} ||\partial f^{m+1}(s)||_p^p + \int_0^t |\partial f^{m+1}|_{\gamma_+,p}^p \\
\lesssim\ & ||\partial f_0||_p^p + \int_0^t |\partial f^{m+1}|_{\gamma_-,p}^p + \int_0^t \iint_{\Omega\times\mathbb{R}^3} |\partial H + [\partial v]\nabla_x f^{m+1} + [\partial\nu] f^{m+1}||\partial f^{m+1}|^{p-1} \qquad (7.77)\\
\lesssim\ & ||\partial f_0||_p^p + \int_0^t |\partial f^{m+1}|_{\gamma_-,p}^p + P(||e^{\theta|v|^2} f_0||_\infty)\Big\{\int_0^t ||\partial f^{m+1}(s)||_p^p + \int_0^t ||\partial f^m(s)||_p^p\Big\},
\end{aligned}$$

where we have used (7.67) and (7.68). Using furthermore estimates (7.71), (7.72), (7.73) and (7.75) for the incoming boundary contribution, and choosing sufficiently small $0<\varepsilon\ll 1$, $0<T'_*\ll 1$, we deduce that for all $0\le t<T'_*$,

$$\begin{aligned}
&\sup_{0\le s\le t} ||\partial f^{m+1}(s)||_p^p + \int_0^t |\partial f^{m+1}|_{\gamma_+,p}^p \\
&\le C_{t,\Omega}\left\{||\partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty)\right\} + \frac{1}{8}\max_{i=m,m-1}\left\{\sup_{0\le s\le t} ||\partial f^i(s)||_p^p + \int_0^t |\partial f^i|_{\gamma_+,p}^p\right\}.
\end{aligned}$$

To conclude the proof we use the following fact from [67] : Suppose $a_i\ge 0, D\ge 0$ and $A_i = \max\{a_i, a_{i-1},\cdots,a_{i-(k-1)}\}$ for fixed $k\in\mathbb{N}$.

$$If\ \ a_{m+1} \le \frac{1}{8}A_m + D \ \text{ then } \ A_m \ \le\ \frac{1}{8}A_0 + \left(\frac{8}{7}\right)^2 D, \ \text{ for } \frac{m}{k}\gg 1. \tag{7.78}$$

Proof of (7.78) : In fact, we can iterate for $m, m-1, ...$ to get

$$\begin{aligned}
a_m &\le \frac{1}{8}\max\{\frac{1}{8}A_{m-2} + D, A_{m-2}\} + D \le \frac{1}{8}A_{m-2} + (1+\frac{1}{8})D \\
&\le \frac{1}{8}\max\{\frac{1}{8}A_{m-3} + D, A_{m-3}\} + (1+\frac{1}{8})D \le \frac{1}{8}A_{m-3} + (1+\frac{1}{8}+\frac{1}{8^2})D \\
&\le \frac{1}{8}A_{m-k} + \frac{8}{7}D.
\end{aligned}$$

Similarly $a_{m-i} \le \frac{1}{8}A_{m-k} + \frac{8}{7}D$ for all $i = 0, 1, \cdots, k-1$. Therefore if $1 \ll m/k \in \mathbb{N}$,

$$\begin{aligned} A_m &= \max\{a_m, a_{m-1}, \cdots, a_{m-(k-1)}\} \le \frac{1}{8}A_{m-k} + \frac{8}{7}D \\ &\le \frac{1}{8^2}A_{m-2k} + \frac{8}{7}(1+\frac{1}{8})D \le \frac{1}{8^3}A_{m-3k} + \frac{8}{7}(1+\frac{1}{8}+\frac{1}{8^2})D \\ &\le \left(\frac{1}{8}\right)^{[\frac{m}{k}]} A_{m-[\frac{m}{k}]k} + \left(\frac{8}{7}\right)^2 D \le \left(\frac{1}{8}\right)^{\frac{m}{k}} A_0 + \left(\frac{8}{7}\right)^2 D \ \le \ \frac{1}{8}A_0 + \left(\frac{8}{7}\right)^2 D. \end{aligned}$$

This completes the proof of (7.78).

In (7.78), setting $k = 2$ and for $0 \le t < T'_*$,

$$a_i = \sup_{0\le s\le t} ||\partial f^i(t)||_p^p + \int_0^t |\partial f^i|^p_{\gamma_+,p}, \qquad D = C_{t,\Omega}\big\{||\partial f_0||_p^p + P(||\langle v\rangle^\beta f_0||_\infty)\big\},$$

and applying (7.78), we complete the proof of the claim, and this concludes the proof of Theorem 7.1. $\square$

The following result indicates that Theorem 7.1 is optimal :

Lemma 7.8. *Let $\Omega = B(0;1)$ with $B(0;1) = \{x \in \mathbb{R}^3 : |x| < 1\}$. There exists an initial datum $f_0(x,v) \in C^\infty$ with $f_0 \subset\subset B(0;1)\times B(0;1)$ so that the solution f to*

$$\begin{aligned} &\partial_t f + v\cdot\nabla_x f = 0, \quad f|_{t=0} = f_0, \\ &f(t,x,v)|_{\gamma_-} = c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \end{aligned} \tag{7.79}$$

satisfies

$$\int_0^1\int_{\gamma_-} |\nabla_x f(s,x,v)|^2 \mathrm{d}\gamma\mathrm{d}s \ = \ +\infty,$$

so that the estimate (7.15) of Theorem 7.1 fails for $p = 2$.

Proof. We prove by contradiction. Suppose $\int_0^1\int_{\gamma_-} |\partial f(s,x,v)|^2\mathrm{d}\gamma\mathrm{d}s < +\infty$. Then

$$\partial_n f(t,x,v) = \frac{1}{n\cdot v}\Big\{ -\partial_t f - (\tau_1\cdot v)\partial_{\tau_1} f - (\tau_2\cdot v)\partial_{\tau_2} f\Big\}, \quad for\ (x,v)\in\gamma_-.$$

We use the boundary condition to define :

$$\begin{aligned} \partial_t f(t,x,v)|_{\gamma_-} &= c_\mu\sqrt{\mu(v)}A(t,x) \equiv c_\mu\sqrt{\mu}\int_{n\cdot u>0}\partial_t f\sqrt{\mu}\{n\cdot u\}\mathrm{d}u, \\ \partial_{\tau_i} f(t,x,v)|_{\gamma_-} &= c_\mu\sqrt{\mu(v)}B_i(t,x) \\ &\equiv c_\mu\sqrt{\mu}\int_{n\cdot u>0}\partial_{\tau_i} f\sqrt{\mu}\{n\cdot u\}\mathrm{d}u + c_\mu\sqrt{\mu}\int_{n\cdot u>0}\nabla_v f\frac{\partial\mathcal{T}}{\partial\tau_i}\mathcal{T}^{-1}u\sqrt{\mu}\{n\cdot u\}\mathrm{d}u. \end{aligned}$$

We make a change of variables $v_n = v\cdot n(x),\ v_{\tau_1} = v\cdot\tau_1(x),\ v_{\tau_2} = v\cdot\tau_2(x)$ to compute

$$\begin{aligned} &\int_{\partial\Omega}\mathrm{d}S_x\int_0^\infty \mathrm{d}v_n\iint_{\mathbb{R}^2}\mathrm{d}v_{\tau_1}\mathrm{d}v_{\tau_2} \\ &\quad\times\frac{\mu(v)}{v_\perp}\Big\{(A)^2 + (v_{\tau_1})^2(B_1)^2 + (v_{\tau_2})^2(B_2)^2 + 2v_{\tau_1}AB_1 + 2v_{\tau_2}AB_2 + 2v_{\tau_1}v_{\tau_2}B_1B_2\Big\} \\ &= \int_0^\infty \mathrm{d}v_n\frac{e^{-\frac{|v_n|^2}{2}}}{v_n}\int_{\partial\Omega}\mathrm{d}S_x\big\{(A)^2 + 2\pi(B_1)^2 + 2\pi(B_2)^2\big\}. \end{aligned}$$

Note that the integration over $\partial\Omega$ is a function of t only (independent of v). Since $\int_0^\infty \frac{\mathrm{d}v_n}{v_n} = \infty$, we conclude that $A = B_1 = B_2 \equiv 0$ for $(t,x)\in[0,\infty)\times\partial\Omega$. In particular from $A(t,x) = 0$ we have for all $t \ge 0$

$$\int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u = \int_{n(x)\cdot u>0} f(0,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u. \tag{7.80}$$

We now choose the initial datum to vanish near $\partial\Omega$:

$$f_0(x,v) = \phi(|x|)\phi(|v|),$$

where $\phi \in C^\infty([0,\infty))$ and $\phi \geq 0$ and supp$\phi \subset\subset [0,1)$ and $\phi \equiv 1$ on $[0,\frac{1}{2}]$. Clearly

$$c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u>0} f_0(x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u = 0.$$

Hence $f(t,x,v) \geq 0$ from $f_0 \geq 0$ and the zero inflow boundary condition from (7.80) and the above equality. Moreover following the backward trajectory to the initial plane for $t \in [\frac{1}{8},\frac{1}{4}]$ and $(x,v) \in \gamma_+$ and $|v - \frac{x}{|x|}| < \frac{1}{64}$, and $|v| \in [\frac{1}{8},\frac{1}{2}]$,

$$f(t,x,v) = f_0(x-tv,v) = 1,$$

which contradicts to $c_\mu\sqrt{\mu(v)}\int_{n\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u = 0$ for $(t,x,v) \in [0,\infty)\times\gamma_-$ from (7.80). □

7.5.2 Weighted $W^{1,p}$ $(2 \leq p < \infty)$ Estimate

We now establish the weighted $W^{1,p}$ estimate for $2 \leq p < \infty$ with the same iteration (7.31). From Lemma 7.5 for $0 < \theta < \frac{1}{4}$, we have a uniform bound (7.29) and (7.30). Recall the notation $\partial = [\nabla_x, \nabla_v]$. Then $e^{-\varpi\langle v\rangle t}[\alpha(x,v)]^\beta \partial f^m$ satisfies

$$\begin{aligned}
[\partial_t + v\cdot\nabla_x + \nu_{\varpi,\beta} + \nu(\sqrt{\mu}f^m)](e^{-\varpi\langle v\rangle t}\alpha(x,v)^\beta\partial f^{m+1}) &= e^{-\varpi\langle v\rangle t}\alpha(x,v)^\beta\mathcal{G}^m, \\
\alpha(x,v)^\beta\partial f^{m+1}(0,x,v) &= \alpha(x,v)^\beta\partial f_0(x,v).
\end{aligned} \tag{7.81}$$

Here $\nu_{\varpi,\beta}$ is defined in (7.55) and $\mathcal{G}^m$ is defined by

$$\mathcal{G}^m \;=\; -[\partial v]\cdot\nabla_x f^{m+1} - \partial[\nu(\sqrt{\mu}f^m)]f^{m+1} + \partial[\Gamma_{\text{gain}}(f^m,f^m)], \tag{7.82}$$

and satisfies by (7.67) and (7.68)

$$|\mathcal{G}^m| \;\lesssim\; |\nabla_x f^{m+1}| + e^{-\frac{\theta'}{2}|v|^2}||e^{\theta|v|^2}f_0||_\infty^2 + P(||e^{\theta|v|^2}f_0||_\infty)\int_{\mathbb{R}^3}\frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}}|\partial f^m(u)|\mathrm{d}u, \tag{7.83}$$

so that

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}\alpha(x,v)^\beta|\mathcal{G}^m| \\
&\lesssim e^{-\varpi\langle v\rangle t}\alpha(x,v)^\beta\Big\{|\nabla_x f^{m+1}| + P(||e^{\theta|v|^2}f_0||_\infty)\Big[e^{-\frac{\theta'}{2}|v|^2} + \int_{\mathbb{R}^3}\frac{e^{-C_{\theta'}|v-u|^2}}{|v-u|^{2-\kappa}}|\partial f^m(u)|\mathrm{d}u\Big]\Big\}.
\end{aligned}$$

For $(x,v) \in \gamma$, from (7.70), the boundary condition is bounded for $\beta < \frac{p-1}{2p}$ by

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}[\alpha(x,v)]^\beta|\partial f^{m+1}(t,x,v)| \\
&\lesssim\; e^{-\varpi\langle v\rangle t}[\alpha(x,v)]^\beta\sqrt{\mu(v)}\Big(1+\frac{\langle v\rangle}{|n(x)\cdot v|}\Big)\int_{n\cdot u>0}|\partial f^m(t,x,u)|\langle u\rangle\sqrt{\mu}\{n\cdot u\}\mathrm{d}u \\
&\quad+\frac{e^{-\varpi\langle v\rangle t}[\alpha(x,v)]^\beta}{|n(x)\cdot v|}e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned} \tag{7.84}$$

Set $f^0 = f_0$ and $\partial f^0 = [\partial_t f^0, \nabla_x f^0, \nabla_v f^0] = [0,0,0]$. The main estimate is the following :

Proof of Theorem 7.2. Fix $p \geq 2$, $\frac{p-2}{2p} < \beta < \frac{p-1}{2p}$ and $\varpi \gg_\Omega 1$. We claim that there exists $0 < T_* \ll 1$ such that we have the following uniformly-in-m,

$$\sup_{0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f^m(t)||_p^p + \int_0^{T_*}|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^m|_{\gamma,p}^p \lesssim_{\Omega,T_*} P(||e^{\theta|v|^2}f_0||_\infty)||\alpha^\beta\partial f_0||_p^p, \tag{7.85}$$

where P is some polynomial.

Once we have (7.85) then we pass to the limit, $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f^m \rightharpoonup e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f$ weakly with norms $\sup_{t\in[0,T_*]}||\cdot||_p^p$ and $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f^m|_\gamma \rightharpoonup e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|_\gamma$ in $\int_0^{T_*}|\cdot|_{\gamma,p}^p$ and $e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f$ satisfies (7.85). Repeat the same procedure for $[T_*,2T_*],[2T_*,3T_*],\cdots$, up to the local existence time interval $[0,T^*]$ in Lemma 7.5 to conclude Theorem 7.2.

We prove (7.85) by induction. From Proposition 7.2, ∂f^1 exits. More precisely we construct $\partial_t f^1, \nabla_x f^1$ first and then $\nabla_v f^1$. Because of our choice of ∂f^0, the estimate (7.85) is valid for $m=1$. Now assume that ∂f^i exists and (7.85) is valid for all $i=1,2,\cdots,m$. Applying the weighted inflow estimate (Proposition 7.2) we deduce that ∂f^{m+1} exists. From the Green's identity (Lemma 7.7) we have

$$\begin{aligned}
&\sup_{0\le s\le t}||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}(s)||_p^p+\int_0^t|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}|^p_{\gamma_+,p}\\
&+\int_0^t||\langle v\rangle^{1/p}e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}||_p^p\\
\lesssim\;& ||\alpha^\beta\partial f_0||_p+tP(||e^{\theta|v|^2}f_0||_\infty)+\int_0^t|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}|^p_{\gamma_-,p}\\
&+(t+\varepsilon)\sup_{0\le s\le t}||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}(s)||_p^p+\int_0^t\iint_{\Omega\times\mathbb{R}^3}[e^{-\varpi\langle v\rangle s}\alpha^\beta]^p|\mathcal{G}_m||\partial f^{m+1}|^{p-1}\\
\lesssim\;& ||\alpha^\beta\partial f_0||_p+tP(||e^{\theta|v|^2}f_0||_\infty)+\int_0^t|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}|^p_{\gamma_-,p}\\
&+(t+\varepsilon)\sup_{0\le s\le t}||e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^{m+1}(s)||_p^p\\
&+P(||e^{\theta|v|^2}f_0||_\infty)\int_0^t\iint_{\Omega\times\mathbb{R}^3}[e^{-\varpi\langle v\rangle s}\alpha^\beta]^p|\partial f^{m+1}|^{p-1}\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|\partial f^m(u)|.
\end{aligned}\tag{7.86}$$

Step 1. Estimate for the nonlocal term : The key estimate is the following : For $0<\beta<\frac{p-1}{2p}$, $0<\theta<\frac14$, and some $C_{\varpi,\beta,p}>0$,

$$\sup_{x\in\Omega}\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{[e^{-\frac{\varpi}{\beta}\langle v\rangle s}\alpha(x,v)]^{\frac{\beta p}{p-1}}}{[e^{-\frac{\varpi}{\beta}\langle u\rangle s}\alpha(x,u)]^{\frac{\beta p}{p-1}}}\mathrm{d}u\ \lesssim_{\Omega,\theta}\ \langle v\rangle^{\frac{\beta p}{p-1}}e^{C_{\varpi,\beta,p}s^2}.\tag{7.87}$$

First we assume $|\xi(x)|<\delta_\Omega$ so that $n(x):=\frac{\nabla\xi(x)}{|\nabla\xi(x)|}$ is well-defined. We decompose $u_n=u\cdot n(x)=u\cdot\frac{\nabla\xi(x)}{|\nabla\xi(x)|}$ and $u_\tau=u-u_n n(x)$. For $0\le\kappa\le1$ is bounded by

$$\begin{aligned}
&|v|^{\frac{\beta p}{p-1}}\int_{\mathbb{R}^3}\frac{1}{|v-u|^{2-\kappa}}e^{-C_\theta|v-u|^2}\frac{e^{-\frac{\varpi p}{p-1}\langle v\rangle t}}{e^{-\frac{\varpi p}{p-1}\langle u\rangle t}}\frac{1}{|u\cdot\nabla\xi(x)|^{\frac{\beta p}{p-1}}}\mathrm{d}u\\
\lesssim_\Omega\;& |v|^{\frac{\beta p}{p-1}}\int_{\mathbb{R}^3}|v-u|^{-2+\kappa}e^{-\frac{C_\theta|v-u|^2}{2}}e^{\frac{\varpi p}{p-1}t|v-u|}|u_n|^{\frac{-\beta p}{p-1}}\mathrm{d}u\\
\lesssim_\Omega\;& |v|^{\frac{\beta p}{p-1}}e^{C_{\varpi,\beta,p}t^2}\int_{\mathbb{R}^2}\mathrm{d}u_\tau\int_{\mathbb{R}}\mathrm{d}u_n|v-u|^{-2+\kappa}e^{-\frac{C_\theta|v-u|^2}{4}}|u_n|^{-\frac{\beta p}{p-1}}\\
\lesssim_\Omega\;& C_\kappa|v|^{\frac{\beta p}{p-1}}e^{C_{\varpi,\beta,p}t^2},
\end{aligned}$$

where we have used

$$e^{\frac{\varpi\beta p}{p-1}t|v-u|}\lesssim e^{C_{\varpi,\beta,p}t^2}\times e^{-\frac{C_\theta|v-u|^2}{4}},\tag{7.88}$$

for some $C_{\varpi,\beta,p}>0$. Furthermore we split the last integration as

$$\int_{|u_n|/2\le|v_n-u_n|}+\int_{|u_n|/2\ge|v_n-u_n|}.$$

Both of them are bounded by

$$C\left[\int\frac{e^{-\frac{C_\theta|v_n-u_n|^2}{8}}}{|u_n|^{\frac{\beta p}{p-1}}}\mathrm{d}u_n+\int\frac{e^{-\frac{C_\theta|v_n-u_n|^2}{8}}}{|v_n-u_n|^{\frac{\beta p}{p-1}}}\mathrm{d}u_n\right]\lesssim\langle v_n\rangle^{-\frac{\beta p}{p-1}}+1.$$

If $|\xi(x)|\ge\delta_\Omega$ then

$$\alpha(x,v)\ge2|\xi(x)|\{v\cdot\nabla^2\xi(x)\cdot v\}\gtrsim\delta_\Omega|v|^2\gtrsim\delta_\Omega|v_3|^2,$$

where $v=(v_1,v_2,v_3)$ is the standard coordinate. We set $v_3=v_n$ and $v_\tau=(v_1,v_2)$ and follow the exactly same proof. Therefore we conclude (7.87).

Therefore

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle s}\alpha^\beta\Big|\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\partial f^m(u)\mathrm{d}u\Big| \\
\lesssim_\theta\ & \Big(\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{[e^{-\frac{\varpi}{\beta}\langle u\rangle s}\alpha]^{\beta q}}{[e^{-\frac{\varpi}{\beta}\langle u\rangle s}\alpha]^{\beta q}}\mathrm{d}u\Big)^{\frac1q}\Big(\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|[e^{-\varpi\langle u\rangle s}\alpha]^\beta\partial f^m(u)|^p\mathrm{d}u\Big)^{\frac1p} \\
\lesssim_\theta\ & \langle v\rangle^\beta e^{Cs^2}\Big(\int_{\mathbb{R}^3}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}|e^{-\varpi\langle u\rangle s}\alpha^\beta\partial f^m(u)|^p\mathrm{d}u\Big)^{\frac1p},
\end{aligned}
$$

where at the last line we used $\frac{p-2}{2p}<\beta<\frac{p-1}{2p}$ so that $\langle v\rangle^\beta\le\langle v\rangle$.

Finally we use Hölder estimate to bound the last term (nonlocal term) of (7.86) by

$$
\begin{aligned}
& Cte^{C_{\varpi,\beta,p}t^2}P(||e^{\theta|v|^2}f_0||_\infty)\sup_{0\le s\le t}\iint_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^m|^p \\
&\quad+(\delta+\varepsilon)P(||e^{\theta|v|^2}f_0||_\infty)\max_{i=m,m+1}\int_0^t\iint_{\Omega\times\mathbb{R}^3}\langle v\rangle|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^i|^p.
\end{aligned}
\tag{7.89}
$$

Step 2. Boundary Estimate : Recall (7.21). We use (7.84) to estimate the contribution of γ_-

$$
\begin{aligned}
& \int_0^t\int_{\gamma_-}|e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta\partial f^{m+1}(s,x,v)|^p \\
\lesssim_p & \int_0^t\int_{\gamma_-}[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\sqrt{\mu}^p\Big(1+\frac{\langle v\rangle}{|n(x)\cdot v|}\Big)^p\left[\int_{n(x)\cdot u>0}|\partial f^m(s,x,u)|\mu^{1/4}\{n\cdot u\}\mathrm{d}u\right]^p \\
& +P(||e^{\theta|v|^2}f_0||_\infty)\int_0^t\int_{\gamma_-}\frac{[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p}{|n(x)\cdot v|^p}e^{-\frac{\theta p}{4}|v|^2}\mathrm{d}\gamma\mathrm{d}s.
\end{aligned}
\tag{7.90}
$$

Using $e^{-\varpi\langle v\rangle s}\alpha(x,v)\le e^{-\frac{\varpi\langle v\rangle}{2}s}|\nabla_x\xi(x)\cdot v|^2$ for $x\in\partial\Omega$, the last term is bounded by

$$
C_\Omega P(||e^{\theta|v|^2}f_0||_\infty)\int_0^t\int_{\partial\Omega}\int_{\mathbb{R}^3}|n(x)\cdot v|^{\beta p-p+1}e^{-\frac{\theta p}{4}|v|^2}\mathrm{d}v\mathrm{d}S_x\mathrm{d}s\lesssim_{\Omega,p,\zeta}tP(||e^{\theta|v|^2}f_0||_\infty),
$$

for $\beta>\frac{p-2}{2p}$ so that $2\beta p-p+1>-1$.

For the first term in (7.90) we split as

$$
\left[\int_{n(x)\cdot u>0}\cdots\mathrm{d}u\right]^p\lesssim_p\left[\int_{(x,u)\in\gamma_+^\varepsilon}\cdots\mathrm{d}u\right]^p+\left[\int_{(x,u)\in\gamma_+\setminus\gamma_+^\varepsilon}\cdots\mathrm{d}u\right]^p.
$$

The γ_+^ε contribution (grazing part) of (7.90) is bounded by

$$
\begin{aligned}
& C_p\int_0^t\int_{\gamma_-}[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\sqrt{\mu}^p\Big(|n\cdot v|+\frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\Big) \\
& \times\left|\int_{(x,u)\in\gamma_+^\varepsilon}e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta\partial f^m\{n\cdot u\}^{1/p}\frac{\{n\cdot u\}^{1/q}\mu^{1/4}}{e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta}\mathrm{d}u\right|^p\mathrm{d}v\mathrm{d}S_x\mathrm{d}s \\
\lesssim_{\Omega,p} & \int_0^t\int_{\gamma_-}[e^{-\varpi\langle v\rangle s}\alpha(v)^\beta]^p\Big(|n\cdot v|+\frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\Big)\sqrt{\mu}^p \\
& \times\left[\int_{(x,u)\in\gamma_+}[e^{-\varpi\langle v\rangle s}\alpha(u)^\beta]^p|\partial f^m|^p\{n\cdot u\}\mathrm{d}u\right] \\
& \times\left[\int_{(x,u)\in\gamma_+^\varepsilon}[e^{-\varpi\langle u\rangle s}\alpha(u)^\beta]^{-q}\mu^{q/4}\{n\cdot u\}\mathrm{d}u\right]^{p/q}\mathrm{d}v\mathrm{d}S_x\mathrm{d}s, \\
\lesssim_{\Omega,p,\varpi,\beta} & \ \varepsilon^a e^{C_{\varpi,\beta,p}t^2}\int_0^t|e^{-\varpi\langle v\rangle s}\alpha^\beta\partial f^m(s)|^p_{\gamma_+,p}\mathrm{d}s,
\end{aligned}
$$

where we used $[e^{-\varpi\langle v\rangle s}\alpha(x,v)] \leq |\nabla\xi(x)\cdot v|^2 \lesssim_\Omega |n(x)\cdot v|^2$ and, for $\beta > \frac{p-2}{2p}$ $(2\beta p - p + 1 > -1)$,

$$
\begin{aligned}
&[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\Big(|n\cdot v| + \frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\Big)\sqrt{\mu}^p \\
&\lesssim_\Omega \Big(|n(x)\cdot v|^{1+2\beta p} + \langle v\rangle^p |n(x)\cdot v|^{2\beta p - p+1}\Big)\sqrt{\mu(v)}^p \in L^1(\{v\in\mathbb{R}^3\}),
\end{aligned}
$$

and, here, $a>0$ is determined via, with $\frac{p-1}{p} = \frac{1}{q}$,

$$
\begin{aligned}
&\int_{\gamma_+^\varepsilon} [e^{-\frac{\varpi}{\beta}\langle u\rangle s}\alpha(x,u)]^{-\frac{\beta p}{p-1}} \mu^{\frac{p}{4(p-1)}}\{n\cdot u\}\mathrm{d}u \\
&\lesssim_\Omega \int_{\gamma_+^\varepsilon}\Big[e^{-\frac{\frac{\varpi}{\beta}\langle u\rangle s}{2}}|u\cdot\nabla\xi(x)|\Big]^{-\frac{\beta p}{p-1}} e^{-\frac{p}{4(p-1)}|u|^2}|n\cdot u|\mathrm{d}u \\
&\lesssim_\Omega \int_{\gamma_+^\varepsilon} |u\cdot n|^{1-\frac{\beta p}{p-1}} e^{\frac{\varpi}{2(p-1)}\langle u\rangle s} e^{-\frac{p}{4(p-1)}|u|^2}\mathrm{d}u \\
&\lesssim_\Omega e^{C_{\varpi,\beta,p}s^2}\int_{\gamma_+^\varepsilon} |u\cdot n|^{1-\frac{\beta p}{p-1}} e^{-\frac{p}{8(p-1)}|u|^2}\mathrm{d}u \\
&\lesssim_{\Omega,p} \varepsilon^a e^{C_{\varpi,\beta,p}t^2},
\end{aligned}
$$

for some $a>0$ since $1-\frac{2\beta p}{p-1} > -1$.

On the other hand, for the non-grazing contribution $\gamma_+\backslash\gamma_+^\varepsilon$, we use a similar estimate to get

$$
\begin{aligned}
&\int_0^t\int_{\gamma_-}[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\sqrt{\mu}^p\Big(1+\frac{\langle v\rangle}{|n(x)\cdot v|}\Big)^p\left[\int_{\gamma_+\backslash\gamma_+^\varepsilon}|\partial f^m(s,x,u)|\mu(u)^{1/4}\{n(x)\cdot u\}\mathrm{d}u\right]^p\mathrm{d}\gamma\mathrm{d}s \\
&\lesssim_\Omega \int_0^t\int_{\partial\Omega}\int_{\mathbb{R}^3}[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\Big(|n\cdot v| + \frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\Big)\sqrt{\mu}^p \\
&\quad\times\left[\int_{\gamma_+\backslash\gamma_+^\varepsilon} e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta|\partial f^m(s,x,u)|\{n\cdot u\}^{1/p}\frac{\{n\cdot u\}^{1/q}\mu(u)^{1/4}}{[e^{-\varpi\langle u\rangle s}\alpha(x,u)]^\beta}\mathrm{d}u\right]^p\mathrm{d}v\mathrm{d}S_x\mathrm{d}s \\
&\lesssim_\Omega \int_0^t\int_{\gamma_-}[e^{-\varpi\langle v\rangle s}\alpha(x,v)^\beta]^p\Big(|n\cdot v| + \frac{\langle v\rangle^p}{|n\cdot v|^{p-1}}\Big)\sqrt{\mu}^p \\
&\quad\times\left[\int_{\gamma_+\backslash\gamma_+^\varepsilon}[e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta]^p|\partial f^m|^p\{n\cdot u\}\mathrm{d}u\right] \\
&\quad\times\left[\int_{\gamma_+}[e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta]^{-q}\mu^{q/4}\{n\cdot u\}\mathrm{d}u\right]^{p/q}\mathrm{d}v\mathrm{d}S_x\mathrm{d}s \\
&\lesssim_\Omega e^{C_{\varpi,\beta,p}t^2}\int_0^t\int_{\gamma_+\backslash\gamma_+^\varepsilon}[e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta]^p|\partial f^m(s)|^p\mathrm{d}\gamma\mathrm{d}s,
\end{aligned}
$$

where we used $\frac{p-2}{2p} < \beta < \frac{p-1}{2p}$ and

$$
\begin{aligned}
&\int_{\gamma_+}[e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta]^{-q}\mu(u)^{q/4}\{n(x)\cdot u\}\mathrm{d}u \\
&= \int_{\gamma_+}[e^{-\varpi\langle u\rangle s}\alpha(x,u)^\beta]^{-\frac{p}{p-1}}\mu(u)^{\frac{p}{4(p-1)}}\{n\cdot u\}\mathrm{d}u \lesssim_{\Omega,p} e^{C_{\varpi,\beta,p}t^2}.
\end{aligned}
$$

By Lemma 7.6 and (7.81), and (7.89) the non-grazing part is further bounded by

$$
\begin{aligned}
&\int_0^t \int_{\gamma_+\setminus\gamma_+^\varepsilon} \\
&\lesssim_\varepsilon \int_0^t ||\alpha^\beta \partial f_0||_p^p + \int_0^t ||e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m||_p^p + \int_0^t \iint_{\Omega\times\mathbb{R}^3} |\mathcal{G}^m| [e^{-\varpi\langle v\rangle s}\alpha^\beta]^p |\partial f^m|^{p-1} \\
&\lesssim \int_0^t ||\alpha^\beta \partial f_0||_p^p + \int_0^t ||e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m||_p^p + t \sup_{0\le s\le t} ||e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m(s)||_p^p + (1+t)P(||e^{\theta|v|^2} f_0||_\infty) \\
&\quad + Cte^{C_{\varpi,\beta,p}t^2} P(||e^{\theta|v|^2} f_0||_\infty) \sup_{0\le s\le t} \iint_{\Omega\times\mathbb{R}^3} |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m|^p \\
&\quad + (\delta+\varepsilon) P(||e^{\theta|v|^2} f_0||_\infty) \max_{i=m,m+1} \int_0^t \iint_{\Omega\times\mathbb{R}^3} \langle v\rangle |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^i|^p.
\end{aligned}
$$

In summary, the boundary contribution of (7.86) is controlled by, for all $0 \le t \le T$,

$$
\begin{aligned}
&\int_0^t |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m(s)|_{\gamma_-,p}^p \mathrm{d}s \\
&\lesssim \int_0^T ||\alpha(v)^\beta \partial f_0||_p^p + \varepsilon^a \int_0^T |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m|_{\gamma_+,p}^p \\
&\quad + T \max_{i=m-1,m} \sup_{0\le t\le T_*} ||e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^i(t)||_p^p + P(||e^{\theta|v|^2} f_0||_\infty) \\
&\quad + Cte^{C_{\varpi,\beta,p}t^2} P(||e^{\theta|v|^2} f_0||_\infty) \sup_{0\le s\le t} \iint_{\Omega\times\mathbb{R}^3} |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^m|^p \\
&\quad + (\delta+\varepsilon) P(||e^{\theta|v|^2} f_0||_\infty) \max_{i=m,m+1} \int_0^t \iint_{\Omega\times\mathbb{R}^3} \langle v\rangle |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^i|^p.
\end{aligned}
$$

Finally we collect the terms to deduce

$$
\begin{aligned}
&\sup_{0\le t\le T} ||e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^{m+1}(t)||_p^p + \int_0^T ||\langle v\rangle^{1/p} e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^{m+1}||_p^p \\
&+ \int_0^T |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^{m+1}|_{\gamma_+,p}^p \mathrm{d}s \\
&\le C_{T,\Omega}\big\{||\alpha^\beta \partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty)\big\} + \big\{\varepsilon + \delta + Te^{C_{\varpi,\beta,p}(T)^2}\big\} P(||e^{\theta|v|^2} f_0||_\infty) \\
&\times \max_{i=m,m-1} \Big\{ \sup_{0\le t\le T} ||\alpha^\beta \partial f^i(t)||_p^p + \int_0^T |e^{-\varpi\langle v\rangle s}\alpha^\beta \partial f^i|_{\gamma_+,p}^p + \int_0^T ||\langle v\rangle^{1/p} e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^i||_p^p \Big\}.
\end{aligned}
$$

Recall $C_{\varpi,\beta,p}$ from (7.87). Choose $0 < T \ll 1$, and $0 < \varepsilon \ll 1,\ 0 < \delta \ll 1$ and hence

$$
\begin{aligned}
&\sup_{0\le t\le T} ||e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^{m+1}(t)||_p^p + \int_0^T |e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^{m+1}|_{\gamma_+,p}^p \\
&\le C_{T,\Omega}\big\{||\alpha^\beta \partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty)\big\} \\
&\quad + \frac{1}{8} \max_{i=m,m-1} \Big\{ \sup_{0\le t\le T} ||e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^i(t)||_p^p + \int_0^T |e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^i|_{\gamma_+,p}^p \Big\}.
\end{aligned}
$$

Set

$$
\begin{aligned}
a_i &= \sup_{0\le t\le T_*} ||e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^{m+1}(t)||_p^p + \int_0^T |e^{-\varpi\langle v\rangle t}\alpha^\beta \partial f^{m+1}|_{\gamma_+,p}^p, \\
D &= C_{T,\Omega}\big\{||\alpha^\beta \partial f_0||_p^p + P(||e^{\theta|v|^2} f_0||_\infty)\big\}.
\end{aligned}
$$

Apply (7.78) with $k = 2$ to complete the proof. □

4.3. Weighted $\mathbf{C^1}$ Estimate

We start with the same iterative sequences (7.81) with $\beta=\frac{1}{2}$. For $(x,v)\in\gamma$, note that $\sqrt{\alpha(x,v)}=|n(x)\cdot v|$. Recall $\mathcal{G}$ in (7.82). We define

$$\mathcal{N}^m(t,x,v):=e^{-\varpi\langle v\rangle t}\sqrt{\alpha(x,v)}\mathcal{G}^m(t,x,v). \tag{7.91}$$

From (7.84) with $\beta=\frac{1}{2}$, we have, for $(x,v)\in\gamma_-$,

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}|\sqrt{\alpha(x,v)}\partial f^{m+1}(t,x,v)|\\
&\lesssim \langle v\rangle c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0}e^{-\varpi\langle u\rangle t}\sqrt{\alpha(x,u)}|\partial f^m(t,x,u)|e^{\varpi\langle u\rangle t}\langle u\rangle\sqrt{\mu(u)}\mathrm{d}u\\
&\quad+e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}\tag{7.92}$$

Recall the stochastic cycles in Definition 7.1 : For (t,x,v) with $(x,v)\notin\gamma_0$ and let $(t^0,x^0,v^0)=(t,x,v)$. For $v^\ell\cdot n(x^{\ell+1})>0$ we define the $(\ell+1)-$component of the back-time cycle as

$$(t^{\ell+1},x^{\ell+1},v^{\ell+1})=(t^k-t_{\mathbf{b}}(x^\ell,v^\ell),x_{\mathbf{b}}(x^\ell,v^\ell),v^{\ell+1}).$$

Lemma 7.9. *If $t^1<0$ then*

$$|e^{-\varpi\langle v\rangle t}\alpha(x,v)^{1/2}\partial f^{m+1}(t,x,v)|\lesssim\ ||\alpha(x,v)^{1/2}\partial f_0||_\infty+\int_0^t|\mathcal{N}^m(s,x-(t-s)v,v)|\mathrm{d}s. \tag{7.93}$$

If $t^1>0$ then

$$\begin{aligned}
&|e^{-\varpi\langle v\rangle t}\alpha(x,v)^{1/2}\partial f^{m+1}(t,x,v)|\\
\lesssim&\int_{t^1}^t|\mathcal{N}^m(s,x-(t-s)v,v)|\mathrm{d}s+e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty)\\
&+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\sum_{i=1}^{\ell-1}1_{\{t^{\ell+1}<0<t^\ell\}}\ |\alpha^{1/2}\partial f^{m+1-i}(0,x^i-t^iv^i,v^i)|\ \mathrm{d}\Sigma_i^{\ell-1}\\
&+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\sum_{i=1}^{\ell-1}1_{\{t^{i+1}<0<t^i\}}\int_0^{t^i}|\mathcal{N}^{m-i}(s,x^i-(t^i-s)v^i,v^i)|\ \mathrm{d}s\ \mathrm{d}\Sigma_i^{\ell-1}\\
&+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\sum_{i=1}^{\ell-1}1_{\{t^{i+1}<0\}}\int_{t^{i+1}}^{t^i}|\mathcal{N}^{m-i}(s,x^i-(t^i-s)v^i,v^i)|\ \mathrm{d}s\ \mathrm{d}\Sigma_i^{\ell-1}\\
&+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\sum_{i=2}^{\ell-1}1_{\{t^{i-1}<0\}}e^{-\frac{\theta}{4}|v^{i-1}|^2}P(||e^{\theta|v|^2}f_0||_\infty)\ \mathrm{d}\Sigma_{i-1}^{\ell-1}\\
&+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\mathbf{1}_{\{t^\ell>0\}}|e^{-\varpi\langle v^{\ell-1}\rangle t^\ell}\alpha(x^\ell,v^{\ell-1})^{1/2}\partial f^{m+1-\ell}(t^\ell,x^\ell,v^{\ell-1})|\ \mathrm{d}\Sigma_{\ell-1}^{\ell-1},
\end{aligned}\tag{7.94}$$

where $\mathcal{V}_j=\{v^j\in\mathbb{R}^3:n(x^j)\cdot v^j>0\}$ and

$$w(v)=\frac{c_\mu}{\langle v\rangle\sqrt{\mu(v)}},$$

and

$$\begin{aligned}
&\mathrm{d}\Sigma_i^{\ell-1}\\
&=\Big\{\Pi_{j=i+1}^{\ell-1}\quad\mu(v^j)c_\mu|n(x^j)\cdot v^j|\mathrm{d}v^j\Big\}\Big\{w(v^i)e^{\varpi\langle v^i\rangle t^i}\langle v^i\rangle^2c_\mu\mu(v^i)\mathrm{d}v^i\Big\}\Big\{\Pi_{j=1}^{i-1}e^{\varpi\langle v^j\rangle t^j}\langle v^j\rangle^2c_\mu\mu(v^j)\mathrm{d}v^j\Big\}.
\end{aligned}$$

Remark that $\mathrm{d}\Sigma_i^{\ell-1}$ is not a probability measure!

Proof. For $t^1<0$ we use (7.81) with $\beta=1$ to obtain

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}\alpha(x,v)^{1/2}\partial f^{m+1}(t,x,v)\\
&\lesssim\alpha(x-tv,v)^{1/2}\partial f_0(x-tv,v)+\int_0^te^{-\nu_{\varpi,1}(v)(t-s)}\mathcal{N}^m(s,x-(t-s)v,v)\mathrm{d}s.
\end{aligned}$$

Consider the case of $t^1 > 0$. We prove by the induction on ℓ, the number of iterations. First for $\ell = 1$, along the characteristics, for $t^1 > 0$, we have

$$\begin{aligned}
& e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t,x,v) \\
\lesssim \;& e^{-\nu_{\varpi,1}(t-t_1)}e^{-\varpi\langle v\rangle t^1}\alpha^{1/2}\partial f^{m+1}(t^1,x^1,v) + \int_{t^1}^t e^{-\nu_{\varpi,1}(t-s)}\mathcal{N}^m(s,x-(t-s)v,v)\mathrm{d}s.
\end{aligned}$$

Now we apply (7.92) to the first term above to further estimate

$$\begin{aligned}
& e^{-\varpi\langle v\rangle t}\alpha^{1/2}|\partial f^{m+1}(t,x,v)| \\
\lesssim \;& e^{-\nu_{\varpi,1}(v)(t-t^1)}e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty) + \int_{t^1}^t e^{-\nu_{\varpi,1}(v)(t-s)}|\mathcal{N}^m(s,x-(t-s)v,v)|\mathrm{d}s \\
& + e^{-\nu_{\varpi,1}(v)(t-t^1)}\langle v\rangle c_\mu\sqrt{\mu(v)}\int_{\mathcal{V}_1} e^{-\varpi\langle v^1\rangle t^1}\alpha^{1/2}|\partial f^m(t^1,x^1,v^1)|e^{\varpi\langle v^1\rangle t^1}\langle v^1\rangle\sqrt{\mu(v^1)}\mathrm{d}v^1 \\
\lesssim \;& e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty) + \int_{t^1}^t |\mathcal{N}^m(s,x-(t-s)v,v)| \\
& + \frac{c_\mu}{w(v)}\int_{\mathcal{V}_1} e^{-\varpi\langle v^1\rangle t^1}\alpha^{1/2}|\partial f^m(t^1,x^1,v^1)|e^{\varpi\langle v^1\rangle t^1}w(v^1)\langle v^1\rangle^2\mu(v^1)\mathrm{d}v^1,
\end{aligned}\tag{7.95}$$

where $w(v)$ is defined in (7.95). Now we continue to express $\partial f^m(t^1,x^1,v^1)$ via backward trajectory to get

$$\begin{aligned}
& e^{-\varpi\langle v^1\rangle t^1}\alpha(x^1,v^1)^{1/2}|\partial f^m(t^1,x^1,v^1)| \\
\leq \;& \mathbf{1}_{\{t^2<0<t^1\}}\Big\{\alpha^{1/2}|\partial f^m(0,x^1-t^1v^1,v^1)| + \int_0^{t^1}|\mathcal{N}^{m-1}(s,x^1-(t^1-s)v^1,v^1)|\mathrm{d}s\Big\} \\
& + \mathbf{1}_{\{t^2>0\}}\Big\{e^{-\varpi\langle v^1\rangle t^2}\alpha^{1/2}|\partial f^m(t^2,x^2,v^1)| + \int_{t^2}^{t^1}|\mathcal{N}^{m-1}(s,x^1-(t^1-s)v^1,v^1)|\mathrm{d}s\Big\}.
\end{aligned}$$

Therefore we conclude from (7.95) that

$$\begin{aligned}
& e^{-\varpi\langle v\rangle t}\alpha(x,v)^{1/2}|\partial f^{m+1}(t,x,v)| \\
\lesssim & \int_{t^1}^t |\mathcal{N}^m(s,x-(t-s)v,v)|\mathrm{d}s + e^{-\frac{\theta}{4}|v|^2}P(||e^{\theta|v|^2}f_0||_\infty) \\
& + \frac{1}{w(v)}\int_{\mathcal{V}_1}\mathbf{1}_{\{t^2<0<t^1\}}\alpha(x^1-t^1v^1,v^1)^{1/2}|\partial f_0(x^1-t^1v^1,v^1)|e^{\varpi\langle v^1\rangle t^1}w(v^1)\langle v^1\rangle^2c_\mu\mu(v^1)\mathrm{d}v^1 \\
& + \frac{1}{w(v)}\int_{\mathcal{V}_1}\mathbf{1}_{\{t^2<0<t^1\}}\int_0^{t^1}|\mathcal{N}^{m-1}(s,x^1-(t^1-s)v^1,v^1)|\mathrm{d}s e^{\varpi\langle v^1\rangle t^1}w(v^1)\langle v^1\rangle^2c_\mu\mu(v^1)\mathrm{d}v^1 \\
& + \frac{1}{w(v)}\int_{\mathcal{V}_1}\mathbf{1}_{\{t^2>0\}}\int_{t^2}^{t^1}|\mathcal{N}^{m-1}(s,x^1-(t^1-s)v^1,v^1)|\mathrm{d}s e^{\varpi\langle v^1\rangle t^1}w(v^1)\langle v^1\rangle^2c_\mu\mu(v^1)\mathrm{d}v^1 \\
& + \frac{1}{w(v)}\int_{\mathcal{V}_1}\mathbf{1}_{\{t^2>0\}}e^{-\varpi\langle v^1\rangle t^2}\alpha(x^2,v^1)^{1/2}|\partial f^m(t^2,x^2,v^1)|e^{\varpi\langle v^1\rangle t^1}w(v^1)\langle v^1\rangle^2c_\mu\mu(v^1)\mathrm{d}v^1,
\end{aligned}$$

and it equals (7.94) for $\ell = 2$.

Assume (7.94) is valid for $\ell \in \mathbb{N}$. We use (7.92) and express the last term of (7.94) as

$$\begin{aligned}
& \mathbf{1}_{\{t^\ell>0\}}e^{-\varpi\langle v^{\ell-1}\rangle t^\ell}\alpha(x^\ell,v^{\ell-1})|\partial f^{m+1-k}(t^\ell,x^\ell,v^{\ell-1})| \\
\lesssim \;& \langle v^{\ell-1}\rangle c_\mu\sqrt{\mu(v^{\ell-1})}\int_{\mathcal{V}_\ell}\mathbf{1}_{\{t^\ell>0\}}e^{-\varpi\langle v^\ell\rangle t^\ell}\alpha^{1/2}|\partial f^{m+1-(k+1)}(t^\ell,x^\ell,v^\ell)|e^{\varpi\langle v^\ell\rangle t^\ell}\langle v^\ell\rangle\sqrt{\mu(v^\ell)}\mathrm{d}v^\ell \\
& + e^{-\frac{\theta}{4}|v_{k-1}|^2}P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}\tag{7.96}$$

Then we decompose $\mathbf{1}_{\{t^\ell>0\}}e^{-\varpi\langle v^\ell\rangle t^\ell}\alpha^{1/2}|\partial f^{m+1-(\ell+1)}(t^\ell,x^\ell,v^\ell)| = \mathbf{1}_{\{t^{\ell+1}<0<t^\ell\}} + \mathbf{1}_{\{t^{\ell+1}>0\}}$, where the first part hits the initial plane as

$$\begin{aligned}
& \mathbf{1}_{\{t^{\ell+1}<0<t^\ell\}}e^{-\varpi\langle v^\ell\rangle t^\ell}\alpha^{1/2}|\partial f^{m+1-(\ell+1)}(t^\ell,x^\ell,v^\ell)| \\
\lesssim \;& \alpha^{1/2}|\partial f_0(x^\ell-t^\ell v^\ell,v^\ell)| + \int_0^{t^\ell}|\mathcal{N}^{m+1-(\ell+2)}(s,x^\ell-(t^\ell-s)v^\ell,v^\ell)|\mathrm{d}s,
\end{aligned}\tag{7.97}$$

and the second part hits at the boundary as

$$\begin{aligned}
&\mathbf{1}_{\{t^{\ell+1}>0\}}e^{-\varpi\langle v\rangle t}\alpha^{1/2}|\partial f^{m+1-(\ell+1)}(t^\ell,x^\ell,v^\ell)| \\
&\lesssim e^{-\varpi\langle v^\ell\rangle t^{\ell+1}}\alpha^{1/2}|\partial f^{m+1-(\ell+1)}(t^{\ell+1},x^{\ell+1},v^\ell)| \\
&\quad+\int_{t^{\ell+1}}^{t^\ell}|\mathcal{N}^{m+1-(\ell+2)}(s,x^\ell-(t^\ell-s)v^\ell,v^\ell)|\mathrm{d}s.
\end{aligned} \tag{7.98}$$

To summarize, from (7.96) upon integrating over $\prod_{j=1}^{\ell-1}\mathcal{V}_j$, we obtain a bound for the last term of (7.94) as

$$\begin{aligned}
&\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\mathbf{1}_{\{t^\ell>0\}}|e^{-\varpi\langle v^{\ell-1}\rangle t^\ell}\alpha^{1/2}\partial f^{m+1-\ell}(t^\ell,x^\ell,v^{\ell-1})|\mathrm{d}\Sigma_{\ell-1}^{\ell-1} \\
&\lesssim P(||e^{\theta|v|^2}f_0||_\infty)\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\mathbf{1}_{\{t^\ell>0\}}e^{-\frac{\theta}{4}|v^{\ell-1}|^2}\mathrm{d}\Sigma_{\ell-1}^{\ell-1} \\
&\quad+\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell}\mathcal{V}_j}\mathbf{1}_{\{t^\ell>0\}}e^{-\varpi\langle v^\ell\rangle t^\ell}\sqrt{\alpha}|\partial f^{m+1-(\ell+1)}(t^\ell,x^\ell,v^\ell)|\mathrm{d}\Sigma_\ell^\ell,
\end{aligned}$$

where by (7.97) and (7.98), the last term is bounded by

$$\begin{aligned}
&\frac{1}{w(v)}\int_{\prod_{j=1}^{\ell}\mathcal{V}_j}\langle v^{\ell-1}\rangle c_\mu\sqrt{\mu(v^{\ell-1})}\sqrt{\mu(v^\ell)}\langle v^\ell\rangle e^{\varpi\langle v^\ell\rangle t^\ell}\mathrm{d}v^\ell \\
&\times\prod_{j=1}^{\ell-2}\Big\{e^{\varpi\langle v^j\rangle t^j}\langle v^j\rangle^2c_\mu\mu(v^j)\mathrm{d}v^j\Big\}\Big\{w(v^{\ell-1})e^{\varpi\langle v^{\ell-1}\rangle t^{\ell-1}}\langle v^{\ell-1}\rangle^2\mu(v^{\ell-1})\mathrm{d}v^{\ell-1}\Big\} \\
&\times\Big\{\mathbf{1}_{\{t^{\ell+1}<0<t^\ell\}}\Big[\alpha^{1/2}|\partial f(0,x^\ell-t^\ell v^\ell,v^\ell)|+\int_0^{t^\ell}|\mathcal{N}^{m-\ell-2}(s,x^\ell-(t^\ell-s)v^\ell,v^\ell)|\mathrm{d}s\Big] \\
&\quad+\mathbf{1}_{\{t^{\ell+1}>0\}}\Big[e^{-\varpi\langle v^\ell\rangle t^{\ell+1}}\alpha^{1/2}|\partial f^{m-\ell-1}(t^{\ell+1},x^{\ell+1},v^\ell)| \\
&\quad+\int_{t^{\ell+1}}^{t^\ell}|\mathcal{N}^{m-\ell-2}(s,x^\ell-(t^\ell-s)v^\ell,v^\ell)|\mathrm{d}s\Big]\Big\}.
\end{aligned}$$

Now we use (7.95) to conclude Lemma 7.9. $\square$

Lemma 7.10. *There exists $\ell_0(\varepsilon)>0$ such that for $\ell\geq\ell_0$ and for all $(t,x,v)\in[0,1]\times\bar{\Omega}\times\mathbb{R}^3$, we have*

$$\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j}\mathbf{1}_{\{t^\ell(t,x,v,v^1,\cdots,v^{\ell-1})>0\}}\mathrm{d}\Sigma_{\ell-1}^{\ell-1}\quad\lesssim_\Omega\quad\left(\frac{1}{2}\right)^{-\ell/5}.$$

Proof. The proof is based on Lemma 23 of [75]. We note that, for some fixed constant $C_0>0$,

$$\begin{aligned}
d\Sigma_{\ell-1}^{\ell-1}&\leq w(v^{\ell-1})e^{\varpi\langle v^{\ell-1}\rangle t^{\ell-1}}\langle v^{\ell-1}\rangle^2c_\mu\mu(v^{\ell-1})\Pi_{j=1}^{\ell-2}e^{\varpi\langle v^j\rangle t^j}\langle v^j\rangle^2c_\mu\mu(v^j)\mathrm{d}v^1\dots\mathrm{d}v^{\ell-1} \\
&\leq\Pi_{j=1}^{\ell-1}\{C'e^{C't^2}\mu(v^j)^{\frac14}\}\ \mathrm{d}v^1\dots\mathrm{d}v^{\ell-1}\leq\{C_0\}^\ell\Pi_{j=1}^{\ell-1}\mu(v^j)^{\frac14}\mathrm{d}v^j.
\end{aligned}$$

Choose $\delta=\delta(C_0)>0$ small and define

$$\mathcal{V}_j^\delta\equiv\{v^j\in\mathcal{V}_j:v^j\cdot n(x^j)\geq\delta,\ |v^j|\leq\delta^{-1}\},$$

where we have $\int_{\mathcal{V}_j\backslash\mathcal{V}_j^\delta}C_0\mu(v^j)^{\frac14}\lesssim\delta$ for some $C_0>0$. Choose sufficiently small $\delta>0$.

On the other hand if $v^j\in\mathcal{V}_j^\delta$ then by Lemma 6 of [75], $(t^j-t^{j+1})\geq\delta^3/C_\Omega$. Therefore if $t^\ell\geq0$ then there can be at most $\big\{\big[\frac{C_\Omega}{\delta^3}\big]+1\big\}$ numbers of $v^m\in\mathcal{V}_m^\delta$ for $1\leq m\leq\ell-1$. Equivalently there are at least $\ell-2-\big[\frac{C_\Omega}{\delta^3}\big]$ numbers of $v^{m_i}\in\mathcal{V}_{m_i}\backslash\mathcal{V}_{m_i}^\delta$. Hence from $\{C_0\}^\ell=\{C_0\}^m\times\{C_0\}^{\ell-1-m}$, we have

$$
\begin{aligned}
&\int_{\prod_{j=1}^{\ell-1}\mathcal{V}_j} 1_{\{t^\ell(t,x,v,v^1,\cdots,v^{\ell-1})>0\}} d\Sigma_{\ell-1}^{\ell-1} \\
\leq\ & \sum_{m=1}^{\left[\frac{C_\Omega}{\delta^3}\right]+1} \int_{\left\{\begin{array}{l}\text{there are exactly } m \text{ of } v_{m_i}\in\mathcal{V}_{m_i}^\delta \\ \text{and } \ \ell-1-m \ of \ v_{m_i}\in\mathcal{V}_{m_i}\backslash\mathcal{V}_{m_i}^\delta\end{array}\right\}} \prod_{j=1}^{\ell-1} C_0\mu(v^j)^{1/4}\mathrm{d}v^j \\
\leq\ & \sum_{m=1}^{\left[\frac{C_\Omega}{\delta^3}\right]+1} \begin{pmatrix} \ell-1 \\ m \end{pmatrix} \left\{\int_{\mathcal{V}} C_0\mu(v)^{1/4}\mathrm{d}v\right\}^m \left\{\int_{\mathcal{V}\backslash\mathcal{V}^\delta} C_0\mu(v)^{1/4}\mathrm{d}v\right\}^{\ell-1-m} \\
\leq\ & \left(\left[\frac{C_\Omega}{\delta^3}\right]+1\right)\{\ell-1\}^{\left[\frac{C_\Omega}{\delta^3}\right]+1}\{\delta\}^{\ell-2-\left[\frac{C_\Omega}{\delta^3}\right]}\left\{\int_{\mathcal{V}} C_0\mu(v)^{1/4}dv\right\}^{\left[\frac{C_\Omega}{\delta^3}\right]+1} \\
\lesssim\ & \frac{\ell}{N}\{Ck\}^{\frac{\ell}{N}}\left(\frac{\ell}{N}\right)^{-\frac{N\ell}{10}} \\
\leq\ & \{CN\}^{\frac{\ell}{N}}\left(\frac{\ell}{N}\right)^{\frac{\ell}{N}}\left(\frac{\ell}{N}\right)^{-\frac{\ell}{N}\frac{N^2}{20}} \leq \left(\frac{\ell}{N}\right)^{\frac{\ell}{N}\left(-\frac{N^2}{20}+3\right)} \leq \left(\frac{1}{\ell/N}\right)^{\frac{-\frac{N^2}{20}+3}{N}\ell} \leq \left(\frac{1}{2}\right)^{-\ell},
\end{aligned}
$$

where we have chosen $\ell = N\times\left(\left[\frac{C_\Omega}{\delta^3}\right]+1\right)$ and $N = \left(\left[\frac{C_\Omega}{\delta^3}\right]+1\right) \gg C > 1$. $\square$

Now we are ready to prove the weighted C^1 part of the main theorem :

Proof of weighted C^1 part in Theorem 7.2. First we show $W^{1,\infty}$ estimate. Recall that we use the same sequences (7.81) with $\beta = \frac{1}{2}$ used for the weighted $W^{1,p}$ estimate ($2\leq p<\infty$). We estimate along the stochastic cycles with (7.93) and (7.94). For $t^1 < 0$, the backward trajectory first hits $t = 0$. From Lemma 7.9 and Lemma 7.4 for (7.91), we deduce

$$
\begin{aligned}
&\sup_{0\leq t\leq T} ||\mathbf{1}_{\{t_1<0\}}e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t)||_\infty \\
&\lesssim ||\alpha^{1/2}\partial f_0||_\infty + P(||e^{\theta|v|^2}f_0||_\infty) + T\sup_{0\leq t\leq T}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t)||_\infty \\
&+ \underbrace{\int_{t^1}^t\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle(t-s)}\frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{\alpha(x,v)^{1/2}}{\alpha(x,u)^{1/2}}\mathrm{d}u\mathrm{d}s} \ P(||e^{\theta|v|^2}f_0||_\infty)\sup_{m,\,0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t)||_\infty,
\end{aligned}
$$

where we have used (7.88). Note that, for any $\beta > \frac{1}{2}$,

$$
\frac{1}{\alpha(x,u)^{1/2}} \lesssim \frac{1}{\alpha(x,u)^\beta} + 1 \tag{7.99}
$$

We apply (7.23) to bound the underbrace term as, for $1\geq\beta>\frac{1}{2}$,

$$
\begin{aligned}
&\left\{\mathbf{1}_{|v|\lesssim 1}\frac{\alpha(x,v)^{\frac{1}{2}+\frac{3}{4}-\frac{\beta}{2}}t_Z^{\frac{3}{2}-\beta}}{|v|^{2\beta-1}} + \mathbf{1}_{|v|\gtrsim 1}\frac{\varepsilon^{\frac{3}{2}-\beta}\alpha(x,v)^{\frac{1}{2}}}{|v|^2\alpha(x,v)^{\beta-1}}\right\} + \frac{\alpha(x,v)^{\frac{1}{2}}}{\varpi\langle v\rangle\varepsilon^2\alpha(x,v)^{\beta-\frac{1}{2}}} \\
&\lesssim\ t^{\frac{3}{2}-\beta} + \varepsilon^{\frac{3}{2}-\beta} + \frac{1}{\varepsilon^2\varpi},
\end{aligned}
\tag{7.100}
$$

where we used $\alpha(x,v)\lesssim|v|^2$.

If $t^1(t,x,v)\geq 0$, the backward trajectory first hits the boundary, then from (7.94) we have the following line-by-line estimate

$$
\begin{aligned}
&|\mathbf{1}_{\{t_1>0\}}e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t,x,v)| \\
\leq\ & \underbrace{\int_{t^1}^{t}\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle (t-s)}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2\kappa}}\frac{\alpha(X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))^{\frac{1}{2}}}{\alpha(X_{\mathbf{cl}}(s),u)^{\frac{1}{2}}}\mathrm{d}u\mathrm{d}s}\, ||e^{-\varpi\langle v\rangle s}\alpha^{1/2}\partial f^m(s)||_\infty \\
&+ P(||e^{\theta|v|^2}f_0||_\infty) + \ell(Ce^{Ct^2})^\ell \max_{1\leq i\leq \ell-1}||\alpha^{\frac{1}{2}}\partial f_0^{m+1-i}||_\infty \\
&+ \ell(Ce^{Ct^2})^\ell\langle v\rangle\sqrt{\mu(v)}\times\max_i \underbrace{\int_0^{t^i}\int_{\mathbb{R}^3} e^{-\varpi\langle v^i\rangle (t-s)}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2\kappa}}\frac{\alpha(X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))^{\frac{1}{2}}}{\alpha(X_{\mathbf{cl}}(s),u)^{\frac{1}{2}}}\mathrm{d}u\mathrm{d}s} \\
&\times \max_{1\leq i\leq k-1}\sup_{0\leq s\leq t}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1-i}(t)||_\infty \\
&+ \ell(Ce^{Ct^2})^\ell P(||e^{\theta|v|^2}f_0||_\infty) + \left(\frac{1}{2}\right)^{-\frac{\ell}{5}}\sup_{0\leq s\leq t}||e^{-\varpi\langle v\rangle s}\alpha^{1/2}\partial f^{m+1-\ell}(s)||_\infty,
\end{aligned}
$$

where we have used (7.81), Lemma 7.10, and Lemma 7.4 for (7.91) and (7.88). For the underbraced terms we apply (7.99) and (7.100). Therefore

$$
\begin{aligned}
&|\mathbf{1}_{\{t_1>0\}}e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t,x,v)| \\
\lesssim\ & C_\ell C^{C\ell t^2}\big\{t^{\frac{3}{2}-\beta}+\varepsilon^{\frac{3}{2}-\beta}+\frac{1}{\varepsilon^2\varpi}\big\}\times\max_{0\leq i\leq m}\sup_{0\leq s\leq t}||e^{-\varpi\langle v\rangle s}\alpha^{1/2}\partial f^i(s)||_\infty \\
&+ C_\ell C^{C\ell t^2}\max_{0\leq i\leq m}||\alpha^{1/2}\partial f_0^i||_\infty + \left(\frac{1}{2}\right)^{-\frac{\ell}{5}}\max_{0\leq i\leq m}\sup_{0\leq s\leq t}||e^{-\varpi\langle v\rangle s}\alpha^{1/2}\partial f^i(s)||_\infty.
\end{aligned}
$$

We choose a large ℓ and then small t and then small ε and then finally large ϖ to conclude

$$
\begin{aligned}
\sup_{0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^{m+1}(t)||_\infty \quad\leq\quad & \frac{1}{8}\max_{m-\ell\leq i\leq m}\sup_{0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^i(t)||_\infty \\
& + ||\alpha^{1/2}\partial f_0||_\infty + P(||e^{\theta|v|^2}\partial f_0||_\infty).
\end{aligned}
$$

Set $D = ||\alpha^{1/2}\partial f_0||_\infty + P(||e^{\theta|v|^2}\partial f_0||_\infty)$,

$$
a_i = \sup_{0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^i(t)||_\infty,\quad A_i = \max\{a_i, a_{i-1},\cdots,a_{i-(\ell-1)}\},
$$

then we have $a_{m+1}\leq \frac{1}{8}A_m + D$. Use (7.78) to conclude

$$
\sup_{0\leq t\leq T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f(t)||_\infty \lesssim ||\alpha^{1/2}\partial f_0||_\infty + P(||e^{\theta|v|^2}f_0||_\infty).
$$

The existence and uniqueness and the estimate in Theorem 7.2 are clear for short time $T_*>0$. We follow the same procedure for $t\in[T_*,2T_*]$ to conclude

$$
\sup_{T_*\leq t\leq 2T_*}||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f(t)||_\infty \lesssim_{\Omega,T_*} ||e^{-\varpi\langle v\rangle T_*}\partial f(T_*)||_\infty + P(||e^{\theta|v|^2}f_0||_\infty).
$$

Then we conclude the weighted $W^{1,\infty}$ part of Theorem 7.2 following the same procedure for $[T_*,2T_*]$, $[2T_*,3T_*]$, $\cdots$.

Now we consider the continuity of $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f$. Remark that for each step $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^m$ satisfies the condition of Proposition 7.2. Therefore we conclude $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^m\in C^1([0,T_*]\times\bar{\Omega}\times\mathbb{R}^3)$. Now we follow $W^{1,\infty}$ estimate part for $e^{-\varpi\langle v\rangle t}\alpha^{1/2}[\partial f^{m+1}-\partial f^m]$ to show that $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^m$ is Cauchy in L^∞. Then $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f^m\to e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f$ strongly in L^∞ so that $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\partial f\in C^0([0,T_*]\times\bar{\Omega}\times\mathbb{R}^3)$. $\square$

7.6 Appendix. Non-Existence of Second Derivatives

In the previous theorem, we consider the *first-order derivative* of the Boltzmann solution with several boundary conditions. Now we show that some second order spatial derivative does not exist up to the boundary in general so that our result is quite optimal.

Assume that all the second order spatial derivatives exist away from the grazing set $\gamma_0 = \{(x,v) \in \partial\Omega \times \mathbb{R}^3 : n(x)\cdot v = 0\}$ but up to some boundary $\partial\Omega\times\mathbb{R}^3$. Taking the normal derivative $\partial_n = n(x)\cdot\nabla_x = \frac{\nabla_x \xi(x)}{|\nabla_x\xi(x)|}\cdot\nabla_x$ to the Boltzmann equation directly yields

$$v\cdot\partial_n\nabla_x f = -\partial_n\partial_t f - \nu(\sqrt{\mu}f)\partial_n f + \underbrace{\partial_n\Gamma_{\text{gain}}(f,f) - \partial_n\nu(\sqrt{\mu}f)f}.$$

From previous Theorem we know that $\partial_n\partial_t f,\ \nu(\sqrt{\mu}f)\partial_n f \sim \frac{1}{\alpha^a}$ with some $a>0$. In this section we show that the underbraced term blows up at the boundary with any velocity for symmetric domains.

Assume $f_0 \sim (\sqrt{\mu})^{1-\delta}$ for some $0<\delta\ll 1$. Then there exists $\mathbf{k}_{f_0}(v,u)$ such that

$$\Gamma_{\text{gain}}(f,f_0) + \Gamma_{\text{gain}}(f_0,f) - \nu(\sqrt{\mu}f)f_0 := \int_{\mathbb{R}^3}\mathbf{k}_{f_0}(v,u)f(u)\mathrm{d}u.$$

First consider the diffuse reflection boundary condition. Theorem 7.2 plays an important role in our proof.

Proposition 7.3 (Diffuse BC)**.** *Assume $\Omega = \{x\in\mathbb{R}^3 : |x|<1\}$ and $\xi(x) = |x|^2-1$. Assume the initial datum f_0 satisfies, for some $x_0\in\partial\Omega$,*

$$\Big[\int_{n(x_0)\cdot u_\tau = 0}\mathbf{k}_{f_0}(v,u)u\cdot n(x_0)\partial_n f_0(x_0,u)\mathrm{d}u_\tau\Big]_{u\cdot n(x_0)=0} > C > 0. \tag{7.101}$$

Then there exist $t>0$ such that for all $v\in\mathbb{R}^3$,

$$\partial_n\Gamma_{\text{gain}}(f,f)(t,x_0,v) - \partial_n\nu(\sqrt{\mu}f)f(t,x_0,v) = \infty. \tag{7.102}$$

We remark that for $0<\theta<\frac14$ we have $\sup_t ||e^{\theta|v|^2}f(t)||_\infty \lesssim ||e^{\theta|v|^2}f_0||_\infty$ due to Lemma 7.5 or [75, 67] and $||\alpha^{1/2}\partial f(t)||_\infty \lesssim 1$ due to Theorem 7.2. We also remark that the condition (7.101) is very natural for the diffuse BC.

Proof. We denote the different quotient

$$\triangle_\varepsilon f(t,x,v) := \frac{f(t,x+\varepsilon[-n(x)],v) - f(t,x,v)}{\varepsilon}.$$

Then

$$\triangle_\varepsilon\{\Gamma_{\text{gain}}(f,f)\} - \nu(\sqrt{\mu}\triangle_\varepsilon f)f = \Gamma_{\text{gain}}(\triangle_\varepsilon f,f) + \Gamma_{\text{gain}}(f,\triangle_\varepsilon f) - \nu(\sqrt{\mu}\triangle_\varepsilon f)f.$$

Assuming $f\sim f_0\sim(\sqrt{\mu})^{1-\delta}$ for $0<\delta\ll 1$, we have

$$\begin{aligned}&\Gamma_{\text{gain}}(\triangle_\varepsilon f,f) + \Gamma_{\text{gain}}(f,\triangle_\varepsilon f) - \nu(\sqrt{\mu}\triangle_\varepsilon f)f\\ &\sim \int_{\mathbb{R}^3}\mathbf{k}_{f_0}(v,u)\triangle_\varepsilon f(x,u)\mathrm{d}u \sim \int_{\mathbb{R}^3}\mathbf{k}_{f_0}(v,u)\frac{f(x-\varepsilon n(x),u) - f(x,u)}{\varepsilon}\mathrm{d}u,\end{aligned} \tag{7.103}$$

where $\mathbf{k}_{f_0}(v,u)\sim\mathbf{k}(v,u)$ in (7.25) with slightly different exponents. For simplicity let us assume $\mathbf{k}_{f_0}(v,u)$ is bounded. We split as

$$\begin{aligned}&\int_{\mathbb{R}^3}\mathbf{k}_{f_0}(v,u)\frac{f(t,x-\varepsilon n(x),u) - f(t,x,u)}{\varepsilon}\mathrm{d}u\\ &= \underbrace{\int_{|n(x)\cdot u|\le\varepsilon}}_{\mathbf{I}} + \underbrace{\int_{\varepsilon\le|n(x)\cdot u|\le\sigma}}_{\mathbf{II}} + \underbrace{\int_{\sigma\le|n(x)\cdot u|}}_{\mathbf{III}}.\end{aligned} \tag{7.104}$$

The first term is bounded as $\mathbf{I}\lesssim O(1)||e^{\theta|v|^2}f||_\infty$. The last term is bounded due to Theorem 7.2. Since $\xi(x) = |x|^2-1$, for all $0<r<\varepsilon\ll 1$,

$$\begin{aligned}\nabla\xi(x-rn(x))\cdot u &= \nabla\xi(x)\cdot u - \int_0^r\big\{\nabla\xi(x)\cdot\nabla^2\xi(x-r'n(x))\cdot u\big\}\mathrm{d}r'\\ &= \nabla\xi(x)\cdot u - 2\int_0^r\nabla\xi(x)\cdot u\mathrm{d}r'\\ &= \nabla\xi(x)\cdot u + O(\varepsilon)|\nabla\xi(x)\cdot u|\\ &\sim \nabla\xi(x)\cdot u.\end{aligned} \tag{7.105}$$

Therefore $\sigma \leq |n(x)\cdot u|$ implies $\sigma \lesssim \sqrt{\alpha(x,u)}$ and

$$\begin{aligned}\mathbf{III} &\lesssim ||e^{-\varpi\langle v\rangle t}\sqrt{\alpha}\nabla_x f(t)||_\infty \int_{\sigma\lesssim\sqrt{\alpha}} \frac{e^{\varpi\langle u\rangle t}}{\sqrt{\alpha}}\mathbf{k}_{f_0}(v,u)\mathrm{d}u \\ &= \int_{\sigma\leq\sqrt{\alpha},|u|\leq N} + \int_{\sigma\leq\sqrt{\alpha},|u|\geq N} \lesssim \frac{O(1)+e^{CNt}}{\sigma}.\end{aligned}$$

For the second term of (7.104) we use (7.105) to conclude, for $0\leq r\leq\varepsilon$,

$$\varepsilon \lesssim |n(x-rn(x))\cdot u| \lesssim \sigma.$$

Therefore $f(t,x-\varepsilon n(x),u)$ is differentiable so that

$$\frac{f(t,x-\varepsilon n(x),u)-f(t,x,u)}{\varepsilon} = \int_0^1 \partial_n f(t,x-\varepsilon rn(x),u)\mathrm{d}r. \tag{7.106}$$

We further split $\mathbf{II}$ as

$$\mathbf{II} = \underbrace{\int_{\substack{\varepsilon\leq|n(x)\cdot u|\leq\sigma\\ \frac{1}{N}\leq|u|\leq N}}}_{\mathbf{II}_a} + \underbrace{\int_{\substack{\varepsilon\leq|n(x)\cdot u|\leq\sigma\\ |u|\leq\frac{1}{N},|u|\geq N}}}_{\mathbf{II}_b}.$$

For the second term we use Theorem 7.2 to have

$$\begin{aligned}\mathbf{II}_b &\lesssim e^{-N}\int_0^1 \mathrm{d}r\int_{\varepsilon\lesssim|u_n|\lesssim\sigma}\mathrm{d}u_n\int_{|u_\tau|\gtrsim N}\mathrm{d}u_\tau\ \mathbf{k}_{f_0}(v,u)\partial_n f(t,x-\varepsilon rn(x),u) \\ &\lesssim e^{-N}\int_0^1 \mathrm{d}r\int_{\varepsilon\lesssim|u_n|\lesssim\sigma}\mathrm{d}u_n\int_{|u_\tau|\gtrsim N}\mathrm{d}u_\tau\ \frac{\mathbf{k}_{f_0}(v,u)}{\sqrt{|u_n|^2+Cr\varepsilon N^2}},\end{aligned} \tag{7.107}$$

where we used

$$\xi(x-\varepsilon rn(x)) = \xi(x)+C\varepsilon r = C\varepsilon r.$$

The main term is $\mathbf{II}_a$:

$$\mathbf{II}_a = \int_0^1 \mathrm{d}r \iint_{\substack{\varepsilon\lesssim|u_n|\lesssim\sigma\\ \frac{1}{N}\leq|u|\leq N}} \mathrm{d}u_\tau\mathrm{d}u_n\ \mathbf{k}_{f_0}(v,u)\partial_n f(t,x-\varepsilon rn(x),u).$$

We claim that if Ω is convex (7.3) then for $(x,v)\in\gamma_-$

$$t_{\mathbf{b}}(x,v) \lesssim_\xi \frac{\sqrt{\alpha(x,v)}}{|v|^2}. \tag{7.108}$$

It suffices to show $t_{\mathbf{b}}(x,v)\lesssim_\xi \frac{|n(x)\cdot v|}{|v|^2}$. Since $\xi(x)=0=\xi(x-t_{\mathbf{b}}(x,v)v)$ for $(x,v)\in\gamma_-$, we have

$$\begin{aligned}0 = \xi(x-t_{\mathbf{b}}(x,v)v) &= \xi(x)+\int_0^{t_{\mathbf{b}}(x,v)}[-v\cdot\nabla_x\xi(x-sv)]\mathrm{d}s \\ &= [-v\cdot\nabla_x\xi(x)]t_{\mathbf{b}}(x,v)+\int_0^{t_{\mathbf{b}}(x,v)}\int_0^s\{v\cdot\nabla_x^2\xi(x-\tau v)\cdot v\}\mathrm{d}\tau\mathrm{d}s.\end{aligned}$$

By the convexity of ξ in (7.3) we have $[v\cdot\nabla_x\xi(x)]t_{\mathbf{b}}(x,v) \geq \frac{(t_{\mathbf{b}}(x,v))^2}{2}C_\xi|v|^2$, and therefore this proves (7.108). From (7.108), for $\varepsilon\lesssim|u_n|\lesssim\sigma$ and $\frac{1}{N}\leq|u|\leq N$,

$$t_{\mathbf{b}}(x-\varepsilon rn(x),u) \lesssim \frac{\sqrt{\alpha(x-\varepsilon rn(x),u)}}{|u|^2} \lesssim \frac{\sqrt{\sigma^2+\varepsilon rN^2}}{\frac{1}{N^2}} \lesssim N^2\sqrt{\sigma^2+\varepsilon N^2}.$$

Let $x(r) = x - \varepsilon r n(x)$. For $\varepsilon \lesssim |u_n| \lesssim \sigma$ and $\frac{1}{N} \leq |u| \leq N$ and $t \gtrsim N^2\sqrt{\sigma^2 + \varepsilon N^2}$,

$$
\begin{aligned}
&\partial_n f(t, x(r), u) \\
&= n(x(r)) \cdot \nabla_x \Big\{ f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) + \int_0^{t_{\mathbf{b}}} [\Gamma_{\text{gain}}(f,f) - \nu(F)f](t-s, x(r) - su, u)\mathrm{d}s \Big\} \\
&= \sum_{i=1}^{2} n(x(r)) \cdot \tau_i(x_{\mathbf{b}}) \partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) + \frac{n(x(r)) \cdot n(x_{\mathbf{b}})}{n(x_{\mathbf{b}}) \cdot u} \underline{u \cdot n(x_{\mathbf{b}}) \partial_n f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)} \\
&+ \int_0^{t_{\mathbf{b}}} n(x(r)) \\
&\quad \cdot \{\Gamma_{\text{gain}}(\nabla_x f, f) + \Gamma_{\text{gain}}(f, \nabla_x f) - \nu(\sqrt{\mu}\nabla_x f) f - \nu(\sqrt{\mu} f)\nabla_x f\}(t-s, x(r) - su, u)\mathrm{d}s.
\end{aligned}
$$

Now we expand in time for the underlined term and choose $0 < t \ll 1$ ($N^2\sqrt{\sigma^2 + \varepsilon N^2} \ll 1$) so that

$$
\begin{aligned}
&u \cdot n(x_{\mathbf{b}}) \partial_n f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) \\
&= u \cdot n(x_{\mathbf{b}}) \partial_n f_0(x_{\mathbf{b}}, u) + \int_0^{t - t_{\mathbf{b}}} \{u \cdot n(x_{\mathbf{b}})\} \partial_t \partial_n f(s, x_{\mathbf{b}}, u)\mathrm{d}s \\
&= u \cdot n(x_{\mathbf{b}}) \partial_n f_0(x_{\mathbf{b}}, u) + O(1) t e^{\varpi N t} ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \partial_t \partial_n f(t)||_\infty.
\end{aligned}
$$

The tangential derivative term is bounded by

$$
\begin{aligned}
&|n(x(r)) \cdot \tau_i(x_{\mathbf{b}}(x(r), u))||\partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim |n(x_{\mathbf{b}}) \cdot \tau_i(x_{\mathbf{b}}) + O(t_{\mathbf{b}}(x(r), u)) u \cdot \nabla_x n(x(r))||\partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim \frac{\sqrt{\alpha(x_{\mathbf{b}}, u)}}{|u|} |\nabla_x f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim N e^{\varpi N t} ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t, x, v)||_\infty,
\end{aligned}
$$

and the time integration terms are bounded by

$$
\begin{aligned}
&||e^{\theta|v|^2} f||_\infty \int_0^{t_{\mathbf{b}}} \int_{\mathbb{R}^3} \frac{e^{-C|u-u'|^2}}{|u-u'|^{2-\kappa}} |\partial_x f(t-s, x(r) - su, u')|\mathrm{d}u'\mathrm{d}s \\
&\quad + N e^{\varpi N t} ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \\
&\lesssim ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \\
&\quad \times e^{\varpi N t} \Big\{ \int_0^{t_{\mathbf{b}}} \int_{\mathbb{R}^3} e^{-\varpi\langle u \rangle (t-s)} \frac{e^{-C|u-u'|^2}}{|u-u'|^{2-\kappa}} \frac{|u'|^\delta}{\alpha(x(r) - su, u')^{\frac{1+\delta}{2}}} \mathrm{d}u'\mathrm{d}s \Big\} \\
&\lesssim ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \frac{e^{\varpi N t} C_N}{[\alpha(x(r), u)]^{\delta/2}}.
\end{aligned}
$$

Now we plug these estimates into $\mathbf{II}_a$ to have

$$
\begin{aligned}
\mathbf{II}_a + \mathbf{II}_b \gtrsim & \int_0^1 \int_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{\alpha(x_0 - \varepsilon r n(x_0), u)}} \\
& \times \Big[\int_{\cdot n(x_0) \cdot u_\tau = 0} \mathbf{k}_{f_0}(v, u) u \cdot n(x_0) \partial_n f_0(x_0, u) \mathrm{d}u_\tau \Big]_{u \cdot n(x_0) = 0} \\
& - \Big\{ O(t) e^{-\varpi N t} ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \partial_t \partial_n f(t)||_\infty + e^{-N} \Big\} \int_0^1 \iint_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{\alpha(x_0 - \varepsilon r n(x_0), u)}} \\
& - O(1) N e^{\varpi N t} ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \\
& - O_N(1) e^{\varpi N t} ||e^{\theta|v|^2} f_0||_\infty ||e^{-\varpi\langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \int_0^1 \iint_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{[\alpha(x_0 - \varepsilon r n(x_0), u)]^{\delta/2}}.
\end{aligned}
$$

Due to (7.101), for $N \gg 1$ and $t \ll 1$ with $N^2\sqrt{\sigma^2 + \varepsilon N^2} \ll 1$

$$\begin{aligned}
\mathbf{II} &\gtrsim \int_0^1 \int_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{|u_n|^2 + C\varepsilon r |u_\tau|^2}} \mathrm{d}u_n \mathrm{d}u_\tau \mathrm{d}r \\
&\gtrsim \int_{\varepsilon \le |u_n| \le \sigma} \frac{N^2}{|u_n| + \sqrt{\varepsilon} N} \mathrm{d}u_\tau \mathrm{d}u_n \\
&\gtrsim N^2 \ln \frac{1}{\varepsilon + \sqrt{\varepsilon} N} - O_{N,\sigma}(1) \\
&\gtrsim \frac{N^2}{2} \ln \frac{1}{\varepsilon} - o(1) \ln \frac{1}{\varepsilon} - O_{N,\sigma}(1) \to \infty.
\end{aligned}$$

$\square$

Chapitre 8

BV-regularity of the Boltzmann equation in non-convex domains

Abstract

This Chapter is an extract from the paper [76] in collaboration with Y. Guo, C. Kim and D. Tonon. Consider the Boltzmann equation in a general non-convex domain with the diffuse boundary condition. We establish optimal BV estimates for the solution. Our method consists of a new $W^{1,1}$ trace estimate for the diffuse boundary condition and a delicate construction of a small $\varepsilon-$tubular neighborhood of the singular set (grazing trajectories). We also illustrate that such $BV-$regularity is rather optimal in the case of strictly non-convex domains.

Sommaire

8.1 Introduction

Boundary effects play an important role in the dynamics of solutions of the Boltzmann equation

$$\partial_t F + v \cdot \nabla_x F = Q(F, F), \tag{8.1}$$

where $F(t, x, v) \geq 0$ denotes the particle distribution in the phase space $\Omega \times \mathbb{R}^3$. Here t stands for the time variable, x for the space variables, and v for the velocity variables.

Throughout this paper, the collision operator takes the form

$$\begin{aligned} Q(F_1, F_2) &:= Q_{\text{gain}}(F_1, F_2) - Q_{\text{loss}}(F_1, F_2) \\ &= \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} |v-u|^\kappa q_0(\theta) \Big[F_1(u') F_2(v') - F_1(u) F_2(v) \Big] \mathrm{d}\omega \mathrm{d}u, \end{aligned} \tag{8.2}$$

where $u' = u + [(v-u)\cdot\omega]\omega,\ v' = v - [(v-u)\cdot\omega]\omega$ and $0 \leq \kappa \leq 1$ (hard potential) and $0 \leq q_0(\theta) \leq C|\cos\theta|$ (angular cutoff) with $\cos\theta = \frac{v-u}{|v-u|} \cdot \omega$ with $\omega \in \mathbb{S}^2$. We denote the global Maxwellian

$$\mu(v) = \exp\Big(- \frac{|v|^2}{2} \Big).$$

Throughout this paper we assume that Ω is a bounded open subset of $\mathbb{R}^3$. The boundary $\partial\Omega$ is locally a graph of a given C^2 function : for each point $x_0 \in \partial\Omega$ there exist $r > 0$ and a C^2 function $\eta : \mathbb{R}^2 \to \mathbb{R}$ such that, up to a rotation and relabeling, we have

$$\begin{aligned} \partial\Omega \cap B(x_0; r) &= \big\{ x \in B(x_0; r) : x_3 = \eta(x_1, x_2) \big\}, \\ \Omega \cap B(x_0; r) &= \big\{ x \in B(x_0; r) : x_3 > \eta(x_1, x_2) \big\}. \end{aligned} \tag{8.3}$$

The boundary of the phase space $\Omega \times \mathbb{R}^3$ is

$$\gamma := \{(x, v) \in \partial\Omega \times \mathbb{R}^3\}. \tag{8.4}$$

We denote $n = n(x)$ the outward normal direction at $x \in \partial\Omega$. We decompose γ as

$$\begin{aligned} \gamma_- &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x) \cdot v < 0\}, && (\textit{the incoming set}), \\ \gamma_+ &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x) \cdot v > 0\}, && (\textit{the outgoing set}), \\ \gamma_0 &= \{(x, v) \in \partial\Omega \times \mathbb{R}^3 : n(x) \cdot v = 0\}, && (\textit{the grazing set}). \end{aligned}$$

In general the boundary condition is imposed only for the incoming set γ_- for general kinetic PDEs. We consider *the diffuse boundary condition* in this paper : for $(x, v) \in \gamma_-$

$$F(t, x, v) = c_\mu \mu(v) \int_{n(x)\cdot u > 0} F(t, x, u) \{n(x) \cdot u\} \mathrm{d}u, \tag{8.5}$$

with $c_\mu \int_{n(x)\cdot u>0} \mu(u)\{n(x) \cdot u\}\mathrm{d}u = 1$.

Despite extensive developments in the study of the Boltzmann equation, many basic questions regarding solutions in a physical bounded domain, such as their regularity, have remained largely open. This is partly due to the characteristic nature of boundary conditions in kinetic theory : Consider the simple transport equation $v \cdot \nabla_x f(x, v) = 0$ with the given boundary condition $f|_{\gamma_-} = g$. It is solved by $f(x, v) = g(x_{\mathbf{b}}(x, v), v) = g(x - t_{\mathbf{b}}(x, v)v, v)$ where $t_{\mathbf{b}}(x, v)$ is the *backward exit time* defined as

$$\begin{aligned} t_{\mathbf{b}}(x, v) &:= \sup(\{0\} \cup \{\tau > 0 : x - sv \in \Omega \text{ for all } 0 < s < \tau\}), \\ x_{\mathbf{b}}(x, v) &:= x - t_{\mathbf{b}}(x, v)v. \end{aligned} \tag{8.6}$$

Similarly the *forward exit time* $t_{\mathbf{f}}$ is defined as

$$\begin{aligned} t_{\mathbf{f}}(x, v) &:= \sup(\{0\} \cup \{\tau > 0 : x + sv \in \Omega \text{ for all } 0 < s < \tau\}), \\ x_{\mathbf{f}}(x, v) &:= x + t_{\mathbf{f}}(x, v)v. \end{aligned} \tag{8.7}$$

Since $x_{\mathbf{b}}(x, v)$ has singular behavior (even not continuous) if $n(x_{\mathbf{b}}(x, v)) \cdot v = 0$, we expect f might be singular on *the singular set* :

$$\mathfrak{S}_{\mathrm{B}} := \{(x, v) \in \bar{\Omega} \times \mathbb{R}^3 : n(x_{\mathbf{b}}(x, v)) \cdot v = 0\}, \tag{8.8}$$

which is the collection of all the characteristics emanating from the grazing set γ_0.

In [75], it is shown that in convex domains, the solutions of the Boltzmann equation are continuous away from the grazing set γ_0. On the other hand, in [81], it is shown that the singularity (discontinuity) does occur for Boltzmann solutions in a non-convex domain, and such singularity propagates along the singular set $\mathfrak{S}_{\mathrm{B}}$. Very recently in [77] the authors were able to establish weighted C^1 estimates in convex domains for all basic boundary conditions. The main purpose of this paper is to establish the first BV regularity estimate for the Boltzmann solution in non-convex domains.

We denote $\|\cdot\|_\infty$ the $L^\infty(\bar\Omega\times\mathbb{R}^3)$ norm, while $\|\cdot\|_p$ is the $L^p(\Omega\times\mathbb{R}^3)$ norm. We denote $|\cdot|_p$ either the $L^p(\partial\Omega\times\mathbb{R}^3, \mathrm{d}S_x \mathrm{d}v)$ norm and $|\cdot|_{\gamma,p}$ the $L^p(\partial\Omega\times\mathbb{R}^3) = L^p(\partial\Omega\times\mathbb{R}^3, \mathrm{d}\gamma)$ norm where $\mathrm{d}\gamma = |n(x)\cdot v| \mathrm{d}S_x \mathrm{d}v$ with the surface measure $\mathrm{d}S_x$ on $\partial\Omega$. We write $|\cdot|_{\gamma_\pm,p} = |\cdot \mathbf{1}_{\gamma_\pm}|_{\gamma,p}$. For a function f on $\Omega\times\mathbb{R}^3$, we denote f_γ to be its trace on γ whenever it exists.

A function $f\in L^1(\Omega\times\mathbb{R}^3)$ has *bounded variation* in $\Omega\times\mathbb{R}^3$ if

$$\sup\Big\{\iint_{\Omega\times\mathbb{R}^3} f \mathrm{div}\varphi \, \mathrm{d}x\,\mathrm{d}v : \varphi\in C_c^1(\Omega\times\mathbb{R}^3;\mathbb{R}^3\times\mathbb{R}^3),\ |\varphi|\le 1\Big\} < \infty.$$

We define

$$\|f\|_{BV} := \|f\|_{L^1(\Omega\times\mathbb{R}^3)} + V(f),$$

where

$$V(f) := \sup\Big\{\iint_{\Omega\times\mathbb{R}^3} f \mathrm{div}\varphi \, \mathrm{d}x\,\mathrm{d}v : \varphi\in C_c^1(\Omega\times\mathbb{R}^3;\mathbb{R}^3\times\mathbb{R}^3),\ |\varphi|\le 1\Big\} < \infty.$$

Theorem 8.1. *Let Ω be a bounded open subset of $\mathbb{R}^3$ with C^2 boundary $\partial\Omega$ as in (8.3). Assume that $0\le\kappa\le 1$ in (8.2), $F_0 = \sqrt{\mu} f_0 \ge 0$, $f_0\in BV(\Omega\times\mathbb{R}^3)$, and $\|e^{\theta|v|^2} f_0\|_\infty < +\infty$ for $0<\theta<\frac14$. Then there exists $T = T(\|e^{\theta|v|^2} f_0\|_\infty) > 0$ such that $F = \sqrt{\mu} f$ solves the Boltzmann equation (8.1) with the diffuse boundary condition (8.5) and $f\in L^\infty([0,T]; BV(\Omega\times\mathbb{R}^3))$ and $\nabla_{x,v} f \mathrm{d}\gamma$ is a Radon measure on $\partial\Omega\times\mathbb{R}^3$.*

Moreover, for all $0\le t\le T$,

$$\|f(t)\|_{BV} \ \lesssim_{T,\Omega} \ \|f_0\|_{BV} + P(\|e^{\theta|v|^2} f_0\|_\infty), \tag{8.9}$$

for some polynomial P and $\nabla_{x,v} f_\gamma(t)$ is a Radon measure σ_t on $\partial\Omega\times\mathbb{R}^3$ such that $\int_0^T |\sigma_t(\partial\Omega\times\mathbb{R}^3)|\,\mathrm{d}t \lesssim_{T,\Omega} \|f_0\|_{BV} + P(\|e^{\theta|v|^2} f_0\|_\infty)$.

We remark that the result holds even without any size restriction for the initial datum within a small time. On the other hand, if $\|e^{\theta|v|^2} g_0\|_\infty \ll 1$ for $F_0 = \mu + \sqrt{\mu} g_0 \ge 0$, then, writing $F = \mu + \sqrt{\mu} g \ge 0$, Theorem 8.1 holds for $g(t)$ for all $t\ge 0$:

$$\|g(t)\|_{BV} \ \lesssim_{t,\Omega} \ \|g_0\|_{BV} + P(\|e^{\theta|v|^2} g_0\|_\infty).$$

Moreover the BV regularity (even in the bulk) is the best regularity we can expect. The reason is that in general the singular set $\mathfrak{S}_{\mathrm{B}}$ is a co-dimension 1 subset in the phase space $\Omega\times\mathbb{R}^3$.

Remark 8.1. *Assume that the domain Ω is non-convex : there exist at least one point $x_0\in\partial\Omega$ and $u\in\mathbb{R}^3$ and $(u_1,u_2)\neq 0$ such that (8.3) and*

$$\sum_{i,j=1,2} u_i u_j \partial_i\partial_j \eta(x_0) < 0, \qquad (\textit{strictly non-convex point}). \tag{8.10}$$

Then the singular set $\mathfrak{S}_{\mathrm{B}}$ is a co-dimension 1 subset of $\Omega\times\mathbb{R}^3$. Moreover if we restrict the singular set to the characteristics emanating from the strictly non-convex points

$$\big\{(x,v)\in\mathfrak{S}_{\mathrm{B}} : (x_{\mathbf{b}}(x,v),v) \ \textit{is a strictly non-convex point}\big\},$$

then this set is a co-dimension 1 submanifold of $\Omega\times\mathbb{R}^3$.

We put the proof of Remark 1 in the appendix. Since discontinuous solutions were constructed for non-convex domains in [81], this remark shows that the Boltzmann solutions are singular on the co-dimensional 1 subset $\mathfrak{S}_{\mathrm{B}}$. Then it is standard to conclude that the best possible regularity space is indeed the BV space ([69]). Hence Theorem 1 is optimal.

The equation for $f = F/\sqrt{\mu}$ where F solves (8.1) is

$$\partial_t f + v \cdot \nabla_x f + \nu(\sqrt{\mu} f) f = \Gamma_{\text{gain}}(f, f), \qquad \text{in } \Omega \times \mathbb{R}^3, \tag{8.11}$$

where

$$\Gamma_{\text{gain}}(f_1, f_2) := \frac{1}{\sqrt{\mu}} Q_{\text{gain}}(\sqrt{\mu} f_1, \sqrt{\mu} f_2), \quad \nu(\sqrt{\mu} f_1) f_2 = \frac{1}{\sqrt{\mu}} Q_{\text{loss}}(\sqrt{\mu} f_1, \sqrt{\mu} f_2). \tag{8.12}$$

The boundary condition for $f = F/\sqrt{\mu}$ where F satisfies (8.5) is

$$f(t, x, v) = c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u > 0} f(t, x, u) \sqrt{\mu(u)} \{n(x) \cdot u\} \mathrm{d}u, \qquad \text{on } (x, v) \in \gamma_-. \tag{8.13}$$

The local-in-time existence of the solution f with $\sup_{0 \le t \le T} \| e^{\theta |v|^2} f(t) \|_\infty \lesssim \| e^{\theta' |v|^2} f_0 \|_\infty$ for $0 < \theta < \theta' < \frac{1}{4}$ is standard (e.g. Lemma 6 in [77]).

We now illustrate the main ideas of the proof of Theorem 1. For simplicity we assume that f satisfies (8.13) but solves the following simpler problem

$$\partial_t f + v \cdot \nabla_x f + \nu f = H, \qquad f|_{t=0} = f_0, \tag{8.14}$$

with the boundary condition (8.13), and where $\nu = \nu(t, x, v) \ge 0$, H, and ν are smooth enough. In general solutions f of (8.14) are discontinuous on $\mathfrak{S}_{\mathrm{B}}$ and (distributional) derivatives do not exist [81]. In order to take (distributional) derivatives we employ the following *approximation scheme* using some smooth cut-off function $\chi_\varepsilon(x, v)$ vanishing on some open neighborhood of $\mathfrak{S}_{\mathrm{B}}$.

$$\begin{aligned} \partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + \nu f^\varepsilon &= \chi_\varepsilon H \quad \text{in } (x, v) \in \Omega \times \mathbb{R}^3, \\ f^\varepsilon|_{t=0} &= \chi_\varepsilon f_0 \quad \text{in } (x, v) \in \Omega \times \mathbb{R}^3, \\ f^\varepsilon(t, x, v) = \chi_\varepsilon c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u > 0} & f^\varepsilon(t, x, u) \sqrt{\mu(u)} \{n(x) \cdot u\} \mathrm{d}u, \quad \text{on } (x, v) \in \gamma_-. \end{aligned} \tag{8.15}$$

Due to the cut-off χ_ε, the solution of (8.15) f^ε vanishes on some open subset of $\bar{\Omega} \times \mathbb{R}^3$ containing the singular set $\mathfrak{S}_{\mathrm{B}}$ defined in (8.8). Therefore f^ε is smooth. Once we can show that f^ε is uniformly bounded in L^∞ and ∂f^ε is uniformly bounded in $L^1(\Omega \times \mathbb{R}^3)$ then we conclude that f^ε converges to f weak$-*$ in L^∞ and $f \in BV$ solves (8.14) with (8.13). We apply (distributional) derivatives $\partial \in \{\nabla_x, \nabla_v\}$ to the equation and have

$$|\partial_t \partial f^\varepsilon + v \cdot \nabla_x \partial f^\varepsilon + \nu \partial f^\varepsilon| \le |\partial f^\varepsilon| + |\partial \nu f^\varepsilon| + |\partial \chi_\varepsilon H| + |\chi_\varepsilon \partial H|.$$

On the other hand at the boundary we use an orthonormal transformation $\mathcal{T}(x)$ flattening the boundary in order to remove a $x-$dependence of the integration range : $\{n(x) \cdot u > 0\} \mapsto \{(\mathcal{T}^{-1} u)_3 > 0\}$ (see (17) $\sim$ (21) in [77]). Instead the geometric $x-$dependence enters into the velocity component and hence after differentiating in x tangentially we have an extra $v-$derivative. For the normal derivative in x we use the equation. Overall the derivatives of the boundary terms are bounded as in [77] :

$$|\partial f^\varepsilon| \sim |\partial \chi_\varepsilon| + \frac{1}{|n \cdot v|} \int_{n\cdot u > 0} |\partial f^\varepsilon| \{n \cdot u\} \mathrm{d}u + \frac{1}{|n \cdot v|} \big\{ |H| + |\nu f| \big\}, \qquad \text{on } \gamma_-.$$

We then apply the energy-type estimate (Green's identity, Lemma .8) and the above boundary control to have

$$\begin{aligned} & \| \partial f^\varepsilon(t) \|_1 + \int_0^t |\partial f^\varepsilon|_{\gamma_+, 1} + \int_0^t \| \nu \partial f^\varepsilon(s) \| \mathrm{d}s \\ \lesssim \quad & \| \partial \chi_\varepsilon f(0) \|_1 + \int_0^t |\partial f^\varepsilon|_{\gamma_-, 1} + \int_0^t \| \partial \chi_\varepsilon H \|_1 + \text{“good terms”} \\ \lesssim_t \quad & \underbrace{\| \partial \chi_\varepsilon \|_1 + |\partial \chi_\varepsilon|_{\gamma_-, 1}}_{(A)} + \underbrace{C \int_0^t |\partial f^\varepsilon|_{\gamma_+, 1}}_{(B)} + \text{“good terms”}. \end{aligned}$$

The first main difficulty is to *construct a smooth cut-off function* χ_ε such that it vanishes on an open neighborhood of $\mathfrak{S}_{\mathrm{B}}$ and makes (A) be finite at the same time. We carefully construct, in Lemma 8.1, an open neighborhood $\mathcal{O}_\varepsilon$ of $\mathfrak{S}_{\mathrm{B}}$. More precisely $\mathcal{O}_\varepsilon$ is a collection of $\varepsilon-$tubular neighborhoods of forward trajectories emanating from the grazing set γ_0. Also we can show that $\mathcal{O}_\varepsilon$ contains all points whose distance from $\mathfrak{S}_{\mathrm{B}}$ is less than ε. Such $\varepsilon-$thickness is important for constructing cut-off functions. In fact we construct smooth cut-off functions χ_ε by convoluting the characteristic function $\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_\varepsilon}$ with some standard mollifier. And the $\varepsilon-$thickness guarantees that the cut-off function vanishes around $\mathfrak{S}_{\mathrm{B}}$. Fortunately χ_ε satisfies the desired bound $(A)<\infty$, that is, χ_ε is uniformly bounded in $W^{1,1}$ (Lemma 8.2 and Proposition 8.1), whose proofs are delicate. Since χ_ε is a standard $\varepsilon-$mollification of $\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_\varepsilon}$ we have $\partial\chi_\varepsilon \sim \partial[1-\chi_\varepsilon] \sim \frac{1}{\varepsilon}(\frac{1}{\varepsilon^6}\mathbf{1}_{|x|+|v|<\varepsilon}) * \mathbf{1}_{\mathcal{O}_\varepsilon}$. For example a desired estimate for $|\partial\chi_\varepsilon|_{\gamma_-,1}$ is

$$\int_{(x,v)\in\gamma_-,\ |v|\lesssim 1} \mathbf{1}_{\mathcal{O}_\varepsilon}(x,v)|n(x)\cdot v|\mathrm{d}v\mathrm{d}S_x \sim \varepsilon.$$

Let us denote $\mathcal{O}_\varepsilon$ a collection of $\varepsilon-$tubular neighborhoods of forward trajectories emanating from γ_0. Unfortunately there could be infinitely many grazing trajectories passing by x, which might lead to

$$\begin{aligned} & \int_{(x,v)\in\gamma_-,\ |v|\lesssim 1} \mathbf{1}_{\mathcal{O}_\varepsilon}(x,v)|n(x)\cdot v|\mathrm{d}v\mathrm{d}S_x \\ \sim\ & \{\text{number of grazing at } x\} \times \int_{|v|\lesssim 1} \mathbf{1}_{\varepsilon-\text{tubular neighborhood}}(v)|n(x)\cdot v|\mathrm{d}v \\ \sim\ & \infty. \end{aligned}$$

Instead we establish a geometric Lemma 8.3 to show that $|n(x)\cdot v| \lesssim \sqrt{\varepsilon}$ if $(x,v)\in\mathcal{O}_\varepsilon$. For the proof, we decompose $\mathcal{O}_\varepsilon$ carefully in position and velocity with varying grazing trajectories. We remark that $|\partial\chi_\varepsilon|_{\gamma_+,1}<\infty$ may not be true in general.

The second main difficulty is to *control the outgoing term* (B). We denote the (outgoing) almost grazing set

$$\gamma_+^\delta := \{(x,v)\in\gamma_+ : v\cdot n(x) < \delta \text{ or } |v| > 1/\delta\}, \tag{8.16}$$

and the (outgoing) non-grazing set

$$\gamma_+\backslash\gamma_+^\delta = \{(x,v)\in\gamma_+ : v\cdot n(x) \geq \delta \text{ and } |v| \leq 1/\delta\}. \tag{8.17}$$

In fact the $\gamma_+\backslash\gamma_+^\delta$ contribution can be controlled by the bulk integration and the initial data by the trace theorem. However the γ_+^δ contribution cannot be bounded by the bulk integration nor $\int_0^t |\partial f^\varepsilon|_{\gamma_+,1}$ in the LHS of the energy-type estimate since the constant $C>0$ of (B) can be large in general. The new idea is to use the Duhamel formula along the trajectory once again (*Double iteration scheme*) to extract an extra small constant to close the estimate. We evaluate ∂f^ε along the characteristics and use the bound of ∂f^ε on γ_- to have

$$\begin{aligned} & \int_0^t |\partial f^\varepsilon|_{\gamma_+^\delta,1} \\ =\ & \int_0^t \int_{(x,v)\in\gamma_+^\delta} |\partial f^\varepsilon(s,x,v)|\{n(x)\cdot v\}\mathrm{d}S_x\mathrm{d}v\mathrm{d}s \\ \sim\ & \int_0^t \mathrm{d}s \int_{(x,v)\in\gamma_+^\delta} |\partial f^\varepsilon(s-t_{\mathbf{b}}(x,v), x_{\mathbf{b}}(x,v),v)|\{n(x)\cdot v\}\mathrm{d}S_x\mathrm{d}v \\ \sim\ & \int_0^t \int_{(x,v)\in\gamma_+^\delta} \{n(x)\cdot v\}|\partial\chi_\varepsilon(x_{\mathbf{b}}(x,v),v)|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s && (8.18) \\ & + \int_0^t \int_{(x,v)\in\gamma_+^\delta} \frac{n(x)\cdot v}{n(x_{\mathbf{b}}(x,v))\cdot v} \int_{n(x_{\mathbf{b}})\cdot u>0} |\partial f^\varepsilon(x_{\mathbf{b}}(x,v),u)|\{n(x_{\mathbf{b}}(x,v))\cdot u\}\mathrm{d}u\mathrm{d}S_x\mathrm{d}v\mathrm{d}s. && (8.19) \end{aligned}$$

In Lemma 8.4, we establish a crucial change of variables $(x,v)\mapsto(x_{\mathbf{b}}(x,v),v)$ with $|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v \lesssim |n(x_{\mathbf{b}})\cdot v|\mathrm{d}S_{x_{\mathbf{b}}}\mathrm{d}v$. Clearly (8.18) is bounded by $|\partial\chi_\varepsilon|_{\gamma_-,1}$. For (8.19) we use Lemma 8.4 to convert $x-$integration into $x_{\mathbf{b}}-$integration and remove the singular factor $\frac{n(x)\cdot v}{n(x_{\mathbf{b}}(x,v))\cdot v}$. Furthermore, since $x\in\partial\Omega$ we have $x = x_{\mathbf{b}}(x_{\mathbf{b}},-v)$ and $(x,v)\in\gamma_+^\delta$ which implies $(x_{\mathbf{b}}(x_{\mathbf{b}},-v),v)\in\gamma_+^\delta$. Then we can bound the last term by

$$\sup_{x_{\mathbf{b}}\in\partial\Omega} \int \mathbf{1}_{(x_{\mathbf{b}}(x_{\mathbf{b}},-v),v)\in\gamma_+^\delta}\mathrm{d}v \times \int_0^t |\partial f^\varepsilon|_{\gamma_+,1}.$$

Using the covering lemma of [75] (Lemma .9), we are able to extract an extra small constant from $\sup_{x_{\mathbf{b}}\in\partial\Omega}\int \mathbf{1}_{(x_{\mathbf{b}}(x_{\mathbf{b}},-v),v)\in\gamma_+^\delta}\mathrm{d}v$.

Finally in order to study the nonlinear problem with diffuse boundary condition we employ some *approximation scheme*. On each sequence the problem is a linear problem with given boundary data but the solutions are vanishing on the singular set $\mathfrak{S}_B$. Thanks to the crucial properties of the smooth cut-off function χ_ε we are able to achieve uniform estimates via energy-type estimates with the new estimate for the outgoing term. The quadratic nonlinear terms are controllable due to the known pointwise estimates of the solutions ([75, 77]).

The plan of the paper is the following : In Section 2 we construct the desired $\varepsilon-$neighborhood of the singular set and its smooth cut-off functions. Then we prove the quantitative estimates of the cut-off functions and their derivatives in the bulk and on the boundary. In Section 3 we establish the new trace theorem using double iteration. In Appendix 1 we recall some basic geometric results. In the Appendix 2 we show that the singular set is codimension 1 in general.

8.2 $\varepsilon-$Neighborhood of the Singular set

In this section, we construct an open covering of the singular set $\mathfrak{S}_\mathrm{B}$ (proof of Lemma 8.1) and a smooth function that cuts off the open covering of $\mathfrak{S}_\mathrm{B}$ (Definition 1). Moreover, we prove their crucial properties in Lemma 8.1, Lemma 8.2, and Proposition 8.1.

8.2.1 Construction of Neighborhoods

Lemma 8.1. *For $0<\varepsilon\le\varepsilon_1\ll 1$ and $\theta>0$, we construct an open set $\mathcal{O}_{\varepsilon,\varepsilon_1}\subset\mathbb{R}^3\times\mathbb{R}^3$, such that,*

$$\mathfrak{S}_\mathrm{B}\ \subset\ \mathcal{O}_{\varepsilon,\varepsilon_1}. \tag{8.20}$$

There exists $C_*=C_*(\Omega)\gg 1$ such that for any $0<\varepsilon\le\varepsilon_1\ll 1$

$$\overline{\mathcal{O}_{\varepsilon,\varepsilon_1}}\ \subset\ \mathcal{O}_{\varepsilon,C_*\varepsilon_1}. \tag{8.21}$$

Moreover there exist $C_1=C_1(\theta,\Omega,C_*)>0,\ C_2=C_2(\Omega,C_*)>0,$ such that

$$\iint_{\Omega\times\mathbb{R}^3}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x,v)e^{-\theta|v|^2}\mathrm{d}v\mathrm{d}x<C_1\varepsilon, \tag{8.22}$$

and

$$\mathrm{dist}\big(\bar\Omega\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon},\mathfrak{S}_\mathrm{B}\big)>C_2\varepsilon. \tag{8.23}$$

Proof. Construction of $\mathcal{O}_{\varepsilon,\varepsilon_1}$: Let us fix $\delta>0$ (δ will be chosen later in (8.26)). Since the boundary $\partial\Omega$ is locally a graph of smooth functions, there exists a finite number $M_{\Omega,\delta}$ of small open balls $\mathcal{U}_1,\mathcal{U}_2,..,\mathcal{U}_{M_{\Omega,\delta}}\subset\mathbb{R}^3$ with $\mathrm{diam}(\mathcal{U}_m)<2\delta$ for all m, such that

$$\partial\Omega\ \subset\ \bigcup_{m=1}^{M_{\Omega,\delta}}[\,\mathcal{U}_m\ \cap\ \partial\Omega\,]\quad\text{with}\quad M_{\Omega,\delta}=O(\frac{1}{\delta^2}), \tag{8.24}$$

and for every m, inside $\mathcal{U}_m$ the boundary $\mathcal{U}_m\cap\partial\Omega$ is exactly described by a smooth function η_m defined on a (small) open set $\mathcal{A}_m\subset\mathbb{R}^2$.

For all m, without loss of generality (up to rotations and translations *depending on* m, and up to reducing the size of the ball $\mathcal{U}_m$) we will always assume that

$$\begin{aligned}\mathcal{U}_m\cap\partial\Omega &= \big\{(x_1,x_2,\eta_m(x_1,x_2))\in\mathcal{A}_m\times\mathbb{R}\big\},\\ \mathcal{U}_m\cap\Omega &= \big\{(x_1,x_2,x_3)\in\mathcal{A}_m\times\mathbb{R}:x_3>\eta_m(x_1,x_2)\big\},\end{aligned} \tag{8.25}$$

and

$$(0,0)\in\mathcal{A}_m\ \subset_{\text{open}}\ [-\delta,\delta]\times[-\delta,\delta],$$
$$\partial_1\eta_m(0,0)=0=\partial_2\eta_m(0,0).$$

Therefore

$$n(0,0,\eta_m(0,0))=\frac{1}{\sqrt{1+|\partial_1\eta_m(0,0)|^2+|\partial_2\eta_m(0,0)|^2}}(\partial_1\eta_m(0,0),\partial_2\eta_m(0,0),-1)=(0,0,-1).$$

Recall that $\partial\Omega$ is locally C^2. Then we can choose $\delta > 0$ small enough to satisfy for all $m \in \{1, .., M_{\Omega,\delta}\}$

$$\begin{aligned}&|\partial_1 \eta_m(x_1,x_2) - \partial_1 \eta_m(0,0)| + |\partial_2 \eta_m(x_1,x_2) - \partial_2 \eta_m(0,0)| \\ =&|\partial_1 \eta_m(x_1,x_2)| + |\partial_2 \eta_m(x_1,x_2)| \leq \frac{1}{8} \quad \text{for } (x_1,x_2) \in \mathcal{A}_m,\end{aligned} \tag{8.26}$$

and

$$|\partial_1^2 \eta_m(x_1,x_2)| + |\partial_2^2 \eta_m(x_1,x_2)| + |\partial_1\partial_2 \eta_m(x_1,x_2)| \leq C_\eta \quad \text{for } (x_1,x_2) \in \mathcal{A}_m. \tag{8.27}$$

Now we define the lattice point on $\mathcal{A}_m$ as

$$c_{m,i,j,\varepsilon} := (\varepsilon i, \varepsilon j) \quad \text{for } -N_\varepsilon \leq i,j \leq N_\varepsilon = O(\frac{\delta}{\varepsilon}). \tag{8.28}$$

Then we define the (i,j)-*rectangular* $\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1}$ which is centered at $c_{m,i,j,\varepsilon}$ and whose side is $2\varepsilon_1$:

$$\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1} := \Big\{(x_1,x_2) : \varepsilon i - \varepsilon_1 < x_1 < \varepsilon i + \varepsilon_1 \text{ and } \varepsilon j - \varepsilon_1 < x_2 < \varepsilon j + \varepsilon_1\Big\} \ \cap \ \mathcal{A}_m. \tag{8.29}$$

Note that if $\varepsilon_1 \geq \varepsilon$ then $\{\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1}\}$ is open covering of $\mathcal{A}_m$, i.e.

$$\mathcal{A}_m \subset \bigcup_{-N_\varepsilon \leq i,j \leq N_\varepsilon} \mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1} \quad \text{with} \quad N_\varepsilon = O(\frac{\delta}{\varepsilon}). \tag{8.30}$$

For each rectangle we define the representative outward normal

$$n_{m,i,j,\varepsilon} := \frac{1}{\sqrt{1 + |\partial_1\eta_m(c_{m,i,j,\varepsilon})|^2 + |\partial_2\eta_m(c_{m,i,j,\varepsilon})|^2}}(\partial_1\eta_m(c_{m,i,j,\varepsilon}), \partial_2\eta_m(c_{m,i,j,\varepsilon}), -1).$$

Let $\{\hat{x}_{1,m,i,j,\varepsilon}, \hat{x}_{2,m,i,j,\varepsilon}\} \subset \mathbb{S}^2$ be an orthonormal basis of the tangent space of $\partial\Omega$ at $(c_{m,i,j,\varepsilon}, \eta_m(c_{m,i,j,\varepsilon}))$. Remark that the three vectors $\hat{x}_{1,m,i,j,\varepsilon}$, $\hat{x}_{2,m,i,j,\varepsilon}$, and $n_{m,i,j,\varepsilon}$ are fixed for each m,i,j,ε and that $\{\hat{x}_{1,m,i,j,\varepsilon}, \hat{x}_{2,m,i,j,\varepsilon}, n_{m,i,j,\varepsilon}\}$ is an orthonormal basis of $\mathbb{R}^3$.

We split the tangent velocity space at $(c_{m,i,j,\varepsilon}, \eta_m(c_{m,i,j,\varepsilon})) \in \partial\Omega$ as

$$\big\{v \in \mathbb{R}^3 : v \cdot n_{m,i,j,\varepsilon} = 0\big\} \ \subseteq \ \bigcup_{\ell=0}^{L_\varepsilon} \Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell}, \quad \text{with} \quad L_\varepsilon = O(\frac{1}{\varepsilon}),$$

where

$$\begin{aligned}&\Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell} \\ &:= \Big\{ r_v \cos\theta_v \cos\phi_v \hat{x}_{1,m,i,j,\varepsilon} + r_v \sin\theta_v \cos\phi_v \hat{x}_{2,m,i,j,\varepsilon} + r_v \sin\phi_v n_{m,i,j,\varepsilon} \in \mathbb{R}^3 : \\ &\qquad\qquad |r_v \sin\phi_v| < 8C_\eta\varepsilon_1 \text{ for } r_v \in [0,1], \quad |\sin\phi_v| < 8C_\eta\varepsilon_1 \text{ for } r_v \in [1,\infty), \\ &\qquad\qquad |\theta_v - \varepsilon\ell| < \varepsilon_1 \text{ for } r_v \in [0,\infty)\Big\},\end{aligned} \tag{8.31}$$

with the constant $C_\eta > 0$ from (8.27).

Remark that for $\varepsilon_1 \geq \varepsilon$,

$$\bigcup_{\ell=0}^{L_\varepsilon} \Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell} = \left\{ v \in \mathbb{R}^3 : \begin{array}{c} |v \cdot n_{m,i,j,\varepsilon}| < 8C_\eta\varepsilon_1 \text{ for } |v| \leq 1, \\ \text{or } \left|\frac{v}{|v|} \cdot n_{m,i,j,\varepsilon}\right| < 8C_\eta\varepsilon_1 \text{ for } |v| \geq 1 \end{array} \right\}. \tag{8.32}$$

Now we are ready to construct the desired open cover corresponding to $\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1} \times \Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell}$ as

$$\mathcal{O}_{m,i,j,\varepsilon,\varepsilon_1,\ell} \ := \Big[\bigcup_{x \in \mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1) \Big] \times \Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell}, \tag{8.33}$$

where

$$\begin{aligned}\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell} := \Big\{ &(x_1,x_2,\eta_m(x_1,x_2)) + \tau[\cos\theta \hat{x}_{1,m,i,j,\varepsilon} + \sin\theta \hat{x}_{2,m,i,j,\varepsilon}] + s n_{m,i,j,\varepsilon} \in \mathbb{R}^3 : \\ &(x_1,x_2) \in \mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1}, \ \theta \in \big(\varepsilon\ell - \varepsilon_1, \varepsilon\ell + \varepsilon_1\big), \ s \in (-\varepsilon,\varepsilon) \\ &\tau \in \big[0, t_{\mathbf{f}}\big((x_1,x_2,\eta_m(x_1,x_2)), \cos\theta \hat{x}_{1,m,i,j,\varepsilon} + \sin\theta \hat{x}_{2,m,i,j,\varepsilon}\big)\big]\Big\}.\end{aligned} \tag{8.34}$$

We note that $\mathcal{O}_{m,i,j,\varepsilon,\varepsilon_1,\ell}$ is an infinite union of open sets and hence is an open set.

Finally we define

$$\mathcal{O}_{\varepsilon,\varepsilon_1} := \bigcup_{m,i,j,\ell} \mathcal{O}_{m,i,j,\varepsilon,\varepsilon_1,\ell} \ \cup \ \big[\mathbb{R}^3 \times B_{\mathbb{R}^3}(0;\varepsilon_1)\big], \tag{8.35}$$

where $1 \leq m \leq M_{\Omega,\delta} = O(\frac{1}{\delta^2}),\ -N_\varepsilon \leq i,j \leq N_\varepsilon = O(\frac{\delta}{\varepsilon}),\ 0 \leq \ell \leq L_\varepsilon = O(\frac{1}{\varepsilon})$. Since $\mathcal{O}_{\varepsilon,\varepsilon_1}$ is a union of open sets, it is an open set.

Proof of (8.20) : Suppose there exists $(x,v) \in \mathfrak{S}_{\mathrm{B}}$. By the definition of $\mathfrak{S}_{\mathrm{B}}$ in (8.8) there exists $y = x_{\mathbf{b}}(x,v) \in \partial\Omega$, such that $x = y + t_{\mathbf{b}}(y,v)v$ and $v \cdot n(y) = 0$ from (8.6) and (8.7). Then $y \in \mathcal{U}_m$ for some m. Without loss of generality (up to rotations and translations) we may assume that $y = (y_1, y_2, \eta_m(y_1,y_2))$ and $(y_1,y_2) \in \mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1}$ for some i,j.

Firstly we consider the case of $|v| \geq 1$. Then we check that

$$\begin{aligned}
\big|n_{m,i,j,\varepsilon} \cdot \frac{v}{|v|}\big| &\leq \Big|n(y_1,y_2,\eta_m(y_1,y_2)) \cdot \frac{v}{|v|}\Big| + \Big|[n_{m,i,j,\varepsilon} - n(y_1,y_2,\eta_m(y_1,y_2))] \cdot \frac{v}{|v|}\Big| \\
&= 0 + \big|n(c_{m,i,j,\varepsilon}, \eta_m(c_{m,i,j,\varepsilon})) - n(y_1,y_2,\eta_m(y_1,y_2))\big| \\
&\leq |\nabla\eta_m(c_{m,i,j,\varepsilon}) - \nabla\eta_m(y_1,y_2)| + \frac{\big|\sqrt{1+|\nabla\eta_m(y_1,y_2)|^2} - \sqrt{1+|\nabla\eta_m(c_{m,i,j,\varepsilon})|^2}\big|}{\sqrt{1+|\nabla\eta_m(c_{m,i,j,\varepsilon})|^2}} \\
&\leq 2|\nabla\eta_m(c_{m,i,j,\varepsilon}) - \nabla\eta_m(y_1,y_2)|,
\end{aligned}$$

where we used the Taylor expansion at the last line. Using (8.27), we have

$$\begin{aligned}
|\nabla\eta_m(c_{m,i,j,\varepsilon}) - \nabla\eta_m(y_1,y_2)| &\leq 4\varepsilon_1 \times \|\eta_m\|_{C^2(\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1})} \\
&\leq 4\varepsilon_1 \times \|\eta_m\|_{C^2(\mathcal{A}_m)} \\
&\leq 4C_\eta\varepsilon_1.
\end{aligned}$$

Therefore we conclude

$$\big|n_{m,i,j,\varepsilon} \cdot \frac{v}{|v|}\big| \leq 8C_\eta\varepsilon_1.$$

By (8.32), $v \in \bigcup_{\ell=0}^{L_\varepsilon} \Theta_{m,i,j,\varepsilon,\ell}$ and hence $(x,v) \in \mathcal{O}_{\varepsilon,\varepsilon_1}$.

Secondly we consider the case of $|v| \leq 1$. Then from (8.27) and following the similar estimate of $|v| \geq 1$ case

$$\begin{aligned}
|v \cdot n_{m,i,j,\varepsilon}| &\leq |v \cdot n(y)| + |v \cdot (n(y) - n_{m,i,j,\varepsilon})| \\
&\leq 4\varepsilon_1\|\eta\|_{C^2(\mathcal{R}_{m,i,j,\varepsilon,\varepsilon_1})} \ \leq \ 4\varepsilon_1\|\eta\|_{C^2(\mathcal{A}_m)} \\
&\leq 8C_\eta\varepsilon_1.
\end{aligned}$$

By the statement of (8.32), $v \in \bigcup_{\ell=0}^{L_\varepsilon} \Theta_{m,i,j,\varepsilon,\ell}$ and hence $(x,v) \in \mathcal{O}_{m,i,j,\varepsilon,\varepsilon_1,\ell} \subset \mathcal{O}_{\varepsilon,\varepsilon_1}$.

Proof of (8.21) : It suffices to show that there exists a constant $C_* \gg 1$ such that if $(x,v) \in \overline{\mathcal{O}_{\varepsilon,\varepsilon_1}}$ then $(x,v) \in \mathcal{O}_{\varepsilon,C_*\varepsilon_1}$.

Since in the definition (8.35) the union on m,i,j,ℓ is finite, we have

$$\begin{aligned}
\overline{\mathcal{O}_{\varepsilon,\varepsilon_1}} &= \bigcup_{m,i,j,\ell} \overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} \ \cup \ \big[\mathbb{R}^3 \times \big\{v \in \mathbb{R}^3 : |v| \leq \varepsilon_1\big\}\big] \\
&= \bigcup_{m,i,j,\ell} \Bigg[\underbrace{\overline{\Big(\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1)\Big)}} \times \overline{\Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell}}\Bigg] \ \cup \ \big[\mathbb{R}^3 \times \big\{v \in \mathbb{R}^3 : |v| \leq \varepsilon_1\big\}\big].
\end{aligned}$$

First we define an open set including the underbraced set (a closed set). For $0 < \varsigma$, we define

$$\begin{aligned}
&\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} \ \bigcup_{y\in B_{\mathbb{R}^3}(x;\varepsilon_1)} B_{\mathbb{R}^3}(y;\varsigma) \\
&= \Big\{z \in \mathbb{R}^3 : \text{there exists } x \in \mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell} \text{ and } y \in B_{\mathbb{R}^3}(x;\varepsilon_1) \text{ such that } z \in B_{\mathbb{R}^3}(y;\varsigma)\Big\}.
\end{aligned} \tag{8.36}$$

Since it is an infinite union of open balls, (8.36) is open and the underbraced set is contained in (8.36) for any $\varsigma > 0$.

Now we claim that, there exists $C_* = C_*(\Omega) \gg 1$ such that for $0 < \varepsilon \leq \varepsilon_1 \ll 1$, there exists $0 < \varsigma = \varsigma(\varepsilon_1, C^*) \ll 1$ such that

$$\bigcup_{x \in \mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} \bigcup_{y \in B_{\mathbb{R}^3}(x;\varepsilon_1)} B_{\mathbb{R}^3}(y;\varsigma) \subset \bigcup_{x \in \mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x; C_*\varepsilon_1). \tag{8.37}$$

Choose $z \in \bigcup_{x \in \mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} \bigcup_{y \in B_{\mathbb{R}^3}(x;\varepsilon_1)} B_{\mathbb{R}^3}(y;\varsigma)$. From (8.36) there exist $x \in \mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}$ and $y \in B_{\mathbb{R}^3}(x;\varepsilon_1)$ such that $z \in B_{\mathbb{R}^3}(y;\varsigma)$. If we choose $\varsigma < \varepsilon_1$ then $|x-z| \leq |x-y| + |y-z| \leq 2\varepsilon_1 < C_*\varepsilon_1$ and therefore $z \in B_{\mathbb{R}^3}(x; C_*\varepsilon_1)$. Clearly $x \in \mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon_1,\ell}$. This proves our claim (8.37).

On the other hand, from (8.31), $C_* \gg 1$ and the fact that the vectors $\hat{x}_{1,m,i,j,\varepsilon}$, $\hat{x}_{2,m,i,j,\varepsilon}$, and $n_{m,i,j,\varepsilon}$ are fixed for given m, i, j,

$$\begin{aligned}
\overline{\Theta_{m,i,j,\varepsilon,\varepsilon_1,\ell}} \;=\; & \Big\{ v = r_v \cos\theta_v \cos\phi_v \hat{x}_{1,m,i,j,\varepsilon} + r_v \sin\theta_v \cos\phi_v \hat{x}_{2,m,ij,\varepsilon} + r_v \sin\phi_v n_{m,i,j,\varepsilon} \in \mathbb{R}^3 : \\
& \quad |r_v \sin\phi_v| \leq 8C_\eta \varepsilon_1 \text{ for } r_v \in [0,1], \quad |\sin\phi_v| \leq 8C_\eta\varepsilon_1 \text{ for } r_v \in [1,\infty), \\
& \quad |\theta_v - \varepsilon\ell| \leq \varepsilon_1 \text{ for } r_v \in [0,\infty) \Big\} \\
\subset\; & \Big\{ v = r_v \cos\theta_v \cos\phi_v \hat{x}_{1,m,i,j,\varepsilon} + r_v \sin\theta_v \cos\phi_v \hat{x}_{2,m,ij,\varepsilon} + r_v \sin\phi_v n_{m,i,j,\varepsilon} \in \mathbb{R}^3 : \\
& \quad |r_v \sin\phi_v| < 8C_\eta C_* \varepsilon_1 \text{ for } r_v \in [0,1], \quad |\sin\phi_v| < 8C_\eta C_*\varepsilon_1 \text{ for } r_v \in [1,\infty), \\
& \quad |\theta_v - \varepsilon\ell| < C_*\varepsilon_1 \text{ for } r_v \in [0,\infty) \Big\} \\
=\; & \Theta_{m,i,j,\varepsilon,C_*\varepsilon_1,\ell}.
\end{aligned} \tag{8.38}$$

Finally we conclude, from (8.37) and (8.38),

$$\begin{aligned}
\overline{\mathcal{O}_{\varepsilon,\varepsilon_1}} \;\subset\; & \bigcup_{m,i,j,\ell} \Big[\bigcup_{x \in \mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon_1}} B_{\mathbb{R}^3}(x; C_*\varepsilon_1) \times \Theta_{m,i,j,\varepsilon,C_*\varepsilon_1,\ell} \Big] \;\cup\; \big[\mathbb{R}^3 \times B_{\mathbb{R}^3}(0; C_*\varepsilon_1) \big] \\
=\; & \mathcal{O}_{\varepsilon,C_*\varepsilon_1}.
\end{aligned}$$

Proof of (8.22) : From (8.35), we deduce

$$\begin{aligned}
& \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x,v) e^{-\theta|v|^2} \mathrm{d}v\mathrm{d}x \\
\leq\; & \sum_{m,i,j,\ell} \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(x,v) e^{-\theta|v|^2} \mathrm{d}v\mathrm{d}x + \mathrm{m}_3(\Omega) O(|\varepsilon|^3) \\
\leq\; & M_{\Omega,\delta} (2N_\varepsilon)^2 L_\varepsilon \times \sup_{m,i,j,\ell} \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(x,v) e^{-\theta|v|^2} \mathrm{d}v\mathrm{d}x + \mathrm{m}_3(\Omega) O(|\varepsilon|^3) \\
\lesssim_\Omega\; & O(\frac{1}{\varepsilon^3}) \times \sup_{m,i,j,\ell} \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(x,v) e^{-\theta|v|^2} \mathrm{d}v\mathrm{d}x + O(|\varepsilon|^3).
\end{aligned}$$

Therefore, to prove (8.22), it suffices to show

$$\sup_{m,i,j,\ell} \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(x,v) e^{-\theta|v|^2} \mathrm{d}v\mathrm{d}x \;\lesssim_{\delta,\Omega}\; \varepsilon^4. \tag{8.39}$$

From (8.31),

$$\begin{aligned}
& \int_{\mathbb{R}^3} \mathbf{1}_{\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(v) e^{-\theta|v|^2} \mathrm{d}v \\
=\; & \int_{|v|\leq 1} + \int_{|v|\geq 1} \\
\leq\; & \int_{|r_v \sin\phi_v| \leq 8C_\eta C_*\varepsilon} \mathrm{d}|r_v \sin\phi_v| \int_0^\infty |r_v \cos\phi_v| e^{-\theta|r_v\cos\phi_v|^2} \mathrm{d}|r_v\cos\phi_v| \int_{|\theta_v - \varepsilon\ell| < C_*\varepsilon} \mathrm{d}\theta_v \\
& + \int_1^\infty |r_v|^2 e^{-\theta|r_v|^2} \mathrm{d}r_v \int_{|\sin\phi_v| < 8C_\eta C_*\varepsilon} \mathrm{d}\phi_v \int_{|\theta_v - \varepsilon\ell| < C_*\varepsilon} \mathrm{d}\theta_v \\
\lesssim_\Omega\; & \varepsilon^2.
\end{aligned}$$

Now we claim that, for $\varepsilon_1 \geq \varepsilon$,

$$\mathrm{m}_3\Big(\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1)\Big) \lesssim_\Omega \varepsilon_1^2. \tag{8.40}$$

Without loss of generality we assume that $i=j=0$ and $l=0$. Therefore $c_{m,i,j,\varepsilon}=0$ in (8.28) and

$$\begin{aligned}\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell} \subset \Big\{&(x_1,x_2,\eta_m(x_1,x_2)) + \tau[\cos\theta\mathbf{e}_1 + \sin\theta\mathbf{e}_2] + s\mathbf{e}_3 \in \mathbb{R}^3 :\\ &(x_1,x_2)\in(-\varepsilon_1,\varepsilon_1)^2,\ \theta\in(-\varepsilon_1,\varepsilon_1),\\ &\tau\in\big[0, t_{\mathbf{f}}((x_1,x_2,\eta(x_1,x_2)),\cos\theta\mathbf{e}_1+\sin\theta\mathbf{e}_2)\big],\ s\in(-\varepsilon_1,\varepsilon_1)\Big\}.\end{aligned}$$

Since Ω is bounded, we have that $\mathrm{diam}(\Omega) = \sup_{x,y\in\Omega}|x-y| < +\infty$ and hence

$$t_{\mathbf{f}}((x_1,x_2,\eta(x_1,x_2)),\cos\theta\mathbf{e}_1+\sin\theta\mathbf{e}_2) \leq \mathrm{diam}(\Omega).$$

We have

$$\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1) \subset \bigcup_{\tau=0}^{2\mathrm{diam}(\Omega)} B_{\mathbb{R}^3}(\tau\mathbf{e}_1;[10+\|\eta\|_{C^1(\mathcal{A}_m)}+\tau\|\eta\|_{C^2(\mathcal{A}_m)}]\varepsilon_1).$$

More precisely $\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1)$ is included in the truncated cone with height $\mathrm{diam}(\Omega)$, top radius $[10+\|\eta\|_{C^1(\mathcal{A}_m)}]\varepsilon_1$, and the bottom radius $[10+\|\eta\|_{C^1(\mathcal{A}_m)}+\mathrm{diam}(\Omega)\|\eta\|_{C^2(\mathcal{A}_m)}]\varepsilon_1$.

Therefore, using (8.26) and (8.27), we conclude (8.40)

$$\begin{aligned}\mathrm{m}_3\Big(\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon_1,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1)\Big) &\leq \mathrm{m}_3\Big(\bigcup_{\tau=0}^{2\mathrm{diam}(\Omega)} B_{\mathbb{R}^3}(\tau\mathbf{e}_1;[10+\|\eta\|_{C^1(\mathcal{A}_m)}+\tau\|\eta\|_{C^2(\mathcal{A}_m)}]\varepsilon_1)\Big)\\ &\leq 3\,\mathrm{diam}(\Omega)\Big[10+\|\eta\|_{C^1(\mathcal{A}_m)}+\mathrm{diam}(\Omega)\|\eta\|_{C^2(\mathcal{A}_m)}\Big]^2\times(\varepsilon_1)^2\\ &\leq 3\,\mathrm{diam}(\Omega)\big[10+\frac{1}{8}+C_\eta\mathrm{diam}(\Omega)\big]^2(\varepsilon_1)^2\\ &\lesssim_\Omega \varepsilon_1^2.\end{aligned}$$

Finally selecting $\varepsilon_1 = C_*\varepsilon$ in (8.40) we conclude (8.39) as

$$\begin{aligned}&\mathrm{m}_3\Big(\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(x;C_*\varepsilon)\Big)\times\int_{\mathbb{R}^3}\mathbf{1}_{\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}(v)e^{-\theta|v|^2}\mathrm{d}v\\ &\lesssim \mathrm{m}_3\Big(\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\varepsilon_1)\Big)\times(\varepsilon)^2\\ &\lesssim \varepsilon^4.\end{aligned}$$

Proof of (8.23) : Due to (8.20), it suffices to show that there exists $C_2 = C_2(C_*) > 0$ such that

$$\mathrm{dist}\big(\bar\Omega\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon},\ \overline{\mathcal{O}_{\varepsilon,\varepsilon}}\big) > C_2\varepsilon. \tag{8.41}$$

By the definition of $\mathcal{O}_{\varepsilon,\varepsilon}$ in (8.35),

$$\begin{aligned}&\mathrm{dist}(\bar\Omega\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon},\overline{\mathcal{O}_{\varepsilon,\varepsilon}})\\ =\ &\inf\big\{|(x,v)-(y,u)| : (x,v)\in(\mathcal{O}_{\varepsilon,C_*\varepsilon})^c,\ (y,u)\in\overline{\mathcal{O}_{\varepsilon,\varepsilon}}\big\}\\ =\ &\inf_{m,i,j,\ell}\inf\big\{|(x,v)-(y,u)| : (x,v)\in(\mathcal{O}_{\varepsilon,C_*\varepsilon})^c,\ (y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\cup[\mathbb{R}^3\times\overline{B_{\mathbb{R}^3}(0;\varepsilon)}]\big\}\\ \geq\ &\inf_{m,i,j,\ell}\inf\big\{|(x,v)-(y,u)| : (x,v)\in(\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c\cap[\mathbb{R}^3\times B_{\mathbb{R}^3}(0,C_*\varepsilon)^c],\\ &\qquad (y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\cup[\mathbb{R}^3\times B_{\mathbb{R}^3}(0;\varepsilon)]\big\}\\ =\ &\inf_{m,i,j,\ell}\min\Big\{\inf\big\{|(x,v)-(y,u)| : (x,v)\in(\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c\cap[\mathbb{R}^3\times B_{\mathbb{R}^3}(0;C_*\varepsilon)^c],\\ &\qquad (y,u)\in\mathbb{R}^3\times B_{\mathbb{R}^3}(0;\varepsilon)\big\},\end{aligned} \tag{8.42}$$

$$\begin{aligned}&\inf\big\{|(x,v)-(y,u)| : (x,v)\in(\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c\ \cap\ [\mathbb{R}^3\times B_{\mathbb{R}^3}(0,C_*\varepsilon)^c],\\ &\qquad (y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\ \cap\ [\mathbb{R}^3\times B_{\mathbb{R}^3}(0,\varepsilon)^c]\big\}\ \Big\}.\end{aligned} \tag{8.43}$$

Clearly,

$$
\begin{aligned}
(8.42) \quad &\geq \inf\left\{|(x,v)-(y,u)| : (x,v)\in\mathbb{R}^3\times B_{\mathbb{R}^3}(0;C_*\varepsilon)^c,\ (y,u)\in\mathbb{R}^3\times B_{\mathbb{R}^3}(0;\varepsilon)\right\}\\
&\geq \inf\left\{|v-u| : v\in B_{\mathbb{R}^3}(0;C_*\varepsilon)^c,\ u\in B_{\mathbb{R}^3}(0;\varepsilon)\right\}\\
&= (C_*-1)\varepsilon.
\end{aligned}
$$

Now we claim that (8.43) is bounded below by the minimum of (8.44) and (8.45) :

$$
\begin{aligned}
&(8.43)\\
\geq\ &\min\Bigg(\inf\Big\{|(x,v)-(y,u)| :\\
&\qquad (x,v)\in\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(x,C_*\varepsilon)\times\left[\left(\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}\right)^c\backslash B_{\mathbb{R}^3}(0;C_*\varepsilon)\right],\\
&\qquad (y,u)\in\Big[\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\frac{C_*}{2}\varepsilon)\Big]\times\left[\,\overline{\Theta_{m,i,j,\varepsilon,\varepsilon,\ell}}\backslash B_{\mathbb{R}^3}(0;\varepsilon)\right]\Big\}, \qquad (8.44)\\
&\quad\inf\Big\{|(x,v)-(y,u)| :\\
&\qquad (x,v)\in\Big[\bigcap_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}\left(B_{\mathbb{R}^3}(x;C_*\varepsilon)\right)^c\Big]\times\left[\mathbb{R}^3\backslash B_{\mathbb{R}^3}(0;C_*\varepsilon)\right],\\
&\qquad (y,u)\in\Big[\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\frac{C_*}{2}\varepsilon)\Big]\times\left[\,\overline{\Theta_{m,i,j,\varepsilon,\varepsilon,\ell}}\backslash B_{\mathbb{R}^3}(0;\varepsilon)\right]\Big\}\Bigg). \qquad (8.45)
\end{aligned}
$$

Firstly, we divide $\{(x,v)\in(\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c\}$ in (8.43) into two parts : from the definition of $\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}$ in (8.33), we deduce that

$$
\begin{aligned}
(\mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c &= \Big[\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(x;C_*\varepsilon)\Big]\times\left(\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}\right)^c\\
&\quad\cup\Big[\bigcap_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}\left(B_{\mathbb{R}^3}(x;C_*\varepsilon)\right)^c\Big]\times\mathbb{R}^3.
\end{aligned}
$$

Therefore, (8.43) is bounded below by the minimum of following two numbers :

$$
\begin{aligned}
&\inf\Big\{|(x,v)-(y,u)| : (x,v)\in\Big[\bigcup_{x\in\mathcal{X}_{m,i,j,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(x;C_*\varepsilon)\Big]\times[(\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell})^c\backslash B_{\mathbb{R}^3}(0,C_*\varepsilon)^c],\\
&\qquad (y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\cap[\mathbb{R}^3\times B_{\mathbb{R}^3}(0,\varepsilon)^c]\Big\},\\
&\inf\Big\{|(x,v)-(y,u)| : (x,v)\in\Big[\bigcap_{x\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}\left(B_{\mathbb{R}^3}(x;C_*\varepsilon)\right)^c\Big]\times[\mathbb{R}^3\backslash B_{\mathbb{R}^3}(0,C_*\varepsilon)],\\
&\qquad (y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\cap[\mathbb{R}^3\times B_{\mathbb{R}^3}(0,\varepsilon)^c]\Big\}.
\end{aligned} \qquad (8.46)
$$

Secondly, we consider $\{(y,u)\in\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}}\}$. From (8.37) with $\varepsilon_1=\varepsilon$, for some $\varsigma=\varsigma(\varepsilon,C_*)>0$

$$
\overline{\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\varepsilon)}\subset\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon,\ell}}\bigcup_{y\in B_{\mathbb{R}^3}(x;\varepsilon)} B_{\mathbb{R}^3}(y;\varsigma)\subset\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\frac{C_*}{2}\varepsilon),
$$

and from the definition of $\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}$ in (8.33), we conclude

$$
\begin{aligned}
\overline{\mathcal{O}_{m,i,j,\varepsilon,\varepsilon,\ell}} &= \overline{\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\varepsilon)}\times\overline{\Theta_{m,i,j,\varepsilon,\varepsilon,\ell}}\\
&\subset\Big[\bigcup_{x\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(x;\frac{C_*}{2}\varepsilon)\Big]\times\overline{\Theta_{m,i,j,\varepsilon,\varepsilon,\ell}}.
\end{aligned}
$$

Therefore, the first number of (8.46) is bounded below by (8.44) and the second of (8.46) by (8.45). This proves the claim.

Now we claim that

$$(8.44) \gtrsim \varepsilon, \quad \text{and } (8.45) \gtrsim \varepsilon.$$

Firstly, we prove (8.44) $\gtrsim \varepsilon$. Let $v \in \big(\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}\big)^c \backslash B_{\mathbb{R}^3}(0; C_*\varepsilon)$. By (8.31)

$$v = r_v \cos\theta_v \cos\phi_v \hat{x}_{1,m,i,j,\varepsilon} + r_v \sin\theta_v \cos\phi_v \hat{x}_{2,m,i,j,\varepsilon} + r_v \sin\phi_v n_{m,i,j,\varepsilon},$$

where

$$\begin{aligned} & |r_v \sin\phi_v| \geq 8C_\eta C_*\varepsilon \quad \text{and} \quad |r_v| \leq 1, \\ \text{or} \quad & |\sin\phi_v| \geq 8C_\eta C_*\varepsilon \quad \text{and} \quad |r_v| \geq 1, \\ \text{or} \quad & |\theta_v - \varepsilon\ell| \geq C_*\varepsilon. \end{aligned} \tag{8.47}$$

Let $u \in \overline{\Theta_{m,i,j,\varepsilon,\varepsilon,\ell}} \backslash B_{\mathbb{R}^3}(0, \varepsilon)$. Again from (8.31) we have

$$u = r_u \cos\theta_u \cos\phi_u \hat{x}_{1,m,i,j,\varepsilon} + r_u \sin\theta_u \cos\phi_u \hat{x}_{2,m,i,j,\varepsilon} + r_u \sin\phi_u n_{m,i,j,\varepsilon},$$

where

$$\begin{aligned} & |\theta_u - \varepsilon\ell| \leq \varepsilon, \\ \text{and} \quad & |r_u \sin\phi_u| \leq 8C_\eta\varepsilon \quad \text{for } |r_u| \leq 1, \\ \text{and} \quad & |\sin\phi_u| \leq 8C_\eta\varepsilon \quad \text{for } |r_u| \geq 1. \end{aligned} \tag{8.48}$$

If $|\theta_v - \varepsilon\ell| \geq C_*\varepsilon$ then clearly $|v-u| \gtrsim \varepsilon$ since $|\theta_u - \varepsilon\ell| \leq \varepsilon$.

Now we consider the case of $|\theta_v - \varepsilon\ell| \leq C_*\varepsilon$.

If $|r_v| \leq 1$ (therefore $|r_v \sin\phi_v| \geq 8C_\eta C_*\varepsilon$ from (8.47)) and $|r_u| \leq 1$ (therefore $|r_u \sin\phi_u| \leq 8C_\eta\varepsilon$ from (8.48)). Therefore

$$\begin{aligned} |v-u| &\geq |(v-u)\cdot n_{m,i,j,\varepsilon}| \geq |v \cdot n_{m,i,j,\varepsilon}| - |u \cdot n_{m,i,j,\varepsilon}| \\ &\geq |r_v \sin\phi_v| - |r_u \sin\phi_u| \geq 8C_\eta C_*\varepsilon - 8C_\eta\varepsilon \\ &\gtrsim \varepsilon. \end{aligned}$$

On the other hand if $|r_v| \geq 1$ and $|r_u| \leq 1$ (therefore $|\sin\phi_v| \geq 8C_\eta C_*\varepsilon$ from (8.47) and $|r_u \sin\phi_u| \leq 8C_\eta\varepsilon$ from (8.48)), then

$$\begin{aligned} |v-u| &\geq |(v-u)\cdot n_{m,i,j,\varepsilon}| \geq |r_v \sin\phi_v - r_u \sin\phi_u| \geq |r_v \sin\phi_v| - |r_u \sin\phi_u| \\ &\geq |\sin\phi_v| - 8C_\eta\varepsilon \\ &\geq 8C_\eta C_*\varepsilon - 8C_\eta\varepsilon \\ &\gtrsim \varepsilon. \end{aligned}$$

If $|r_v| \leq 1$ and $|r_u| \geq 1$, then $|r_v \sin\phi_v| \geq 8C_\eta C_*\varepsilon$ from (8.47) and $|\sin\phi_u| \leq 8C_\eta\varepsilon$ from (8.48).

Fix $0 < c_* \ll 1 \ll C_*$. If $C_* - c_* \geq |r_u|$, then

$$\begin{aligned} |v-u| &\geq |(v-u)\cdot n_{m,i,j,\varepsilon}| \geq |v \cdot n_{m,i,j,\varepsilon}| - |u \cdot n_{m,i,j,\varepsilon}| \\ &= |r_v \sin\phi_v| - |r_u \sin\phi_u| \\ &\geq 8C_\eta C_*\varepsilon - |r_u| \times 8C_\eta\varepsilon \geq 8C_\eta\varepsilon(C_* - |r_u|) \\ &\geq 8C_\eta\varepsilon \times c_*. \end{aligned}$$

On the other hand, if $C_* - c_* \leq |r_u|$, then

$$\begin{aligned} |v-u| &\geq \big|[u - (u\cdot n_{m,i,j,\varepsilon})n_{m,i,j,\varepsilon}] - [v - (v\cdot n_{m,i,j,\varepsilon})n_{m,i,j,\varepsilon}]\big| \\ &\geq |r_u||\cos\phi_u| - |r_v||\cos\phi_v| \\ &\geq |r_u|\sqrt{1 - 64(C_\eta)^2\varepsilon^2} - |\cos\phi_v| \\ &\geq (C_* - c_*)\sqrt{1 - 64(C_\eta)^2\varepsilon^2} - 1 \\ &\gtrsim 1. \end{aligned}$$

If $|r_v| \geq 1$ and $|r_u| \geq 1$ then $|\sin \phi_v| \geq 8C_\eta C_* \varepsilon$ and $|\sin \phi_u| \leq 8C_\eta \varepsilon$ from (8.47) and (8.48). Then

$$\begin{aligned} |v-u| &\geq |(v-u)\cdot n_{m,i,j,\ell}| \\ &\gtrsim |r_v||\sin\phi_v - \sin\phi_u| \\ &\gtrsim C_\eta(C_*-1)\varepsilon. \end{aligned}$$

Combining all cases, we deduce (8.44) $\gtrsim \varepsilon$.
Secondly, we prove (8.45) $\gtrsim \varepsilon$. The proof is due to

$$\begin{aligned} (8.45) &\geq \inf\Big\{|x-y| : x \in \bigcap_{z\in\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} (B_{\mathbb{R}^3}(z;C_*\varepsilon))^c,\ y \in \bigcup_{z\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(z;\frac{C_*}{2}\varepsilon)\Big\} \\ &\geq \inf\Big\{|x-y| : x \in \bigcap_{z\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} (B_{\mathbb{R}^3}(z;C_*\varepsilon))^c,\ y \in \bigcup_{z\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} B_{\mathbb{R}^3}(z;\frac{C_*}{2}\varepsilon)\Big\} \\ &\geq \inf_{z\in\mathcal{X}_{m,i,j,\varepsilon,\frac{C_*}{2}\varepsilon,\ell}} \inf\Big\{|x-y| : x\in (B_{\mathbb{R}^3}(z;C_*\varepsilon))^c,\ y\in B_{\mathbb{R}^3}(z;\frac{C_*}{2}\varepsilon)\Big\} \\ &\geq \frac{C_*}{2}\varepsilon. \end{aligned}$$

□

8.2.2 Construction of Cut-off functions

Recall the standard mollifier $\varphi : \mathbb{R}^3\times\mathbb{R}^3 \to [0,\infty)$,

$$\varphi(x,v) := C\exp\Big(\frac{1}{|x|^2+|v|^2-1}\Big),\ \text{for } \sqrt{|x|^2+|v|^2}<1, \qquad \varphi(x,v):=0,\ \text{for } \sqrt{|x|^2+|v|^2}\geq 1,$$

where the constant $C>0$ is selected so that $\int_{\mathbb{R}^3\times\mathbb{R}^3}\varphi(x,v)\mathrm{d}v\mathrm{d}x = 1$.
For each $\varepsilon>0$, set

$$\varphi_\varepsilon(x,v) := (\varepsilon/\tilde{C})^{-6}\varphi(\frac{\sqrt{|x|^2+|v|^2}}{\varepsilon/\tilde{C}}), \tag{8.49}$$

where $\tilde{C}\gg C_*\gg 1$. Clearly φ_ε is smooth and bounded and satisfies

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varphi_\varepsilon(x,v)\mathrm{d}v\mathrm{d}x = 1, \quad \mathrm{spt}(\varphi_\varepsilon)\subset B_{\mathbb{R}^3\times\mathbb{R}^3}(0;\varepsilon/\tilde{C}).$$

Definition 8.1. *We define a smooth cut-off function $\chi_\varepsilon : \bar{\Omega}\times\mathbb{R}^3\to[0,2]$ as*

$$\begin{aligned} \chi_\varepsilon(x,v) &:= \mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\setminus\mathcal{O}_{\varepsilon,C_*\varepsilon}} * \varphi_\varepsilon(x,v) \\ &= \iint_{\mathbb{R}^3\times\mathbb{R}^3}\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\setminus\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)\varphi_\varepsilon(x-y,v-u)\mathrm{d}u\mathrm{d}y. \end{aligned} \tag{8.50}$$

The following properties of the cut-off function are crucial for our analysis.

Lemma 8.2. *For $\theta>0$, there exist $\tilde{C}\gg C_*\gg 1$ in (8.49) and (8.50) and $\varepsilon_0=\varepsilon_0(\Omega)>0$ such that if $0<\varepsilon<\varepsilon_0$ then*

$$\mathfrak{S}_{\mathrm{B}} \subset \big\{(x,v)\in\bar{\Omega}\times\mathbb{R}^3 : \chi_\varepsilon(x,v)=0\big\}, \tag{8.51}$$

and, for either $\partial=\nabla_x$ or $\partial=\nabla_v$,

$$\iint_{\Omega\times\mathbb{R}^3}[1-\chi_\varepsilon(x,v)]e^{-\theta|v|^2}\mathrm{d}v\mathrm{d}x \lesssim_\Omega \varepsilon, \tag{8.52}$$

$$\iint_{\Omega\times\mathbb{R}^3}|\partial\chi_\varepsilon(x,v)|e^{-\theta|v|^2}\mathrm{d}v\mathrm{d}x \lesssim_\Omega 1. \tag{8.53}$$

Proof. Firstly we prove (8.51). Let $(x,v) \in \mathfrak{S}_{\mathrm{B}}$. Due to (8.49) if $|(x,v)-(y,u)| \geq \varepsilon/\tilde{C}$ then $\varphi_\varepsilon(x-y, v-u) = 0$. Therefore

$$(8.50) = \iint_{B_{\mathbb{R}^6}((x,v);\varepsilon/\tilde{C})} \mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)\varphi_\varepsilon(x-y,v-u)\mathrm{d}y\mathrm{d}u.$$

On the other hand, due to (8.23) with $\varepsilon_1 = \varepsilon$ and $\tilde{C} \gg C_*$, we have $(y,u) \in \mathcal{O}_{\varepsilon,C_*\varepsilon}$ and

$$\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u) \equiv 0, \quad \text{on} \quad (y,u) \in B_{\mathbb{R}^6}((x,v);\varepsilon/\tilde{C}).$$

Therefore we conclude $\chi_\varepsilon(x,v) = 0$ and (8.51).

Secondly we deduce (8.52). We use (8.22) with $\varepsilon_1 = \varepsilon$ to have

$$\begin{aligned}
&\iint_{\mathbb{R}^3\times\mathbb{R}^3}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\big[1-\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)\big]\varphi_\varepsilon(x-y,v-u)e^{-\theta|v|^2}\mathrm{d}u\mathrm{d}y\mathrm{d}v\mathrm{d}x\\
&\leq \iint_{\mathbb{R}^3\times\mathbb{R}^3}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)e^{-\frac{\theta}{2}|u|^2}\mathrm{d}u\mathrm{d}y\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varphi_\varepsilon(x-y,v-u)e^{\theta|v-u|^2}\mathrm{d}v\mathrm{d}x\\
&\leq\ C_1\frac{\varepsilon}{2}\iint_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}\varphi_\varepsilon(x,v)e^{\theta\varepsilon^2/\tilde{C}^2}\mathrm{d}v\mathrm{d}x\\
&\lesssim\ \varepsilon,
\end{aligned}$$

where we used

$$-\theta|v|^2 = \theta|v-u|^2 - \theta|v-u|^2 - \theta|v|^2 \leq \theta|v-u|^2 - \frac{\theta}{2}|u|^2. \tag{8.54}$$

Thirdly we prove (8.53). Note that from a standard scaling argument and (8.49)

$$|\partial\varphi_\varepsilon(x,v)| \ \lesssim\ \frac{\tilde{C}^6}{\varepsilon^7}\mathbf{1}_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}(x,v).$$

We also note that $\partial\chi_\varepsilon = -\partial[1-\chi_\varepsilon]$. Therefore, by Lemma 1,

$$\begin{aligned}
&\iint_{\bar{\Omega}\times\mathbb{R}^3}|\partial\chi_\varepsilon(x,v)|e^{-\theta|v|^2}\mathrm{d}v\mathrm{d}x\\
=\ &\iint\Big|\iint[1-\mathbf{1}_{\bar{\Omega}\times\mathbb{R}^3\backslash\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)]\partial\varphi_\varepsilon(x-y,v-u)e^{-\theta|v|^2}\mathrm{d}u\mathrm{d}y\Big|\mathrm{d}v\mathrm{d}x\\
\leq\ &\iint_{\mathbb{R}^3\times\mathbb{R}^3}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)e^{-\frac{\theta}{2}|u|^2}\mathrm{d}u\mathrm{d}y\iint_{\mathbb{R}^3\times\mathbb{R}^3}O(\varepsilon^{-7}\tilde{C}^6)\mathbf{1}_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}(x,v)\mathrm{d}v\mathrm{d}x\\
\leq\ &O(\varepsilon)\times O(\varepsilon^{-1})\\
\lesssim\ &1.
\end{aligned}$$

□

Proposition 8.1. *With the same constants $\tilde{C} \gg C_* \gg 1$ as in Lemma 8.2 and $0 < \varepsilon < \varepsilon_0$,*

$$\mathfrak{S}_{\mathrm{B}} \cap [\partial\Omega\times\mathbb{R}^3] \ \subset\ \big\{(x,v)\in\partial\Omega\times\mathbb{R}^3 : \chi_\varepsilon(x,v) = 0\big\}. \tag{8.55}$$

Moreover if $|(y,u)| \leq \varepsilon/\tilde{C}$ for $\tilde{C} \gg C_* \gg 1$ then

$$\int_{\partial\Omega}\int_{n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\theta|v-u|^2}|n(x-y)\cdot(v-u)|\mathrm{d}v\mathrm{d}S_x \ \lesssim\ \varepsilon, \tag{8.56}$$

and

$$\int_{\gamma_-}[1-\chi_\varepsilon(x,v)]e^{-\theta|v|^2}\mathrm{d}\gamma \quad \lesssim_\Omega \quad \varepsilon, \tag{8.57}$$

$$\int_{\gamma_-}|\partial\chi_\varepsilon(x,v)|e^{-\theta|v|^2}\mathrm{d}\gamma \quad \lesssim_\Omega \quad 1. \tag{8.58}$$

The following fact is crucial to prove Proposition 8.1 and especially (8.56) :

Lemma 8.3. *We fix $m_0 = 1, 2, \cdots, M_{\Omega,\delta}$ in (8.24). From (8.25), we may assume (up to rotations and translations) there exists a C^2-function $\eta_{m_0} : [-\delta, \delta] \times [-\delta, \delta] \to \mathbb{R}$, whose graph is the boundary $\mathcal{U}_{m_0} \cap \partial\Omega$.*

Let $(x_1, x_2) \in \mathcal{A}_{m_0} \cap [-\delta/2, \delta/2] \times [-\delta/2, \delta/2]$ and $(x_1, x_2) \in \mathcal{R}_{m_0,i_0,j_0,\varepsilon,C_*\varepsilon}$ for $|i_0|, |j_0| \le N_\varepsilon$. (see (8.28), (8.29), and (8.30))

Suppose i) $|y| \le \varepsilon/\tilde{C}$ and

$$\big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y, v\big) \ \in \ \mathcal{O}_{\varepsilon,C_*\varepsilon}, \tag{8.59}$$

and ii) for large but fixed $s_* \gg 1$.

$$-1 \le n_{m_0}(0,0) \cdot \frac{v}{|v|} \le -s_* C_2 \sqrt{\varepsilon}, \quad \text{with } C_2 := \sqrt{\frac{8C_*}{3}} \big[1 + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}\big]^{1/2}. \tag{8.60}$$

Then either $|v| < \varepsilon^{1/3}$ or there exists $(i, j) \in [-N_1 + i_0, N_1 + i_0] \times [-N_1 + j_0, N_1 + j_0]$, with

$$N_1 := \lfloor \frac{8C_3}{\sqrt{\varepsilon}} \rfloor, \quad C_3 := \frac{4C_* + 8C_* \big[1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}\big]^{1/2} + 2/\tilde{C}}{s_* C_2}, \tag{8.61}$$

such that

$$\big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y, v\big) \ \in \bigcup_{0 \le \ell \le L_\varepsilon} \mathcal{O}_{m_0,i,j,\varepsilon,C_*\varepsilon,\ell} \ \cap \ \bar{\Omega} \times \{v \in \mathbb{R}^3 : |v| \ge \varepsilon^{1/3}\},$$

and

$$\big|n_{m_0}(0,0) \cdot \frac{v}{|v|}\big| \ \le \ C_4 \sqrt{\varepsilon} \quad \text{with } C_4 = C_3 \big[1 + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}\big]. \tag{8.62}$$

Remark that the constant N_1 in (8.61) does not depend on x, y, v.

Proof of Lemma 8.3. Without loss of generality (up to rotations and translations), we may assume

$$(i_0, j_0) = (0, 0) \ \text{ and } \ \eta_{m_0}(0,0) = 0 \ \text{ and } \ \nabla \eta_{m_0}(0,0) = 0. \tag{8.63}$$

Consider the case of $|v| \ge \varepsilon^{1/3}$. Since $\big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y, v\big) \in \mathcal{O}_{\varepsilon,C_*\varepsilon}$ we use the definition of $\mathcal{O}_{\varepsilon,C_*\varepsilon}$ in (8.35) to have

$$\text{either} \quad \underbrace{|v| < C_*\varepsilon}_{(8.64)-(i)} \quad \text{or} \quad \underbrace{(x - y, v) \in \bigcup_{m,i,j,\ell} \mathcal{O}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}}_{(8.64)-(ii)}. \tag{8.64}$$

For small $0 < \varepsilon \ll 1$, we can exclude the case of $(8.64) - (i)$ since $|v| > \varepsilon^{1/3} \gg C_*\varepsilon$.

Consider the case of $(8.64) - (ii)$. In this case, we claim that

$$\big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y, v\big) \ \in \ \bigcup_{i,j,\ell} \mathcal{O}_{m_0,i,j,\varepsilon,C_*\varepsilon,\ell}. \tag{8.65}$$

From $(8.64) - (ii)$ and the definition of $\mathcal{O}_{m_0,i,j,\varepsilon,C_*\varepsilon,\ell}$ in (8.33), there exist m, i, j, ℓ such that

$$\big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y, v\big) \ \in \ \Big[\bigcup_{p \in \mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}} B_{\mathbb{R}^3}(p; C_*\varepsilon)\Big] \times \Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}.$$

In particular, there exists $p \in \mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}$ satisfying

$$\big|p - \big((x_1, x_2, \eta_{m_0}(x_1, x_2)) - y\big)\big| < C_*\varepsilon.$$

By the definition of $\mathcal{X}_{m,i,j,\varepsilon,C_*\varepsilon,\ell}$ in (8.34),

$$p = (\bar{p}_1, \bar{p}_2, \eta_m(\bar{p}_1, \bar{p}_2)) + \bar{\tau}\big[\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon}\big] + \bar{s} n_{m,i,j,\varepsilon},$$

for some

$$\begin{array}{rcl}(\bar{p}_1,\bar{p}_2) & \in & \mathcal{R}_{m,i,j,\varepsilon,C_*\varepsilon},\\ \bar{\theta} & \in & (\varepsilon\ell - C_*\varepsilon, \varepsilon\ell + C_*\varepsilon),\\ \bar{\tau} & \in & [0, t_{\mathbf{f}}((\bar{p}_1,\bar{p}_2,\eta_m(\bar{p}_1,\bar{p}_2)), \cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon})],\\ \bar{s} & \in & [-\varepsilon,\varepsilon].\end{array}$$

By the definition of $t_{\mathbf{f}}$ in (8.7),

$$z := p - \bar{s} n_{m,i,j,\varepsilon} = (\bar{p}_1,\bar{p}_2,\eta_m(\bar{p}_1,\bar{p}_2)) + \bar{\tau}\big[\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon}\big] \in \Omega.$$

And

$$\begin{aligned}&|z - \big((x_1,x_2,\eta_{m_0}(x_1,x_2)) - y\big)|\\ &\leq |z-p| + |p - \big((x_1,x_2,\eta_{m_0}(x_1,x_2)) - y\big)|\\ &\leq 2C_*\varepsilon.\end{aligned} \tag{8.66}$$

From (8.63), (8.66), and $|y| \leq \varepsilon/\tilde{C}$, we deduce

$$\begin{aligned}&|z - (0,0,\eta_{m_0}(0,0))|\\ &\leq |z - \big((x_1,x_2,\eta_{m_0}(x_1,x_2)) - y\big)| + |(x_1,x_2,\eta_{m_0}(x_1,x_2)) - (0,0,\eta_{m_0}(0,0))| + |y|\\ &\leq 2C_*\varepsilon + 4C_*\varepsilon(1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}) + \varepsilon/\tilde{C}.\end{aligned}$$

Denote $(\bar{z}_1,\bar{z}_2) = (\bar{p}_1,\bar{p}_2)$. By the definition of $t_{\mathbf{b}}$ and $t_{\mathbf{f}}$ in (8.6) and (8.7)

$$x_{\mathbf{b}}(z, \cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon} + 0n_{m,i,j,\varepsilon}) = (\bar{z}_1,\bar{z}_2,\eta_{m_0}(\bar{z}_1,\bar{z}_2)). \tag{8.67}$$

On the other hand, by the definition of $\Theta_{m,i,j,\varepsilon,C_*\varepsilon,\ell}$ in (8.31),

$$\frac{v}{|v|} = \cos\theta_v\cos\phi_v\hat{x}_{1,m,i,j,\varepsilon} + \sin\theta_v\cos\phi_v\hat{x}_{2,m,i,j,\varepsilon} + \sin\phi_v n_{m,i,j,\varepsilon}, \quad \text{with} \quad |\theta_v - \varepsilon\ell| < C_*\varepsilon, \tag{8.68}$$

and

$$\begin{aligned}|v\cdot n_{m,i,j,\varepsilon}| &< 8C_\eta C_*\varepsilon, \quad \text{for} \quad \varepsilon^{1/3} \leq |v| \leq 1,\\ \Big|\frac{v}{|v|}\cdot n_{m,i,j,\varepsilon}\Big| &< 8C_\eta C_*\varepsilon, \quad \text{for} \quad 1 \leq |v|.\end{aligned}$$

Therefore, for $0 < \varepsilon \ll 1$,

$$\Big|\frac{v}{|v|}\cdot n_{m,i,j,\varepsilon}\Big| = |\sin\phi_v| < \max\big\{8C_\eta C_*\varepsilon^{2/3}, 8C_\eta C_*\varepsilon\big\} \leq 16C_\eta C_*\varepsilon^{2/3}. \tag{8.69}$$

Now we estimate as

$$\begin{aligned}&n_{m_0}(0,0)\cdot(\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon} + 0n_{m,i,j,\varepsilon})\\ &\leq n_{m_0}(0,0)\cdot\frac{v}{|v|} + n_m(0,0)\cdot\underbrace{\Big(\frac{v}{|v|} - (\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon} + 0n_{m,i,j,\varepsilon})\Big)}_{(\mathbf{a})}.\end{aligned}$$

We use (8.68), (8.69), and $\bar{\theta} \in (\varepsilon\ell - C_*\varepsilon, \varepsilon\ell + C_*\varepsilon)$ to conclude that, for $0 < \varepsilon \ll 1$,

$$\begin{array}{rcl}(\mathbf{a}) & \leq & 2\big\{|\cos\theta_v - \cos\bar{\theta}| + |\cos\theta_v||\cos\phi_v - 1| + |\sin\theta_v - \sin\bar{\theta}| + |\sin\theta_v||\cos\phi_v - 1| + |\sin\phi_v|\big\}\\ & \leq & 2\{4C_*\varepsilon + 16C_\eta C_*\varepsilon^{2/3} + 2(16)^2C_\eta^2C_*^2\varepsilon^{4/3}\}\\ & \leq & 200C_\eta C_*\varepsilon^{2/3}.\end{array}$$

Finally from (8.60), for $0 < \varepsilon \ll 1$,

$$\begin{array}{rcl}-1 & \leq & n_{m_0}(0,0)\cdot(\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon} + 0n_{m,i,j,\varepsilon})\\ & \leq & -s_*\times C_2\sqrt{\varepsilon} + 400C_\eta C_*\varepsilon^{2/3}\\ & \leq & -\dfrac{s_*C_2}{2}\sqrt{\varepsilon}.\end{array} \tag{8.70}$$

Now we are ready to prove the first claim (8.65). Denote

$$\hat{u} := \cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon}.$$

Recall that $|z| \leq (2C_* + 4C_*[1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}] + 1/\tilde{C})\varepsilon$ and $z \in \Omega$. Therefore for $0 < \varepsilon \ll 1$ the function η_{m_0} is defined around (z_1, z_2) and $z_3 > \eta_{m_0}(z_1, z_2)$.

We define, for $|\tau| \ll 1$,

$$\Phi(\tau) = z_3 - \hat{u}_3\tau - \eta_{m_0}(z_1 - \hat{u}_1\tau, z_2 - \hat{u}_2\tau). \tag{8.71}$$

Clearly $\Phi(0) > 0$. Expanding $\Phi(\tau)$ in τ, from $-\hat{u}_3 = n_{m_0}(0,0)\cdot(\cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon})$, and (8.70), we have

$$\begin{aligned}
\Phi(\tau) &\leq -\hat{u}_3\tau + |z_3| + |\eta_{m_0}(z_1 - \hat{u}_1\tau, z_2 - \hat{u}_2\tau)| \\
&\leq -s_* \times \frac{C_2}{2}\sqrt{\varepsilon}\tau \\
&\quad + (2C_* + 4C_*[1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}] + 1/\tilde{C})\varepsilon \\
&\quad + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}(2C_* + 4C_*[1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}] + 1/\tilde{C})^2\varepsilon^2 \\
&\quad + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}|\tau|^2,
\end{aligned}$$

where we have used

$$\begin{aligned}
&\eta_{m_0}(z_1 - \hat{u}_1\tau, z_2 - \hat{u}_2\tau) \\
&= \eta_{m_0}(z_1, z_2) + \int_0^\tau \frac{d}{ds}\eta_{m_0}(z_1 - \hat{u}_1 s, z_2 - \hat{u}_2 s)\mathrm{d}s \\
&= \eta_{m_0}(z_1, z_2) - (\hat{u}_1, \hat{u}_2)\cdot\nabla\eta_{m_0}(z_1, z_2)\tau + \int_0^\tau\int_0^s \frac{d}{d{s_1}^2}\eta_m(z_1 - \hat{u}_1 s_1, z_2 - \hat{u}_2 s_1)\mathrm{d}s_1\mathrm{d}s \\
&\leq \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}\frac{|z|^2}{2} - (\hat{u}_1, \hat{u}_2)\cdot\nabla\eta_{m_0}(0,0)|\tau| + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}|z||\tau| + \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}\frac{|\tau|^2}{2} \\
&\leq \|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}\Big(|z|^2 + |\tau|^2\Big).
\end{aligned}$$

Now we plug $\tau = \frac{1}{s_*}\times C_3\sqrt{\varepsilon}$ with the constant C_3 in (8.61) to have, for $s_* \gg 1$ and $0 < \varepsilon \ll 1$,

$$\begin{aligned}
\Phi(\tau) &\leq -\Big[\frac{C_2C_3}{2} - \big(2C_* + 4C_*[1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_{m_0})}] + 1/\tilde{C}\big) - \frac{\|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})}C_3^2}{(s_*)^2}\Big]\varepsilon + O(\varepsilon^2) \\
&< 0.
\end{aligned}$$

By the mean value theorem, there exists at least one $\tau \in (0, C_3\sqrt{\varepsilon}]$ satisfying $\Phi(\tau) = 0$. We choose the smallest one of them and denote it as $\tau_0 \in (0, C_3\sqrt{\varepsilon}]$. By this definition and (8.67), for $0 < \varepsilon \ll 1$,

$$\begin{aligned}
x_{\mathbf{b}}(z, \hat{u}) &= x_{\mathbf{b}}(z, \cos\bar{\theta}\hat{x}_{1,m,i,j,\varepsilon} + \sin\bar{\theta}\hat{x}_{2,m,i,j,\varepsilon}) \\
&= z - \tau_0\hat{u} \\
&= \big(z_1 - \tau_0\hat{u}_1, z_2 - \tau_0\hat{u}_2, z_3 - \tau_0\hat{u}_3\big).
\end{aligned}$$

Therefore, $x_{\mathbf{b}}(z, \hat{u}) \in \partial\Omega \cap \mathcal{U}_{m_0}$ and this proves (8.65).

For $0 < \varepsilon \ll 1$

$$\begin{aligned}
|\big(z_1 - \tau_0\hat{u}_1, z_2 - \tau_0\hat{u}_2\big)| &\leq \big(2C_* + 4C_*(1 + \|\eta_{m_0}\|_{C^1(\mathcal{A}_m)} + 1/\tilde{C})\big)\varepsilon + C_3\sqrt{\varepsilon} \\
&\leq 2C_3\sqrt{\varepsilon}.
\end{aligned}$$

Moreover,

$$\big(z_1 - \tau_0\hat{u}_1, z_2 - \tau_0\hat{u}_2\big) \in \mathcal{R}_{m_0,i,j,\varepsilon,C_*\varepsilon},$$

for

$$|i - i_0|, |j - j_0| \ \leq \ (2C_3\sqrt{\varepsilon})/\varepsilon \ \leq \ 2C_3\frac{1}{\sqrt{\varepsilon}} \leq N_1.$$

We only need to prove (8.62). From (8.69) and (8.61)

$$\begin{aligned}
\big|n_{m_0}(0,0)\cdot\frac{v}{|v|}\big| \leq\ & \big|n_{m_0,i,j,\varepsilon,C_*\varepsilon}\cdot\frac{v}{|v|}\big| + \big|(n_{m_0}(0,0)-n_{m_0,i,j,\varepsilon,C_*\varepsilon})\cdot\frac{v}{|v|}\big| \\
\leq\ & 16C_\eta C_*\varepsilon^{2/3} + \|n_{m_0}\|_{C^1(\mathcal{A}_{m_0})}|N_1\varepsilon + C_*\varepsilon| \\
\leq\ & 16C_\eta C_*\varepsilon^{2/3} + \|n_{m_0}\|_{C^1(\mathcal{A}_{m_0})}\big\{2C_3\sqrt{\varepsilon}+C_*\varepsilon\big\} \\
\leq\ & 10C_3(1+\|\eta_{m_0}\|_{C^2(\mathcal{A}_{m_0})})\sqrt{\varepsilon} \\
\leq\ & C_4\sqrt{\varepsilon},
\end{aligned}$$

and (8.62) follows. □

Proof of Proposition 8.1. The first statement (8.55) is clear from (8.51). Once we assume (8.56) then it is easy to prove (8.57), (8.58) :

Firstly we prove (8.57). Due to properties of the standard mollifier (8.49), we obtain

$$\begin{aligned}
&\iint_{x\in\partial\Omega,n(x)\cdot v<0}\big[1-\chi_\varepsilon(x,v)\big]e^{-\theta|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v \\
=\ &\iint_{x\in\partial\Omega,n(x)\cdot v<0}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\big[1-\mathbf{1}_{\bar\Omega\times\mathbb{R}^3\setminus\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)\big]\varphi_\varepsilon(y,u)e^{-\theta|v|^2}\mathrm{d}u\mathrm{d}y|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v \\
\leq\ &\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varphi_\varepsilon(y,u)e^{\theta|u|^2}\mathrm{d}u\mathrm{d}y\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{2}|v-u|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v \\
=\ &\iint_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde C)}\varphi_\varepsilon(y,u)e^{\frac{\theta}{2}|u|^2}\mathrm{d}u\mathrm{d}y \\
&\times\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{4}|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v,
\end{aligned}$$

where we used

$$\begin{aligned}
-\theta|v|^2 \ \leq\ & -\frac{\theta}{2}|v|^2-\Big(\frac{\theta}{2}|v|^2-\frac{\theta}{4}|v-u|^2\Big)-\frac{\theta}{4}|v-u|^2 \\
\leq\ & -\frac{\theta}{2}|v|^2-\Big(\frac{\theta}{2}|v|^2-\frac{\theta}{2}|v|^2-\frac{\theta}{2}|u|^2\Big)-\frac{\theta}{4}|v-u|^2 \\
\leq\ & -\frac{\theta}{2}|v|^2+\frac{\theta}{2}|u|^2-\frac{\theta}{4}|v-u|^2.
\end{aligned}$$

Since $|y|+|u|\leq\varepsilon/\tilde C$ and $n(x)\cdot v<0$, we have

$$\begin{aligned}
n(x)\cdot v &= n(x)\cdot v-n(x-y)\cdot(v-u)+n(x-y)\cdot(v-u) \\
&= n(x-y)\cdot(v-u)+[n(x)-n(x-y)]\cdot v+n(x-y)\cdot u \\
&= n(x-y)\cdot(v-u)+O(\frac{\varepsilon}{\tilde C})(1+|v|).
\end{aligned}$$

Therefore, we use (8.56) to bound (8.57) further as

$$\begin{aligned}
(8.57)\leq\ &\iint_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde C)}\varphi_\varepsilon(y,u)e^{\frac{\theta}{2}|u|^2}\mathrm{d}u\mathrm{d}y \\
&\times\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{4}|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n(x-y)\cdot(v-u)|\mathrm{d}S_x\mathrm{d}v \\
&+O(\frac{\varepsilon}{\tilde C})e^{\frac{\theta\varepsilon^2}{2\tilde C^2}}\times\mathrm{m}_3(\partial\Omega)\times\int_{\mathbb{R}^3}(1+|v|)e^{-\frac{\theta}{2}|v|^2}\mathrm{d}v \\
\lesssim_\Omega\ &\varepsilon\times e^{\frac{\theta\varepsilon^2}{2(\tilde C)^2}} \\
\lesssim_\Omega\ &\varepsilon.
\end{aligned}$$

Secondly we prove (8.58). Following the same proof of (8.57) , we deduce

$$\begin{aligned}
&\Big|\iint_{x\in\partial\Omega,n(x)\cdot v<0}\partial\chi_\varepsilon(x,v)e^{-\theta|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\Big|\\
&=\Big|\iint_{x\in\partial\Omega,n(x)\cdot v<0}\partial\big[\chi_\varepsilon(x,v)-1\big]e^{-\theta|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\Big|\\
&=\Big|\iint_{x\in\partial\Omega,n(x)\cdot v<0}\partial\Big[\iint_{\mathbb{R}^3\times\mathbb{R}^3}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(y,u)\varphi_\varepsilon(x-y,v-u)\mathrm{d}u\mathrm{d}y\Big]e^{-\theta|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\Big|\\
&\le\Big|\iint_{x\in\partial\Omega,n(x)\cdot v<0}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)|\partial\varphi_\varepsilon(y,u)|\mathrm{d}u\mathrm{d}y|n(x)\cdot v|e^{-\theta|v|^2}\mathrm{d}S_x\mathrm{d}v\Big|\\
&=\iint_{B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}|\partial\varphi_\varepsilon(y,u)|e^{\frac{\theta}{2}|u|^2}\mathrm{d}u\mathrm{d}y\\
&\quad\times\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{4}|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\\
&\lesssim\sup_{(y,u)\in B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{4}|v-u|^2}e^{-\frac{\theta}{2}|v|^2}(1+|v|)\mathrm{d}S_x\mathrm{d}v\\
&+O(\frac{1}{\varepsilon})\sup_{(y,u)\in B_{\mathbb{R}^6}(0;\varepsilon/\tilde{C})}\iint_{x\in\partial\Omega,n(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\frac{\theta}{4}|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n(x-y)\cdot(v-u)|\mathrm{d}S_x\mathrm{d}v\\
&\lesssim 1.
\end{aligned}$$

Proof of (8.56). Let $|(y,u)|\le\varepsilon/\tilde{C}$. We use (8.24) to decompose

$$\begin{aligned}
(8.56)&\le\sum_{m=1}^{M_{\Omega,\delta}}\int_{\mathcal{U}_m\cap\partial\Omega}\int_{n_m(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\mathrm{d}S_x\\
&\le M_{\Omega,\delta}\times\sup_m\int_{\mathcal{U}_m\cap\partial\Omega}\int_{n_m(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\mathrm{d}S_x\\
&\lesssim_\Omega\frac{1}{\delta^2}\sup_m\int_{\mathcal{U}_m\cap\partial\Omega}\int_{n_m(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\mathrm{d}S_x.
\end{aligned}$$

For fixed $m=1,2,\cdots,M_{\Omega,\delta}$, we use (8.25) and (8.30) again to decompose

$$\begin{aligned}
&\int_{\mathcal{U}_m\cap\partial\Omega}\int_{n_m(x)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x-y,v-u)e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\mathrm{d}S_x\\
&=\int_{\mathcal{A}_m}\int_{n_m(x_1,x_2)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x_1-y_1,x_2-y_2,\eta_m(x_1,x_2)-y_3,v-u)\\
&\qquad\times e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\sqrt{1+|\nabla\eta_m(x_1,x_2)|^2}\mathrm{d}x_1\mathrm{d}x_2\\
&\le\sum_{-N_\varepsilon\le i,j\le N_\varepsilon}\int_{\mathcal{R}_{m,i,j,\varepsilon,C_*\varepsilon}}\int_{n_m(x_1,x_2)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x_1-y_1,x_2-y_2,\eta_m(x_1,x_2)-y_3,v-u)\\
&\qquad\times e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\sqrt{1+|\nabla\eta_m(x_1,x_2)|^2}\mathrm{d}x_1\mathrm{d}x_2\\
&\lesssim\frac{\delta^2}{\varepsilon^2}\sup_{-N_\varepsilon\le i,j\le N_\varepsilon}\int_{\mathcal{R}_{m,i,j,\varepsilon,C_*\varepsilon}}\int_{n_m(x_1,x_2)\cdot v<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x_1-y_1,x_2-y_2,\eta_m(x_1,x_2)-y_3,v-u)\\
&\qquad\times e^{-\theta|v-u|^2}e^{-\frac{\theta}{2}|v|^2}|n_m(x-y)\cdot(v-u)|\mathrm{d}v\sqrt{1+|\nabla\eta_m(x_1,x_2)|^2}\mathrm{d}x_1\mathrm{d}x_2,
\end{aligned}$$

where $n_m(x_1,x_2)=\frac{1}{\sqrt{1+|\partial_1\eta_m(x_1,x_2)|^2+|\partial_1\eta_m(x_1,x_2)|^2}}\big(\partial_1\eta_m(x_1,x_2),\partial_2\eta_m(x_1,x_2),-1\big)$.

We fix i,j. Without loss of generality (up to rotations and translations), we may assume

$$c_{m,i,j,\varepsilon}=(0,0),\quad\partial_1\eta_m(0,0)=0=\partial_2\eta_m(0,0),\quad n_{m,i,j,\varepsilon}=(0,0,-1).$$

We claim

$$\begin{aligned}&\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{n_m(x_1,x_2)\cdot(v+u)<0}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x_1-y_1,x_2-y_2,\eta_m(x_1,x_2)-y_3,v)\\&\qquad\qquad\times e^{-\theta|v|^2}e^{-\frac{\theta}{2}|v+u|^2}|n_m(x-y)\cdot v|\mathrm{d}v\sqrt{1+|\nabla\eta_m(x_1,x_2)|^2}\mathrm{d}x_1\mathrm{d}x_2\\&\lesssim\varepsilon^3.\end{aligned}\tag{8.72}$$

Once we prove (8.72), due to the above estimates for the decomposition, we conclude (8.56) directly.

For $(x_1,x_2)\in[-C_*\varepsilon,C_*\varepsilon]^2$, $|(y,u)|<\varepsilon/\tilde{C}$, and $n_m(x_1,x_2)\cdot(v+u)<0$, we deduce

$$\begin{aligned}n_{m,i,j,\varepsilon}\cdot v&=n_m(0,0)\cdot v\\&=n_m(x_1,x_2)\cdot(v+u)+\big[n_m(0,0)\cdot v-n_m(x_1,x_2)\cdot(v+u)\big]\\&<0+|n_m(x_1,x_2)||u|+|n_m(0,0)-n_m(x_1,x_2)||v|\\&\le\varepsilon/\tilde{C}+2C_*\varepsilon\|\eta_m\|_{C^2([-C_*\varepsilon,C_*\varepsilon]^2)}|v|\\&\le C_5(1+|v|)\varepsilon,\end{aligned}\tag{8.73}$$

where $C_5=\max\big\{1/\tilde{C},2C_*\|\eta_m\|_{C^2([-C_*\varepsilon,C_*\varepsilon]^2)}\big\}$. Therefore

$$(8.72)\ \le\ \int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{n_{m,i,j,\varepsilon}\cdot v<C_5(1+|v|)\varepsilon}\cdots.$$

According to Lemma 8.3, we decompose

$$\begin{aligned}&\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{n_m(0,0)\cdot v\le C_5(1+|v|)\varepsilon}\mathbf{1}_{\mathcal{O}_{\varepsilon,C_*\varepsilon}}(x_1-y_1,x_2-y_2,\eta_m(x_1,x_2)-y_3,v)\\&\qquad\qquad\times e^{-\theta|v|^2}e^{-\frac{\theta}{2}|v+u|^2}|n_m(x-y)\cdot v|\mathrm{d}v\sqrt{1+|\nabla\eta_m(x_1,x_2)|^2}\mathrm{d}x_1\mathrm{d}x_2\\&=\underbrace{\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{\big\{-s_*C_2\sqrt{\varepsilon}\le n_m(0,0)\cdot\frac{v}{|v|}\le C_5\frac{1+|v|}{|v|}\varepsilon\big\}}\cdots}_{(\mathbf{I})}\\&\quad+\underbrace{\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{\big\{-1\le n_m(0,0)\cdot\frac{v}{|v|}\le-s_*C_2\sqrt{\varepsilon}\big\}}\cdots}_{(\mathbf{II})}.\end{aligned}\tag{8.74}$$

First we consider (**I**). If $-s_*C_2\sqrt{\varepsilon}\le n_m(0,0)\cdot\frac{v}{|v|}\le 0$ then $0\le v_3=-n_m(0,0)\cdot v\le s_*C_2|v|\sqrt{\varepsilon}$ and for $0<\varepsilon\ll 1$

$$0\ \le\ v_3\ \le\ 2s_*C_2\sqrt{|v_1|^2+|v_2|^2}\sqrt{\varepsilon}.$$

Moreover

$$\begin{aligned}|n_m(x-y)\cdot v|&\le|n_m(0,0)\cdot v|+\|n_m\|_{C^1([-C_*\varepsilon,C_*\varepsilon]^2)}(C_*+1/\tilde{C})|v|\varepsilon\\&\le s_*C_2|v|\sqrt{\varepsilon}+4\|\eta_m\|_{C^2([-C_*\varepsilon,C_*\varepsilon]^2)}(C_*+1/\tilde{C})|v|\varepsilon.\end{aligned}$$

If $n_m(0,0)\cdot\frac{v}{|v|}\le C_5\frac{1+|v|}{|v|}\varepsilon$ then for $0<\varepsilon\ll 1$

$$|v_3|=|n_m(0,0)\cdot v|\le 2C_5(1+\sqrt{|v_1|^2+|v_2|^2})\varepsilon.$$

Therefore,

$$\begin{aligned}(\mathbf{I})&=\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{0\le v_3\le 2s_*C_2\sqrt{|v_1|^2+|v_2|^2}\sqrt{\varepsilon}}e^{-\theta|v|^2}\big\{s_*C_2|v|\sqrt{\varepsilon}+4\|\eta_m\|_{C^2([-C_*\varepsilon,C_*\varepsilon]^2)}(C_*+1/\tilde{C})|v|\varepsilon\big\}\\&\quad+\int_{[-C_*\varepsilon,C_*\varepsilon]^2}\int_{|v_3|\le 2C_5(1+\sqrt{|v_1|^2+|v_2|^2})\varepsilon}e^{-\theta|v|^2}\\&\lesssim\mathrm{m}_2([-C_*\varepsilon,C_*\varepsilon]^2)\times\sqrt{\varepsilon}\iint_{\mathbb{R}^2}\mathrm{d}v_1\mathrm{d}v_2\ e^{-\frac{\theta}{2}|v_1|^2}e^{-\frac{\theta}{2}|v_2|^2}\int_0^{2s_*C_2\sqrt{|v_1|^2+|v_2|^2}\sqrt{\varepsilon}}\mathrm{d}v_3\\&\quad+\mathrm{m}_2([-C_*\varepsilon,C_*\varepsilon]^2)\times\iint_{\mathbb{R}^2}\mathrm{d}v_1\mathrm{d}v_2\ e^{-\theta|v_1|^2}e^{-\theta|v_2|^2}\int_0^{2C_5(1+\sqrt{|v_1|^2+|v_2|^2})\varepsilon}\mathrm{d}v_3\\&\lesssim\varepsilon^3.\end{aligned}\tag{8.75}$$

We decompose (**II**), according to Lemma 8.3 :

$$(\mathbf{II}) = \int_{[-C_*\varepsilon, C_*\varepsilon]^2} \int_{|v|<\varepsilon^{1/3}} + \int_{[-C_*\varepsilon, C_*\varepsilon]^2} \int_{\left\{-1 \le n_m(0,0)\cdot \frac{v}{|v|} \le -s_* C_2 \sqrt{\varepsilon} \text{ and } |v| \ge \varepsilon^{1/3}\right\}}.$$

The first term is clearly bounded by $O(1)\varepsilon^3$. For the second term we use (8.62) to have

$$\begin{aligned} &\big\{ -1 \le n_m(0,0)\cdot \frac{v}{|v|} \le -s_* C_2\sqrt{\varepsilon} \text{ and } |v| \ge \varepsilon^{1/3}\big\} \\ \subset \quad &\big\{ |n_m(0,0)\cdot \frac{v}{|v|}| \le C_4\sqrt{\varepsilon} \text{ and } |v| \ge \varepsilon^{1/3}\big\}. \end{aligned}$$

Therefore we follow the same proof as for (8.75) to obtain

$$\begin{aligned} (\mathbf{II}) \ &\lesssim \ \varepsilon^3 + \int_{[-C_*\varepsilon, C_*\varepsilon]^2} \int_{|v_3| \le 2C_4\sqrt{|v_1|^2+|v_2|^2}\sqrt{\varepsilon}} \\ &\qquad\qquad \times e^{-\theta|v|^2}\big\{ C_4|v|\sqrt{\varepsilon} + 4\|\eta_m\|_{C^2([-C_*\varepsilon, C_*\varepsilon]^2)}(C_* + 1/\tilde{C})|v|\varepsilon \big\} \\ &\lesssim \ \varepsilon^3. \end{aligned} \tag{8.76}$$

We conclude (8.74) from (8.75) and (8.76). □

8.3 New Trace Theorem via the Double Iteration

In this section we prove the following geometric result. For the later purpose (this will be used in the approximation scheme for the nonlinear problem with diffuse BC) we state the result for the sequence of solutions.

Proposition 8.2. *Let $h_0 \in L^1(\Omega\times\mathbb{R}^3)$. Let $(h^m)_{m\ge 0} \subset L^\infty([0,T]; L^1(\Omega\times\mathbb{R}^3)) \cap L^1([0,T]; L^1(\gamma_+, \mathrm{d}\gamma))$ solve*

$$\{\partial_t + v\cdot\nabla_x + \nu\} h^{m+1} = H^m, \quad h^{m+1}|_{t=0} = h_0, \tag{8.77}$$

where $\nu = \nu(t,x,v) \ge 0$, and such that the following inequality holds for all $(x,v)\in\gamma_-$

$$\begin{aligned} |h^{m+1}(t,x,v)| \le C_1\sqrt{\mu(v)}\Big(1 + \frac{\langle v\rangle}{|n(x)\cdot v|}\Big) \int_{n(x)\cdot u>0} |h^m(t,x,u)|\mu(u)^{\frac14}\{n(x)\cdot u\}\mathrm{d}u \\ + \Big(1 + \frac{e^{-C_2|v|^2}}{|n(x)\cdot v|}\Big) R^m, \end{aligned} \tag{8.78}$$

where $H^m \in L^1([0,T]; L^1(\Omega\times\mathbb{R}^3))$ and $R^m \in L^1([0,T]; L^1(\partial\Omega\times\mathbb{R}^3, \langle v\rangle\, \mathrm{d}S_x\, \mathrm{d}v))$.

Then for all $m\ge 1$, $h^{m+1}_{\gamma_-} \in L^1([0,T]; L^1(\gamma_-, \mathrm{d}\gamma))$ and satisfies, for $t\in[0,T]$ and $0<\delta\ll 1$,

$$\begin{aligned} \int_0^t |h^{m+1}(s)|_{\gamma_-,1} \le \ O(\delta)\int_0^t |h^{m-1}(s)|_{\gamma_+,1} + C_\delta\|h_0\|_1 \\ + C_\delta \max_{i=m,m-1}\Big\{ \int_0^t \|h^i(s)\|_1 + \int_0^t |\langle v\rangle R^i(s)|_1 + \int_0^t \|H^i(s)\|_1 \Big\}. \end{aligned} \tag{8.79}$$

Our proof requires the following lemma :

Lemma 8.4. *Let $\Omega\subset\mathbb{R}^3$ be an open bounded set with a smooth boundary $\partial\Omega$.*

For $k\in\mathbb{N}$, consider the map

$$\begin{aligned} \Phi_k : \{(x,v)\in\gamma_+ : \ n(x_{\mathbf{b}}(x,v))\cdot v < -1/k\} \ &\to \ \{(x_{\mathbf{b}}, v)\in\gamma_- : n(x_{\mathbf{b}})\cdot v < -1/k\}, \\ (x,v) \ &\mapsto \ \Phi_k(x,v) := (\tilde{x}, v) := (x_{\mathbf{b}}(x,v), v). \end{aligned}$$

Then Φ_k is one-to-one and we have a change of variables formula for all $k\in\mathbb{N}$:

$$\mathbf{1}_{\{n(\tilde{x})\cdot v<-1/k\}}\, |n(\tilde{x})\cdot v|\, \mathrm{d}v\mathrm{d}S_{\tilde{x}} \ = \ \mathbf{1}_{\{n(x_{\mathbf{b}}(x,v))\cdot v<-1/k\}}\, |n(x)\cdot v|\, \mathrm{d}v\mathrm{d}S_x.$$

Proof of Lemma 8.4. Let (x,v), $(x',v') \in \gamma_+$ such that $n(x_{\mathbf{b}}(x,v))\cdot v,\ \ n(x_{\mathbf{b}}(x',v'))\cdot v' < -1/k$. If $\Phi_k(x,v) = \Phi_k(x',v')$ then $v=v'$ and $x_{\mathbf{b}}(x,v) = x_{\mathbf{b}}(x',v)$. Since $x = x_{\mathbf{f}}(x_{\mathbf{b}}(x,v),v) = x_{\mathbf{f}}(x_{\mathbf{b}}(x',v),v) = x'$ the mapping Φ_k is one-to-one.

Now we prove the change of variables formula. It suffices to consider a small neighborhood of $\partial\Omega$ around x. Without loss of generality we may assume $x_3 = \eta(x_1,x_2)$ for some $\eta:\mathbb{R}^2\to\mathbb{R}$. First we consider the case $n_3(x_{\mathbf{b}}(x,v))\neq 0$ so that

$$\tilde{x} = x_{\mathbf{b}}(x,v) = (\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = (\tilde{x}_1,\tilde{x}_2,\varphi(\tilde{x}_1,\tilde{x}_2)) \in \partial\Omega,$$

for some function $\varphi:\mathbb{R}^2\to\mathbb{R}$.

The change of variable is given by

$$\begin{aligned} \mathrm{d}S_{\tilde{x}}\mathrm{d}v &= \sqrt{1+|\nabla\varphi|^2}\mathrm{d}\tilde{x}_1\mathrm{d}\tilde{x}_2\mathrm{d}v \\ &= \frac{\sqrt{1+|\nabla\varphi|^2}}{\sqrt{1+|\nabla\eta|^2}} J\sqrt{1+|\nabla\eta|^2}\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}v \\ &= \frac{\sqrt{1+|\nabla\varphi|^2}}{\sqrt{1+|\nabla\eta|^2}} J\mathrm{d}S_x\mathrm{d}v. \end{aligned} \tag{8.80}$$

where J is the Jacobian,

$$J = \left|\frac{\partial(\tilde{x}_1,\tilde{x}_2,v_1,v_2,v_3)}{\partial(x_1,x_2,v_1,v_2,v_3)}\right| = \left|\begin{array}{cc} \partial_{x_1}\tilde{x}_1 & \partial_{x_2}\tilde{x}_1 \\ \partial_{x_1}\tilde{x}_2 & \partial_{x_2}\tilde{x}_2 \end{array}\right|.$$

By the definition of $x_{\mathbf{b}}(x,v)$, we have the following identity : $v|x-\tilde{x}| = |v|(x-\tilde{x})$, i.e.

$$\begin{aligned} &\{(x_1-\tilde{x}_1)^2 + (x_2-\tilde{x}_2)^2 + [\eta(x_1,x_2)-\varphi(\tilde{x}_1,\tilde{x}_2)]^2\}^{\frac{1}{2}} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \\ &= |v| \begin{pmatrix} x_1-\tilde{x}_1 \\ x_2-\tilde{x}_2 \\ \eta(x_1,x_2)-\varphi(\tilde{x}_1,\tilde{x}_2) \end{pmatrix}. \end{aligned} \tag{8.81}$$

Denote $D = \{(x_1-\tilde{x}_1)^2 + (x_2-\tilde{x}_2)^2 + [\eta(x_1,x_2)-\varphi(\tilde{x}_1,\tilde{x}_2)]^2\}$. Directly from (8.81)

$$\begin{aligned} &\begin{bmatrix} \Big[(x_1-\tilde{x}_1)+(\eta-\varphi)\partial_{\tilde{x}_1}\varphi\Big]D^{-\frac{1}{2}}v_1 - |v| & \Big[(x_2-\tilde{x}_2)+(\eta-\varphi)\partial_{\tilde{x}_2}\varphi\Big]D^{-\frac{1}{2}}v_1 \\ \Big[(x_1-\tilde{x}_1)+(\eta-\varphi)\partial_{\tilde{x}_1}\varphi\Big]D^{-\frac{1}{2}}v_2 & \Big[(x_2-\tilde{x}_2)+(\eta-\varphi)\partial_{\tilde{x}_2}\varphi\Big]D^{-\frac{1}{2}}v_2 - |v| \end{bmatrix} \\ &\times \begin{bmatrix} \partial_{x_1}\tilde{x}_1 & \partial_{x_2}\tilde{x}_1 \\ \partial_{x_1}\tilde{x}_2 & \partial_{x_2}\tilde{x}_2 \end{bmatrix} \\ &= \begin{bmatrix} v_1 D^{-\frac{1}{2}}\big((x_1-\tilde{x}_1)+(\eta-\varphi)\partial_{x_1}\eta\big) - |v| & v_1 D^{-\frac{1}{2}}\big((x_2-\tilde{x}_2)+(\eta-\varphi)\partial_{x_2}\eta\big) \\ v_2 D^{-\frac{1}{2}}\big((x_1-\tilde{x}_1)+(\eta-\varphi)\partial_{x_1}\eta\big) & v_2 D^{-\frac{1}{2}}\big((x_2-\tilde{x}_2)+\partial_{x_2}\eta(\eta-\varphi)\big) - |v| \end{bmatrix}. \end{aligned}$$

Direct computations yield

$$\begin{aligned} J &= \frac{|v| - D^{-\frac{1}{2}}\Big[v_1(x_1-\tilde{x}_1) + v_1(\eta-\varphi)\partial_{x_1}\eta + v_2(x_2-\tilde{x}_2) + v_2(\eta-\varphi)\partial_{x_2}\eta\Big]}{|v| - D^{-\frac{1}{2}}\Big[v_2(x_2-\tilde{x}_2) + v_2(\eta-\varphi)\partial_{\tilde{x}_2}\varphi + v_1(x_1-\tilde{x}_1) + v_1(\eta-\varphi)\partial_{\tilde{x}_1}\varphi\Big]} \\ &= \frac{|v|^2 - \big[(v_1)^2+(v_2)^2+(v_3)(v_1\partial_{x_1}\eta + v_2\partial_{x_2}\eta)\big]}{|v|^2 - \big[(v_1)^2+(v_2)^2+(v_3)(v_1\partial_{\tilde{x}_1}\varphi + v_2\partial_{\tilde{x}_2}\varphi)\big]} = \frac{(\partial_{x_1}\eta,\partial_{x_2}\eta,-1)\cdot v}{(\partial_{\tilde{x}_1}\varphi,\partial_{\tilde{x}_2}\varphi,-1)\cdot v} \\ &= \frac{\sqrt{1+|\nabla\eta|^2}}{\sqrt{1+|\nabla\varphi|^2}} \times \frac{n(x)\cdot v}{n(\tilde{x})\cdot v}. \end{aligned}$$

Then we use (8.80) to conclude the proof.

Secondly we consider the case of $n_1(x_{\mathbf{b}}(x,v))\neq 0$ or $n_2(x_{\mathbf{b}}(x,v))\neq 0$. Without loss of generality we may assume $n_2(x_{\mathbf{b}}(x,v))\neq 0$ so that

$$\tilde{x} = x_{\mathbf{b}}(x,v) = (\tilde{x}_1,\tilde{x}_2,\tilde{x}_3) = (\tilde{x}_1,\varphi(\tilde{x}_1,\tilde{x}_3),\tilde{x}_3),$$

for some function $\varphi : \mathbb{R}^2 \to \mathbb{R}$. Notice that (8.80) still holds with $\tilde{x}_2$ replaced by $\tilde{x}_3$. From the fact $v|x-\tilde{x}| = |v|(x-\tilde{x})$ we have

$$\{(x_1-\tilde{x}_1)^2 + (x_2-\varphi(\tilde{x}_1,\tilde{x}_3))^2 + [\eta(x_1,x_2)-\tilde{x}_3]^2\}^{\frac{1}{2}} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = |v| \begin{pmatrix} x_1-\tilde{x}_1 \\ x_2-\varphi(\tilde{x}_1,\tilde{x}_3) \\ \eta(x_1,x_2)-\tilde{x}_3. \end{pmatrix}. \tag{8.82}$$

We define $\tilde{D} = \{(x_1-\tilde{x}_1)^2 + (x_2-\varphi(\tilde{x}_1,\tilde{x}_3))^2 + [\eta(x_1,x_2)-\tilde{x}_3]^2\}$.

By direct computation

$$\begin{aligned}
&\begin{bmatrix} \Big[(x_1-\tilde{x}_1)+(x_2-\varphi)\partial_{\tilde{x}_1}\varphi\Big]v_1\tilde{D}^{-\frac{1}{2}} - |v| & \Big[(x_2-\varphi)\partial_{\tilde{x}_3}\varphi + (\eta-\tilde{x}_3)\Big]v_1\tilde{D}^{-\frac{1}{2}} \\ \Big[(x_1-\tilde{x}_1)+(x_2-\varphi)\partial_{\tilde{x}_1}\varphi\Big]v_3\tilde{D}^{-\frac{1}{2}} & \Big[(x_2-\varphi)\partial_{\tilde{x}_3}\varphi + (\eta-\tilde{x}_3)\Big]v_3\tilde{D}^{-\frac{1}{2}} - |v| \end{bmatrix} \\
&\times \begin{bmatrix} \partial_{x_1}\tilde{x}_1 & \partial_{x_2}\tilde{x}_1 \\ \partial_{x_1}\tilde{x}_3 & \partial_{x_2}\tilde{x}_3 \end{bmatrix} \\
&= \begin{bmatrix} \Big[(x_1-\tilde{x}_1)+(\eta-\tilde{x}_3)\partial_{x_1}\eta\Big]v_1\tilde{D}^{-1/2} - |v| & \Big[(x_2-\varphi)+(\eta-\tilde{x}_3)\partial_{x_2}\eta\Big]v_1\tilde{D}^{-1/2} \\ \Big[(x_1-\tilde{x}_1)+(\eta-\tilde{x}_3)\partial_{x_1}\eta\Big]v_3\tilde{D}^{-1/2} - |v|\partial_{x_1}\eta & \Big[(x_2-\varphi)+(\eta-\tilde{x}_3)\partial_{x_2}\eta\Big]v_3\tilde{D}^{-1/2} - |v|\partial_{x_2}\eta \end{bmatrix},
\end{aligned}$$

and

$$\begin{aligned}
&\det \begin{bmatrix} \partial_{x_1}\tilde{x}_1 & \partial_{x_2}\tilde{x}_1 \\ \partial_{x_1}\tilde{x}_3 & \partial_{x_2}\tilde{x}_3 \end{bmatrix} \\
&= \frac{|v|^2\partial_{x_2}\eta - \Big[(x_1-\tilde{x}_1)+(\eta-\tilde{x}_3)\partial_{x_1}\eta\Big]v_1|v|\tilde{D}^{-\frac{1}{2}}\partial_{x_2}\eta + \Big[(x_2-\varphi)+(\eta-\tilde{x}_3)\partial_{x_2}\eta\Big]\tilde{D}^{-\frac{1}{2}}|v|(v_1\partial_{x_1}\eta - v_3)}{|v|^2 - \Big[(x_1-\tilde{x}_1)+(x_2-\varphi)\partial_{\tilde{x}_1}\varphi\Big]|v|v_1\tilde{D}^{-\frac{1}{2}} - \Big[(x_2-\varphi)\partial_{\tilde{x}_3}\varphi+(\eta-\tilde{x}_3)\Big]|v|v_3\tilde{D}^{-\frac{1}{2}}} \\
&= \frac{v_1\partial_{x_1}\eta + v_2\partial_{x_2}\eta - v_3}{-v_1\partial_{\tilde{x}_1}\varphi + v_2 - v_3\partial_{\tilde{x}_3}\varphi} = \frac{\big(\partial_{x_1}\eta, \partial_{x_2}\eta, -1\big)\cdot v}{-\big(\partial_{\tilde{x}_1}\varphi, -1, \partial_{\tilde{x}_3}\varphi\big)\cdot v} \\
&= -\frac{\sqrt{1+|\nabla\eta|^2}}{\sqrt{1+|\nabla\varphi|^2}} \times \frac{n(x)\cdot v}{n(\tilde{x})\cdot v}.
\end{aligned}$$

Then we use (8.80) (with $\tilde{x}_2$ replaced by $\tilde{x}_3$) to conclude the proof. □

Proof of Proposition 8.2. It suffices to prove the estimate (8.79).

Using (8.78), we obtain

$$\int_0^t |h^{m+1}(s)|_{\gamma_-,1} := \int_0^t \iint_{n(x)\cdot v<0} |h^{m+1}(s,x,v)||n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s \;\lesssim\; (A)+(B),$$

where

$$\begin{aligned}
(A) &:= \int_0^t \iint_{n(x)\cdot v>0} |h^m(s,x,v)|\mu(v)^{\frac{1}{4}}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s \\
(B) &:= \int_0^t \iint_{n(x)\cdot v<0} |R^m(s,x,v)|\{1+|n(x)\cdot v|\}\mathrm{d}S_x\mathrm{d}v\mathrm{d}s
\end{aligned}$$

Clearly the last term (B) is bounded by the RHS of (8.79).

Focus on (A). Recall the almost grazing set γ_+^δ and the non-grazing set $\gamma_+\backslash\gamma_+^\delta$ in (8.16) and (8.17). We split the outgoing part as

$$\gamma_+ \;=\; \gamma_+^\delta \;\cup\; \gamma_+\backslash\gamma_+^\delta.$$

Due to Lemma .7 in the appendix, the non-grazing part $\gamma_+\backslash\gamma_+^\delta$ of the integral is bounded as

$$\begin{aligned}
\int_0^t \iint_{\gamma_+\backslash\gamma_+^\delta} &\lesssim_{t,\delta,\Omega} \|h_0\|_1 + \int_0^t \big\{\big|\big|h^m(s)\big|\big|_1 + \big|\big|[\partial_t + v\cdot\nabla_x + \nu]h^m(s)\big|\big|_1\big\}\mathrm{d}s \\
&\lesssim_{t,\delta,\Omega} \|h_0\|_1 + \int_0^t \|h^m\|_1 + \int_0^t \|H^{m-1}\|_1.
\end{aligned} \tag{8.83}$$

For the almost grazing set γ_+^δ, we claim that the following truncated term with a number $k\in\mathbb{N}$ is uniformly bounded in k as follows :

Claim :

$$\begin{aligned}&\int_0^t\iint_{\substack{x\in\partial\Omega,\\ n(x)\cdot v>0}}\mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}|h^m(s,x,v)|\mu(v)^{\frac14}\{n(x)\cdot v\}\mathrm{d}v\mathrm{d}S_x\mathrm{d}s\\&\leq O(\delta)\int_0^t|h^{m-1}(s)|_{\gamma_+,1}+C_\delta\Big\{\|h_0\|_1+\int_0^t\|h^{m-1}(s)\|_1+\int_0^t\|H^{m-1}\|_1+t|R^{m-1}|_1\Big\}.\end{aligned}\tag{8.84}$$

Proof of Claim (8.84) : In order to show (8.84) we use the Duhamel formula of the equation (8.77) together with (8.78) : for $(x,v)\in\gamma_+^\delta$ and $\frac1k<|n(x_{\mathbf{b}}(x,v))\cdot v|$

$$\begin{aligned}&|h^m(s,x,v)|\mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}\\
\leq\;&\mathbf{1}_{\{s<t_{\mathbf{b}}(x,v)\}}|h_0(x-sv,v)|+\int_{\max\{0,s-t_{\mathbf{b}}(x,v)\}}^s|H^{m-1}(\tau,x-(s-\tau)v,v)|\mathrm{d}\tau\\
&+\mathbf{1}_{\{s>t_{\mathbf{b}}(x,v)\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}C_1\sqrt{\mu(v)}\left(1+\frac{\langle v\rangle}{|n(x_{\mathbf{b}}(x,v))\cdot v|}\right)\\
&\qquad\times\int_{n(x_{\mathbf{b}}(x,v))\cdot v_1>0}|h^{m-1}(s-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v_1)|\mu(v_1)^{\frac14}\{n(x_{\mathbf{b}}(x,v))\cdot v_1\}\mathrm{d}v_1\\
&+\mathbf{1}_{\{s>t_{\mathbf{b}}(x,v)\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}\Big(1+\frac{e^{-C_2|v|^2}}{|n(x_{\mathbf{b}}(x,v))\cdot v|}\Big)|R^{m-1}(s-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v)|.\end{aligned}$$

We plug this estimate into the left hand side of (8.84) to have

$$\int_0^t\iint_{\substack{x\in\partial\Omega,\\ n(x)\cdot v>0}}\mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}|h^m(s,x,v)|\mu(v)^{\frac14}\{n(x)\cdot v\}\mathrm{d}v\mathrm{d}S_x\mathrm{d}s$$

$$\leq\int_0^t\iint_{\gamma_+^\delta}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}|h_0(x-sv,v)|\mu(v)^{\frac14}|n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s\tag{8.85}$$

$$\begin{aligned}+&\int_0^t\iint_{\gamma_+^\delta}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}\mu(v)^{\frac14}|n(x)\cdot v|\\&\qquad\times\int_{\max\{0,s-t_{\mathbf{b}}(x,v)\}}^s|H^{m-1}(\tau,x-(s-\tau)v,v)|\mathrm{d}\tau\mathrm{d}S_x\mathrm{d}v\mathrm{d}s\end{aligned}\tag{8.86}$$

$$\begin{aligned}+&\int_0^t\iint_{\gamma_+^\delta}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}\mu(v)^{\frac12}\frac{|n(x)\cdot v|}{|n(x_{\mathbf{b}}(x,v))\cdot v|}\int_{n(x_{\mathbf{b}}(x,v))\cdot v_1>0}\mathbf{1}_{\{s>t_{\mathbf{b}}(x,v)\}}\\&\qquad\times|h^{m-1}(s-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v_1)|\mu(v_1)^{\frac14}\{n(x_{\mathbf{b}}(x,v))\cdot v_1\}\mathrm{d}v_1\mathrm{d}S_x\mathrm{d}v\mathrm{d}s\end{aligned}\tag{8.87}$$

$$\begin{aligned}+&\int_0^t\iint_{\gamma_+^\delta}\mathbf{1}_{\{s>t_{\mathbf{b}}(x,v)\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}\mu(v)^{\frac14}\frac{|n(x)\cdot v|}{|n(x_{\mathbf{b}}(x,v))\cdot v|}\\&\qquad\times|R^{m-1}(s-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v)|\mathrm{d}S_x\mathrm{d}v\mathrm{d}s.\end{aligned}\tag{8.88}$$

Estimate of (8.85) : Note that $x\in\partial\Omega$ in (8.85). Without loss of generality we may assume that there exists $\eta:\mathbb{R}^2\to\mathbb{R}$ such that $x^3=\eta(x^1,x^2)$. We apply the following change of variables : for fixed $v\in\mathbb{R}^3$,

$$(x^1,x^2;s)\in\mathbb{R}^2\times\{0\leq s\leq t_{\mathbf{b}}(x,v)\}\;\mapsto\;y=(x^1-sv^1,x^2-sv^2,\eta(x^1,x^2)-sv^3)\in\bar{\Omega}.$$

Clearly such mapping is one-to-one.

We compute the Jacobian :

$$\begin{aligned}\det\left(\frac{\partial(y^1,y^2,y^3)}{\partial(x^1,x^2,s)}\right)&=\det\begin{pmatrix}1&0&-v^1\\0&1&-v^2\\\partial_{x^1}\eta(x^1,x^2)&\partial_{x^2}\eta(x^1,x^2)&-v^3\end{pmatrix}\\&=v\cdot\begin{pmatrix}\partial_{x^1}\eta\\\partial_{x^2}\eta\\-1\end{pmatrix}=v\cdot n\sqrt{1+|\partial_{x^1}\eta|^2+|\partial_{x^2}\eta|^2}.\end{aligned}$$

Therefore

$$\{v\cdot n(x)\}\mathrm{d}S_x\mathrm{d}s=\{v\cdot n(x)\}\sqrt{1+|\partial_{x^1}\eta|^2+|\partial_{x^2}\eta|^2}\mathrm{d}x^1\mathrm{d}x^2\mathrm{d}s=\mathrm{d}y=\ \mathrm{d}y^1\,\mathrm{d}y^2\,\mathrm{d}y^3,$$

and

$$\begin{aligned}(8.85)&\le\int_{\mathbb{R}^3}\mathrm{d}v\int_0^t\mathrm{d}s\int_{\partial\Omega}\mathrm{d}S_x\mathbf{1}_{\{(x,v)\in\gamma_+\}}\mathbf{1}_{\{1/k<|n(x_{\mathbf{b}}(x,v))\cdot v|\}}|h_0(x-sv,v)|\mu(v)^{\frac14}|n(x)\cdot v|\\&\le\int_{\mathbb{R}^3}\mathrm{d}v\int_\Omega\mathrm{d}y|h_0(y,v)|\mu(v)^{\frac14}\\&\le\|h_0\|_1.\end{aligned}\tag{8.89}$$

Estimate of (8.86) : Considering the region of $\big\{(\tau,s)\in[0,t]\times[0,t]:\max\{0,s-t_{\mathbf{b}}(x,v)\}\le\tau\le s\big\}$,

$$(8.86)\le\int_{\mathbb{R}^3}\mathrm{d}v\int_0^t\mathrm{d}\tau\int_\tau^{\min\{t,\tau+t_{\mathbf{b}}(x,v)\}}\mathrm{d}s\int_{\partial\Omega}\mathrm{d}S_x|H^{m-1}(\tau,x-(s-\tau)v,v)|\mu(v)^{\frac14}|n(x)\cdot v|.\tag{8.90}$$

Note that $x\in\partial\Omega$. Without loss of generality we may assume that $x^3=\eta(x^1,x^2)$ for $\eta:\mathbb{R}^2\to\mathbb{R}$. We apply the change of variables : for fixed $v\in\mathbb{R}^3$ and $\tau\in[0,t]$,

$$(x^1,x^2;s)\in\mathbb{R}^2\times[\tau,\min\{t,\tau+t_{\mathbf{b}}(x,v)\}]\ \mapsto\ y\equiv(x^1-(s-\tau)v^1,x^2-(s-\tau)v^2,\eta(x^1,x^2)-(s-\tau)v^3).$$

The Jacobian is $\{v\cdot n(x)\}\sqrt{1+|\partial_{x^1}\eta|^2+|\partial_{x^2}\eta|^2}$ and $\{v\cdot n(x)\}\mathrm{d}s\mathrm{d}S_x\ \le\ \mathrm{d}y$. Applying the change of variables to (8.90) to have

$$(8.86)\le\int_0^t\int_{\mathbb{R}^3}\int_\Omega|H^{m-1}(\tau,y,v)|\mu(v)^{\frac14}\mathrm{d}y\mathrm{d}v\mathrm{d}\tau.\tag{8.91}$$

Estimate of (8.87) : This part is the most delicate among (8.85)$\sim$(8.88). Rewrite (8.87) as

$$\begin{aligned}&\int_0^t\mathrm{d}s\int_{\partial\Omega}\mathrm{d}S_x\int_{\mathbb{R}^3}\mathrm{d}v\int_{\mathbb{R}^3}\mathrm{d}v_1\ \mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}\mathbf{1}_{\{n(x_{\mathbf{b}}(x,v))\cdot v_1>0\}}\mathbf{1}_{\{s>t_{\mathbf{b}}(x,v)\}}\mathbf{1}_{\{|n(x_{\mathbf{b}}(x,v))\cdot v|>1/k\}}\\&\qquad\times\mu(v_1)^{\frac14}\mu(v)^{\frac12}\frac{|n(x)\cdot v|}{|n(x_{\mathbf{b}}(x,v))\cdot v|}|n(x_{\mathbf{b}}(x,v))\cdot v_1||h^{m-1}(s-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v_1)|.\end{aligned}\tag{8.92}$$

First we apply the following change of variables

$$s\in[0,t]\ \mapsto\ \tilde{s}=s-t_{\mathbf{b}}(x,v)\in[0,t-t_{\mathbf{b}}(x,v)],\tag{8.93}$$

where we have used the fact that s is integrated over $[t_{\mathbf{b}}(x,v),t]$. Clearly the Jacobian is 1 so that $\mathrm{d}\tilde{s}=\mathrm{d}s$ and hence

$$\begin{aligned}(8.92)\le&\int_0^t\mathrm{d}\tilde{s}\int_{\partial\Omega}\mathrm{d}S_x\int_{\mathbb{R}^3}\mathrm{d}v\int_{\mathbb{R}^3}\mathrm{d}v_1\ \underbrace{\mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}}\ \mathbf{1}_{\{n(x_{\mathbf{b}}(x,v))\cdot v_1>0\}}\mathbf{1}_{\{|n(x_{\mathbf{b}})\cdot v|>1/k\}}\\&\qquad\times\mu(v_1)^{\frac14}\mu(v)^{\frac12}\frac{|n(x)\cdot v|}{|n(x_{\mathbf{b}}(x,v))\cdot v|}|n(x_{\mathbf{b}}(x,v))\cdot v_1||h^{m-1}(\tilde{s},x_{\mathbf{b}}(x,v),v_1)|.\end{aligned}\tag{8.94}$$

Let us denote

$$\tilde{x}:=x_{\mathbf{b}}(x,v).\tag{8.95}$$

Note that since $(x,v)\in\gamma_+$ and $|n(x_{\mathbf{b}}(x,v))\cdot v|>1/k$, from Lemma 8.4, the mapping $(x,v)\mapsto(\tilde{x},v)$ is one-to-one and

$$\begin{aligned}t_{\mathbf{b}}(x,v)\ &=t_{\mathbf{b}}(x_{\mathbf{b}}(x,v),-v),\\x\ &=x_{\mathbf{b}}(x,v)+t_{\mathbf{b}}(x,v)v=x_{\mathbf{b}}(x,v)+t_{\mathbf{b}}(x_{\mathbf{b}}(x,v),-v)v=x_{\mathbf{b}}(x,v)-t_{\mathbf{b}}(x_{\mathbf{b}}(x,v),-v)(-v)\\&=\tilde{x}-t_{\mathbf{b}}(\tilde{x},-v)(-v),\end{aligned}$$

and hence we can rewrite the underbraced term in (8.94) as

$$\mathbf{1}_{\{(x,v)\in\gamma_+^\delta\}}\ =\ \mathbf{1}_{\{0<n(\tilde{x}-t_{\mathbf{b}}(\tilde{x},-v)(-v))\cdot v<\delta\ \text{or}\ |v|>1/\delta\}}.\tag{8.96}$$

Now we apply the change of variables of Lemma 8.4 : for $(x,v)\in\gamma_+$ and $|n(x_{\mathbf{b}}(x,v))\cdot v| = |n(\tilde{x})\cdot v| > 1/k$, we apply the change of variables

$$(x,v)\mapsto(\tilde{x},v) := (x_{\mathbf{b}}(x,v),v). \tag{8.97}$$

From Lemma 8.4, the Jacobian is

$$\det\left(\frac{\partial(\tilde{x},v)}{\partial(x,v)}\right) = \det\left(\frac{\partial\tilde{x}}{\partial x}\right) = \left|\frac{n(x)\cdot v}{n(\tilde{x})\cdot v}\right| \frac{\sqrt{1+|\nabla\eta|^2}}{\sqrt{1+|\nabla\varphi|^2}}, \quad \text{and} \quad \mathrm{d}S_{\tilde{x}} := \left|\frac{n(x)\cdot v}{n(\tilde{x})\cdot v}\right| \mathrm{d}S_x.$$

Then from (8.94) and (8.96),

$$\begin{aligned}
(8.92) \leq & \int_0^t \mathrm{d}\tilde{s}\int_{\mathbb{R}^3}\mathrm{d}v_1\int_{\mathbb{R}^3}\mathrm{d}v\int_{\partial\Omega}\mathrm{d}S_{\tilde{x}}\big\{\mathbf{1}_{0<n(\tilde{x}-t_{\mathbf{b}}(\tilde{x},-v)(-v))\cdot v<\delta} + \mathbf{1}_{|v|>1/\delta}\big\} \\
& \qquad \times \mathbf{1}_{\{n(\tilde{x})\cdot v_1>0\}}\mathbf{1}_{\{|n(\tilde{x})\cdot v|>1/k\}}\mu(v)^{\frac12}\mu(v_1)^{\frac14}|n(\tilde{x})\cdot v_1|\;|h^{m-1}(\tilde{s},\tilde{x},v_1)| \\
\leq & \int_0^t\iint_{\gamma_+}|h^{m-1}(\tilde{s},\tilde{x},v_1)|\mu(v_1)^{\frac14}|n(\tilde{x})\cdot v_1|\mathrm{d}S_{\tilde{x}}\mathrm{d}v_1\,\mathrm{d}\tilde{s} \\
& \qquad \times \underbrace{\sup_{\tilde{x}\in\partial\Omega}\int_{\mathbb{R}^3}\mathbf{1}_{\{-\delta<n(\tilde{x}-t_{\mathbf{b}}(\tilde{x},-v)(-v))\cdot(-v)<0\}}\mu(v)^{\frac12}\,\mathrm{d}v} \\
& + O(\delta)\int_0^t\iint_{\gamma_+}|h^{m-1}(\tilde{s},\tilde{x},v_1)|\mu(v_1)^{\frac14}|n(\tilde{x})\cdot v_1|\mathrm{d}S_{\tilde{x}}\mathrm{d}v_1\,\mathrm{d}\tilde{s},
\end{aligned} \tag{8.98}$$

where we extracted $O(\delta)$ from $\int_{\mathbb{R}^3}\mathbf{1}_{|v|>1/\delta}\mu(v)^{\frac12}\mathrm{d}v \lesssim e^{-\frac{1}{10\delta}}\int_{\mathbb{R}^3}\mu(v)^{\frac14}\mathrm{d}v$.

We claim the following :

Claim : For any small $0<\delta'\ll 1$, we can choose sufficiently small $0<\delta\ll 1$ such that

$$\sup_{\tilde{x}\in\partial\Omega}\int_{\mathbb{R}^3}\mathbf{1}_{\{-\delta<n(\tilde{x}-t_{\mathbf{b}}(\tilde{x},-v)(-v))\cdot(-v)<0\}}\mu(v)^{\frac12}\,\mathrm{d}v \leq \delta'. \tag{8.99}$$

This is consequence of Lemma .9. For given $\delta'>0$, we choose a sufficiently large $N\gg\frac{1}{\delta'}$ and we take $\delta_{\delta',N}>0$ as in Lemma .9. Then we choose a sufficiently small $\delta=\delta(\delta',N)>0$ such that $\delta\ll\delta_{\delta',N}$ in Lemma .9. Due to Lemma .9 and (121),

$$\max_i \sup_{\tilde{x}\in B(x_i;r_i)} \mathrm{m}_3\{v\in\mathbb{R}^3 : |v|\leq N,\ |n(x_{\mathbf{b}}(\tilde{x},-v))\cdot(-v)|\leq\delta\} \ \leq\ \max_i \mathrm{m}_3(\mathcal{O}_{x_i})\leq\delta'.$$

Finally we conclude the claim (8.99) by

$$\begin{aligned}
& \int_{\mathbb{R}^3}\mathbf{1}_{\{-\delta<n(x_{\mathbf{b}}(\tilde{x},-v))\cdot(-v)<0\}}\mu(v)^{\frac12}\mathrm{d}v \\
= & \int_{|v|\geq N}+\int_{|v|\leq N} \\
\leq & \ e^{-N^2/4}+\max_i \mathrm{m}_3(\mathcal{O}_i) \\
\leq & \ e^{-\frac{1}{4(\delta')^2}}+\delta'.
\end{aligned}$$

Therefore, from (8.94), (8.98), (8.99), we have, for $0<\delta,\delta'\ll 1$,

$$(8.87) \lesssim [O(\delta)+O(\delta')]\times\int_0^t\int_{\gamma_+}|h^{m-1}(\tilde{s},\tilde{x},v_1)|\mu(v_1)^{\frac14}|n(\tilde{x})\cdot v_1|\,\mathrm{d}S_{\tilde{x}}\,\mathrm{d}v_1\,\mathrm{d}\tilde{s}. \tag{8.100}$$

Estimate of (8.88) : We apply the change of variables (8.93) and then apply (8.97) and use Lemma 8.4 to bound

$$(8.88) \lesssim \int_0^t\int_{\partial\Omega}\int_{\mathbb{R}^3}\mu(v)^{\frac14}|R^{m-1}(\tilde{s},\tilde{x},v)|\mathrm{d}S_{\tilde{x}}\mathrm{d}v\mathrm{d}\tilde{s}. \tag{8.101}$$

Finally from (8.89), (8.91), (8.100) and (8.101), we prove our claim (8.84).

The last step is to pass a limit $k \to \infty$. Clearly the sequence is non-decreasing in k :

$$0 \leq \mathbf{1}_{\{\frac{1}{k} < |n(x_{\mathbf{b}}(x,v))\cdot v|\}} |h^m(s,x,v)| \leq \mathbf{1}_{\{\frac{1}{k+1} < |n(x_{\mathbf{b}}(x,v))\cdot v|\}} |h^m(s,x,v)|.$$

We claim the following :
Claim : As $k \to \infty$,

$$\mathbf{1}_{\{\frac{1}{k} < |n(x_{\mathbf{b}}(x,v))\cdot v|\}} \mu(v)^{\frac14} |h^m(s,x,v)| \ \to \ \mu(v)^{\frac14} |h^m(s,x,v)| \quad \text{a.e. } (x,v) \in \gamma_+ \text{ with } \mathrm{d}\gamma.$$

It suffices to show $\mathbf{1}_{\{\frac{1}{k} < |n(x_{\mathbf{b}}(x,v))\cdot v|\}} \mu(v)^{\frac14} \to \mu(v)^{\frac14}$ a.e. on γ_+. For $\varepsilon > 0$ and $N \gg \varepsilon^{-1} \gg 1$, choose $k \gg 1$ such that $\frac{1}{k} < \delta_{\varepsilon,N}$ in Lemma .9. Then

$$\begin{aligned}
&\Big[1 - \mathbf{1}_{\{|n(x_{\mathbf{b}}(x,v))\cdot v| > \frac1k\}}(x,v)\Big] \mu(v)^{\frac14} \\
&\leq \max_{1\leq i \leq l_{\varepsilon,N,\Omega}} \mathbf{1}_{B(x_i;r_i)}(x) \times \mathbf{1}_{\{|n(x_{\mathbf{b}}(x,v))\cdot v| \leq \frac1k\}} \mu(v)^{\frac14} \\
&\leq \max_{1\leq i \leq l_{\varepsilon,N,\Omega}} \mathbf{1}_{B(x_i;r_i)}(x) \times \mathbf{1}_{\{|n(x_{\mathbf{b}}(x,v))\cdot v| \leq \delta_{\varepsilon,N}\}} \mu(v)^{\frac14} \\
&\leq \max_{1\leq i \leq l_{\varepsilon,N,\Omega}} \mathbf{1}_{B(x_i;r_i)}(x) \times \Big\{ \mathbf{1}_{\{|v|\leq N, v\in \mathcal{O}_i\}}(v)\mu(v)^{\frac14} + \mathbf{1}_{|v|\geq N}(v) e^{-\frac{N^2}{16}} \mu(v)^{\frac18} \Big\},
\end{aligned}$$

and hence

$$\begin{aligned}
&\int_{\gamma_+} |1 - \mathbf{1}_{\{|n(x_{\mathbf{b}}(x,v))\cdot v| > \frac1k\}}(x,v)| \mu(v)^{\frac12}\, \mathrm{d}\gamma \\
&\leq \max_{1\leq i \leq l_{\varepsilon,N,\Omega}} \int_{\partial\Omega}\int_{n\cdot v>0} \mathbf{1}_{\{|v|\leq N, v\in\mathcal{O}_i\}}\, \mathrm{d}v\, \mathrm{d}S_x + O(\frac{1}{N}) \\
&\lesssim \varepsilon + O(\frac1N) \lesssim \varepsilon,
\end{aligned}$$

which concludes the claim.

Now we use the monotone convergence theorem to conclude

$$\int_0^t \int_{\gamma_+^\delta} \mathbf{1}_{\{1/k < |n(x_{\mathbf{b}}(x,v))\cdot v|\}} |h^m(s,x,v)| \mu(v)^{\frac14} \mathrm{d}\gamma \mathrm{d}s \to \int_0^t \int_{\gamma_+^\delta} |h^m(s,x,v)| \mu(v)^{\frac14} \mathrm{d}\gamma \mathrm{d}s,$$

as $k \to \infty$ and therefore $\int_0^t \int_{\gamma_+^\delta} |h^m(s,x,v)| \mu(v)^{\frac14} \mathrm{d}\gamma \mathrm{d}s$ has the same upper bound of (8.84). Together with (8.83) we conclude (8.79). $\square$

8.4 Linear and Nonlinear Estimates

The main purpose of this section is to prove the main theorem (Theorem 1). To estimate solutions of the nonlinear equation (8.1) with the diffuse boundary condition (8.5) we use the following approximation scheme.

For $f_0 \in BV(\Omega\times\mathbb{R}^3)$ and $\|e^{\theta|v|^2} f_0\|_\infty < \infty$ we choose $f_0^\varepsilon \in BV(\Omega\times\mathbb{R}^3) \cap C^\infty(\Omega\times\mathbb{R}^3)$ satisfying $\|e^{\theta|v|^2}[f_0^\varepsilon - f_0]\|_\infty \to 0$ and $\|\nabla_{x,v} f_0^\varepsilon\|_1 \to \|f_0\|_{\widetilde{BV}}$.

Consider the sequence $f^{\varepsilon,m}$ defined by $f^{\varepsilon,0} = \chi_\varepsilon f_0^\varepsilon$ and for all $m \geq 0$,

$$\begin{aligned}
\partial_t f^{\varepsilon,m+1} + v\cdot\nabla_x f^{\varepsilon,m+1} + \nu(\sqrt{\mu} f^{\varepsilon,m}) f^{\varepsilon,m+1} &= \chi_\varepsilon \Gamma_{\text{gain}}(f^{\varepsilon,m}, f^{\varepsilon,m}), \ \text{ in } \ \Omega\times\mathbb{R}^3, \\
f^{\varepsilon,m+1}(0,x,v) &= \chi_\varepsilon f_0^\varepsilon(x,v), \ \text{ in } \ \Omega\times\mathbb{R}^3, \\
f^{\varepsilon,m+1}(t,x,v) = \chi_\varepsilon(x,v) c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u>0} & f^{\varepsilon,m}(t,x,u)\sqrt{\mu}\{n\cdot u\} \mathrm{d}u, \ \text{ on } \ \gamma_-,
\end{aligned} \tag{8.102}$$

where χ_ε is defined in (8.50).

In order to study such sequences, we first consider a linear equation with the in-flow boundary condition

$$f(t,x,v)|_{\gamma_-} = g(t,x,v). \tag{8.103}$$

Let $\{\tau_1(x), \tau_2(x)\}$ be a basis of the tangent space at $x \in \partial\Omega$ (therefore $\{\tau_1(x), \tau_2(x), n(x)\}$ is an orthonormal basis of $\mathbb{R}^3$). Denote ∂_{τ_i} to be the (tangential) τ_i-directional derivative and ∂_n to be the normal derivative.

Lemma 8.5. *Assume $\mathcal{U}$ is an open subset of $\mathbb{R}^3\times\mathbb{R}^3$ such that $\mathfrak{S}_{\mathrm{B}}\subset\mathcal{U}$. Assume*

$$f_0(x,v)\equiv 0,\ \ g(t,x,v)\equiv 0,\ \ H(t,x,v)\equiv 0,\quad \textit{for}\quad (t,x,v)\in[0,T]\times\{\mathcal{U}\cap(\bar{\Omega}\times\mathbb{R}^3)\}. \tag{8.104}$$

Assume further that for $0<\theta<\frac{1}{4}$,

$$e^{\theta|v|^2}f_0\in L^\infty(\Omega\times\mathbb{R}^3),\ \ e^{\theta|v|^2}g\in L^\infty([0,T]\times\gamma_-),\ \ e^{\theta|v|^2}H\in L^\infty([0,T]\times\Omega\times\mathbb{R}^3),$$

and

$$\begin{aligned}
&\nabla_x f_0,\ \nabla_v f_0\in\ L^1(\Omega\times\mathbb{R}^3),\\
&\partial_{\tau_i}g,\ \frac{1}{n(x)\cdot v}\Big\{-\partial_t g-\sum_i(v\cdot\tau_i)\partial_{\tau_i}g-\nu g+H\Big\},\ \nabla_v g, e^{-\theta|v|^2}\nabla_x\nu, e^{-\theta|v|^2}\nabla_v\nu\ \in\ L^1([0,T]\times\gamma_-),\\
&\nabla_x H,\ \nabla_v H,\ e^{-\theta|v|^2}\nabla_x\nu,\ e^{-\theta|v|^2}\nabla_v\nu\ \in\ L^1([0,T]\times\Omega\times\mathbb{R}^3).
\end{aligned}$$

Then there exists a unique solution f to the transport equation (8.14) with in-flow boundary condition (8.103) such that $e^{\theta|v|^2}f\in C^0([0,T]\times\bar{\Omega}\times\mathbb{R}^3)$ and $\nabla_x f,\ \nabla_v f\in C^0([0,T];L^1(\Omega\times\mathbb{R}^3))$ and the traces satisfy

$$\begin{aligned}
&\nabla_x f=\nabla_x g,\quad \nabla_v f=\nabla_v g,\quad \textit{on } \gamma_-,\\
&\nabla_x f(0,x,v)=\nabla_x f_0,\quad \nabla_v f(0,x,v)=\nabla_v f_0,\quad \textit{in } \Omega\times\mathbb{R}^3,
\end{aligned}$$

where $\nabla_x g$ is defined by

$$\nabla_x g=\sum_{i=1,2}\tau_i\partial_{\tau_i}g+\frac{n}{n\cdot v}\big\{-\partial_t g-\sum_i(v\cdot\tau_i)\partial_{\tau_i}g-\nu g+H\big\}.$$

Moreover

$$\begin{aligned}
&\|\nabla_x f(t)\|_1+\int_0^t|\nabla_x f|_{\gamma_+,1}+\int_0^t\|\nu\nabla_x f\|_1\\
&\qquad=\|\nabla_x f_0\|_1+\int_0^t|\nabla_x g|_{\gamma_-,1}+\int_0^t\iint_{\Omega\times\mathbb{R}^3}\mathrm{sgn}(\nabla_x f)\big\{\nabla_x H-\nabla_x\nu f\big\},
\end{aligned}\tag{8.105}$$

$$\begin{aligned}
&\|\nabla_v f(t)\|_1+\int_0^t|\nabla_v f|_{\gamma_+,1}+\int_0^t\|\nu\nabla_v f\|_1\\
&\qquad=\|\nabla_v f_0\|_1+\int_0^t|\nabla_v g|_{\gamma_-,1}+\int_0^t\iint_{\Omega\times\mathbb{R}^3}\mathrm{sgn}(\nabla_v f)\big\{\nabla_v H-\nabla_x f-\nabla_v\nu f\big\}.
\end{aligned}\tag{8.106}$$

Proof. We use the Duhamel formula of f :

$$\begin{aligned}
f(t,x,v)=\ &\mathbf{1}_{\{t<t_{\mathbf{b}}(x,v)\}}e^{-\int_0^t\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau}f_0(x-tv,v)\\
&+\mathbf{1}_{\{t>t_{\mathbf{b}}(x,v)\}}e^{-\int_0^{t_{\mathbf{b}}(x,v)}\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau}g(t-t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v),v)\\
&+\int_0^{\min\{t,t_{\mathbf{b}}(x,v)\}}e^{-\int_0^s\nu(t-\tau,x-\tau v,v)\mathrm{d}\tau}H(t-s,x-sv,v)\mathrm{d}s.
\end{aligned}\tag{8.107}$$

Following Proposition 1 of [77], we have, on $\{t\neq t_{\mathbf{b}}\}$

$$
\begin{aligned}
&\nabla_x f(t,x,v)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\\
&= \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left\{ \nabla_x f_0(x-tv,v) - \left(\int_0^t \nabla_x \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau \right) f_0(x-tv,v) \right\}\\
&\quad + \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \Big\{ \sum_{i=1}^2 \tau_i \partial_{\tau_i} g - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})} \big\{ \partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H \big\} \Big\} (t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&\quad - \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^{t_{\mathbf{b}}} \nabla_x \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau \right) g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&\quad + \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \nabla_x H(t-s,x-vs,v)\,\mathrm{d}s\\
&\quad - \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \left(\int_0^s \nabla_x \nu(s-\tau,x-\tau v,v)\mathrm{d}\tau \right) H(t-s,x-vs,v)\,\mathrm{d}s,
\end{aligned}
\tag{8.108}
$$

$$
\begin{aligned}
&\nabla_v f(t,x,v)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\\
&= \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} [-t\nabla_x f_0 + \nabla_v f_0](x-tv,v)\\
&\quad - \mathbf{1}_{\{t<t_{\mathbf{b}}\}} e^{-\int_0^t \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \int_0^t \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau f_0(x-tv,v)\\
&\quad - \mathbf{1}_{\{t>t_{\mathbf{b}}\}} t_{\mathbf{b}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \Big\{ \sum_{i=1}^2 \tau_i \partial_{\tau_i} g - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})} \big\{ \partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H \big\} \Big\} (t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&\quad + \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \Big\{ \nabla_v g(t-t_{\mathbf{b}},x_{\mathbf{b}},v) \Big\}\\
&\quad - \mathbf{1}_{\{t>t_{\mathbf{b}}\}} e^{-\int_0^{t_{\mathbf{b}}} \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \Big\{ \int_0^{t_{\mathbf{b}}} \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau \Big\} g(t-t_{\mathbf{b}},x_{\mathbf{b}},v)\\
&\quad + \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \{\nabla_v H - s\nabla_x H\}(t-s,x-vs,v)\,\mathrm{d}s\\
&\quad - \int_0^{\min(t,t_{\mathbf{b}})} e^{-\int_0^s \nu(t-\tau,x-\tau v,v)\mathrm{d}\tau} \{ \int_0^s \{-\tau\nabla_x\nu + \nabla_v\nu\}(t-\tau,x-\tau v,v)\mathrm{d}\tau \} H(t-s,x-vs,v)\,\mathrm{d}s
\end{aligned}
\tag{8.109}
$$

Therefore, we have

$$
\begin{aligned}
\|\nabla_x f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_1 &\lesssim \|\nabla_x f_0\|_1 + t\{\|e^{\theta|v|^2} f_0\|_\infty + \|e^{\theta|v|^2} g\|_\infty\}\\
&\quad + \int_0^t \Big| \sum_{i=1}^2 \tau_i\partial_{\tau_i} g - \frac{n}{v\cdot n} \big\{ \partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H \big\} \Big|_{\gamma_-,1}\\
&\quad + \int_0^t \|\nabla_x H(s)\|_1 + \int_0^t s\|e^{\theta|v|^2} H(s)\|_\infty
\end{aligned}
\tag{8.110}
$$

$$
\begin{aligned}
\|\nabla_v f(t)\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}\|_1 &\lesssim t\|\nabla_x f_0\|_1 + \|\nabla_v f_0\|_1 + t\|e^{\theta|v|^2} f_0\|_\infty\\
&\quad + t\int_0^t \Big| \Big\{ \sum_{i=1}^2 \tau_i\partial_{\tau_i} g - \frac{n}{v\cdot n} \big\{ \partial_t g + \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i} g + \nu g - H \big\} \Big\} \Big|_{\gamma_-,1}\\
&\quad + \int_0^t |\nabla_v g|_{\gamma_-,1} + t^2 \sup_{0\le s\le t} |e^{\theta|v|^2} g(s)|_{\gamma_-,\infty}\\
&\quad + \int_0^t \|\nabla_x H\|_1 + \int_0^t \|\nabla_v H\|_1 + C\int_0^t \|e^{\theta|v|^2} H\|_\infty.
\end{aligned}
$$

From our assumption, f_0, g, and H have compact supports and the RHS are bounded. Therefore

$$
\partial f \mathbf{1}_{\{t\neq t_{\mathbf{b}}\}} = [\partial_t f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}},\ \nabla_x f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}},\ \nabla_v f\mathbf{1}_{\{t\neq t_{\mathbf{b}}\}}] \in\ L^\infty([0,T];L^1(\Omega\times\mathbb{R}^3)).
$$

Since $\partial f \equiv 0$ around $\{t = t_{\mathbf{b}}\}$ clearly $\partial f \mathbf{1}_{\{t \neq t_{\mathbf{b}}\}}$ is the distributional derivative of f. Therefore $\nabla_x f$ and $\nabla_v f$ lie in $L^\infty([0,T]; L^1(\Omega \times \mathbb{R}^3))$; this allows us to apply Lemma .7 to compute the traces on the incoming boundary in $L^1([0,T]; L^1(\gamma_-, \mathrm{d}\gamma))$ (by taking limits of the flow along the characteristics : see the proof of Proposition 1 in [77] for details). Then, by Green's identity (Lemma .8) we know that $\nabla_x f$ and $\nabla_v f$ lie in $C^0([0,T]; L^1(\Omega \times \mathbb{R}^3))$ and we get (8.105) and (8.106).

□

Before going to the proof of main theorem we recall the standard estimate from [67] :
Suppose $a_i \geq 0, D \geq 0$ and $A_i = \max\{a_i, \cdots, a_{i-(k-1)}\}$ for fixed $k \in \mathbb{N}$.

$$\text{If } a_{m+1} \leq \frac{1}{8} A_m + D \text{ then } A_m \leq \frac{1}{8} A_0 + \left(\frac{8}{7}\right)^2 D \text{ for } m/k \gg 1. \tag{8.111}$$

Now we are ready to prove the main theorem.

Proof of Theorem 1. Consider the approximation scheme (8.102). For a fixed $0 < \varepsilon \ll 1$, it is clear that $(f^{\varepsilon,m})_m$ is Cauchy for the norm $\sup_{0 \leq t \leq T} \|e^{\theta' |v|^2} \cdot \|_\infty$ for $0 < \theta' < \theta < \frac{1}{4}$ and some $0 < T \ll 1$. The key element of the proof is to utilize the exponential weight in v to suppress the $|v|$ growth in the gain term estimate at least for some short time. For details, see Lemma 6 in [77].

Therefore $f^{\varepsilon,m} \to f^\varepsilon$ up to subsequence for the norm $\sup_{0 \leq t \leq T} \|e^{\theta|v|^2} \cdot \|_\infty$ and f^ε satisfies (8.102) with $f^{\varepsilon,m+1}$ and $f^{\varepsilon,m}$ replaced by f^ε by the trace theorem. Since $|\chi_\varepsilon| \leq 1$ for $0 < \varepsilon \ll 1$, $\sup_{0 \leq t \leq T} \|e^{\theta|v|^2} f^\varepsilon(t)\|_\infty$ is uniformly bounded in ε for $0 < \varepsilon \ll 1$ and $0 < T \ll 1$. Therefore $f^\varepsilon \to f$ weak$-*$ up to a subsequence and the limiting function f solves the Boltzmann equation with the diffuse boundary condition in the sense of distributions.

Now we consider the derivatives of the solution $f^{\varepsilon,m}$ of (8.102). Recall that $BV(\Omega \times \mathbb{R}^3)$ has $i)$ a *compactness* property :

$$\begin{aligned} &\text{Suppose } g^k \in BV \text{ and } \sup_k \|g^k\|_{BV} < \infty \\ &\qquad \text{then } \exists\, g \in BV \text{ with } g^k \to g \text{ in } L^1 \text{ up to subsequence,} \end{aligned} \tag{8.112}$$

and $ii)$ a *lower semicontinuity* property :

$$\text{Suppose } g^k \in BV \text{ and } g^k \to g \text{ in } L^1_{loc} \text{ then } \|f\|_{\widetilde{BV}} \leq \liminf_{k \to \infty} \|g^k\|_{\widetilde{BV}}. \tag{8.113}$$

Due to the smooth approximation f_0^ε of the initial datum f_0 and the cut-off χ_ε, $f^{\varepsilon,m}$ is smooth by Lemma 8.5. We take derivatives $\partial \in \{\nabla_x, \nabla_v\}$ to have

$$\begin{aligned} &\left[\partial_t + v \cdot \nabla_x + \nu(\sqrt{\mu} f^{\varepsilon,m})\right] \partial f^{\varepsilon,m+1} \\ &= -\partial v \cdot \nabla_x f^{\varepsilon,m+1} - \nu(\partial[\sqrt{\mu} f^{\varepsilon,m}]) f^{\varepsilon,m+1} + \partial \chi_\varepsilon \Gamma_{\text{gain}}(f^{\varepsilon,m}, f^{\varepsilon,m}) + \chi_\varepsilon \partial[\Gamma_{\text{gain}}(f^{\varepsilon,m}, f^{\varepsilon,m})] \\ &\quad + (error) \\ &\partial f^{\varepsilon,m+1}(0,x,v) = \partial \chi_\varepsilon f_0^\varepsilon(x,v) + \chi_\varepsilon \partial f_0^\varepsilon(x,v), \end{aligned}$$

where $(error) \leq e^{-\theta|v|^2} \partial \nu \|e^{\theta|v|^2} f^{\varepsilon,m}\|_\infty \|e^{\theta|v|^2} f^{\varepsilon,m+1}\|_\infty$. For all $(x,v) \in \gamma_-$,

$$\begin{aligned} |\partial f^{\varepsilon,m+1}(t,x,v)| &\lesssim \sqrt{\mu(v)} \left(1 + \frac{\langle v \rangle}{|n(x) \cdot v|}\right) \int_{n(x) \cdot u > 0} |\partial f^{\varepsilon,m}(t,x,u)| \mu(u)^{\frac{1}{4}} \{n(x) \cdot u\} \mathrm{d}u \\ &\quad + \frac{\langle v \rangle^\kappa e^{-C_\theta |v|^2}}{|n(x) \cdot v|} \|e^{\theta|v|^2} f_0\|_\infty + |\partial \chi_\varepsilon(x,v) \sqrt{\mu(v)}| P(\|e^{\theta|v|^2} f_0\|_\infty), \end{aligned}$$

for some polynomial P. Due to quadratic nonlinear term Γ we require $P(s) = s(1+s)$.

Then by Proposition 8.5 and $\sqrt{\mu} f^{\varepsilon,m} \geq 0$,

$$\begin{aligned} &\|\partial f^{\varepsilon,m+1}(t)\|_1 + \int_0^t |\partial f^{\varepsilon,m+1}(s)|_{\gamma_+,1} \\ &\lesssim \|e^{-\theta'|v|^2} \partial \chi_\varepsilon\|_1 \|e^{\theta'|v|^2} f_0\|_\infty + \|\partial f_0^\varepsilon\|_1 + \int_0^t |\partial f^{\varepsilon,m+1}(s)|_{\gamma_-} \\ &\quad + \int_0^t \|\partial f^{\varepsilon,m+1}(s)\|_1 \mathrm{d}s + P(\|e^{\theta|v|^2} f^{\varepsilon,m}\|_\infty) \\ &\quad\quad \times \left\{t + t \iint_{\Omega \times \mathbb{R}^3} e^{-C_\theta |v|^2} |\partial \chi_\varepsilon| + \int_0^t \|\partial f^{\varepsilon,m}(s)\|_1 \mathrm{d}s\right\}, \end{aligned} \tag{8.114}$$

where we have used Lemma .10 in Appendix 1.

Applying Lemma 8.2 and Proposition 8.1 to (8.114), we obtain

$$\begin{aligned}
&\|\partial f^{\varepsilon,m+1}(t)\|_1 + \int_0^t |\partial f^{\varepsilon,m+1}(s)|_{\gamma_+,1} \\
&\lesssim \|e^{\theta'|v|^2} f_0\|_\infty + \|f_0\|_{BV} + \int_0^t |\partial f^{\varepsilon,m+1}(s)|_{\gamma_-,1} \\
&\quad + t[1+P(\|e^{\theta'|v|^2} f_0\|_\infty)] \sup_{0\leq s\leq t} \|\partial f^{\varepsilon,m+1}(s)\|_1 \mathrm{d}s + tP(\|e^{\theta'|v|^2} f_0\|_\infty).
\end{aligned} \tag{8.115}$$

On the other hand, we apply Proposition 8.2 and Lemma .7 to bound

$$\begin{aligned}
\int_0^t |\partial f^{\varepsilon,m+1}|_{\gamma_-,1} &\lesssim O(\delta) \int_0^t |\partial f^{\varepsilon,m-1}|_{\gamma_+,1} + C_\delta\{\|f_0\|_{BV} + tP(\|e^{\theta'|v|^2} f_0\|_\infty)\} \\
&\quad + C_\delta t[1+P(\|e^{\theta'|v|^2} f_0\|_\infty)] \max_{i=m,m-1} \sup_{0\leq s\leq t} \|\partial f^{\varepsilon,i}(s)\|_1.
\end{aligned} \tag{8.116}$$

Finally from (8.115) and (8.116), chosing $\delta \ll 1$ and $T := T(f_0)$ small enough, we have for all $0 \leq t \leq T$

$$\begin{aligned}
&\sup_{0\leq s\leq t} \|\partial f^{\varepsilon,m+1}(s)\|_1 + \int_0^t |\partial f^{\varepsilon,m+1}(s)|_{\gamma,1} \\
&\leq C\{\|f_0\|_{BV} + P(\|e^{\theta'|v|^2} f_0\|_\infty)\} + \frac{1}{8} \max_{i=m,m-1} \Big\{ \sup_{0\leq s\leq t} \|\partial f^{\varepsilon,i}(s)\|_1 + \int_0^t |\partial f^{\varepsilon,i}|_{\gamma,1} \Big\}.
\end{aligned}$$

Now using (8.111) we conclude

$$\sup_{0\leq s\leq t} \|\partial f^{\varepsilon,m}(s)\|_1 + \int_0^t |\partial f^{\varepsilon,m}(s)|_{\gamma,1} \ \lesssim\ \|f_0\|_{BV} + P(\|e^{\theta|v|^2} f_0\|_\infty) \quad \text{for all } m \in \mathbb{N}. \tag{8.117}$$

Now we pass the to limit in m and then in ε to conclude the main theorem. From the compactness (8.112) and a lower semicontinuity (8.113) we conclude

$$\sup_{0\leq s\leq t} \|f(s)\|_{BV} \ \lesssim\ \|f_0\|_{BV} + P(\|e^{\theta|v|^2} f_0\|_\infty).$$

For the boundary term we use the *weak compactness of measures* : If σ^k is a signed Radon measures on $\partial\Omega \times \mathbb{R}^3$ satisfying $\sup_k \sigma^k(\partial\Omega \times \mathbb{R}^3) < \infty$ then there exists a Radon measure σ such that $\sigma^k \rightharpoonup \sigma$ in $\mathcal{M}$.

More precisely we define, for almost-every s, and for any Lebesgue-measurable set $A \subset \partial\Omega \times \mathbb{R}^3$,

$$\begin{aligned}
\sigma_s^{\varepsilon,m}(A) &= \Big(\sigma_{s,x^1}^{\varepsilon,m}(A), \sigma_{s,x^2}^{\varepsilon,m}(A), \sigma_{s,x^3}^{\varepsilon,m}(A), \sigma_{s,v^1}^{\varepsilon,m}(A), \sigma_{s,v^2}^{\varepsilon,m}(A), \sigma_{s,v^3}^{\varepsilon,m}(A)\Big)^T \\
&:= \int_A \nabla_{x,v} f^{\varepsilon,m}(s) \mathrm{d}\gamma \in \mathbb{R}^6.
\end{aligned}$$

Then there exists a Radon measure σ_s such that $\sigma_s^{\varepsilon,m} \rightharpoonup \sigma_s$ in $\mathcal{M}$, i.e.

$$\int_{\partial\Omega\times\mathbb{R}^3} g \partial f^{\varepsilon,m}(s) \mathrm{d}\gamma \to \int_{\partial\Omega\times\mathbb{R}^3} g \mathrm{d}\sigma_s \quad \text{for all } \ g \in C_c^0(\partial\Omega \times \mathbb{R}^3). \tag{8.118}$$

It is standard (Hahn's decomposition theorem) to decompose $\sigma_s = \sigma_{s,+} - \sigma_{s,-}$ with $\sigma_{s,\pm} \geq 0$. Denote $|\sigma_s|_{\mathcal{M}(\gamma)} = \sigma_{s,+}(\partial\Omega \times \mathbb{R}^3) + \sigma_{s,-}(\partial\Omega \times \mathbb{R}^3)$. Then by the lower semicontinuity property of measures we have $|\sigma_s|_{\mathcal{M}(\gamma)} \leq \liminf |\sigma_s^{\varepsilon,m}|_{\mathcal{M}(\gamma)} = \liminf |\partial f_s^{\varepsilon,m}|_{L^1(\gamma)}$, so that by (8.117) $\int_0^t |\sigma_s|_{\mathcal{M}(\gamma)} \,\mathrm{d}s \lesssim \|f_0\|_{BV} + P(\|e^{\theta|v|^2} f_0\|_\infty)$. Due to (8.118), the (distributional) derivatives $\nabla_{x,v} f(s)|_\gamma$ equal the Radon measure σ_s on $\partial\Omega \times \mathbb{R}^3$ in the sense of distributions.

□

Appendix 1. Some Basic Results

We collect some basic known results such as the derivatives of $t_{\mathbf{b}}$ and $x_{\mathbf{b}}$, the standard trace theorem, integration by parts formula, and the size of singular set.

Lemma .6 ([75, 67]). *If*

$$v\cdot n(x_{\mathbf{b}}(x,v))<0, \tag{119}$$

then $(t_{\mathbf{b}}(x,v),x_{\mathbf{b}}(x,v))$ *are smooth functions of* (x,v) *such that*

$$\nabla_x t_{\mathbf{b}}=\frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})},\qquad \nabla_v t_{\mathbf{b}}=-\frac{t_{\mathbf{b}}n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})},$$
$$\nabla_x x_{\mathbf{b}}=I-\frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\otimes v,\qquad \nabla_v x_{\mathbf{b}}=-t_{\mathbf{b}}I+\frac{t_{\mathbf{b}}n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\otimes v.$$

Recall the almost grazing set γ_+^δ defined in (8.16). We first estimate the outgoing trace on $\gamma_+\setminus\gamma_+^\delta$. We remark that for the outgoing part, our estimate is global in time without cut-off, in contrast to the general trace theorem.

Lemma .7 (Outgoing trace theorem, [77]). *Assume that* $\varphi\geq 0$. *For any small parameter* $\delta>0$, *there exists a constant* $C_{\delta,T,\Omega}>0$ *such that for any* h *in* $L^1([0,T]\times\Omega\times\mathbb{R}^3)$ *with* $\partial_t h+v\cdot\nabla_x h+\varphi h$ *lying in* $L^1([0,T]\times\Omega\times\mathbb{R}^3)$, *we have for all* $0\leq t\leq T$,

$$\int_0^t\int_{\gamma_+\setminus\gamma_+^\delta}|h|\mathrm{d}\gamma\mathrm{d}s\leq C_{\delta,T,\Omega}\left[\ \|h_0\|_1+\int_0^t\big\{\|h(s)\|_1+\big\|[\partial_t+v\cdot\nabla_x+\varphi]h(s)\big\|_1\big\}\mathrm{d}s\ \right].$$

Furthermore, for any (s,x,v) *in* $[0,T]\times\Omega\times\mathbb{R}^3$ *the function* $h(s+s',x+s'v,v)$ *is absolutely continuous in* s' *in the interval* $[-\min\{t_{\mathbf{b}}(x,v),s\},\min\{t_{\mathbf{b}}(x,-v),T-s\}]$.

Lemma .8 (Green's Identity, [75, 67]). *For* $p\in[1,\infty)$ *assume that* $f,\partial_t f+v\cdot\nabla_x f+\varphi f\in L^p([0,T]\times\Omega\times\mathbb{R}^3)$ *with* $\varphi\geq 0$ *and* $f_{\gamma_-}\in L^p([0,T]\times\partial\Omega\times\mathbb{R}^3;\mathrm{d}t\mathrm{d}\gamma)$. *Then* $f\in C^0([0,T];L^p(\Omega\times\mathbb{R}^3))$ *and* $f_{\gamma_+}\in L^p([0,T]\times\partial\Omega\times\mathbb{R}^3;\mathrm{d}t\mathrm{d}\gamma)$ *and for almost every* $t\in[0,T]$ *:*

$$\|f(t)\|_p^p+\int_0^t|f|_{\gamma_+,p}^p=\|f(0)\|_p^p+\int_0^t|f|_{\gamma_-,p}^p+\int_0^t\iint_{\Omega\times\mathbb{R}^3}\{\partial_t f+v\cdot\nabla_x f+\varphi f\}p|f|^{p-2}f.$$

Lemma .9 (Lemma 17 and Lemma 18 of [75]). *Let* $\Omega\subset\mathbb{R}^3$ *be an open bounded set with a smooth boundary* $\partial\Omega$. *Then, for all* $x\in\bar{\Omega}$, *we have*

$$\mathrm{m}_3\{v\in\mathbb{R}^3:\ n(x_{\mathbf{b}}(x,v))\cdot v=0\}=0, \tag{120}$$

Moreover, for any $\varepsilon>0$ *and* $N\gg 1$, *there exist* $\delta_{\varepsilon,N}>0$ *and* $l=l_{\varepsilon,N,\Omega}$ *balls* $B(x_1;r_1),B(x_2;r_2),\cdots,B(x_l;r_l)$ *with* $x_i\in\bar{\Omega}$ *and covering* $\bar{\Omega}$ *(i.e.* $\bar{\Omega}\subset\bigcup B(x_i;r_i)$*), as well as* l *open sets* $\mathcal{O}_{x_1},\mathcal{O}_{x_2},\cdots,\mathcal{O}_{x_l}\subset B_N:=\{v\in\mathbb{R}^3:|v|\leq N\}$, *with* $\mathrm{m}_3(\mathcal{O}_{x_i})<\varepsilon$ *for all* $1\leq i\leq l_{\varepsilon,N,\Omega}$, *such that for any* $x\in\bar{\Omega}$, *there exists* $i=1,2,\cdots,l_{\varepsilon,N,\Omega}$ *such that* $x\in B(x_i;r_i)$ *and*

$$|v\cdot n(x_{\mathbf{b}}(x,v))|\ >\delta_{\varepsilon,N},\quad \textit{for all } v\notin\mathcal{O}_{x_i}.$$

In particular,

$$\mathcal{O}_{x_i}\ \supset\bigcup_{x\in B(x_i;r_i)}\{v\in B_N:|v\cdot n(x_{\mathbf{b}}(x,v))|\leq\delta_{\varepsilon,N}\}. \tag{121}$$

Proof. The details of the proof are recorded in [75]. The proof of (120) is due to Sard's theorem : For fixed $x\in\bar{\Omega}$ we consider the following mapping

$$\phi_x:\partial\Omega\to\mathbb{S}^2,\quad \phi_x:y\in\partial\Omega\mapsto-\frac{y-x}{|y-x|}.$$

If $n(x_{\mathbf{b}}(x,v))\cdot v=0$ then $\frac{v}{|v|}$ is a critical value of ϕ_x at $y=x_{\mathbf{b}}(x,v)$. Then by Sard's theorem the Lebesgue measure of such set on $\mathbb{S}^2$ is zero.

Now we fix $0<\varepsilon\ll 1$ and $x\in\bar{\Omega}$. Due to (120) there exists an open set $\mathcal{O}_x\in\mathbb{R}^3$ such that $\mathrm{m}_3(\mathcal{O}_x)<\varepsilon$ and $|v\cdot n(x_{\mathbf{b}}(x,v))|\neq 0$ for $v\notin\mathcal{O}_x$. By Lemma .6, $v\mapsto v\cdot n(x_{\mathbf{b}}(x,v))$ is smooth on the compact set $\{\mathbb{R}^3\backslash\mathcal{O}_x\}\cap B_N$. Then by the compactness we have a positive lower bound $2\delta_{\varepsilon,N,x}>0$ of $|v\cdot n(x_{\mathbf{b}}(x,v))|$. Then by Lemma .6 again, there exists a ball $B(x;r_x)$ such that for all y in this ball and all $v\in\{\mathbb{R}^3\backslash\mathcal{O}_x\}\cap B_N$ we have $|v\cdot n(x_{\mathbf{b}}(y,v))|\geq\delta_{\varepsilon,N,x}$. Then we use the compactness of $\bar{\Omega}$ to extract the finite covering which satisfies (121). $\square$

Lemma .10 (Lemma 5 of [77]). *For any smooth function $g = g(x,v)$ and $\partial \in \{\nabla_x, \nabla_v\}$ and $0 < \theta < \frac{1}{4}$,*

$$\begin{aligned} \|\partial \Gamma_{\text{gain}}(g,g)\|_1 &\lesssim \|e^{\theta|v|^2} g\|_\infty \Big\{ |\partial x| \|\nabla_x g\|_1 + |\partial v| \|\nabla_v g\|_1 \Big\} + \langle v \rangle^\kappa e^{-\theta|v|^2} |\partial v| \|e^{\theta|v|^2} g\|_\infty^2, \\ \iint_{\Omega\times\mathbb{R}^3} |\nu(\partial[\sqrt{\mu} g]) g| \mathrm{d}v\mathrm{d}x &\lesssim \|e^{\theta|v|^2} g\|_\infty \int_\Omega \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} e^{-\frac{\theta}{4}|v-u|^2} |\partial g(u)| \mathrm{d}u\mathrm{d}v\mathrm{d}x \lesssim \|e^{\theta|v|^2} g\|_\infty \|\partial g\|_1. \end{aligned}$$

Appendix 2. $\mathfrak{S}_\mathrm{B}$ is a Co-Dimension 1 subset

We prove **Remark 1**. It suffices to show that $\mathfrak{S}_\mathrm{B} \cap \bar{\Omega} \times \mathbb{R}^3$ is a co-dimension 1 submanifold of $\bar{\Omega} \times \mathbb{R}^3$. More precisely we will show that if $(x_0, v_0) \in \Omega \times \mathbb{R}^3$ satisfies $n(x_{\mathbf{b}}(x_0, v_0)) \cdot v_0 = 0$ and the boundary is strictly non-convex (8.10) at $(x_{\mathbf{b}}(x_0,v_0), v_0)$ then there exists $0 < \varepsilon \ll 1$ such that the following set is a 5 dimensional submanifold :

$$\big\{ (x,v) \in \mathfrak{S}_\mathrm{B} \cap B((x_0,v_0);\varepsilon) : x_{\mathbf{b}}(x,v) \sim x_{\mathbf{b}}(x_0,v_0) \big\} \subset \bar{\Omega} \times \mathbb{R}^3. \tag{122}$$

Without loss of generality we may assume $x_{\mathbf{b}}(x_0,v_0) = (0,0,0) = \mathbf{0}$ and $v_0 = \mathbf{e}_1$ and $n(0,0,0) = -\mathbf{e}_3$ so that $\partial\Omega$ is locally a graph of a function $\eta : \mathbb{R}^2 \to \mathbb{R}$ and $\nabla \eta(0,0) = \mathbf{0}$. Therefore the strictly non-convex condition (8.10) at $(x_{\mathbf{b}}(x_0,v_0), v_0) = (\mathbf{0}, \mathbf{e}_1)$ implies

$$\partial_1 \partial_1 \eta(0,0) \neq 0. \tag{123}$$

Clearly, (122) is contained in

$$\big\{ (x+sv, v) \in \bar{\Omega} \times \mathbb{R}^3 : x \in \partial\Omega,\ n(x)\cdot v = 0,\ (x,v) \sim (x_0,v_0),\ s \in [0,\infty) \big\}. \tag{124}$$

Consider $(x,v) \sim (x_0,v_0)$. We choose a basis for the tangent space :

$$\begin{aligned} \tau_1 &= \frac{1}{\sqrt{1+|\nabla\eta|^2}} \begin{pmatrix} 1 \\ 0 \\ \partial_1 \eta \end{pmatrix}, \\ \tau_2 &= \frac{1}{\sqrt{1+|\nabla\eta|^2}\sqrt{1+(\partial_1\eta)^2}} \begin{pmatrix} -\partial_1\eta\partial_2\eta \\ 1 + (\partial_1\eta)^2 \\ \partial_2\eta \end{pmatrix}. \end{aligned}$$

For $(x_1, x_2, \theta, r_v, s) \in \mathbb{R}^2 \times [0,2\pi) \times [0,\infty) \times [0,\infty)$ we write $(x+sv, v)$ in (124) as

$$\begin{aligned} X(x_1,x_2,\theta,r_v,s) &:= \begin{pmatrix} x_1 \\ x_2 \\ \eta(x_1,x_2) \end{pmatrix} + sr_v \cos\theta\ \tau_1(x_1,x_2) + sr_v \sin\theta\ \tau_2(x_1,x_2), \\ V(x_1,x_2,\theta,r_v,s) &:= r_v \cos\theta\ \tau_1(x_1,x_2) + r_v \sin\theta\ \tau_2(x_1,x_2). \end{aligned}$$

In order to prove Remark 1 it suffices to show that the followings are linearly independent

$$\begin{pmatrix} \partial_{x_1} X \\ \partial_{x_1} V \end{pmatrix}, \begin{pmatrix} \partial_{x_2} X \\ \partial_{x_2} V \end{pmatrix}, \begin{pmatrix} \partial_\theta X \\ \partial_\theta V \end{pmatrix}, \begin{pmatrix} \partial_s X \\ \partial_s V \end{pmatrix}, \begin{pmatrix} \partial_{r_v} X \\ \partial_{r_v} V \end{pmatrix} \in \mathbb{R}^6.$$

It suffices to show that the normal is non-vanishing :

$$\mathcal{N} := \det \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 & \mathbf{e}_4 & \mathbf{e}_5 & \mathbf{e}_6 \\ \partial_{x_1} X_1 & \partial_{x_1} X_2 & \partial_{x_1} X_3 & \partial_{x_1} V_1 & \partial_{x_1} V_2 & \partial_{x_1} V_3 \\ \partial_{x_2} X_1 & \partial_{x_2} X_2 & \partial_{x_2} X_3 & \partial_{x_2} V_1 & \partial_{x_2} V_2 & \partial_{x_2} V_3 \\ \partial_\theta X_1 & \partial_\theta X_2 & \partial_\theta X_3 & \partial_\theta V_1 & \partial_\theta V_2 & \partial_\theta V_3 \\ \partial_s X_1 & \partial_s X_2 & \partial_s X_3 & 0 & 0 & 0 \\ \partial_{r_v} X_1 & \partial_{r_v} X_2 & \partial_{r_v} X_3 & \partial_{r_v} V_1 & \partial_{r_v} V_2 & \partial_{r_v} V_3 \end{pmatrix}.$$

To compute the normal we need to know

$$\partial_1\tau_1(x_1,x_2) = \frac{\partial_1^2\eta}{[1+(\nabla\eta)^2]^{3/2}}\begin{pmatrix} -\partial_1\eta \\ 0 \\ 1 \end{pmatrix} + \frac{\partial_2\eta}{[1+(\nabla\eta)^2]^{3/2}}\begin{pmatrix} 0 \\ 0 \\ \partial_2\eta\partial_1^2\eta - \partial_1\eta\partial_1\partial_2\eta \end{pmatrix},$$

$$\partial_2\tau_1(x_1,x_2) = \frac{1}{[1+(\nabla\eta)^2]^{1/2}}\begin{pmatrix} 0 \\ 0 \\ \partial_1\partial_2\eta \end{pmatrix} - \frac{1}{[1+(\nabla\eta)^2]^{3/2}}\begin{pmatrix} \nabla\eta\cdot\nabla\partial_2\eta \\ 0 \\ \partial_1\eta\nabla\eta\cdot\nabla\partial_2\eta \end{pmatrix},$$

$$\begin{aligned}
\partial_1(\tau_2)_1 &= \frac{(\partial_1\eta)^2\partial_2\eta\partial_1^2\eta}{[1+(\partial_1\eta)^2]^{3/2}[1+|\nabla\eta|^2]^{1/2}} + \frac{(\partial_1\eta)^2\partial_2\eta\partial_1^2\eta + \partial_1\eta(\partial_2\eta)^2\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{3/2}} \\
&\quad - \frac{\partial_1^2\eta\partial_2\eta + \partial_1\eta\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}}, \\
\partial_2(\tau_2)_1 &= \frac{\partial_1\eta\partial_2\eta\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{3/2}[1+|\nabla\eta|^2]^{1/2}} + \frac{(\partial_1\eta)^2\partial_2\eta\partial_1\partial_2\eta + \partial_1\eta(\partial_2\eta)^2\partial_2^2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{3/2}} \\
&\quad - \frac{\partial_1\partial_2\eta\partial_2\eta + \partial_1\eta\partial_2^2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}}, \\
\partial_1(\tau_2)_2 &= \frac{\partial_1\eta\partial_1^2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}} - \frac{[1+(\partial_1\eta)^2]^{1/2}[\partial_1\eta\partial_1^2\eta + \partial_2\eta\partial_1\partial_2\eta]}{[1+|\nabla\eta|^2]^{3/2}}, \\
\partial_2(\tau_2)_2 &= \frac{\partial_1\eta\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}} - \frac{[1+(\partial_1\eta)^2]^{1/2}[\partial_1\eta\partial_1\partial_2\eta + \partial_2\eta\partial_2^2\eta]}{[1+|\nabla\eta|^2]^{3/2}}, \\
\partial_1(\tau_2)_3 &= -\frac{\partial_1\eta\partial_2\eta\partial_1^2\eta}{[1+(\partial_1\eta)^2]^{3/2}[1+|\nabla\eta|^2]^{1/2}} - \frac{\partial_1\eta\partial_2\eta\partial_1^2\eta + (\partial_2\eta)^2\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{3/2}} \\
&\quad + \frac{\partial_1\partial_2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}}, \\
\partial_2(\tau_2)_3 &= -\frac{\partial_1\eta\partial_2\eta\partial_2^2\eta}{[1+(\partial_1\eta)^2]^{3/2}[1+|\nabla\eta|^2]^{1/2}} - \frac{\partial_1\eta\partial_2\eta\partial_1\partial_2\eta + (\partial_2\eta)^2\partial_2^2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{3/2}} \\
&\quad + \frac{\partial_2^2\eta}{[1+(\partial_1\eta)^2]^{1/2}[1+|\nabla\eta|^2]^{1/2}}.
\end{aligned}$$

We evaluate the normal at $(x_1,x_2,\theta,s,r_v) = (0,0,0,s,r_v)$. Since $\partial_1\eta(0,0) = 0 = \partial_2\eta(0,0)$,

$$\begin{aligned}
&n(0,0) = \mathbf{e}_3, \quad \tau_1(0,0) = \mathbf{e}_1, \quad \tau_2(0,0) = \mathbf{e}_2, \\
&\partial_1\tau_1(0,0) = \partial_1\partial_1\eta(0,0)\mathbf{e}_3, \quad \partial_2\tau_1(0,0) = \partial_1\partial_2\eta(0,0)\mathbf{e}_3, \\
&\partial_1\tau_2(0,0) = \partial_1\partial_2\eta(0,0)\mathbf{e}_3, \quad \partial_2\tau_2(0,0) = \partial_2\partial_2\eta(0,0)\mathbf{e}_3.
\end{aligned}$$

Due to (123) we have

$$\mathcal{N}(0,0,0,s,r_v) = \det\begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 & \mathbf{e}_4 & \mathbf{e}_5 & \mathbf{e}_6 \\ 1 & 0 & -s\partial_1\partial_1\eta & 0 & 0 & -r_v\partial_1\partial_1\eta \\ 0 & 1 & -s\partial_1\partial_2\eta & 0 & 0 & -r_v\partial_1\partial_2\eta \\ 0 & s & 0 & 0 & r_v & 0 \\ r_v & 0 & 0 & 0 & 0 & 0 \\ s & 0 & 0 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ r_v^2\partial_1\partial_1\eta(0,0) \\ 0 \\ 0 \\ sr_v\partial_1\partial_1\eta(0,0) \end{pmatrix} \neq 0.$$

Therefore $\mathcal{N}(x_1,x_2,\theta,s,r_v) \neq 0$ for $(x_1,x_2,\theta) \sim (0,0,0)$. This proves the claim.

Quatrième partie

Annexe

Annexe A

The Boltzmann equation in convex domains with specular and bounce-back boundary conditions

Abstract

This Chapter is the sequel of Chapter 7. Put together, their contents form the paper [77] in collaboration with Y. Guo, C. Kim and D. Tonon. The basic question of the regularity of the solution of the Boltzmann equation in the presence of physical boundary conditions has long been open due to two effects in competition : on the one hand, the characteristic nature of the boundary ; on the other hand, the non-local mixing of the collision operator. We consider the Boltzmann equation in a strictly convex domain with the specular and bounce-back boundary conditions. As for the diffuse reflexion case, we use a distance function towards the grazing boundary to construct classical C^1 solutions away from the grazing boundary. To complete the theory, we show that second derivatives do not exist up to the boundary in general by constructing counterexamples for both boundary conditions.

Sommaire

A.1 Introduction

This text is the sequel of Chapter 7. As in Chapter 7, consider the Boltzmann equation

$$\partial_t F + v \cdot \nabla_x F = Q(F, F), \tag{A.1}$$

with the collisional operator

$$\begin{aligned} Q(F_1, F_2) &:= Q_{\text{gain}}(F_1, F_2) - Q_{\text{loss}}(F_1, F_2) \\ &= \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} |v-u|^\kappa q_0(\theta) \Big[F_1(u')F_2(v') - F_1(u)F_2(v) \Big] \mathrm{d}\omega \mathrm{d}u, \end{aligned} \tag{A.2}$$

where $u' = u + [(v-u)\cdot\omega]\omega$, $v' = v - [(v-u)\cdot\omega]\omega$ and $0 \le \kappa \le 1$ (hard potential) and $0 \le q_0(\theta) \le C|\cos\theta|$ (angular cutoff) with $\cos\theta = \frac{v-u}{|v-u|} \cdot \omega$.

Throughout this paper we assume that Ω is a bounded open subset of $\mathbb{R}^3$ and there exists $\xi : \mathbb{R}^3 \to \mathbb{R}$ such that $\Omega = \{x \in \mathbb{R}^3 : \xi(x) < 0\}$, and $\partial\Omega = \{x \in \mathbb{R}^3 : \xi(x) = 0\}$. Moreover for all $x \in \bar{\Omega} = \Omega \cup \partial\Omega$ (therefore $\xi(x) \le 0$) we assume the domain is *strictly convex* :

$$\sum_{i,j} \partial_{ij}\xi(x)\zeta_i\zeta_j \ge C_\xi |\zeta|^2 \quad \text{for all} \quad \zeta \in \mathbb{R}^3. \tag{A.3}$$

We assume that $\nabla\xi(x) \ne 0$ when $|\xi(x)| \ll 1$ and we define the *outward normal* as $n(x) \equiv \frac{\nabla\xi(x)}{|\nabla\xi(x)|}$.

In Chapter 7, we focused on the diffuse boundary condition

(i) Diffuse boundary condition : Let $c_\mu \int_{n(x)\cdot u>0} \mu(u)\{n(x)\cdot u\}\mathrm{d}u = 1$,

$$F(t,x,v) = c_\mu \mu(v) \int_{n(x)\cdot u>0} F(t,x,u)\{n(x)\cdot u\}\mathrm{d}u.$$

We here consider the two other basic boundary conditions on $(x,v) \in \gamma_-$:

(ii) Specular reflection boundary condition :

$$F(t,x,v) = F(t,x,R_x v), \qquad \text{where } R_x v := v - 2n(x)(n(x)\cdot v).$$

(iii) Bounce-back reflection boundary condition :

$$F(t,x,v) = F(t,x,-v).$$

For $(x,v) \in \bar{\Omega} \times \mathbb{R}^3$ recall *the backward exit time* $t_{\mathbf{b}}(x,v)$ defined as

$$t_{\mathbf{b}}(x,v) = \inf\{\tau > 0 : x - sv \notin \Omega\}, \tag{A.4}$$

and $x_{\mathbf{b}}(v) = x - t_{\mathbf{b}} v$.

The characteristics ODE of the Boltzmann equation (A.1) is

$$\frac{\mathrm{d}X(s)}{\mathrm{d}s} = V(s), \quad \frac{\mathrm{d}V(s)}{\mathrm{d}s} = 0.$$

Before the trajectory hits the boundary, $t - s < t_{\mathbf{b}}(x,v)$, we have $[X(s;t,x,v), V(s;t,x,v)] = [x - (t-s)v, v]$ with the initial condition $[X(t;t,x,v), V(t;t,x,v)] = [x,v]$. On the other hand, when the trajectory hits the boundary we define the generalized characteristics as follows :

Definition A.1 ([75]). *Let $(x,v) \notin \gamma_0$ and $(t^0, x^0, v^0) = (t,x,v)$.*

(i) Define the stochastic (diffuse) cycles : see Chapter 7.

(ii) Define the specular cycles, $\ell \ge 1$,

$$(t^{\ell+1}, x^{\ell+1}, v^{\ell+1}) = (t^\ell - t_{\mathbf{b}}(x^\ell, v^\ell), x_{\mathbf{b}}(x^\ell, v^\ell), v^\ell - 2n(x^\ell)(v^\ell \cdot n(x^\ell))).$$

(iii) Define the bounce-back cycles, $\ell \ge 1$,

$$(t^{\ell+1}, x^{\ell+1}, v^{\ell+1}) = (t^\ell - t_{\mathbf{b}}(x^\ell, v^\ell), x_{\mathbf{b}}(x^\ell, v^\ell), -v^\ell).$$

Then for $\ell \geq 1$

$$t^{\ell} = t^1 - (\ell-1)t_{\mathbf{b}}(x^1, v^1), \quad x^{\ell} = \frac{1-(-1)^{\ell}}{2}x^1 + \frac{1+(-1)^{\ell}}{2}x^2, \quad v^{\ell+1} = (-1)^{\ell+1}v.$$

(iv) We define the backward trajectory as

$$X_{\mathbf{cl}}(s;t,x,v) \;=\; \sum_{\ell} \mathbf{1}_{[t^{\ell+1},t^{\ell})}(s)\big\{x^{\ell} - (t^{\ell}-s)v^{\ell}\big\}, \quad V_{\mathbf{cl}}(s;t,x,v) \;=\; \sum_{\ell} \mathbf{1}_{[t^{\ell+1},t^{\ell})}(s)v^{\ell}.$$

Note that if $G(t,x,v)$ solves $\partial_t G + v \cdot \nabla_x G = 0$ with a boundary condition (either diffuse, specular, or bounce-back boundary condition) then

$$G(t,x,v) = G(s, X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)),$$

where $[X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)]$ is defined respectively([75]).

In this paper we establish the first C^1 regularity away from the grazing set γ_0 for Boltzmann solutions in convex domains. This is achieved thanks to the distance function towards the grazing set γ_0 α, whose definition is recalled below.

Definition A.2 (Kinetic Distance)**.** *For* $(x,v) \in \bar{\Omega} \times \mathbb{R}^3$,

$$\alpha(x,v) := |v \cdot \nabla\xi(x)|^2 - 2\{v \cdot \nabla^2\xi(x) \cdot v\}\xi(x).$$

Due to (A.3), the kinetic distance $\alpha(x,v)$ vanishes if and only if $(x,v) \in \gamma_0$. The important technique to treat α along the trajectory is based on the geometric lemma :

Lemma A.1 (Velocity lemma, Lemma 1 of [75])**.** *Along the backward trajectory we define*

$$\alpha(s;t,x,v) := \alpha(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)).$$

Then there exists $\mathcal{C} = \mathcal{C}(\xi) > 0$ *such that, for all* $0 \leq s_1, s_2 \leq t$,

$$e^{-\mathcal{C}|v||s_1-s_2|}\alpha(s_1;t,x,v) \;\leq\; \alpha(s_2;t,x,v) \;\leq\; e^{\mathcal{C}|v||s_1-s_2|}\alpha(s_1;t,x,v).$$

The proof of Lemma A.1 is performed in Chapter 7.

This crucial invariant property of α under operator $v \cdot \nabla_x$ is the key for our analysis. On the other hand, unless $\nabla^3\xi \equiv 0$ (for example the domain is a ball or an ellipsoid), a growth factor $|v|$ creates a geometric effect which is out of control for our analysis. To overcome such a geometric effect, we introduce a strong decay factor $e^{-\varpi\langle v\rangle t}$ with sufficiently large $\varpi > 0$ (see Chapter 7 for details) :

$$\varpi > \max \frac{2v\{v \cdot \nabla^3\xi(x) \cdot v\}\xi}{\alpha\langle v\rangle}. \tag{A.5}$$

Remark that if ξ is quadratic (for example if the domain is a ball or an ellipsoid) then we are able to set $\varpi = 0$ and $\{\partial_t + v \cdot \nabla_x\}\alpha \equiv 0$.

We denote $F = \sqrt{\mu}f$ (f could be large) where $\mu = e^{-\frac{|v|^2}{2}}$ is a global normalized Maxwellian. Then f satisfies

$$\partial_t f + v \cdot \nabla_x f = \Gamma_{\text{gain}}\,(f,f) - \nu(\sqrt{\mu}f)f. \tag{A.6}$$

Here

$$\begin{aligned} \nu(\sqrt{\mu}f)(v) = \nu(F)(v) &:= \frac{1}{\sqrt{\mu(v)}}Q_{\text{loss}}(\sqrt{\mu}f, \sqrt{\mu}f)(v) \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-u,\omega)\sqrt{\mu(u)}f(u)\mathrm{d}\omega\mathrm{d}u, \end{aligned} \tag{A.7}$$

and the gain term of the nonlinear Boltzmann operator is given by

$$\begin{aligned} \Gamma_{\text{gain}}(f_1,f_2)(v) &:= \frac{1}{\sqrt{\mu}}Q_{\text{gain}}(\sqrt{\mu}f_1, \sqrt{\mu}f_2)(v) \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-u,\omega)\sqrt{\mu(u)}f_1(u')f_2(v')\mathrm{d}\omega\mathrm{d}u. \end{aligned} \tag{A.8}$$

The corresponding boundary conditions for f are followings :

(i) Diffuse boundary condition :

$$f(t,x,v) = c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f(t,x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \quad \text{on } \gamma_-. \tag{A.9}$$

(ii) Specular reflection boundary condition :

$$f(t,x,v) = f(t,x,R_x v), \quad \text{on } \gamma_-. \tag{A.10}$$

(iii) Bounce-back reflection boundary condition :

$$f(t,x,v) = f(t,x,-v), \quad \text{on } \gamma_-. \tag{A.11}$$

We denote $||\cdot||_p$ the $L^p(\Omega\times\mathbb{R}^3)$ norm, while $|\cdot|_{\gamma,p}$ is the $L^p(\partial\Omega\times\mathbb{R}^3;\mathrm{d}\gamma)$ norm and $|\cdot|_{\gamma_\pm,p} = |\cdot\mathbf{1}_{\gamma_\pm}|_{\gamma,p}$ where $\mathrm{d}\gamma = |n(x)\cdot v|\mathrm{d}S_x\mathrm{d}v$ with the surface measure $\mathrm{d}S_x$ on $\partial\Omega$. Denote $\langle v\rangle = \sqrt{1+|v|^2}$. We define

$$\partial_t f(0) = \partial_t f_0 \equiv -v\cdot\nabla_x f_0 + \Gamma_{\text{gain}}(f_0,f_0) - \nu(\sqrt{\mu}f_0)f_0. \tag{A.12}$$

Throughout this paper we always assume

$$F_0 = \sqrt{\mu}f_0 \geq 0.$$

A.1.1 Diffuse Reflection BC

For completeness of the C^1 theory, we briefly recall the result of C^1 propagation in the case of the diffuse reflection boundary condition.

Theorem A.1. *Assume the compatibility condition*

$$f_0(x,v) = c_\mu\sqrt{\mu(v)}\int_{n(x)\cdot u>0} f_0(x,u)\sqrt{\mu(u)}\{n(x)\cdot u\}\mathrm{d}u, \tag{A.13}$$

and $0<\kappa\leq 1$ *and recall (A.12). If* $||\alpha^{1/2}\nabla_{x,v}f_0||_\infty + ||e^{\theta|v|^2}f_0||_\infty < +\infty$ *for some* $0<\theta<\frac{1}{4}$*, then* $e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v}f \in L^\infty([0,T];L^\infty(\Omega\times\mathbb{R}^3))$ *such that for all* $0\leq t\leq T$*,*

$$||e^{-\varpi\langle v\rangle t}\alpha^{1/2}\nabla_{x,v}f(t)||_\infty \lesssim_t ||\alpha^{1/2}\nabla_{x,v}f_0||_\infty + P(||e^{\theta|v|^2}f_0||_\infty).$$

If $\alpha^{1/2}\nabla f_0 \in C^0(\bar{\Omega}\times\mathbb{R}^3)$ *and*

$$v\cdot\nabla_x f_0 - \Gamma(f_0,f_0) = c_\mu\sqrt{\mu}\int_{n\cdot u>0}\big\{u\cdot\nabla_x f_0 - \Gamma(f_0,f_0)\big\}\sqrt{\mu}\{n\cdot u\}\mathrm{d}u, \tag{A.14}$$

is valid for $\gamma_-\cup\gamma_0$*, then* $f\in C^1$ *away from the grazing set* γ_0*.*

Furthermore, if $F_0 = \mu+\sqrt{\mu}g_0$ *with* $||e^{\theta|v|^2}g_0||_\infty \ll 1$*, then the theorem holds with* $\nabla_x g(t)$ *and* $\nabla_v g(t)$ *for all* $t\geq 0$*.*

There can be no size restriction on initial data $F_0 = \sqrt{\mu}f_0$. On the other hand, we also remark that from [75, 67], the assumption $||e^{\theta|v|^2}g_0||_\infty \ll 1$ for $F_0 = \mu+\sqrt{\mu}g_0$ without a mass constraint $\iint_{\Omega\times\mathbb{R}^3} g_0\sqrt{\mu}\mathrm{d}v\mathrm{d}x = 0$ ensures a uniform-in-time bound as $\sup_{0\leq t\leq\infty}||e^{\theta|v|^2}g(t)||_\infty \lesssim ||e^{\theta|v|^2}g_0||_\infty$ (not a decay).

We refer to Chapter 7 for an explanation of the main ideas, results of Sobolev regularity propagation, and proofs.

A.1.2 Dynamical non-local to local estimates

As in the diffuse case, the analysis relies on the following dynamical non-local to local estimates.

Lemma A.2. *Let* $(t,x,v)\in[0,\infty)\times\bar{\Omega}\times\mathbb{R}^3$ *and* $\frac{1}{2}<\beta<\frac{3}{2}$ *and* $0<\kappa\leq 1$ *and* $r\in\mathbb{R}$ *and* $Z(s,x,v)\geq 0$*.*

(1) Let $X_{\mathbf{cl}}(s;t,x,v) = x-(t-s)v$ *on* $s\in[t-t_{\mathbf{b}}(x,v),t]$*.*

For any $\varepsilon > 0$, there exist $l \gg_\xi 1$ such that

$$\begin{aligned}
&\int_{t-t_{\mathbf{b}}(x,v)}^{t}\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)]^{\beta}}\frac{\langle u\rangle^r}{\langle v\rangle^r}Z(s,x,v)\mathrm{d}u\mathrm{d}s\\
\lesssim\ &\min\left\{\frac{\varepsilon^{\frac{3}{2}-\beta}}{|v|^2\{\alpha(x,v)\}^{\beta-1}},\frac{\{\alpha(x,v)\}^{\frac{1}{4}-\frac{\beta}{2}}|t_Z|^{\frac{3}{2}-\beta}}{|v|^{2\beta-1}}\right\}\sup_{s\in[t-t_{\mathbf{b}}(x,v),t]}\{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\}\\
&+\frac{C_\varepsilon}{\{\alpha(x,v)\}^{\beta-1/2}}\int_{t-t_{\mathbf{b}}(x,v)}^{t}e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s,
\end{aligned}\tag{A.15}$$

where $t_Z = \sup\{s : Z(s,x,v) \neq 0\}$.

(2) Let $[X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)]$ be the specular backward trajectory or the bounce-back trajectory in Definition A.1.

For any $\varepsilon > 0$, there exist $l \gg_\xi 1$ such that

$$\begin{aligned}
&\int_0^t\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|V_{\mathbf{cl}}(s;t,x,v)-u|^2}}{|V_{\mathbf{cl}}(s;t,x,v)-u|^{2-\kappa}}\frac{\langle u\rangle^r}{\langle v\rangle^r}\frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^{\beta}}\mathrm{d}u\mathrm{d}s\\
\lesssim\ &\frac{O(\varepsilon)}{\langle v\rangle\big[\alpha(x,v)\big]^{\beta-1/2}}\sup_{0\le s\le t}\big\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\big\}.
\end{aligned}\tag{A.16}$$

Again, see 7 for mains ideas. Recall that our estimates not only retain the local structure for α, but they *gain* $\sqrt{\alpha}$ order of regularity. Such a precise gain of regularity is exactly enough to balance out the singularity in α appeared in $\partial X_{\mathbf{cl}}(s;t,x,v)$ and $\partial V_{\mathbf{cl}}(s;t,x,v)$ in both the specular and bounce-back cycles.

A.1.3 Specular Reflection BC

Recall the specular reflection boundary condition in (A.10) and the specular cycles in Definition A.1. Our main theorem is as follow.

Theorem A.2. *Assume $F_0 = \sqrt{\mu}f_0 \geq 0$ and $f_0 \in W^{1,\infty}(\Omega\times\mathbb{R}^3)$ and $0<\kappa\leq 1$ for $1<\beta<\frac{3}{2}$, $0<\theta<\frac{1}{4}$, and $b\in\mathbb{R}$,*

$$||\frac{\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_x f_0||_\infty + ||\frac{|v|^2\alpha^{\beta-1}}{\langle v\rangle^b}\partial_v f_0||_\infty + ||e^{\theta|v|^2}f_0||_\infty < \infty,$$

and the compatibility condition

$$f_0(x,v) = f_0(x,R_xv) \quad \text{on } (x,v)\in\gamma_-. \tag{A.17}$$

Then for all $0\le t\le T$ with $T = T(||e^{\theta|v|^2}f_0||_\infty) > 0$

$$\begin{aligned}
&||e^{-\varpi\langle v\rangle t}\frac{\alpha^\beta}{\langle v\rangle^{b+1}}\partial_x f(t)||_\infty + ||e^{-\varpi\langle v\rangle t}\frac{|v|\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_v f(t)||_\infty\\
\lesssim_{\xi,t}\ &||\frac{\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_x f_0||_\infty + ||\frac{|v|^2\alpha^{\beta-1}}{\langle v\rangle^b}\partial_v f_0||_\infty + P(||\partial_t f_0||_\infty) + P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}\tag{A.18}$$

Moreover, if Ω is real analytic (ξ is real analytic on $\mathbb{R}^3$) and $F_0 = \mu+\sqrt{\mu}g_0 \geq 0$ with $||e^{\theta|v|^2}g_0||_\infty \ll 1$ then this theorem holds for the arbitrarily large time $t\geq 0$.

Furthermore, if $f_0 \in C^1$ and

$$v\cdot\nabla_x f_0(x,v) = R_xv\cdot\nabla_x f_0(x,R_xv) \quad \text{on } (x,v)\in\gamma_-. \tag{A.19}$$

then $f\in C^1$ away from the grazing set γ_0.

There can be no size restriction on initial data $F_0 = \sqrt{\mu}f_0$. We remark from the local existence theorem, $T>0$. The analyticity is a crucial assumption to ensure global stability in [75]. We also remark that the specular theorem is drastically different from the diffusive theorem : in addition to the loss of moments, there is a loss of regularity of α with respect to the initial data. This makes it impossible to use the continuity argument to choose small time interval to close the estimates. We need to use large

ϖ in $e^{-\varpi\langle v\rangle t}$ to extract a small constant to close, which requires extra precise estimates. We note that in 3D case, $\beta > 1/2$, due to the failure of the proof of the non-local to local estimates for the critical $\beta = 1/2$(Lemma A.2). On the other hand, in 2D, due to boundedness of $\partial_{v_3} f$ from x_3-invariance, we are able to estimate $\partial_v \Gamma_{\text{gain}}$ for the critical case $\beta = 1/2$ by Lemma A.12.

In additional to the dynamical non-local to local estimate, the second important ingredient for the specular reflection BC is the following crucial estimate for the derivatives of specular cycles $[X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)]$.

Theorem A.3. *There exists $C = C(\Omega) > 0$ such that for all $(s;t,x,v) \in \mathbb{R}\times\mathbb{R}\times\bar{\Omega}\times\mathbb{R}^3$ with $s \neq t^\ell$ for $\ell = 1,2,\cdots,\ell_*$*

$$
\begin{aligned}
|\partial_x X_{\mathbf{cl}}(s;t,x,v)| &\lesssim e^{C|v|(t-s)}\frac{|v|}{\sqrt{\alpha(x,v)}},\\
|\partial_v X_{\mathbf{cl}}(s;t,x,v)| &\lesssim e^{C|v|(t-s)}\frac{1}{|v|},\\
|\partial_x V_{\mathbf{cl}}(s;t,x,v)| &\lesssim e^{C|v|(t-s)}\frac{|v|^3}{\alpha(x,v)},\\
|\partial_v V_{\mathbf{cl}}(s;t,x,v)| &\lesssim e^{C|v|(t-s)}\frac{|v|}{\sqrt{\alpha(x,v)}}.
\end{aligned}
\tag{A.20}
$$

Our estimates are optimal in terms of the order of $\frac{1}{\alpha}$, and $e^{C|v|(t-s)}$ relates to the $|v|$ growth in the Velocity lemma (Lemma A.1). We remark that these precise orders of singularity, play a critical role for our design of the anisotropic norms in Theorem A.2. In fact, if $|\partial_x X_{\mathbf{cl}}(s;t,x,v)| \backsim \frac{1}{\alpha}$, it would have been too singular for the half power gain of α from the dynamical non-local to local estimates (Lemma A.2), and our method should fail. Moreover, it is also crucial to have precise $|v|$ growth in both $|\partial_x X_{\mathbf{cl}}(s;t,x,v)|$ and $|\partial_x V_{\mathbf{cl}}(s;t,x,v)|$ to be controlled by $e^{-\varpi\langle v\rangle t}$.

We remark that $|\partial_x X_{\mathbf{cl}}(s;t,x,v)| \backsim \frac{1}{\sqrt{\alpha}}$ is unexpected, even after one bounce we would have $\partial_x x^1 \backsim \frac{1}{\sqrt{\alpha}}$ and it is natural to expect $\partial_x X_{\mathbf{cl}}(s;t,x,v)$ picks up additional power of $\frac{1}{\sqrt{\alpha}}$ in the accumulation of $\frac{1}{\sqrt{\alpha}}$ number of bounces. However, via direct computations in 2D disk, we discover that even though

$$\partial_x t^\ell \backsim \frac{1}{\alpha}, \text{ and } \partial_x x^\ell \backsim \frac{1}{\alpha},$$

but surprisingly

$$\partial_x X_{\mathbf{cl}}(s;t,x,v) = \partial_x[x^\ell - (t^\ell - s)v^\ell] \backsim \frac{1}{\sqrt{\alpha}}\ !$$

Clearly, certain cancellations take place in the disk, which is difficult to even expect for general domains.

The proof of our theorem is split into 10 steps, and it is the most delicate proof throughout this paper. We first remark that, due to the 'discontinuous behaviors' of the normal component of $v\cdot n$ at each specular reflection, it is impossible to apply the standard techniques for ODE to estimate $|\partial X_{\mathbf{cl}}(s;t,x,v)|$ and $|\partial V_{\mathbf{cl}}(s;t,x,v)|$. We have to develop different strategies to overcome several analytical difficulties to finally complete the proof.

Topological obstruction and moving frames. It turns out that we only need to consider the most delicate case in which all the bounces are almost grazing and staying near the boundary for $\mathbf{r}^\ell = \frac{|v^\ell\cdot n|}{|v^\ell|} \ll 1$. It is important for us to introduce the spherical co-ordinate system to cover the whole cycle and transform it into the ODE (A.57). Unfortunately, due to the 'hair-ball' theorem in Topology, such a change of coordinate system (or any change of coordinates) can not be smooth everywhere in the 2D surface $\partial\Omega$. In the case of a ball, all the trajectories are confined in a plane, so that one may choose a single chart to cover the whole trajectories. However, in other convex domains except the ball case, with large t, the specular trajectories are extremely complicated, which can reach almost every point on $\partial\Omega$. Hence, choosing a single chart is all but impossible. On the other hand, a 'sudden' change of a chart may create new order of singularity of α from the matrix $\mathcal{P}$ as in (A.98), which will ruin the estimates. It is therefore important to design a 'continuous' changes of charts associated with the almost grazing bounces. Given $n(x)$, we need to construct another globally defined, orthogonal, and continuous vector field. This would have been impossible if we were to seek it only in the physical space, in light of the 'hair-ball' theorem. The key observation is that, we need continuity not from just $\partial\Omega$, but from the phase space $\partial\Omega\times\mathbb{R}^3$. In fact, for almost grazing bounces, the velocity field v is almost perpendicular to $n(x)$, which provides a natural choice for construction of the desired moving frames. These continuous moving frames cost manageable errors for each bounce, which are controlled by the next method.

Matrix Method for normal parts of $\partial X_{\mathbf{cl}}(s)$ and $\partial V_{\mathbf{cl}}(s)$. With such a well-defined moving charts, via the chain rule, one can represent $\partial X_{\mathbf{cl}}(s;t,x,v)$ and $\partial V_{\mathbf{cl}}(s;t,x,v)$ via a multiplication of Jacobian matrices $(t^\ell, x^\ell, v^\ell) \to (t^{\ell-1}, x^{\ell-1}, v^{\ell-1})$ in the spherical coordinate system. The 'matrix method' refers to the study of each discrete Jacobian matrix and precise estimates of their multiplication ($\frac{1}{\sqrt{\alpha}}$ of them !). One important step is to bound such a matrix by $J(\mathbf{r}^\ell)$ in (A.91) which can be diagonalized as $J(\mathbf{r}^\ell) = \mathcal{P}^{-1}\Lambda\mathcal{P}$, with a diagonal matrix Λ. Based on the crucial cancellation property (**A.96**), we can extract a crucial second order of $\mathbf{r}^\ell \ll 1$ appeared in $J(\mathbf{r}^\ell)$. Therefore, over the interval $t|v| \backsim 1$, we are able to estimate $\Pi_{\ell=1}^{\frac{1}{\sqrt{\alpha}}} J(\mathbf{r}^\ell) \sim \frac{1}{\sqrt{\alpha}}$. Together with $\frac{1}{\sqrt{\alpha}}$ from the initial bounce, we expect $\frac{1}{\alpha}$−singularity for both $\partial X_{\mathbf{cl}}(s;t,x,v)$ and $\partial V_{\mathbf{cl}}(s;t,x,v)$ as in (A.107). Even though such estimate is too singular for our purpose we can improve it. Upon a closed inspection,

$$|\partial_x \mathbf{X}_\perp(s;t,x,v)| \lesssim \frac{1}{\sqrt{\alpha}},$$

for the normal component of $X_{\mathbf{cl}}(s)$. This is based on the fact $v_\perp^\ell \sim \sqrt{\alpha}$ via the Velocity lemma (Lemma 1, [75]). Unfortunately, the tangential part $\partial_x \mathbf{X}_{||}(s;t,x,v) \backsim \frac{1}{\alpha}$ is still too singular.

ODE Method for tangential parts of $\partial X_{\mathbf{cl}}(s)$ and $\partial V_{\mathbf{cl}}(s)$. To improve such an estimate, we observe that given the estimates for the normal parts $[\mathbf{X}_\perp(s;t,x,v),\ \mathbf{V}_\perp(s;t,x,v)]$, the sub-system of ODE for $[\mathbf{X}_{||}(s;t,x,v), \mathbf{V}_{||}(s;t,x,v)]$, enjoys much better property. In fact, at each specular reflection, $[\mathbf{X}_{||}(s;t,x,v), \mathbf{V}_{||}(s;t,x,v)]$ are continuous, unlike the the normal velocity $\mathbf{V}_\perp(s;t,x,v)$. Upon integrating over time as $\mathbf{V}_\perp(s;t,x,v) = \dot{\mathbf{X}}_\perp(s;t,x,v)$ (position $\mathbf{X}_\perp(s;t,x,v)$ is still continuous at specular reflection), we are able to derive an integral equations of $[\mathbf{X}_{||}(s;t,x,v), \mathbf{V}_{||}(s;t,x,v)]$ without broken into small discontinuous pieces (A.115) at each specular reflection. In other words, we can use the standard ODE theory to estimate these tangential parts. Our ODE method refers such ODE (Gronwall) estimates (A.111) which lead to the final conclusion of the theorem.

With such crucial estimates, we are able to design anisotropic norms in terms of singularity of $\frac{1}{\alpha}$. Thanks to $\int_0^t\int_u \frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{1}{\alpha(X(s),u)^\beta} \lesssim \alpha^{-\beta+1/2}$ and $\int_0^t\int_u \frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}}\frac{1}{\alpha(X(s),u)^{\beta-1/2}} \lesssim \alpha^{-\beta+1}$ from the dynamical non-local to local estimates for $\beta > 1$, we have exact cancellations of the power of α in the coefficients on the right hand side, and we are able to close the estimates. For $|v|$ either small or large, more careful analysis is needed. In particular, it is important to use the weight function of $e^{-\varpi\langle v\rangle t}$ to control both the growth in Theorem A.3 as well as $|v|$ in front of $\partial_x X_{\mathbf{cl}}$ and $\partial_v V_{\mathbf{cl}}$ to control singularity of $|v|$ in (A.20).

A.1.4 Bounce-back Reflection BC

Recall the bounce-back reflection boundary condition (A.11) and the bounce-back cycles in Definition A.1. Our main theorem is

Theorem A.4. *Assume* $f_0 \in W^{1,\infty}(\Omega\times\mathbb{R}^3)$ *and* $0<\kappa\le 1$ *for* $0<\theta<\frac14$,

$$||\langle v\rangle\partial_x f_0||_\infty + ||\partial_v f_0||_\infty + ||e^{\theta|v|^2}\partial_t f_0||_\infty + ||e^{\theta|v|^2} f_0||_\infty < +\infty,$$

and the compatibility conditions

$$f_0(x,v) = f_0(x,-v), \quad v\cdot\nabla_x f_0(x,v) = -v\cdot\nabla_x f_0(x,-v) \quad \text{on } \gamma_-. \tag{A.21}$$

Then there is $T = T(||e^{\theta|v|^2} f_0||_\infty) > 0$ *so that for all* $0\le t\le T$

$$\begin{aligned} &||e^{-\varpi\langle v\rangle t}\frac{\alpha}{\langle v\rangle^2}\partial_x f(t)||_\infty + ||e^{-\varpi\langle v\rangle t}\frac{|v|\alpha^{1/2}}{\langle v\rangle^2}\partial_v f(t)||_\infty + ||e^{\theta|v|^2}\partial_t f(t)||_\infty \\ &\lesssim_{\xi,t} ||\langle v\rangle\partial_x f_0||_\infty + ||\partial_v f_0||_\infty + P(||e^{\theta|v|^2}\partial_t f_0||_\infty) + P(||e^{\theta|v|^2} f_0||_\infty), \end{aligned} \tag{A.22}$$

for some polynomial P.

Moreover, if $f_0\in C^1$ *then* $f\in C^1$ *away from the grazing set* γ_0. *Furthermore, if* $F_0 = \mu + \sqrt{\mu}g_0 \ge 0$ *with* $||e^{\theta|v|^2}g_0||_\infty \ll 1$ *then this theorem holds for the arbitrarily large time* $t\ge 0$.

There can be no size restriction on initial data $F_0 = \sqrt{\mu} f_0$. We remark that the bounce-back case enjoys explicit expressions of $\partial X_{\mathbf{cl}}(s;t,x,v)$ and $\partial V_{\mathbf{cl}}(s;t,x,v)$. Since $\partial_x t^\ell \sim \frac{1}{\alpha}$ and $\partial_x x^\ell \sim \frac{1}{\sqrt{\alpha}}$, a new difficulty arises in the estimate

$$\partial_x X_{\mathbf{cl}}(s;t,x,v) \sim \frac{1}{\alpha},$$

which is too singular to control by our non-local to local estimates (Lemma A.2). Roughly speaking, the new difficulty is exactly the opposite to the specular case : ∂x^ℓ and ∂v^ℓ are in desired form but not $\partial_x X_{\mathbf{cl}}(s;t,x,v)$! The crucial observation is the following :

Lemma A.3. *In the sense of distribution,*

$$\begin{aligned}
&\partial_{\mathbf{e}}\Big[\int_{t^{j+1}}^{t^j} f(\tau, x^j - (t^j-\tau)v^j, v^j)\mathrm{d}\tau\Big] \\
&= \int_{t^{j+1}}^{t^j} \big[\partial_{\mathbf{e}} t^j, \partial_{\mathbf{e}} x^j + \tau \partial_{\mathbf{e}} v^j, \partial_{\mathbf{e}} v^j\big] \cdot \nabla_{t,x,v} f(\tau, x^j - (t^j-\tau)v^j, v^j)\mathrm{d}\tau \\
&\quad + \lim_{\tau \downarrow t^{j+1}} \big[\partial_{\mathbf{e}} t^j - \partial_{\mathbf{e}} t^{j+1}\big] f(\tau, x^j - (t^j-\tau)v^j, v^j)\big].
\end{aligned}$$

The key idea is to make a change of variable to transform

$$\partial_x X_{\mathbf{cl}}(s;t,x,v) \backsim v^\ell \partial_x t^\ell + \partial_x x^\ell,$$

while $\partial_x t^\ell$ captures the worst singulairty of $\frac{1}{\alpha}$. Fortunately, $\partial_x t^\ell$ is paired with $\partial_t f$, which is bounded, from the time-invariance of the problem and we are able to close the estimate.

A.1.5 Non-existence of $\nabla^2 f$ up to the boundary

In the appendix, we demonstrate that, our estimates can not be valid for higher order derivatives. Otherwise, if $\partial^2 f$ exists up to the boundary, we observe that from taking second derivatives of the Boltzmann equation :

$$v_n \partial_n^2 f = -\partial_{tn} f - (\partial_n v_n)\partial_n f - \sum_{i=1}^2 \partial_n(v_{\tau_i})\partial_{\tau_i} f - \sum_{i=1}^2 v_{\tau_i}\partial_{n\tau_i} f - \nu(F)\partial_n f + \partial_n K(f) + \partial_n \Gamma_{\text{gain}}(f,f).$$

If $|\partial_n f| \geq \frac{1}{\sqrt{\alpha}}$ and $\partial_n K(f) \sim K(\partial_n f)$ then at the boundary we have

$$|\partial_n f| \geq \frac{1}{|v_n|} \notin L^1_{loc}(\mathbb{R}^1),$$

so that $\partial_n K(f)$ is not defined. Since $|\partial_n f|$ is expected to behave at least as bad as $\frac{1}{\sqrt{\alpha}}$ for all diffusive, specular and bounce-back cases, we are able to identify initial conditions such that $|\partial_n f| \geq \frac{1}{|v_n|}$ for some future time.

A.2 Preliminary

Recall Γ_{gain} and ν in Due to the Grad estimate [70]

$$\begin{aligned}
\Gamma_{\text{gain}}(\sqrt{\mu}, g) + \Gamma_{\text{gain}}(g, \sqrt{\mu}) &= \int_{\mathbb{R}^3} \mathbf{k}_2(v,u) g(u)\mathrm{d}u, \\
\nu(\sqrt{\mu} g) &= \int_{\mathbb{R}^3} \mathbf{k}_1(v,u) g(u)\mathrm{d}u,
\end{aligned} \tag{A.23}$$

where

$$\begin{aligned}
\mathbf{k}_1(u,v) &= |u-v|^\kappa e^{-\frac{|v|^2+|u|^2}{2}} \int_{\mathbb{S}^2} q_0\Big(\frac{v-u}{|v-u|}\cdot\omega\Big)\mathrm{d}\omega, \\
\mathbf{k}_2(u,v) &= \frac{2}{|u-v|^2} e^{-\frac{1}{8}|u-v|^2 - \frac{1}{8}\frac{(|u|^2-|v|^2)^2}{|u-v|^2}} \\
&\quad \times \int_{w\cdot(u-v)=0} q_0\Big(\frac{u-v}{\sqrt{|u-v|^2+|w|^2}} \cdot \frac{u-v}{|u-v|}\Big) e^{-|w+\varsigma|^2}(|w|^2+|u-v|^2)^{\frac{\kappa}{2}}\mathrm{d}w,
\end{aligned} \tag{A.24}$$

where $\varsigma := \left(\frac{v+u}{2} \cdot \frac{w}{|w|}\right)\frac{w}{|w|}$. See page 315 of [74] for details.

Lemma A.4. *For $0 \le \kappa \le 1$,*

$$\begin{aligned}|\mathbf{k}_1(u,v)| + |\mathbf{k}_2(u,v)| \;&\lesssim\; \{|v-u|^{\kappa} + |v-u|^{-2+\kappa}\}e^{-\frac{1}{8}|v-u|^2 - \frac{1}{8}\frac{(|v|^2-|u|^2)^2}{|v-u|^2}} \\ &\lesssim\; \frac{e^{-\frac{1}{10}|v-u|^2 - \frac{1}{10}\frac{(|v|^2-|u|^2)^2}{|v-u|^2}}}{|v-u|^{2-\kappa}}.\end{aligned}$$

For $\varrho > 0$ and $-2\varrho < \theta < 2\varrho$ and $\zeta \in \mathbb{R}$, we have for $0 < \kappa \le 1$,

$$\int_{\mathbb{R}^3} \{|v-u|^{\kappa} + |v-u|^{-2+\kappa}\}e^{-\varrho|v-u|^2 - \varrho\frac{(|v|^2-|u|^2)^2}{|v-u|^2}} \frac{\langle v\rangle^{\zeta} e^{\theta|v|^2}}{\langle u\rangle^{\zeta} e^{\theta|u|^2}} \mathrm{d}u \;\lesssim\; \langle v\rangle^{-1}.$$

We define

$$\Gamma_{\mathrm{gain},v}(g_1,g_2)(v) := \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-u,\omega)\nabla_v(\sqrt{\mu})(u) g_1(u')g_2(v')\mathrm{d}\omega\mathrm{d}u, \tag{A.25}$$

where $u' = u - [(u-v)\cdot\omega]\omega$ and $v' = v + [(u-v)\cdot\omega]\omega$.

Lemma A.5. *(i) For $0 < \theta < \frac{1}{4}$ and $0 \le \kappa \le 1$, there exists $C_\theta > 0$ such that, for $(i,j) = (1,2)$ or $(2,1)$,*

$$|\Gamma_{\mathrm{gain}}(g_1,g_2)(v)| \;\lesssim_\theta\; ||e^{\theta|v|^2} g_i||_\infty \int_{\mathbb{R}^3} \frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}} |g_j(u)|\mathrm{d}u, \tag{A.26}$$

and

$$\begin{aligned}\big|\Gamma_{\mathrm{gain}}(g_1,g_2)(v)\big| \;&\lesssim_\theta\; \langle v\rangle^{\kappa} e^{-\theta|v|^2} ||e^{\theta|v|^2} g_1||_\infty ||e^{\theta|v|^2} g_2||_\infty, \\ |\Gamma_{\mathrm{gain},v}(g_1,g_2)(v)| \;&\lesssim_\theta\; \langle v\rangle^{\kappa} e^{-\theta|v|^2} ||e^{\theta|v|^2} g_1||_\infty ||e^{\theta|v|^2} g_2||_\infty, \\ |\nu(\sqrt{\mu} g_1) g_2(v)| \;&\lesssim_\theta\; ||e^{\theta|v|^2} g_2||_\infty \int_{\mathbb{R}^3} \frac{e^{-C_\theta|v-u|^2}}{|v-u|^{2-\kappa}} |g_1(u)|\mathrm{d}u.\end{aligned}$$

(ii) For $p \in [1,\infty)$ and $0 < \theta < \frac{1}{4}$, and for $(i,j) = (1,2)$ or $(i,j) = (2,1)$,

$$\begin{aligned}\|\Gamma_{\mathrm{gain}}(g_1,g_2)\|_p \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_i||_\infty \|g_j\|_p, \\ \|\nu(\sqrt{\mu} g_1) g_2\|_p \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_2||_\infty \|g_1\|_p, \\ \Big|\iint_{\Omega\times\mathbb{R}^3} \Gamma_{\mathrm{gain}}(g_1,g_2) g_3 \mathrm{d}v\mathrm{d}x\Big| \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_i||_\infty \|g_j\|_p \|g_3\|_q, \\ \Big|\iint_{\Omega\times\mathbb{R}^3} \nu(\sqrt{\mu} g_1) g_2 g_3 \mathrm{d}v\mathrm{d}x\Big| \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_2||_\infty \|g_1\|_p \|g_3\|_q.\end{aligned}$$

(iii) For $p \in [1,\infty)$ and $0 < \theta < \frac{1}{4}$, and for $(i,j) = (1,2)$ or $(i,j) = (2,1)$,

$$\begin{aligned}\|\nabla_v[\Gamma_{\mathrm{gain}}(g_1,g_2)]\|_p \;&\lesssim_{\theta,p}\; \sum_{(i,j)} ||e^{\theta|v|^2} g_i||_\infty \|\nabla_v g_j\|_p, \\ \|\nu(\sqrt{\mu}\nabla_v g_1) g_2\|_p \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_2||_\infty \|\nabla_v g_1\|_p, \\ \Big|\iint_{\Omega\times\mathbb{R}^3} \nabla_v \Gamma_{\mathrm{gain}}(g_1,g_2) g_3 \mathrm{d}v\mathrm{d}x\Big| \;&\lesssim_{\theta,p}\; \sum_{(i,j)} ||e^{\theta|v|^2} g_i||_\infty ||\nabla_v g_j||_p ||g_3||_q, \\ \Big|\iint_{\Omega\times\mathbb{R}^3} \nu(\sqrt{\mu}\nabla_v g_1) g_2 g_3 \mathrm{d}v\mathrm{d}x\Big| \;&\lesssim_{\theta,p}\; ||e^{\theta|v|^2} g_2||_\infty ||\nabla_v g_1||_p ||g_3||_q.\end{aligned}$$

(iv) Let $[Y,W] = [Y(x,v), W(x,v)] \in \Omega\times\mathbb{R}^3$. For $0 < \theta < \frac{1}{4}$ and $\partial_{\mathbf{e}}$ with $\mathbf{e} \in \{x,v\}$,

$$\begin{aligned}&|\partial_{\mathbf{e}}\Gamma_{\mathrm{gain}}(g,g)(Y,W)| \\ &\lesssim |\partial_{\mathbf{e}} Y| ||e^{\theta|v|^2} g||_\infty \int_{\mathbb{R}^3} \frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}} |\nabla_x g(Y,u)|\mathrm{d}u \\ &\quad + \; |\partial_{\mathbf{e}} W| ||e^{\theta|v|^2} g||_\infty \int_{\mathbb{R}^3} \frac{e^{-C_\theta|u-W|^2}}{|u-W|^{2-\kappa}} |\nabla_v g(Y,u)|\mathrm{d}u + \langle v\rangle^{\kappa} e^{-\theta|v|^2} |\partial_{\mathbf{e}} W| ||e^{\theta|v|^2} g||_\infty^2.\end{aligned}$$

The proofs of both Lemmas above are performed in 7.

Lemma A.6 (Local Existence). *For $0 \leq \theta < 1/4$, if $||e^{\theta|v|^2} f_0||_\infty < +\infty$ then there exists $T > 0$ depending on $||e^{\theta|v|^2} f_0||_\infty$ such that there exists unique $F = \mu + \sqrt{\mu} f$ solves the Boltzmann equation (A.1) in $[0, T]$ and satisfies the initial condition and boundary conditions (A.9), (A.10), (A.11) respectively and $F(t, x, v) \geq 0$ on $[0, T] \times \bar{\Omega} \times \mathbb{R}^3$ and f satisfies, for some $0 < \theta' < \theta$,*

$$\sup_{0 \leq t \leq T} ||e^{\theta'|v|^2} f(t)||_\infty \lesssim P(||e^{\theta|v|^2} f_0||_\infty), \tag{A.27}$$

for some polynomial P. Moreover if f_0 is continuous and satisfies the compatibility conditions (A.13), (A.17), (A.21) respectively then f is continuous away from the grazing set γ_0.

Moreover, for $0 \leq \bar{\theta} < \frac{1}{4}$, if $||e^{\bar{\theta}|v|^2} \partial_t f_0||_\infty \equiv \big|\big| e^{\bar{\theta}|v|^2} \frac{-v\cdot\nabla_x F_0 + Q(F_0, F_0)}{\sqrt{\mu}} \big|\big|_\infty < +\infty$ and compatibility conditions (A.13), (A.17), (A.21) respectively, then

$$\sup_{0 \leq t \leq T^*} ||e^{\bar{\theta}|v|^2} \partial_t f(t)||_\infty \lesssim P(||e^{\bar{\theta}|v|^2} \partial_t f_0||_\infty) + P(||e^{\theta|v|^2} f_0||_\infty), \tag{A.28}$$

for some polynomial P.

Furthermore for the diffuse and bounce-back boundary conditions if $F_0 = \mu + \sqrt{\mu} g_0$ with $||e^{\theta|v|^2} g_0||_\infty \ll 1$ for $0 < \theta < \frac{1}{4}$ then the results hold for all $t \geq 0$. For the specular reflection boundary condition, if ξ is real analytic (ξ is real analytic), and if $||e^{\theta|v|^2} g_0||_\infty \ll 1$ for $0 < \theta < \frac{1}{4}$ then the results hold for all $t \geq 0$.
.

Proof. The proof relies on the positive preserving iteration of [75, 81]

$$\partial_t F^{m+1} + v \cdot \nabla_x F^{m+1} + \nu(F^m) F^{m+1} = Q_{\text{gain}}(F^m, F^m), \quad F^{m+1}|_{t=0} = F_0 \geq 0, \tag{A.29}$$

which is equivalent to, with $F^m := \sqrt{\mu} f^m$,

$$\partial_t f^{m+1} + v \cdot \nabla_x f^{m+1} + \nu(F^m) f^{m+1} = \Gamma_{\text{gain}}(f^m, f^m), \quad f^{m+1}|_{t=0} = f_0. \tag{A.30}$$

See the proof for the diffuse case in Chapter 7. For the two other boundary conditions, follow the same proof by replacing the condition

(i) Diffuse reflection boundary condition, on $(x, v) \in \gamma_-$,

$$f^{m+1}(t, x, v) \;=\; c_\mu \sqrt{\mu(v)} \int_{n(x)\cdot u > 0} f^m(t, x, u) \sqrt{\mu(u)} \{n(x) \cdot u\} \mathrm{d}u. \tag{A.31}$$

acordingly, by

(ii) Specular reflection boundary condition, on $(x, v) \in \gamma_-$,

$$f^{m+1}(t, x, v) \;=\; f^m(t, x, R_x v), \tag{A.32}$$

where $R_x v = v - 2n(x)(n(x) \cdot v)$.

(iii) Bounce-back reflection boundary condition, on $(x, v) \in \gamma_-$,

$$f^{m+1}(t, x, v) \;=\; f^m(t, x, -v). \tag{A.33}$$

□

A.3 Traces and the In-flow Problems

Recall the almost grazing set γ_+^ε defined as

$$\gamma_+^\varepsilon = \{(x, v) \in \gamma_+ : v \cdot n(x) < \varepsilon \text{ or } |v| > 1/\varepsilon\}. \tag{A.34}$$

We first estimate the outgoing trace on $\gamma_+ \setminus \gamma_+^\varepsilon$. We remark that for the outgoing part, our estimate is global in time without cut-off, in contrast to the general trace theorem.

Lemma A.7. *Assume that $\varphi = \varphi(v)$ is $L^\infty_{loc}(\mathbb{R}^3)$. For any small parameter $\varepsilon > 0$, there exists a constant $C_{\varepsilon,T,\Omega} > 0$ such that for any h in $L^1([0,T], L^1(\Omega\times\mathbb{R}^3))$ with $\partial_t h + v\cdot\nabla_x h + \varphi h$ is in $L^1([0,T], L^1(\Omega\times\mathbb{R}^3))$, we have for all $0 \le t \le T$,*

$$\int_0^t \int_{\gamma_+\setminus\gamma_+^\varepsilon} |h| \mathrm{d}\gamma \mathrm{d}s \le C_{\varepsilon,T,\Omega}\left[||h_0||_1 + \int_0^t \left\{\|h(s)\|_1 + \big\|[\partial_t + v\cdot\nabla_x + \varphi]h(s)\big\|_1\right\}\mathrm{d}s \right].$$

Furthermore, for any (s,x,v) in $[0,T]\times\Omega\times\mathbb{R}^3$ the function $h(s+s', x+s'v, v)$ is absolutely continuous in s' in the interval $[-\min\{t_{\mathbf{b}}(x,v), s\}, \min\{t_{\mathbf{b}}(x,-v), T-s\}]$.

The proof is performed in 7.

Lemma A.8 (Green's Identity)**.** *For $p \in [1,\infty)$ assume that $f, \partial_t f + v\cdot\nabla_x f \in L^p([0,T]; L^p(\Omega\times\mathbb{R}^3))$ and $f_{\gamma_-} \in L^p([0,T]; L^p(\gamma))$. Then $f \in C^0([0,T]; L^p(\Omega\times\mathbb{R}^3))$ and $f_{\gamma_+} \in L^p([0,T]; L^p(\gamma))$ and for almost every $t \in [0,T]$:*

$$||f(t)||_p^p + \int_0^t |f|^p_{\gamma_+,p} = ||f(0)||_p^p + \int_0^t |f|^p_{\gamma_-,p} + \int_0^t \iint_{\Omega\times\mathbb{R}^3} \{\partial_t f + v\cdot\nabla_x f\}|f|^{p-2}f.$$

See [75] for the proof. Now we recall the following propositions for the in-flow problems :

$$\{\partial_t + v\cdot\nabla_x + \nu\}f = H, \quad f(0,x,v) = f_0(x,v), \quad f(t,x,v)|_{\gamma_-} = g(t,x,v), \tag{A.35}$$

where $\nu(t,x,v) \ge 0$. For notational simplicity, we define

$$\partial_t f_0 \equiv -v\cdot\nabla_x f_0 - \nu f_0 + H(0,x,v), \tag{A.36}$$

$$\nabla_x g \equiv \frac{n}{n\cdot v}\Big\{-\partial_t g - \sum_{i=1}^2 (v\cdot\tau_i)\partial_{\tau_i} g - \nu g + H\Big\} + \sum_{i=1}^2 \tau_i \partial_{\tau_i} g. \tag{A.37}$$

We remark that $\partial_t f_0$ is obtained from formally solving (A.35), and $(A.37)$ leads to the usual tangential derivatives of $\partial_{\tau_i} g$, while defines new 'normal derivative' $\partial_n g$ from the equation (A.35).

Proposition A.1. *Assume a compatibility condition*

$$f_0(x,v) = g(0,x,v) \quad \textit{for} \quad (x,v)\in\gamma_-. \tag{A.38}$$

For any fixed $p \in [1,\infty)$, assume

$$\begin{aligned} \nabla_x f_0, \nabla_v f_0, -v\cdot\nabla_x f_0 - \nu f_0 + H(0,x,v) &\in L^p(\Omega\times\mathbb{R}^3),\\ \langle v\rangle g, \partial_t g, \nabla_v g, \partial_{\tau_i} g, \frac{1}{n(x)\cdot v}\{-\partial_t g - \sum_i (v\cdot\tau_i)\partial_{\tau_i} g - \nu(v) g + H\} &\in L^p([0,T]\times\gamma_-), \end{aligned}$$

and, assume $1/p + 1/q = 1$ there exist $TC_T \sim O(T)$ and $\varepsilon \ll 1$ such that for all $t\in[0,T]$

$$\left|\iint_{\Omega\times\mathbb{R}^3} \partial H(t) h(t) \mathrm{d}x\mathrm{d}v\right| \le C_T ||h(t)||_q, \quad \nu \in L^p,$$

Then for sufficiently small $T > 0$ there exists a unique solution f to (A.35) such that $f, \partial_t f, \nabla_x f, \nabla_v f \in C^0([0,T]; L^p(\Omega\times\mathbb{R}^3))$ and the traces satisfy

$$\begin{aligned} \partial_t f|_{\gamma_-} = \partial_t g,\ \nabla_v f|_{\gamma_-} = \nabla_v g,\ \nabla_x f|_{\gamma_-} = \nabla_x g, \quad &on\ \ \gamma_-,\\ \nabla_x f(0,x,v) = \nabla_x f_0,\ \nabla_v f(0,x,v) = \nabla_v f_0,\ \partial_t f(0,x,v) = \partial_t f_0, \quad &in\ \ \Omega\times\mathbb{R}^3, \end{aligned} \tag{A.39}$$

where $\partial_t f_0$ and $\nabla_x g$ are given by (A.36) and (A.37). Moreover

$$||\partial_t f(t)||_p^p + \int_0^t |\partial_t f|^p_{\gamma_+,p} \le ||\partial_t f_0||_p^p + \int_0^t |\partial_t g|^p_{\gamma_-,p} + p\int_0^t \iint_{\Omega\times\mathbb{R}^3} |\partial_t H||\partial_t f|^{p-2}, \tag{A.40}$$

$$||\nabla_x f(t)||_p^p + \int_0^t |\nabla_x f|^p_{\gamma_+,p} \le ||\nabla_x f_0||_p^p + \int_0^t |\nabla_x g|^p_{\gamma_-,p} + p\int_0^t \iint_{\Omega\times\mathbb{R}^3} |\nabla_x H||\nabla_x f|^{p-1}, \tag{A.41}$$

$$\begin{aligned} ||\nabla_v f(t)||_p^p + \int_0^t |\nabla_v f|^p_{\gamma_+,p} \le\ & ||\nabla_v f_0||_p^p + \int_0^t |\nabla_v g|^p_{\gamma_-,p} \\ & + p\int_0^t \iint_{\Omega\times\mathbb{R}^3} |\{\nabla_v H - \nabla_x f - \nabla_v \nu f\}||\nabla_v f|^{p-1}. \end{aligned} \tag{A.42}$$

The proof is performed in 7.

We now study weighted $W^{1,p}$ estimate. We first define an effective collision frequency :

$$\nu_{\varpi,\beta}(t,x,v) = \nu(v) + \varpi\langle v\rangle - \beta\alpha^{-1}[v\cdot\nabla_x\alpha], \tag{A.43}$$

and

$$[\partial_t + v\cdot\nabla_x + \nu_{\varpi,\beta}](e^{-\varpi\langle v\rangle t}\alpha^\beta f) = e^{-\varpi\langle v\rangle t}\alpha^\beta[\partial_t f + v\cdot\nabla_x f + \nu f]. \tag{A.44}$$

Due to (7.6) in Chapter 7 and $\varpi \gg 1$, $\nu_{\varpi,\beta}(t,x,v) \sim \beta\langle v\rangle$.

Proposition A.2. *Let f be a solution of (A.35). Assume (A.38) and $\langle v\rangle g \in L^\infty([0,T]\times\gamma_-)$, and $\nu, \langle v\rangle H \in L^\infty([0,T]\times\Omega\times\mathbb{R}^3)$. For any fixed $p\in[2,\infty]$, assume*

$$\begin{aligned} e^{-\varpi\langle v\rangle t}\alpha^\beta\partial_t g,\ e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_\tau g &\in L^\infty([0,T];L^p(\gamma_-)),\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\big\{|\nabla_\tau g| + \frac{1}{n(x)\cdot v}\big(|\partial_t g| + \langle v\rangle|\nabla_\tau g| + |H|\big)\big\} &\in L^\infty([0,T];L^p(\gamma_-)),\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\big| - v\cdot\nabla_x f_0 - \nu f_0 + H_0\big| &\in L^p(\Omega\times\mathbb{R}^3), \end{aligned}$$

and assume $1/p+1/q=1$ there exist $TC_T = O(T)$ and $\varepsilon \ll 1$ such that for all $t\in[0,T]$

$$\Big|\iint_{\Omega\times\mathbb{R}^3} e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H(t)h(t)\Big| \le C_T\big\{||h(t)||_q + \varepsilon||\nu_{l,\beta}^{1/q}h(t)||_q\big\}.$$

Then $f(t,x,v)$ satisfies

$$||f(t)||_\infty \le ||f_0||_\infty + \sup_{0\le s\le t}||g(s)||_\infty + \Big|\Big|\int_0^t H(s)ds\Big|\Big|_\infty.$$

Recall $\partial = [\partial_t,\nabla_x,\nabla_v]$, then

$$\begin{aligned} \{\partial_t + v\cdot\nabla_x + \nu_{\varpi,\beta}\}[e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f] &= e^{-\varpi\langle v\rangle t}\alpha^\beta\big[-\partial v\cdot\nabla_x f - \partial\nu f + \partial H\big],\\ e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|_{t=0} &= e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0, \quad e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|_{\gamma_-} = e^{-\varpi\langle v\rangle t}\alpha^\beta[\partial g|_{\gamma_-}], \end{aligned}$$

where $[\partial g|_{\gamma_-}]$ is given in (A.39). Moreover, recalling (A.36) and (A.37), we have for $2\le p<\infty$,

$$\begin{aligned} &\int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f(t)|^p + \int_0^t\int_{\Omega\times\mathbb{R}^3}\nu_{\varpi,\beta}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^p + \int_0^t\int_{\gamma_+}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^p\\ &\lesssim \int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0|^p + \int_0^t\int_{\gamma_-}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial g|^p\\ &+\int_0^t\int_{\Omega\times\mathbb{R}^3}|e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H - e^{-\varpi\langle v\rangle t}\alpha^\beta\partial v\cdot\nabla_x f - \partial\nu e^{-\varpi\langle v\rangle t}\alpha^\beta f||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f|^{p-1}, \qquad (A.45)\\ &||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f(t)||_\infty\\ &\lesssim ||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial f_0||_\infty + ||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial g||_\infty\\ &+\int_0^t||e^{-\varpi\langle v\rangle t}\alpha^\beta\partial H - \partial v\cdot e^{-\varpi\langle v\rangle t}\alpha^\beta\nabla_x f - \partial\nu e^{-\varpi\langle v\rangle t}\alpha^\beta f||_\infty, \qquad \text{for } p=\infty. \end{aligned}$$

The proof is performed in 7.

A.4 Dynamical Non-local to Local Estimate

The main purpose of this section is to prove Lemma A.2 and its variants (Lemma A.9).

The dynamical non-local to local estimates for the stochastic (diffuse) cycles ((1) of Lemma A.2) is performed in Chapter 7.

Proof of (2) Lemma A.2. It suffices to consider $r = 0$ case. For the specular cycles and the bounce-back cycles it is important to control the *number of bounces*,

$$\ell_*(s) = \ell_*(s;t,x,v) \in \mathbb{N} \quad \text{if} \quad t^{\ell_*+1} \leq s < t^{\ell_*}.$$

Here we prove $t_{\mathbf{b}}(x,v) \simeq \alpha(x,v)^{1/2}/|v|^2$. Recall (40) of [75] or (2.4) of [67] : if Ω is bounded and $\partial\Omega$(i.e. ξ) is smooth then for $(x,v) \in \gamma_-$

$$t_{\mathbf{b}}(x,v) \gtrsim_\Omega \frac{\sqrt{\alpha(x,v)}}{|v|^2}. \tag{A.46}$$

It suffices to prove $t_{\mathbf{b}}(x,v) \gtrsim_\Omega \frac{|n(x)\cdot v|}{|v|^2}$. For $x \in \partial\Omega$ there exists $0 < \delta \ll 1$ such that

$$\sup_{\substack{y\in\partial\Omega \\ |x-y|<\delta}} \frac{|(x-y)\cdot n(x)|}{|x-y|^2} \lesssim \max_{\substack{y\in\partial\Omega \\ |x-y|<\delta}} |\nabla^2\xi(x)|.$$

If $|x-y| \geq \delta$ then $\frac{|(x-y)\cdot n(x)|}{|x-y|^2} \leq \delta^{-2}|(x-y)\cdot n(x)| \lesssim_{\delta,\Omega} 1$. By the compactness of Ω and $\partial\Omega$ we have $|(x-y)\cdot n(x)| \lesssim |x-y|^2$ for all $x,y \in \partial\Omega$. Taking the inner product of $x - x_{\mathbf{b}}(x,v) = t_{\mathbf{b}}(x,v)v$ with $n(x)$ we have

$$t_{\mathbf{b}}(x,v)|v\cdot n(x)| = |(x - x_{\mathbf{b}}(x,v))\cdot n(x)| \lesssim |x - x_{\mathbf{b}}(x,v)|^2 = C_\Omega |v|^2 |t_{\mathbf{b}}(x,v)|^2,$$

and this proves (A.46).

If Ω is convex (A.3) then for $(x,v) \in \gamma_-$

$$t_{\mathbf{b}}(x,v) \lesssim_\xi \frac{\sqrt{\alpha(x,v)}}{|v|^2}. \tag{A.47}$$

It suffices to show $t_{\mathbf{b}}(x,v) \lesssim_\xi \frac{|n(x)\cdot v|}{|v|^2}$. Since $\xi(x) = 0 = \xi(x - t_{\mathbf{b}}(x,v)v)$ for $(x,v) \in \gamma_-$, we have

$$\begin{aligned} 0 = \xi(x - t_{\mathbf{b}}(x,v)v) &= \xi(x) + \int_0^{t_{\mathbf{b}}(x,v)} [-v\cdot\nabla_x\xi(x-sv)]\mathrm{d}s \\ &= [-v\cdot\nabla_x\xi(x)]t_{\mathbf{b}}(x,v) + \int_0^{t_{\mathbf{b}}(x,v)}\int_0^s \{v\cdot\nabla_x^2\xi(x-\tau v)\cdot v\}\mathrm{d}\tau\mathrm{d}s. \end{aligned}$$

By the convexity of ξ in (A.3) we have $[v\cdot\nabla_x\xi(x)]t_{\mathbf{b}}(x,v) \geq \frac{(t_{\mathbf{b}}(x,v))^2}{2} C_\xi |v|^2$, and therefore this proves (A.47).

An important consequence of Velocity lemma is that for the specular cycles

$$\alpha(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)) \gtrsim e^{-\mathcal{C}|v||t-s|}\alpha(x,v),$$

and therefore for the specular cycles

$$\begin{aligned} \ell_*(s;t,x,v) &\leq \frac{|t-s|}{\min_{0\leq\ell\leq\ell_*(s;t,x,v)} |t^\ell - t^{\ell+1}|} \lesssim \frac{|t-s|}{\min_{0\leq\ell\leq\ell_*(s;t,x,v)} \frac{\sqrt{\alpha(x^\ell,v^\ell)}}{|v^\ell|^2}} \\ &\lesssim \frac{|t-s||v|^2}{\sqrt{\alpha(x,v)}} e^{\mathcal{C}|v|(t-s)}. \end{aligned} \tag{A.48}$$

Remark that for the bounce-back cycles we do not have the growth term $e^{\mathcal{C}|v|(t-s)}$. This is because of the fact $\alpha(X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))$ is either $\alpha(x^1,v^1)$ or $\alpha(x^2,v^2)$, and the fact $|t-t^2| \leq 2|t^1-t^2| \lesssim \frac{C_\Omega}{|v|}$ for the bounded domain.

We consider the specular BC case first. For fixed (x,v) we use the following notation $\alpha(s) := \alpha(s;t,x,v) := \alpha(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v))$.

Firstly we consider the estimate (A.16) for $|v| < \delta$. Using (A.48),

$$\begin{aligned}
&\mathbf{1}_{\{|v|\le\delta\}} \int_0^t \int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)} \frac{e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}} \frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^{\beta}} \mathrm{d}u\mathrm{d}s \\
&\lesssim \sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell} \int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)} \frac{e^{-\theta|v^\ell-u|^2}}{|v^\ell-u|^{2-\kappa}} \frac{Z(s,x,v)}{\big[\alpha(x^\ell-(t^\ell-s)v^\ell,u)\big]^{\beta}} \mathrm{d}u\mathrm{d}s \\
&\lesssim \frac{t|v|^2 e^{\mathcal{C}t\delta}}{\big[\alpha(x,v)\big]^{1/2}} \sup_\ell \Big\{ \frac{O(\tilde{\delta})e^{\mathcal{C}t\delta}}{|v|^2[\alpha(x,v)]^{\beta-1}} \sup_{t^{\ell+1}\le s\le t^\ell} \{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\} \\
&\qquad\qquad + \frac{C_{\tilde{\delta}}e^{\mathcal{C}t\delta}}{[\alpha(x,v)]^{\beta-1/2}} \int_{t^{\ell+1}}^{t^\ell} e^{-l\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s \Big\},
\end{aligned}$$

where we have used (A.15). By (A.46) and (A.47) and the Velocity lemma (Lemma A.1) we have $|t^\ell - t^{\ell+1}| \lesssim_\xi \frac{\sqrt{\alpha(x,v)}}{|v|^2} e^{\mathcal{C}t|v|} \lesssim_{\xi,\delta} \frac{\sqrt{\alpha(x,v)}}{|v|^2} e^{\mathcal{C}t\delta}$ and hence we deduce (A.16) for $|v| < \delta$ by

$$\mathbf{1}_{\{|v|<\delta\}} \int \cdots \lesssim_\xi \frac{O(\tilde{\delta}+l^{-1})te^{2\mathcal{C}t\delta}}{\big[\alpha(x,v)\big]^{\beta-\frac{1}{2}}} \sup_{0\le s\le t} \big\{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\big\}.$$

Now we consider $|v| \ge \delta$. We split the time interval as

$$[0,t] \;=\; [t-\frac{1}{|v|},t] \;\cup\; \bigcup_{j=1}^{[t|v|]+1} [t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}]. \tag{A.49}$$

Consider the first time section $[t-\frac{1}{|v|},t]$. Due to (A.48) we bound

$$\sup_{s\in[t-\frac{1}{|v|},t]} \ell_*(s;t,x,v) \lesssim_\xi \frac{\frac{1}{|v|}|v|^2 e^{\mathcal{C}\frac{1}{|v|}|v|}}{[\alpha(x,v)]^{1/2}} \lesssim \frac{|v|e^{\mathcal{C}}}{[\alpha(x,v)]^{1/2}},$$

and for $s \in [t-\frac{1}{|v|},t]$, $e^{-\mathcal{C}}\alpha(x,v) \lesssim \alpha(X_{\mathbf{cl}}(s;t,x,v),V_{\mathbf{cl}}(s;t,x,v)) \lesssim e^{\mathcal{C}}\alpha(x,v)$, and $|t^\ell - t^{\ell+1}| \lesssim \frac{[\alpha(x,v)]^{1/2}e^{\mathcal{C}}}{|v|^2}$ due to the Velocity lemma. Then we use (A.15) to have

$$\begin{aligned}
&\int_{t-1/|v|}^t \int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)} \frac{e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}} \frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^{\beta}} \mathrm{d}u\mathrm{d}s \\
&\lesssim \sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell} \int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)} \frac{e^{-\theta|v^\ell-u|^2}}{|v^\ell-u|^{2-\kappa}} \frac{Z(s,x,v)}{\big[\alpha(x^\ell-(t^\ell-s)v^\ell,u)\big]^{\beta}} \mathrm{d}u\mathrm{d}s \\
&\lesssim \frac{C_\xi|v|}{[\alpha(x,v)]^{1/2}} \sup_\ell \frac{O(\tilde{\delta})e^{C_\xi}}{|v|^2[\alpha(x,v)]^{\beta-1}} \sup_{t^{\ell+1}\le s\le t^\ell} \{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\} \\
&\quad + \sum_{\ell=0}^{\ell_*(0,t,x,v)} \frac{C_{\tilde{\delta}}e^{C_\xi}}{[\alpha(x,v)]^{\beta-1/2}} \int_{t^{\ell+1}}^{t^\ell} e^{-l\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s \\
&\lesssim \frac{O(\tilde{\delta})}{|v|[\alpha(x,v)]^{\beta-1/2}} \sup_{0\le s\le t} \{e^{-Cl\langle v\rangle(t-s)}Z(s,x,v)\} + \frac{C_{\tilde{\delta},\xi}}{[\alpha(x,v)]^{\beta-1/2}} \int_0^t e^{-Cl\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s \\
&\lesssim \Big(\frac{O(\tilde{\delta})}{|v|[\alpha(x,v)]^{\beta-1/2}} + \frac{C_{\tilde{\delta},\xi}}{l\langle v\rangle[\alpha(x,v)]^{\beta-1/2}} \Big) \sup_{0\le s\le t} \{e^{-Cl\langle v\rangle(t-s)}Z(s,x,v)\}.
\end{aligned}$$

Now we consider time sections $[t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}]$ for $j \ge 1$. Assume that

$$[t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}] \subset [t^{\ell_{j+1}-1}, t^{\ell_{j+1}}] \cup \cdots \cup [t^{\ell_j+1}, t^{\ell_j}],$$

and $[t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}] \cap [t^{\ell_{j+1}-2}, t^{\ell_{j+1}-1}] = \emptyset$ and $[t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}] \cap [t^{\ell_j}, t^{\ell_j-1}] = \emptyset$.

Note that for all $s \in [t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}]$

$$e^{-C_\xi j}\alpha(t) \lesssim \alpha(s) \lesssim e^{C_\xi j}\alpha(t),$$

and

$$\ell_{j+1}-\ell_j \lesssim \frac{(j+1)\frac{1}{|v|}-j\frac{1}{|v|}}{\frac{\sqrt{\alpha(t-j\frac{1}{|v|})}}{|v|^2}} \lesssim \frac{|v|}{\sqrt{\alpha(t)}}e^{C_\xi j},$$

and for $\ell \in [\ell_{j+1}-1, \ell_j]$

$$|t^\ell - t^{\ell+1}| \lesssim \frac{\sqrt{\alpha(t-j\frac{1}{|v|})}}{|v|^2} \lesssim \frac{\sqrt{\alpha(t)}}{|v|^2}e^{C_\xi j}.$$

From (A.15), for all $\ell \in [\ell_{j+1}-1, \ell_j]$

$$\begin{aligned}
&\int_{t^\ell}^{t^{\ell+1}}\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}\frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^\beta}\mathrm{d}u\mathrm{d}s\\
&\lesssim \frac{\tilde\delta}{|v|^2\alpha(t-j/|v|)^{\beta-1}}\sup_{[t^\ell,t^{\ell+1}]}\{e^{-l\langle v\rangle(t-s)}Z\} + \frac{C_{\tilde\delta}}{\alpha(t-j/|v|)^{\beta-1/2}}\int_{t^{\ell+1}}^{t^\ell} e^{-l\langle v\rangle(t-s)}Z,
\end{aligned}$$

is bounded by

$$\begin{aligned}
&\frac{\tilde\delta e^{C_\xi j}}{|v|^2\alpha(t)^{\beta-1}}e^{-\frac{l}{2}j}\sup_{[t^\ell,t^{\ell+1}]}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z\} + \frac{e^{C_\xi j}}{\alpha(t)^{\beta-1/2}}e^{-\frac{l}{2}j}\int_{t^{\ell+1}}^{t^\ell} e^{-\frac{l}{2}\langle v\rangle(t-s)}Z\\
&\lesssim \frac{e^{-Clj}}{|v|^2\alpha(t)^{\beta-1}}\sup_{0\le s\le t}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s)\},
\end{aligned}$$

where we have used the fact $t-s \ge j\frac{1}{|v|}$ for $s \in [t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}]$.

Therefore

$$\begin{aligned}
&\int_{t-(j+1)\frac{1}{|v|}}^{t-j\frac{1}{|v|}}\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}\frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^\beta}\mathrm{d}u\mathrm{d}s\\
&\lesssim |\ell_{j+1}-\ell_j|\sup_{\ell_{j+1}\le\ell\le\ell_j}\int_{t^\ell}^{t^{\ell+1}}\cdots\\
&\lesssim \frac{|v|}{\sqrt{\alpha(t)}}e^{C_\xi j}\times\frac{e^{-lj/4}}{|v|^2\alpha(t)^{\beta-1}}\sup_{0\le s\le t}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\}\\
&\lesssim \frac{e^{-lj/4}}{|v|\alpha(t)^{\beta-1/2}}\sup_{0\le s\le t}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\}.
\end{aligned}$$

Now we sum up all contributions of $[t-(j+1)\frac{1}{|v|}, t-j\frac{1}{|v|}]$ for $j \ge 1$:

$$\begin{aligned}
\sum_{j=1}^{t|v|}\int_{t-(j+1)/|v|}^{t-j/|v|} &\le \sum_{j=1}^{t|v|}\frac{e^{-lj/8}}{|v|\alpha(t)^{\beta-1/2}}\sup_{0\le s\le t}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\}\\
&\lesssim \frac{e^{-l/8}}{|v|[\alpha(x,v)]^{\beta-1/2}}\sup_{0\le s\le t}\{e^{-\frac{l}{2}\langle v\rangle(t-s)}Z(s,x,v)\}.
\end{aligned}$$

where we used $\sum_{j=1}^{t|v|}e^{-lj/8} = e^{-l/16}\sum_{j=2}^{t|v|}e^{-C'lj} \le e^{-l/16}$.

These prove (A.16). For the bounce-back case we set $\mathcal{C}=0$ and we have same conclusion. □

Lemma A.9. *Let $(t,x,v) \in [0,\infty)\times\bar\Omega\times\mathbb{R}^3$ and $Z \ge 0$.*

(1) For $0<\varepsilon\ll 1$ and $\frac{1}{2}<\beta<1$ and $0<\kappa\le 1$, we have

$$\begin{aligned}
&\int_0^{t_{\mathbf{b}}(x,v)}\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|v-u|^2}}{|v-u|^{2-\kappa}[\alpha(x-(t_{\mathbf{b}}(x,v)-s)v,u)]^\beta}\frac{|v|}{|u|}\frac{\langle u\rangle^r}{\langle v\rangle^r}Z(s,x,v)\mathrm{d}u\mathrm{d}s\\
&\lesssim_{\theta,r} \frac{O(\varepsilon)}{|v|^2[\alpha(x,v)]^{\beta-1}}\sup_{s\in[0,t_{\mathbf{b}}(x,v)]}\{e^{-l\langle v\rangle(t-s)}Z(s,x,v)\}\\
&\quad + \frac{C_\varepsilon}{[\alpha(x,v)]^{\beta-1/2}}\int_0^{t_{\mathbf{b}}(x,v)} e^{-Cl\langle v\rangle(t-s)}Z(s,x,v)\mathrm{d}s.
\end{aligned} \tag{A.50}$$

(2) Let $[X_{\mathbf{cl}}(s;t,x,v),V_{\mathbf{cl}}(s;t,x,v)]$ be either the specular backward trajectory or the bounce-back backward trajectory in Definition A.1. For $0<\varepsilon\ll 1$ and $\frac{1}{2}<\beta<1$ and $0<\kappa\leq 1$ and $r\in\mathbb{R}$, there exists $l\gg_{\xi} 1$ and $C=C_{l,\beta,\xi,r}>0$ such that

$$\begin{aligned}&\int_0^t\int_{\mathbb{R}^3} e^{-l\langle v\rangle(t-s)}\frac{e^{-\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}\frac{|v|}{|u|}\frac{\langle u\rangle^r}{\langle v\rangle^r}\frac{Z(s,x,v)}{\big[\alpha(X_{\mathbf{cl}}(s;t,x,v),u)\big]^{\beta}}\mathrm{d}u\mathrm{d}s\\&\lesssim_{\xi,r}\frac{O_{\beta,\kappa,r}(\varepsilon)}{\langle v\rangle\big[\alpha(x,v)\big]^{\beta-1/2}}\sup_{0\leq s\leq t}\big\{e^{-C_{l,\beta,\xi,r}\langle v\rangle(t-s)}Z(s,x,v)\big\}.\end{aligned}\tag{A.51}$$

Now we prove a variant of (1) of Lemma A.2 with extra $\frac{|v|}{|u|}$.

Proof of Lemma A.9. We prove (A.50). Due to *Step 2* and *Step 3* in the proof of *(1)* of Lemma A.2, it suffices to show

$$\int_{\mathbb{R}^3}\frac{|v|e^{-\theta|v-u|^2}\mathrm{d}u}{|v-u|^{2-\kappa}|u|\big[\alpha(x-(t_{\mathbf{b}}(x,v)-s)v,u)\big]^{\beta}}\lesssim\frac{1}{|v|^{2\beta-1}|\xi(x-(t_{\mathbf{b}}(x,v)-s)v)|^{\beta-\frac{1}{2}}}.\tag{A.52}$$

As *Step 1* in the proof of *(1)*, for fixed s and $x-(t_{\mathbf{b}}(x,v)-s)v$, we decompose $u=u_{\tau,1}\tau_1+u_{\tau,2}\tau_2+u_n n$ where $\{\tau_1,\tau_2,n\}$ is the orthonormal basis that we chose in the proof of *(1)*.

Now we split as

$$\begin{aligned}&\int_{\mathbb{R}^3}\frac{|v|e^{-\theta|v-u|^2}\mathrm{d}u}{|v-u|^{2-\kappa}|u|\big[\alpha(x-(t_{\mathbf{b}}(x,v)-s)v,u)\big]^{\beta}}\\&\lesssim_{\xi}\int_{\mathbb{R}^2}\int_{\mathbb{R}}\frac{|v|e^{-\theta|v-u|^2}\mathrm{d}u_n\mathrm{d}u_{\tau}}{|v-u|^{2-\kappa}|u|\big\{|u_n|^2+|\xi(X_{\mathbf{cl}}(s))||u|^2\big\}^{\beta}}\\&=\int_{|u|\geq\frac{|v|}{5}}+\int_{|u|\leq\frac{|v|}{5}}.\end{aligned}$$

For the first term, we have $\frac{|v|}{|u|}\leq 5$ so we reduce it to the previous case (7.60)

$$\int_{|u|\geq\frac{|v|}{5}}\lesssim\int_{\mathbb{R}^3}\frac{e^{-\theta|v-u|^2}\mathrm{d}u_n\mathrm{d}u_{\tau}}{|v-u|^{2-\kappa}\big\{|u_n|^2+|\xi(X_{\mathbf{cl}}(s))||u|^2\big\}^{\beta}},$$

which is bounded by $\frac{1}{|v|^{2\beta-1}|\xi|^{\beta-1/2}}$.

Now we consider the case of $|u|\leq\frac{|v|}{5}$. For fixed $0<\kappa\leq 1$

$$\frac{|v|}{|v-u|^{2-\kappa}}\lesssim\frac{|v|}{|v|^{2-\kappa}}\lesssim|v|^{-1+\kappa},$$

and we have, from $|v-u|^2=\frac{|v-u|^2}{2}+\frac{|v-u|^2}{2}\geq\frac{4^2}{2\cdot 5^2}|v|^2+\frac{4^2}{2}|u|^2$,

$$e^{-\theta|v-u|^2}\leq e^{-C_{\theta}|v|^2}e^{-C_{\theta}|u|^2}.$$

We split $\int_{\mathbb{R}^3} \mathrm{d}u = \int_{|u_n|\geq |\xi|^{1/2}|u_\tau|} + \int_{|u_n|\leq |\xi|^{1/2}|u_\tau|}$ to have (Note $\frac{1}{2}<\beta<1$)

$$
\begin{aligned}
\int_{|u_n|\geq |\xi|^{1/2}|u_\tau|} &\lesssim \frac{e^{-C|v|^2}}{|v|^{1-\kappa}} \int_{\mathbb{R}^2} \frac{e^{-C_\theta |u_\tau|^2}}{|u_\tau|} \int_{|\xi|^{1/2}|u_\tau|}^{|v|/5} |u_n|^{-2\beta} e^{-C_\theta |u_n|^2} \mathrm{d}|u_n| \mathrm{d}u_\tau \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{1-\kappa}} \int_{|u_\tau|\leq \frac{|v|}{5}} \frac{e^{-C_\theta |u_\tau|^2}}{|u_\tau|} \int_{|\xi|^{1/2}|u_\tau|}^{\frac{|v|}{5}} \frac{\mathrm{d}u_n}{|u_n|^{2\beta}} \mathrm{d}u_\tau \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{1-\kappa}} \Big\{ |v| + |v|^{-2\beta+1} \int_{|u_\tau|\leq \frac{|v|}{5}} \frac{\mathrm{d}u_\tau}{|u_\tau|} + \frac{1}{|\xi|^{\beta-\frac{1}{2}}} \int_{|u_\tau|\leq \frac{|v|}{5}} |u_\tau|^{-2\beta} \mathrm{d}u_\tau \Big\} \\
&\lesssim e^{-C|v|^2}|v|^\kappa \big\{ 1 + \frac{1}{|v|^{2\beta-1}} (1+\frac{1}{|\xi|^{\beta-\frac{1}{2}}}) \big\} \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-1}|\xi|^{\beta-\frac{1}{2}}}, \\
\int_{|u_n|\leq |\xi|^{1/2}|u_\tau|} &\lesssim \frac{e^{-C|v|^2}}{|v|^{1-\kappa}} \int_{|u_\tau|\leq \frac{|v|}{5}} \frac{e^{-C_\theta |u_\tau|^2}}{|\xi|^\beta |u_\tau|^{2\beta}|u_\tau|} \int_{|u_n|\leq |\xi|^{1/2}|u_\tau|} \mathrm{d}u_n \mathrm{d}u_\tau \\
&\lesssim \frac{e^{-C|v|^2}}{|v|^{1-\kappa}} \int_{|u_\tau|\leq \frac{|v|}{5}} \frac{e^{-C_\theta |u_\tau|^2}}{|\xi|^{\beta-1/2}|u_\tau|^{2\beta}} \mathrm{d}u_\tau \\
&\lesssim \frac{|v|^{-2\beta+\kappa+1}e^{-C|v|^2}}{|\xi|^{\beta-1/2}} \lesssim \frac{e^{-C|v|^2}}{|v|^{2\beta-1}|\xi|^{\beta-\frac{1}{2}}}.
\end{aligned}
$$

Therefore, combining the cases of $|u|\leq \frac{|v|}{5}$ and $|u|\geq \frac{|v|}{5}$, we conclude (A.52).

The proof of (A.51), (2) of Lemma A.9 is a direct consequence of (A.52) and the proof of (A.16). $\square$

A.5 Specular Reflection BC

We denote the standard spherical coordinate $\mathbf{x}_\parallel = \mathbf{x}_\parallel(\omega) = (\mathbf{x}_{\parallel,1}, \mathbf{x}_{\parallel,2})$ for $\omega\in\mathbb{S}^2$

$$\omega = (\cos \mathbf{x}_{\parallel,1}(\omega) \sin \mathbf{x}_{\parallel,2}(\omega), \sin \mathbf{x}_{\parallel,1}(\omega) \sin \mathbf{x}_{\parallel,2}(\omega), \cos \mathbf{x}_{\parallel,2}(\omega)),$$

where $\mathbf{x}_{\parallel,1}(\omega)\in[0,2\pi)$ is the azimuth and $\mathbf{x}_{\parallel,2}(\omega)\in[0,\pi)$ is the inclination.

We define an orthonormal basis of $\mathbb{R}^3$

$$
\begin{aligned}
\hat{r}(\omega) &:= (\cos \mathbf{x}_{\parallel,1}(\omega) \sin \mathbf{x}_{\parallel,2}(\omega), \sin \mathbf{x}_{\parallel,1}(\omega) \sin \mathbf{x}_{\parallel,2}(\omega), \cos \mathbf{x}_{\parallel,2}(\omega)), \\
\hat{\phi}(\omega) &:= (\cos \mathbf{x}_{\parallel,1}(\omega) \cos \mathbf{x}_{\parallel,2}(\omega), \sin \mathbf{x}_{\parallel,1}(\omega) \cos \mathbf{x}_{\parallel,2}(\omega), -\sin \mathbf{x}_{\parallel,2}(\omega)), \\
\hat{\theta}(\omega) &:= (-\sin \mathbf{x}_{\parallel,1}(\omega), \cos \mathbf{x}_{\parallel,1}(\omega), 0).
\end{aligned}
$$

Moreover, $\hat{r}\times\hat{\phi}=\hat{\theta},\ \hat{\phi}\times\hat{\theta}=\hat{r},\ \hat{\theta}\times\hat{r}=\hat{\phi}$, and

$$\partial_{\mathbf{x}_{\parallel,1}} \hat{r} = \sin \mathbf{x}_{\parallel,2}\ \hat{\theta}, \quad \partial_{\mathbf{x}_{\parallel,2}} \hat{r} = \hat{\phi}, \tag{A.53}$$

where $\partial_{\mathbf{x}_{\parallel,1}} \hat{r}$ does not vanish (non-degenerate) away from $\mathbf{x}_{\parallel,2}=0$ or π.

Lemma A.10. *Assume $\mathbf{0}=(0,0,0)\in\Omega$ and Ω is convex (A.3). Fix*

$$\mathbf{p}=(z,w)\in\partial\Omega\times\mathbb{S}^2 \quad \textit{with} \quad n(z)\cdot w=0.$$

We define the north pole $\mathcal{N}_\mathbf{p}\in\partial\Omega$ and the south pole $\mathcal{S}_\mathbf{p}\in\partial\Omega$ as

$$\mathcal{N}_\mathbf{p} := |\mathcal{N}_\mathbf{p}|(\frac{z}{|z|}\times w)\in\partial\Omega, \quad \mathcal{S}_\mathbf{p} := -|\mathcal{S}_\mathbf{p}|(\frac{z}{|z|}\times w)\in\partial\Omega,$$

where $\partial_{\mathbf{x}_{\parallel,1}}\hat{r}$ is degenerate. We define the straight-line $\mathcal{L}_\mathbf{p}$ passing both poles

$$\mathcal{L}_\mathbf{p} := \{\tau\mathcal{N}_\mathbf{p} + (1-\tau)\mathcal{S}_\mathbf{p} : \tau\in\mathbb{R}\}.$$

(i) There exists a smooth map

$$\begin{aligned} \eta_{\mathbf{p}} \ : \quad [0,2\pi)\times(0,\pi) \quad &\rightarrow \quad \partial\Omega\backslash\{\mathcal{N}_{\mathbf{p}},\mathcal{S}_{\mathbf{p}}\}, \\ \mathbf{x}_{\parallel_{\mathbf{p}}} := (\mathbf{x}_{\parallel_{\mathbf{p}},1},\mathbf{x}_{\parallel_{\mathbf{p}},2}) &\mapsto \quad \eta_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}}), \end{aligned} \tag{A.54}$$

which is one-to-one and onto. Here on $[0,2\pi)\times(0,\pi)$ *we have* $\partial_i\eta_{\mathbf{p}} := \frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},i}} \neq 0$ *and*

$$\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},1}}(\mathbf{x}_{\parallel_{\mathbf{p}}}) \times \frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},2}}(\mathbf{x}_{\parallel_{\mathbf{p}}}) \neq 0. \tag{A.55}$$

We define

$$\mathbf{n}_{\mathbf{p}} := n\circ\eta_{\mathbf{p}} : [0,2\pi)\times(0,\pi)\rightarrow\mathbb{S}^2.$$

(ii) We define the $\mathbf{p}-$*spherical coordinate :*

For $\delta>0,\ \delta_1>0,\ C>0,$ *we have a smooth one-to-one and onto map*

$$\begin{aligned} \Phi_{\mathbf{p}} : [0,C\delta)\times[0,2\pi)\times(\delta_1,\pi-\delta_1)\times\mathbb{R}\times\mathbb{R}^2 \ &\rightarrow \ \{x\in\bar{\Omega} : |\xi(x)|<\delta\}\backslash B_{C\delta_1}(\mathcal{L}_{\mathbf{p}})\times\mathbb{R}^3, \\ (\mathbf{x}_{\perp_{\mathbf{p}}},\mathbf{x}_{\parallel_{\mathbf{p}},1},\mathbf{x}_{\parallel_{\mathbf{p}},2},\mathbf{v}_{\perp_{\mathbf{p}}},\mathbf{v}_{\parallel_{\mathbf{p}},1},\mathbf{v}_{\parallel_{\mathbf{p}},2}) \ &\mapsto \ \Phi_{\mathbf{p}}(\mathbf{x}_{\perp_{\mathbf{p}}},\mathbf{x}_{\parallel_{\mathbf{p}},1},\mathbf{x}_{\parallel_{\mathbf{p}},2},\mathbf{v}_{\perp_{\mathbf{p}}},\mathbf{v}_{\parallel_{\mathbf{p}},1},\mathbf{v}_{\parallel_{\mathbf{p}},2}), \end{aligned}$$

where $B_{C\delta_1}(\mathcal{L}_{\mathbf{p}}) := \{x\in\mathbb{R}^3 : |x-y|<C\delta_1 \text{ for some } y\in\mathcal{L}_{\mathbf{p}}\}.$
Explicitly,

$$\Phi_{\mathbf{p}}(\mathbf{x}_{\perp_{\mathbf{p}}},\mathbf{x}_{\parallel_{\mathbf{p}}},\mathbf{v}_{\perp_{\mathbf{p}}},\mathbf{v}_{\parallel_{\mathbf{p}}}) := \left[\begin{array}{c} \mathbf{x}_{\perp_{\mathbf{p}}}[-\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})]+\eta_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}}) \\ \mathbf{v}_{\perp_{\mathbf{p}}}[-\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})]+\mathbf{v}_{\parallel_{\mathbf{p}}}\cdot\nabla\eta_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})+\mathbf{x}_{\perp_{\mathbf{p}}}\mathbf{v}_{\parallel_{\mathbf{p}}}\cdot\nabla[-\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})] \end{array}\right], \tag{A.56}$$

where $\nabla\eta_{\mathbf{p}} = (\partial_1\eta_{\mathbf{p}},\partial_2\eta_{\mathbf{p}}) = (\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},1}},\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},2}})$ *and* $\nabla\mathbf{n}_{\mathbf{p}} = (\partial_1\mathbf{n}_{\mathbf{p}},\partial_2\mathbf{n}_{\mathbf{p}}) = (\frac{\partial\mathbf{n}_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},1}},\frac{\partial\mathbf{n}_{\mathbf{p}}}{\partial\mathbf{x}_{\parallel_{\mathbf{p}},2}}).$

We fix an inverse map

$$\Phi_{\mathbf{p}}^{-1} : \{x\in\bar{\Omega} : |\xi(x)|<\delta\}\backslash B_{C\delta'}(\mathcal{L}_{\mathbf{p}})\times\mathbb{R}^3 \ \rightarrow \ [0,C\delta)\times[0,2\pi)\times(\delta_1,\pi-\delta_1)\times\mathbb{R}\times\mathbb{R}^2.$$

In general this choice is not unique but once we fix the range as above then an inverse map is uniquely determined.

We denote, for $(x,v)\in\{x\in\bar{\Omega} : |\xi(x)|<\delta\}\backslash B_{C\delta'}(\mathcal{L}_{\mathbf{p}})\times\mathbb{R}^3$

$$(\mathbf{x}_{\perp_{\mathbf{p}}},\mathbf{x}_{\parallel_{\mathbf{p}},1},\mathbf{x}_{\parallel_{\mathbf{p}},2},\mathbf{v}_{\perp_{\mathbf{p}}},\mathbf{v}_{\parallel_{\mathbf{p}},1},\mathbf{v}_{\parallel_{\mathbf{p}},2}) = \Phi_{\mathbf{p}}^{-1}(x,v).$$

(iii) For $|\xi(X_{\mathbf{cl}}(s;t,x,v))|<\delta$ *and* $|X_{\mathbf{cl}}(s;t,x,v)-\mathcal{L}_{\mathbf{p}}|>C\delta_1$ *we define*

$$\begin{aligned} (\mathbf{X}_{\mathbf{p}}(s;t,x,v),\mathbf{V}_{\mathbf{p}}(s;t,x,v)) &:= \Phi_{\mathbf{p}}^{-1}(X_{\mathbf{cl}}(s;t,x,v),V_{\mathbf{cl}}(s;t,x,v)) \\ &:= (\mathbf{x}_{\perp_{\mathbf{p}}}(s;t,x,v),\mathbf{x}_{\parallel_{\mathbf{p}}}(s;t,x,v),\mathbf{v}_{\perp_{\mathbf{p}}}(s;t,x,v),\mathbf{v}_{\parallel_{\mathbf{p}}}(s;t,x,v)). \end{aligned}$$

Then $|v|\simeq|\mathbf{V}_{\mathbf{p}}|$ *and*

$$\begin{aligned} \dot{\mathbf{x}}_{\perp_{\mathbf{p}}}(s;t,x,v) &= \mathbf{v}_{\perp_{\mathbf{p}}}(s;t,x,v), \\ \dot{\mathbf{x}}_{\parallel_{\mathbf{p}}}(s;t,x,v) &= \mathbf{v}_{\parallel_{\mathbf{p}}}(s;t,x,v), \\ \dot{\mathbf{v}}_{\perp_{\mathbf{p}}}(s;t,x,v) &= F_{\perp_{\mathbf{p}}}(\mathbf{x}_{\mathbf{p}}(s;t,x,v),\mathbf{v}_{\mathbf{p}}(s;t,x,v)), \\ \dot{\mathbf{v}}_{\parallel_{\mathbf{p}}}(s;t,x,v) &= F_{\parallel_{\mathbf{p}}}(\mathbf{x}_{\mathbf{p}}(s;t,x,v),\mathbf{v}_{\mathbf{p}}(s;t,x,v)). \end{aligned} \tag{A.57}$$

Here

$$\begin{aligned} F_{\perp_{\mathbf{p}}} &= F_{\perp_{\mathbf{p}}}(\mathbf{x}_{\perp_{\mathbf{p}}},\mathbf{x}_{\parallel_{\mathbf{p}}},\mathbf{v}_{\parallel_{\mathbf{p}}}) \\ &= \sum_{j,k=1}^{2}\mathbf{v}_{\parallel_{\mathbf{p}},k}\mathbf{v}_{\parallel_{\mathbf{p}},j}\ \partial_j\partial_k\eta_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})\cdot\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}}) - \mathbf{x}_{\perp_{\mathbf{p}}}\sum_{k=1}^{2}\mathbf{v}_{\parallel_{\mathbf{p}},k}(\mathbf{v}_{\parallel_{\mathbf{p}}}\cdot\nabla)\partial_k\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})\cdot\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}}), \end{aligned} \tag{A.58}$$

where

$$\sum_{j,k=1}^{2}\mathbf{v}_{\parallel_{\mathbf{p}},k}\mathbf{v}_{\parallel_{\mathbf{p}},j}\ \partial_j\partial_k\eta_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}})\cdot\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\parallel_{\mathbf{p}}}) \lesssim_{\xi} -|\mathbf{v}_{\parallel}|^2,$$

and

$$\begin{aligned} F_{\|_{\mathbf{p}}} &= F_{\|_{\mathbf{p}}}(\mathbf{x}_{\perp_{\mathbf{p}}}, \mathbf{x}_{\|_{\mathbf{p}}}, \mathbf{v}_{\perp_{\mathbf{p}}}, \mathbf{v}_{\|_{\mathbf{p}}}) \\ &= \sum_i G_{\mathbf{p},ij}(\mathbf{x}_{\perp_{\mathbf{p}}}, \mathbf{x}_{\|_{\mathbf{p}}}) \frac{(-1)^i}{\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \cdot (\partial_1 \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \times \partial_2 \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}))} \\ &\quad \times \left\{ 2\mathbf{v}_{\perp_{\mathbf{p}}} \mathbf{v}_{\|_{\mathbf{p}}} \cdot \nabla \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) - \mathbf{v}_{\|_{\mathbf{p}}} \cdot \nabla^2 \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \cdot \mathbf{v}_{\|_{\mathbf{p}}} + \mathbf{x}_{\perp_{\mathbf{p}}} \mathbf{v}_{\|_{\mathbf{p}}} \cdot \nabla^2 \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \cdot \mathbf{v}_{\|_{\mathbf{p}}} \right\} \\ &\quad \cdot \left\{ \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \times \partial_{i+1} \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}}}) \right\}, \end{aligned} \tag{A.59}$$

where a smooth bounded function $G_{\mathbf{p},ij}(\mathbf{x}_{\perp_{\mathbf{p}}}, \mathbf{x}_{\|_{\mathbf{p}}})$ is specified in (A.69).

(iv) Let $\mathbf{q} = (y,u) \in \partial\Omega \times \mathbb{S}^2$ with $n(y) \cdot u = 0$ and $\mathbf{p} \sim \mathbf{q}$ and

$$\Phi_{\mathbf{p}}(\mathbf{x}_{\perp_{\mathbf{p}}}, \mathbf{x}_{\|_{\mathbf{p}}}, \mathbf{v}_{\perp_{\mathbf{p}}}, \mathbf{v}_{\|_{\mathbf{p}}}) = (x,v) = \Phi_{\mathbf{q}}(\mathbf{x}_{\perp_{\mathbf{q}}}, \mathbf{x}_{\|_{\mathbf{q}}}, \mathbf{v}_{\perp_{\mathbf{q}}}, \mathbf{v}_{\|_{\mathbf{q}}}).$$

Then

$$\frac{\partial(\mathbf{x}_{\perp_{\mathbf{p}}}, \mathbf{x}_{\|_{\mathbf{p}}}, \mathbf{v}_{\perp_{\mathbf{p}}}, \mathbf{v}_{\|_{\mathbf{p}}})}{\partial(\mathbf{x}_{\perp_{\mathbf{q}}}, \mathbf{x}_{\|_{\mathbf{q}}}, \mathbf{v}_{\perp_{\mathbf{q}}}, \mathbf{v}_{\|_{\mathbf{q}}})} = \nabla \Phi_{\mathbf{q}}^{-1} \nabla \Phi_{\mathbf{p}} = \mathbf{Id}_{6,6} + O_\xi(|\mathbf{p}-\mathbf{q}|) \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & & & \\ 0 & 1 & 1 & & \mathbf{0}_{3,3} & \\ 0 & 1 & 1 & & & \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & |v| & |v| & 0 & 1 & 1 \\ 0 & |v| & |v| & 0 & 1 & 1 \end{array} \right]. \tag{A.60}$$

Proof of (i) in Lemma A.10. Denote

$$\begin{aligned} \tfrac{z}{|z|} &= \hat{r}(\tfrac{z}{|z|}) := (\cos \mathbf{x}_{\|,1}(\tfrac{z}{|z|}) \sin \mathbf{x}_{\|,2}(\tfrac{z}{|z|}), \sin \mathbf{x}_{\|,1}(\tfrac{z}{|z|}) \sin \mathbf{x}_{\|,2}(\tfrac{z}{|z|}), \cos \mathbf{x}_{\|,2}(\tfrac{z}{|z|})), \\ w &= w_{\mathbf{x}_{\|,2}} \hat{\phi}(\tfrac{z}{|z|}) + w_{\mathbf{x}_{\|,1}} \hat{\theta}(\tfrac{z}{|z|}) := (w \cdot \hat{\phi}(\tfrac{z}{|z|})) \hat{\phi}(\tfrac{z}{|z|}) + (w \cdot \hat{\theta}(\tfrac{z}{|z|})) \hat{\theta}(\tfrac{z}{|z|}), \\ \tfrac{z}{|z|} \times w &= w_{\mathbf{x}_{\|,2}} \hat{\theta}(\tfrac{z}{|z|}) - w_{\mathbf{x}_{\|,1}} \hat{\phi}(\tfrac{z}{|z|}). \end{aligned}$$

We define the rotational matrix which maps $\{\frac{z}{|z|}, w, \frac{z}{|z|} \times w\} \mapsto \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$:

$$\mathcal{O}_{\mathbf{p}} = \begin{bmatrix} \frac{z}{|z|} \\ w \\ \frac{z}{|z|} \times w \end{bmatrix}_{3\times 3} = \begin{bmatrix} \hat{r}(\frac{z}{|z|}) \\ w_{\mathbf{x}_{\|_{\mathbf{p}},2}} \hat{\phi}(\frac{z}{|z|}) + w_{\mathbf{x}_{\|_{\mathbf{p}},1}} \hat{\theta}(\frac{z}{|z|}) \\ -w_{\mathbf{x}_{\|_{\mathbf{p}},1}} \hat{\phi}(\frac{z}{|z|}) + w_{\mathbf{x}_{\|_{\mathbf{p}},2}} \hat{\theta}(\frac{z}{|z|}) \end{bmatrix}_{3\times 3}.$$

For $x \in \partial\Omega$ with $x \neq \mathcal{N}_{\mathbf{p}}$ and $x \neq \mathcal{S}_{\mathbf{p}}$ we define

$$(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) \in [0,2\pi) \times (0,\pi), \quad \text{such that} \quad \hat{r}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) = \mathcal{O}_{\mathbf{p}}\Big(\frac{x}{|x|}\Big).$$

Now we define $R_{\mathbf{p}} : [0,2\pi) \times [0,\pi) \to (0,\infty)$ such that

$$\xi(R_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) \mathcal{O}_{\mathbf{p}}^{-1} \hat{r}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) = 0. \tag{A.61}$$

We also define $\eta_{\mathbf{p}} : [0,2\pi) \times [0,\pi) \to \partial\Omega$ such that

$$\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) = R_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) \mathcal{O}_{\mathbf{p}}^{-1} \hat{r}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}).$$

Directly, from (A.53) and (A.61), with fixed $\mathbf{p} = (z,w)$,

$$\begin{aligned} \frac{\partial R_{\mathbf{p}}}{\partial \mathbf{x}_{\|_{\mathbf{p}},1}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) &= \frac{-\sin(\mathbf{x}_{\|_{\mathbf{p}},2}) R_{\mathbf{p}} \nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{\theta}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}{\nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{r}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})} \\ &= \frac{-\sin(\mathbf{x}_{\|_{\mathbf{p}},2}) [R_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})]^2 \nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{\theta}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}{\nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}, \\ \frac{\partial R_{\mathbf{p}}}{\partial \mathbf{x}_{\|_{\mathbf{p}},2}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) &= \frac{-R_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2}) \nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{\phi}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}{\nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{r}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})} \\ &= \frac{-[R_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})]^2 \nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \mathcal{O}_{\mathbf{p}}^{-1} \hat{\phi}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}{\nabla \xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})) \cdot \eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1}, \mathbf{x}_{\|_{\mathbf{p}},2})}, \end{aligned}$$

where $\nabla\xi(\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1},\mathbf{x}_{\|_{\mathbf{p}},2}))\cdot\eta_{\mathbf{p}}(\mathbf{x}_{\|_{\mathbf{p}},1},\mathbf{x}_{\|_{\mathbf{p}},2})\neq 0$.

And by (A.53)

$$\begin{aligned}\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},1}}(\mathbf{x}_{\|_{\mathbf{p}},1},\mathbf{x}_{\|_{\mathbf{p}},2}) &= \frac{\partial R_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},1}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{r}+\sin(\mathbf{x}_{\|_{\mathbf{p}},2})R_{\mathbf{p}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{\theta},\\ \frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},2}}(\mathbf{x}_{\|_{\mathbf{p}},1},\mathbf{x}_{\|_{\mathbf{p}},2}) &= \frac{\partial R_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},2}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{r}+R_{\mathbf{p}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{\phi}.\end{aligned}$$

Directly we check a non-degenerate condition (A.55)

$$\begin{aligned}&\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},1}}(\mathbf{x}_{\|_{\mathbf{p}}})\times\frac{\partial\eta_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},2}}(\mathbf{x}_{\|_{\mathbf{p}}})\\ &= R_{\mathbf{p}}\frac{\partial R_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},1}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{\theta}+\sin(\mathbf{x}_{\|_{\mathbf{p}},2})R_{p}\frac{\partial R_{\mathbf{p}}}{\partial\mathbf{x}_{\|_{\mathbf{p}},2}}\mathcal{O}_{\mathbf{p}}^{-1}\hat{\phi}-\sin(\mathbf{x}_{\|_{\mathbf{p}},2})R_{\mathbf{p}}^{2}\mathcal{O}_{\mathbf{p}}^{-1}\hat{r}\neq 0.\end{aligned}$$

Proof of (ii) of Lemma A.10. We fix $\mathbf{p}=(z,w)$ and drop $\mathbf{p}-$index (for the chart) in this step. Define

$$\Phi_1:[0,\infty)\times[0,2\pi)\times(0,\pi)\to\bar{\Omega}\backslash\mathcal{L}_{\mathbf{p}},\quad \Phi_1(\mathbf{x}_\perp,\mathbf{x}_\|)=\eta(\mathbf{x}_\|)+\mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\|)]. \tag{A.62}$$

Note that this mapping is surjective : For any $x\in\bar{\Omega}\backslash\mathcal{L}_{\mathbf{p}}$, there exists (could be several) $\mathbf{x}_\|\in[0,2\pi)\times(0,\pi)$ satisfying $|x-\eta(\mathbf{x}_\|)|^2=\min_{\mathbf{y}_\|\in\mathbb{S}^2}|x-\eta(\mathbf{y}_\|)|^2$ ($\mathbb{S}^2$ is compact). Then $(x-\eta(\mathbf{x}_\|^*))\cdot\frac{\partial\eta}{\partial\mathbf{x}_{\|,i}}(\mathbf{x}_\|^*)=0$ for $i=1,2$. Since $\nabla\eta(\mathbf{x}_\|)\neq 0$ from (A.55) and $\xi(\eta(\mathbf{x}_\|))=0$, we have $0\equiv\nabla\xi(\eta(\mathbf{x}_\|))\cdot\frac{\partial\eta}{\partial\mathbf{x}_{\|,i}}(\mathbf{x}_\|)$. Due to (A.55), we conclude $\frac{x-\eta(\mathbf{x}_\|^*)}{|x-\eta(\mathbf{x}_\|^*)|}=[-\mathbf{n}(\mathbf{x}_\|^*)]$ and $x=\eta(\mathbf{x}_\|^*)+(x-\eta(\mathbf{x}_\|^*))=\eta(\mathbf{x}_\|^*)+|x-\eta(\mathbf{x}_\|^*)|[-\mathbf{n}(\mathbf{x}_\|^*)]$.

Since η and ξ (therefore n and $\mathbf{n}$) are smooth, the Φ_1 is smooth. The Jacobian matrix is

$$\frac{\partial\Phi_1(\mathbf{x}_\perp,\mathbf{x}_\|)}{\partial(\mathbf{x}_\perp,\mathbf{x}_\|)}=\begin{bmatrix}-\mathbf{n}(\mathbf{x}_\|) & \begin{smallmatrix}\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)\\ +\mathbf{x}_\perp[-\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)]\end{smallmatrix} & \begin{smallmatrix}\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)\\ +\mathbf{x}_\perp[-\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)]\end{smallmatrix}\end{bmatrix}_{3\times 3}, \tag{A.63}$$

where $\begin{bmatrix}-\mathbf{n}(\mathbf{x}_\|)\end{bmatrix}$, $\begin{bmatrix}\begin{smallmatrix}\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)\\ +\mathbf{x}_\perp[-\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)]\end{smallmatrix}\end{bmatrix}$, $\begin{bmatrix}\begin{smallmatrix}\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)\\ +\mathbf{x}_\perp[-\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)]\end{smallmatrix}\end{bmatrix}$ are column vectors in $\mathbb{R}^3$. By the basic linear algebra, the Jacobian (a determinant of the Jacobian matrix) equals

$$-\mathbf{n}\cdot(\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}}\times\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}})+\mathbf{x}_\perp\mathbf{n}\cdot(\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,1}}\times\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}})-\mathbf{x}_\perp\mathbf{n}\cdot(\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,2}}\times\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}})-|\mathbf{x}_\perp|^2\mathbf{n}\cdot(\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,1}}\times\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\|,2}}).$$

We use the facts $\nabla\eta(\mathbf{x}_\|)\neq 0$ and $\xi(\eta(\mathbf{x}_\|))=0$ and

$$0\equiv\nabla\xi(\eta(\mathbf{x}_\|))\cdot\frac{\partial\eta}{\partial\mathbf{x}_{\|,i}}(\mathbf{x}_\|)=|\nabla\xi(\eta(\mathbf{x}_\|))|\left(\mathbf{n}(\mathbf{x}_\|)\cdot\frac{\partial\eta}{\partial\mathbf{x}_{\|,i}}(\mathbf{x}_\|)\right),$$

and therefore

$$-\mathbf{n}(\mathbf{x}_\|)\cdot\left(\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)\times\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)\right)\neq 0,\quad \text{for all }\mathbf{x}_\|\in[0,2\pi)\times(0,\pi),$$

to conclude that there exists small $\delta>0$ such that if $|\mathbf{x}_\perp|\leq\delta$ and $\mathbf{x}_\|\in[0,2\pi)\times(0,\pi)$ then

$$\det\left(\frac{\partial\Phi_1(\mathbf{x}_\perp,\mathbf{x}_\|)}{\partial(\mathbf{x}_\perp,\mathbf{x}_\|)}\right)=-\mathbf{n}(\mathbf{x}_\|)\cdot\left(\frac{\partial\eta}{\partial\mathbf{x}_{\|,1}}(\mathbf{x}_\|)\times\frac{\partial\eta}{\partial\mathbf{x}_{\|,2}}(\mathbf{x}_\|)\right)+O_\xi(|\mathbf{x}_\perp|)\neq 0.$$

We use the inverse function theorem and we choose an inverse map

$$\Phi_1^{-1}:\Phi_1([0,\delta)\times[0,2\pi)\times(0,\pi))\to[0,\delta)\times[0,2\pi)\times(0,\pi).$$

Note that in general there are infinitely many inverse maps.

If $x\in\Phi_1([0,\delta)\times[0,2\pi)\times(0,\pi))$ then

$$\Phi_1^{-1}(x):=(\mathbf{x}_\perp,\mathbf{x}_\|)\quad\text{and}\quad x=\eta(\mathbf{x}_\|)+\mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\|)].$$

Since Φ_1 is surjective onto $\bar{\Omega}\backslash\mathcal{L}_{\mathbf{p}}$, for $x \in \bar{\Omega}\backslash\mathcal{L}_{\mathbf{p}}$ and $\mathbf{x}_\perp \geq 0$,

$$\begin{aligned}
\xi(x) &= \xi(\eta(\mathbf{x}_\parallel) + \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)]) \\
&= \xi(\eta(\mathbf{x}_\parallel)) + \int_0^{\mathbf{x}_\perp} \frac{d}{ds}\xi(\eta(\mathbf{x}_\parallel) + s[-\mathbf{n}(\mathbf{x}_\parallel)])\mathrm{d}s \\
&= \int_0^{\mathbf{x}_\perp} [-\mathbf{n}(\mathbf{x}_\parallel)] \cdot \nabla\xi(\eta(\mathbf{x}_\parallel) + s[-\mathbf{n}(\mathbf{x}_\parallel)])\mathrm{d}s \\
&= \int_0^{\mathbf{x}_\perp} \Big\{[-\mathbf{n}(\mathbf{x}_\parallel)] \cdot \nabla\xi(\eta(\mathbf{x}_\parallel)) + \int_0^s \mathbf{n}(\mathbf{x}_\parallel) \cdot \nabla^2\xi(\eta(\mathbf{x}_\parallel) + \tau[-\mathbf{n}(\mathbf{x}_\parallel)]) \cdot \mathbf{n}(\mathbf{x}_\parallel)\mathrm{d}\tau\Big\}\mathrm{d}s,
\end{aligned}$$

and by the convexity of ξ we have the following equivalent relation :

For all $x \in \bar{\Omega}$ there exists (not uniquely) $(\mathbf{x}_\perp, \mathbf{x}_\parallel) \in [0,\infty)\times[0,2\pi)\times(0,\pi)$ satisfying $x = \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)] + \eta(\mathbf{x}_\parallel)$. Then for all $(\mathbf{x}_\perp, \mathbf{x}_\parallel)$ with $x = \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)] + \eta(\mathbf{x}_\parallel)$ we have

$$\begin{aligned}
|\nabla\xi(\eta(\mathbf{x}_\parallel))||\mathbf{x}_\perp| - \frac{1}{C_\xi}\frac{|\mathbf{x}_\perp|^2}{2} \ &\leq \ |\xi(x)| = |\xi(\eta(\mathbf{x}_\parallel) + \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)])| \\
&\leq \ |\nabla\xi(\eta(\mathbf{x}_\parallel))||\mathbf{x}_\perp| - C_\xi\frac{|\mathbf{x}_\perp|^2}{2}.
\end{aligned} \tag{A.64}$$

Therefore there exists $0 < C_1 \ll 1$ such that if $|\xi(x)| \leq C_1\delta$ then $|\mathbf{x}_\perp| < \delta$ and hence there exists unique $(\mathbf{x}_\perp, \mathbf{x}_\parallel)$ and all the above computations hold.

Next we define

$$\Phi(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel) = \begin{pmatrix} \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)] + \eta(\mathbf{x}_\parallel) \\ \mathbf{v}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)] + \mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\eta(\mathbf{x}_\parallel) - \mathbf{x}_\perp\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\mathbf{n}(\mathbf{x}_\parallel) \end{pmatrix}.$$

The Jacobian matrix is

$$\frac{\partial\Phi(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel)}{\partial(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel)} = \left[\begin{array}{ccc|c} \multicolumn{3}{c|}{\frac{\partial\Phi_1(\mathbf{x}_\perp,\mathbf{x}_\parallel)}{\partial(\mathbf{x}_\perp,\mathbf{x}_\parallel)}} & \mathbf{0}_{3,3} \\ \hline -\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\mathbf{n}(\mathbf{x}_\parallel) & \begin{array}{c} -\mathbf{v}_\perp \frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\parallel,1}}(\mathbf{x}_\parallel) \\ +\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\frac{\partial\eta}{\partial\mathbf{x}_{\parallel,1}}(\mathbf{x}_\parallel) \\ -\mathbf{x}_\perp\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\parallel,1}}(\mathbf{x}_\parallel) \end{array} & \begin{array}{c} -\mathbf{v}_\perp \frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\parallel,2}}(\mathbf{x}_\parallel) \\ +\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\frac{\partial\eta}{\partial\mathbf{x}_{\parallel,2}}(\mathbf{x}_\parallel) \\ -\mathbf{x}_\perp\mathbf{v}_\parallel \cdot \nabla_{\mathbf{x}_\parallel}\frac{\partial\mathbf{n}}{\partial\mathbf{x}_{\parallel,2}}(\mathbf{x}_\parallel) \end{array} & \frac{\partial\Phi_1(\mathbf{x}_\perp,\mathbf{x}_\parallel)}{\partial(\mathbf{x}_\perp,\mathbf{x}_\parallel)} \end{array}\right]. \tag{A.65}$$

The Jacobian (a determinant of the Jacobian matrix) equals

$$\det\left(\frac{\partial\Phi(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel)}{\partial(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel)}\right) = \left(\det\left(\frac{\partial\Phi_1(\mathbf{x}_\perp, \mathbf{x}_\parallel)}{\partial(\mathbf{x}_\perp, \mathbf{x}_\parallel)}\right)\right)^2 \neq 0,$$

for $|\xi(x)| \leq \delta$ (and therefore $|\mathbf{x}_\perp| \leq C\delta$) and $\mathbf{x}_{\parallel,2} \in (0,\pi)$. By the inverse function theorem we have the inverse mapping Φ^{-1}.

Proof of (iii) of Lemma A.10. From $\dot{v} = 0$ and the second equation of (A.56) equals

$$\begin{aligned}
0 =& \dot{\mathbf{v}}_\perp(s)[-\mathbf{n}(\mathbf{x}_\parallel(s))] - 2\mathbf{v}_\perp(s)\mathbf{v}_\parallel \cdot \nabla\mathbf{n}(\mathbf{x}_\parallel(s)) + \dot{\mathbf{v}}_\parallel(s) \cdot \nabla\eta(\mathbf{x}_\parallel(s)) \\
&+ \mathbf{v}_\parallel \cdot \nabla^2\eta(\mathbf{x}_\parallel) \cdot \mathbf{v}_\parallel - \mathbf{x}_\perp\dot{\mathbf{v}}_\parallel \cdot \nabla\mathbf{n}(\mathbf{x}_\parallel) + \mathbf{x}_\perp\mathbf{v}_\parallel \cdot \nabla^2\mathbf{n}(\mathbf{x}_\parallel) \cdot \mathbf{v}_\parallel.
\end{aligned} \tag{A.66}$$

We take the inner product with $\mathbf{n}(\mathbf{x}_\parallel(s))$ to the above equation to have

$$\dot{\mathbf{v}}_\perp(s) = [\mathbf{v}_\parallel \cdot \nabla^2\eta(\mathbf{x}_\parallel) \cdot \mathbf{v}_\parallel] \cdot \mathbf{n}(\mathbf{x}_\parallel) + \mathbf{x}_\perp[\mathbf{v}_\parallel \cdot \nabla^2\mathbf{n}(\mathbf{x}_\parallel) \cdot \mathbf{v}_\parallel] \cdot \mathbf{n}(\mathbf{x}_\parallel) := F_\perp(\mathbf{v}_\perp, \mathbf{v}_\parallel, \mathbf{x}_\parallel), \tag{A.67}$$

where we have used the fact $\nabla\mathbf{n} \perp \mathbf{n}$ and $\nabla\eta \perp \mathbf{n}$.

Since $0 = \xi(\eta(\mathbf{x}_\parallel))$ we take $\mathbf{x}_{\parallel,i}$ and $\mathbf{x}_{\parallel,j}$ derivatives to have

$$0 = \partial_{\mathbf{x}_{\parallel,j}}\big[\sum_k \partial_k\xi\partial_{\mathbf{x}_{\parallel},i}\eta_k\big] = \sum_{k,m}\partial_k\partial_m\xi\partial_{\mathbf{x}_{\parallel,j}}\eta_m\partial_{\mathbf{x}_{\parallel,i}}\eta_k + \sum_k \partial_k\xi\partial_{\mathbf{x}_{\parallel,i}}\partial_{\mathbf{x}_{\parallel,j}}\eta_k,$$

we have from the convexity (A.3)

$$\big[\mathbf{v}_\parallel \cdot \nabla^2\eta \cdot \mathbf{v}_\parallel\big] \cdot \mathbf{n} = \sum_{i,j,k}\frac{\mathbf{v}_{\parallel,i}\partial_k\xi\partial_i\partial_j\eta_k\mathbf{v}_{\parallel,j}}{|\nabla\xi|} = -\sum_{i,j,k,m}\frac{\{\mathbf{v}_{\parallel,i}\partial_i\eta_m\}\partial_k\partial_m\xi\{\partial_j\eta_m\mathbf{v}_{\parallel,j}\}}{|\nabla\xi|} \lesssim_\xi -|\mathbf{v}_\parallel|^2.$$

Define $a_{ij}(\mathbf{x}_\|)$ via

$$\left[\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right] = \left[\begin{array}{cc} \partial_1\mathbf{n}\cdot\partial_1\mathbf{n} & \partial_1\mathbf{n}\cdot\partial_2\mathbf{n} \\ \partial_2\mathbf{n}\cdot\partial_1\mathbf{n} & \partial_2\mathbf{n}\cdot\partial_2\mathbf{n} \end{array}\right] \left[\begin{array}{cc} \partial_1\eta\cdot\partial_1\eta & \partial_1\eta\cdot\partial_2\eta \\ \partial_2\eta\cdot\partial_1\eta & \partial_2\eta\cdot\partial_2\eta \end{array}\right]^{-1},$$

where $\det(\partial_i\eta\cdot\partial_j\eta) = |\partial_1\eta\times\partial_2\eta|^2 \neq 0$ due to (A.55). Then $\nabla\mathbf{n}$ is generated by $\nabla\eta$:

$$-\partial_i\mathbf{n}(\mathbf{x}_\|) = \sum_k a_{ik}(\mathbf{x}_\|)\partial_k\eta(\mathbf{x}_\|).$$

We take the inner product (A.66) with $(-1)^{i+1}(\mathbf{n}(\mathbf{x}_\|)\times\partial_i\mathbf{n}(\mathbf{x}_\|))$ to have

$$\begin{aligned} &\sum_k(\delta_{ki}+\mathbf{x}_\perp a_{ki})\dot{\mathbf{v}}_{\|,k} \\ &= \frac{(-1)^{i+1}}{-\mathbf{n}(\mathbf{x}_\|)\cdot(\partial_1\eta(\mathbf{x}_\|)\times\partial_2\eta(\mathbf{x}_\|))} \\ &\quad\times\Big\{-2\mathbf{v}_\perp\mathbf{v}_\|\cdot\nabla\mathbf{n}(\mathbf{x}_\|)+\mathbf{v}_\|\cdot\nabla^2\eta(\mathbf{x}_\|)\cdot\mathbf{v}_\| - \mathbf{x}_\perp\mathbf{v}_\|\cdot\nabla^2\mathbf{n}(\mathbf{x}_\|)\cdot\mathbf{v}_\|\Big\}\cdot(-\mathbf{n}(\mathbf{x}_\|)\times\partial_{i+1}\eta(\mathbf{x}_\|)), \end{aligned}$$

where we used the notational convention for $\partial_{i+1}\eta$, the index $i+1$ mod 2 . For $|\xi(x)|\ll 1$(and therefore $|\mathbf{x}_\perp|\ll 1$) the matrix $\delta_{ki}+\mathbf{x}_\perp a_{ki}$ is invertible : there exists the inverse matrix G_{ij} such that $\sum_i(\delta_{ki}+\mathbf{x}_\perp a_{ki}(\mathbf{x}_\|))G_{ij}(\mathbf{x}_\perp,\mathbf{x}_\|)=\delta_{kj}$. Therefore we have

$$\begin{aligned} \dot{\mathbf{v}}_{\|,j} &= \sum_i G_{ij}(\mathbf{x}_\perp,\mathbf{x}_\|)\frac{(-1)^{i+1}}{-\mathbf{n}(\mathbf{x}_\|)\cdot(\partial_1\eta(\mathbf{x}_\|)\times\partial_2\eta(\mathbf{x}_\|))} \\ &\quad\times\Big\{-2\mathbf{v}_\perp\mathbf{v}_\|\cdot\nabla\mathbf{n}(\mathbf{x}_\|)+\mathbf{v}_\|\cdot\nabla^2\eta(\mathbf{x}_\|)\cdot\mathbf{v}_\| - \mathbf{x}_\perp\mathbf{v}_\|\cdot\nabla^2\mathbf{n}(\mathbf{x}_\|)\cdot\mathbf{v}_\|\Big\} \\ &\quad\cdot(-\mathbf{n}(\mathbf{x}_\|)\times\partial_{i+1}\eta(\mathbf{x}_\|)) \\ &:= F_{\|,j}(\mathbf{x}_\perp,\mathbf{x}_\|,\mathbf{v}_\perp,\mathbf{v}_\|). \end{aligned} \tag{A.68}$$

Here

$$\begin{aligned} &\left[\begin{array}{cc} G_{11} & G_{12} \\ G_{21} & G_{22} \end{array}\right] \\ &= \frac{1}{1+\mathbf{x}_\perp(a_{11}+a_{22})+(\mathbf{x}_\perp)^2(a_{11}a_{22}-a_{12}a_{21})}\left[\begin{array}{cc} 1+\mathbf{x}_\perp a_{22} & -\mathbf{x}_\perp a_{12} \\ -\mathbf{x}_\perp a_{21} & 1+\mathbf{x}_\perp a_{11} \end{array}\right], \\ &\left[\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right] \\ &= \frac{1}{|\partial_1\eta|^2|\partial_2\eta|^2-(\partial_1\eta\cdot\partial_2\eta)^2} \\ &\quad\times\left[\begin{array}{cc} |\partial_1\mathbf{n}|^2|\partial_2\eta|^2-(\partial_1\mathbf{n}\cdot\partial_2\mathbf{n})(\partial_1\eta\cdot\partial_2\eta) & -|\partial_1\mathbf{n}|^2(\partial_1\eta\cdot\partial_2\eta)+(\partial_1\mathbf{n}\cdot\partial_2\mathbf{n})|\partial_1\eta|^2 \\ (\partial_1\mathbf{n}\cdot\partial_2\mathbf{n})|\partial_2\eta|^2-|\partial_2\mathbf{n}|^2(\partial_1\eta\cdot\partial_2\eta) & -(\partial_1\mathbf{n}\cdot\partial_2\mathbf{n})(\partial_1\eta\cdot\partial_2\eta)+|\partial_2\mathbf{n}|^2|\partial_1\eta|^2 \end{array}\right]. \end{aligned} \tag{A.69}$$

Proof of (iv) of Lemma A.10. Let $\mathbf{q}=(y,u)\in\partial\Omega\times\mathbb{S}^2$ with $n(y)\cdot u=0$ and $\mathbf{p}\sim\mathbf{q}$. First we claim

$$\begin{aligned} \mathbf{x}_{\perp_\mathbf{p}} &= \mathbf{x}_{\perp_\mathbf{q}}, \\ \eta_\mathbf{p}(\mathbf{x}_{\|_\mathbf{p}}) &= \eta_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}}), \\ \mathbf{v}_{\perp_\mathbf{p}} &= \mathbf{v}_{\perp_\mathbf{q}}, \\ \mathbf{v}_{\|_\mathbf{p}}\cdot\nabla\eta_\mathbf{p}(\mathbf{x}_{\|_\mathbf{p}})-\mathbf{x}_{\perp_\mathbf{p}}\mathbf{v}_{\|_\mathbf{p}}\cdot\nabla\mathbf{n}_\mathbf{p}(\mathbf{x}_{\|_\mathbf{p}}) &= \mathbf{v}_{\|_\mathbf{q}}\cdot\nabla\eta_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}})-\mathbf{x}_{\perp_\mathbf{q}}\mathbf{v}_{\|_\mathbf{q}}\cdot\nabla\mathbf{n}_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}}). \end{aligned} \tag{A.70}$$

Once we show the first two equalities then the third and fourth equalities are clearly valid because $\mathbf{n}_\mathbf{p}\perp\mathbf{v}_\|\cdot\nabla_{\mathbf{x}_\|}\eta_\mathbf{p}$ and $\mathbf{n}_\mathbf{p}\perp\mathbf{v}_\|\cdot\nabla_{\mathbf{x}_\|}\mathbf{n}_\mathbf{p}$ for all $\mathbf{v}_\|\in\mathbb{R}^2$. (Since $\xi(\eta_\mathbf{p})=0$ we have $\mathbf{v}_{\|,i}\partial_{\mathbf{x}_{\|,i}}[\xi(\eta_\mathbf{p}(\mathbf{x}_{\|,1},\mathbf{x}_{\|,2}))] = \mathbf{v}_{\|,i}\partial_{\mathbf{x}_{\|,i}}\eta_\mathbf{p}\cdot\nabla_{\mathbf{x}_\|}\xi=0$, and since $\mathbf{n}_\mathbf{p}\cdot\mathbf{n}_\mathbf{p}=1$ we have $\mathbf{n}_\mathbf{p}\cdot[\mathbf{v}_\|\cdot\nabla_{\mathbf{x}_\|}\mathbf{n}_\mathbf{p}]=0$)

Now we prove the first two equalities of (A.70) and it suffices to prove the second one. And it suffices to show that for $x\in\bar{\Omega}$ with $|\xi(x)|\ll 1$ there exists a unique $x^*\in\partial\Omega\cap B(x,\delta)$ for some $0<\delta\ll 1$ such that

$$|x-x^*|^2 = \min_{y\in\partial\Omega, y\sim x}|x-y|^2. \tag{A.71}$$

By the definition of $(A.62)$ the uniqueness of such x^* in (A.71) implies $\eta_{\mathbf{p}}(\mathbf{x}_{\|_\mathbf{p}}) = x^* = \eta_{\mathbf{q}}(\mathbf{x}_{\|_\mathbf{q}})$.

The existence of such $x^* \in \partial\Omega$ is clear from the compactness of $\partial\Omega$. Without loss of generality (up to rotation) we may assume $\partial_{x_3}\xi(y) \neq 0$ for $y \sim x^*$ and $\partial_{x_1}\xi(x^*) = 0 = \partial_{x_2}\xi(x^*)$. Then we can find the graph $a : (x_1, x_2) \mapsto \mathbb{R}$ but $\xi(x_1, x_2, a(x_1, x_2)) = 0$ when $x^* = (x_1^*, x_2^*, a(x_1^*, x_2^*)) \in \partial\Omega$. By the implicit function theorem,

$$\partial_{x_1} a = -\partial_{x_1}\xi/\partial_{x_3}\xi, \quad \partial_{x_2} a = -\partial_{x_2}\xi/\partial_{x_3}\xi,$$

and $\partial_{x_1} a(x_1^*, x_2^*) = 0 = \partial_{x_2} a(x_1^*, x_2^*)$.

Clearly $x^* = (x_1^*, x_2^*, a(x_1^*, x_2^*))$ satisfies $\big|(x_1, x_2, x_3) - (x_1^*, x_2^*, a(x_1^*, x_2^*))\big| \ll 1$ and

$$\frac{\partial}{\partial x_i^*}\big|(x_1, x_2, x_3) - (x_1^*, x_2^*, a(x_1^*, x_2^*))\big|^2 = -\Big\{(x_i - x_i^*) + (x_3 - a(x_1^*, x_2^*))\frac{\partial a}{\partial x_i^*}(x_1^*, x_2^*)\Big\} = 0, \quad \text{for } i = 1, 2,$$

if and only if (A.71) holds. We take x_i^*-derivative to get

$$1 + \Big(\frac{\partial a}{\partial x_i^*}(x_1^*, x_2^*)\Big)^2 - (x_3 - a(x_1^*, x_2^*))\frac{\partial^2 a}{\partial x_i^* \partial x_i^*}(x_1^*, x_2^*) = 1 - (x_3 - a(x_1^*, x_2^*))\frac{\partial^2 a}{\partial x_i^* \partial x_i^*}(x_1^*, x_2^*) \neq 0,$$

for $|x_3 - a(x_1^*, x_2^*)| \ll_\xi 1$. Using the inverse function theorem we have a uniquely determined $x^* : \{y \in \bar{\Omega} : y \sim x\} \to \partial\Omega \cap B(x, \delta)$. This proves our claim (uniqueness of x^* in (A.71)) and therefore we prove (A.70).

From the second equality of (A.70) and (A.54)

$$\hat{r}(\mathbf{x}_{\|_\mathbf{q},1}, \mathbf{x}_{\|_\mathbf{q},2}) = \mathcal{O}_\mathbf{q}\mathcal{O}_\mathbf{p}^{-1}\hat{r}(\mathbf{x}_{\|_\mathbf{p},1}, \mathbf{x}_{\|_\mathbf{p},2}).$$

Therefore for $i = 1, 2$,

$$\sum_{j=1,2}\frac{\partial \hat{r}}{\partial \mathbf{x}_{\|_\mathbf{q},j}}(\mathbf{x}_{\|_\mathbf{q}})\frac{\partial \mathbf{x}_{\|_\mathbf{q},j}}{\partial \mathbf{x}_{\|_\mathbf{p},i}} = \mathcal{O}_\mathbf{q}\mathcal{O}_\mathbf{p}^{-1}\frac{\partial \hat{r}}{\partial \mathbf{x}_{\|_\mathbf{p},i}}(\mathbf{x}_{\|_\mathbf{p}}),$$

and from (A.53)

$$\begin{aligned}&\left[\begin{array}{c|c|c} -\sin(\mathbf{x}_{\|_\mathbf{q},2})\hat{r}(\mathbf{x}_{\|_\mathbf{q}}) & \sin(\mathbf{x}_{\|_\mathbf{q},2})\hat{\theta}(\mathbf{x}_{\|_\mathbf{q}}) & \hat{\phi}(\mathbf{x}_{\|_\mathbf{q}}) \end{array}\right]\left[\begin{array}{c|c} 0 & \mathbf{0}_{1,2} \\ \hline \mathbf{0}_{2,1} & \frac{\partial \mathbf{x}_{\|_\mathbf{q}}}{\partial \mathbf{x}_{\|_\mathbf{p}}} \end{array}\right]_{3\times 3} \\ &= \mathcal{O}_\mathbf{q}\mathcal{O}_\mathbf{p}^{-1}\left[\begin{array}{c|c|c} \mathbf{0}_{3,1} & \sin(\mathbf{x}_{\|_\mathbf{p},2})\hat{\theta}(\mathbf{x}_{\|_\mathbf{p}}) & \hat{\phi}(\mathbf{x}_{\|_\mathbf{p}}) \end{array}\right],\end{aligned}$$

where we used $\hat{\theta} \times \hat{\phi} = -\hat{r}$.

For $\mathbf{x}_{\|_\mathbf{p},2}, \mathbf{x}_{\|_\mathbf{q},2} \notin \{0, \pi\}$,

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{\partial \mathbf{x}_{\|_\mathbf{q},1}}{\partial \mathbf{x}_{\|_\mathbf{p},1}} & \frac{\partial \mathbf{x}_{\|_\mathbf{q},1}}{\partial \mathbf{x}_{\|_\mathbf{p},2}} \\ 0 & \frac{\partial \mathbf{x}_{\|_\mathbf{q},2}}{\partial \mathbf{x}_{\|_\mathbf{p},1}} & \frac{\partial \mathbf{x}_{\|_\mathbf{q},2}}{\partial \mathbf{x}_{\|_\mathbf{p},2}} \end{bmatrix} = \begin{bmatrix} \frac{-1}{\sin(\mathbf{x}_{\|_\mathbf{q},2})}\hat{r}(\mathbf{x}_{\|_\mathbf{q}})^T \\ \frac{1}{\sin(\mathbf{x}_{\|_\mathbf{q},2})}\hat{\theta}(\mathbf{x}_{\|_\mathbf{q}})^T \\ \hat{\phi}(\mathbf{x}_{\|_\mathbf{q}})^T \end{bmatrix}\mathcal{O}_\mathbf{q}\mathcal{O}_\mathbf{p}^{-1}\left[\begin{array}{c|c|c} \mathbf{0}_{3,1} & \sin(\mathbf{x}_{\|_\mathbf{p},2})\hat{\theta}(\mathbf{x}_{\|_\mathbf{p}}) & \hat{\phi}(\mathbf{x}_{\|_\mathbf{p}}) \end{array}\right].$$

Here $\mathcal{O}_\mathbf{q} = \mathcal{O}_\mathbf{p} + O_\xi(|\mathbf{p} - \mathbf{q}|)$, and $\sin(\mathbf{x}_{\|_\mathbf{p},2})\hat{\theta}(\mathbf{x}_{\|_\mathbf{p}}) = \sin(\mathbf{x}_{\|_\mathbf{q},2})\hat{\theta}(\mathbf{x}_{\|_\mathbf{q}}) + O_\xi(|\mathbf{p} - \mathbf{q}|)$ and $\hat{\phi}(\mathbf{x}_{\|_\mathbf{p}}) = \hat{\phi}(\mathbf{x}_{\|_\mathbf{q}}) + O_\xi(|\mathbf{p} - \mathbf{q}|)$.

Therefore for $\mathbf{x}_{\|_\mathbf{p},2}, \mathbf{x}_{\|_\mathbf{q},2} \notin \{0, \pi\}$

$$\left[\frac{\partial \mathbf{x}_{\|_\mathbf{q}}}{\partial \mathbf{x}_{\|_\mathbf{p}}}\right]_{2\times 2} \lesssim \mathbf{Id}_{2,2} + O_\xi(|\mathbf{p} - \mathbf{q}|). \tag{A.72}$$

From the third equality of (A.70)

$$\left[\begin{array}{c|c|c} -\mathbf{n}_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}}) & \substack{\partial_1\eta_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}}) \\ -\mathbf{x}_{\perp_\mathbf{q}}\partial_1\mathbf{n}_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}})} & \substack{\partial_2\eta_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}}) \\ -\mathbf{x}_{\perp_\mathbf{q}}\partial_2\mathbf{n}_\mathbf{q}(\mathbf{x}_{\|_\mathbf{q}})} \end{array}\right]\left[\begin{array}{c|c} 0 & \mathbf{0}_{1,2} \\ \hline \mathbf{0}_{2,1} & \frac{\partial \mathbf{v}_{\|_\mathbf{q}}}{\partial \mathbf{x}_{\|_\mathbf{p}}} \end{array}\right] = \left[\begin{array}{c|c|c} \mathbf{0}_{3,1} & Z_1 & Z_2 \end{array}\right],$$

and

$$Z_i = \sum_{j=1}^{2} \mathbf{v}_{\|\mathbf{p},j} \sum_{m=1}^{2} \Big(\partial_m \partial_j \eta_{\mathbf{p}} - \mathbf{x}_{\perp_{\mathbf{p}}} \partial_m \partial_j \mathbf{n}_{\mathbf{p}}\Big)\Big(\delta_{mi} - \frac{\partial \mathbf{x}_{\|\mathbf{q},m}}{\partial \mathbf{x}_{\|\mathbf{p},i}}\Big) \lesssim O_\xi(1)|v||\mathbf{p}-\mathbf{q}|,$$

where we have used (A.72).

Therefore

$$\left[\begin{array}{c|c} 0 & \mathbf{0}_{1,2} \\ \hline \mathbf{0}_{2,1} & \frac{\partial \mathbf{v}_{\|\mathbf{q}}}{\partial \mathbf{x}_{\|\mathbf{p}}} \end{array}\right] = \frac{1}{[-\mathbf{n}_{\mathbf{q}}]\cdot\big([\partial_1 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_1 \mathbf{n}_{\mathbf{q}}] \times [\partial_2 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_2 \mathbf{n}_{\mathbf{q}}]\big)}$$
$$\times \left[\begin{array}{c} (\partial_1 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_1 \mathbf{n}_{\mathbf{q}}) \times (\partial_2 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_2 \mathbf{n}_{\mathbf{q}}) \\ (\partial_2 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_2 \mathbf{n}_{\mathbf{q}}) \times (-\mathbf{n}_{\mathbf{q}}) \\ (-\mathbf{n}_{\mathbf{q}}) \times (\partial_1 \eta_{\mathbf{q}} - \mathbf{x}_{\perp_{\mathbf{q}}}\partial_1 \mathbf{n}_{\mathbf{q}}) \end{array}\right] \left[\begin{array}{c|c|c} \mathbf{0}_{3,1} & Z_1 & Z_2 \end{array}\right],$$

and hence from the above estimate of Z_i we have

$$\left[\frac{\partial \mathbf{v}_{\|\mathbf{q}}}{\partial \mathbf{x}_{\|\mathbf{p}}}\right]_{2\times 2} \lesssim_\xi |v||\mathbf{p}-\mathbf{q}|.$$

Again from the third equality of (A.70)

$$\left[\begin{array}{c|c|c} -\mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) & \begin{array}{c}\partial_1 \eta_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) \\ -\mathbf{x}_{\perp_{\mathbf{q}}}\partial_1 \mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}})\end{array} & \begin{array}{c}\partial_2 \eta_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) \\ -\mathbf{x}_{\perp_{\mathbf{q}}}\partial_2 \mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}})\end{array} \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{\partial \mathbf{v}_{\|\mathbf{q}}}{\partial \mathbf{v}_{\|\mathbf{p}}} \end{array}\right]$$
$$= \left[\begin{array}{c|c|c} -\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) & \begin{array}{c}\partial_1 \eta_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) \\ -\mathbf{x}_{\perp_{\mathbf{p}}}\partial_1 \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}})\end{array} & \begin{array}{c}\partial_2 \eta_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) \\ -\mathbf{x}_{\perp_{\mathbf{p}}}\partial_2 \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}})\end{array} \end{array}\right].$$

Since

$$\left[\begin{array}{c|c|c} -\mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) & \begin{array}{c}\partial_1 \eta_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) \\ -\mathbf{x}_{\perp_{\mathbf{p}}}\partial_1 \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}})\end{array} & \begin{array}{c}\partial_2 \eta_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}}) \\ -\mathbf{x}_{\perp_{\mathbf{p}}}\partial_2 \mathbf{n}_{\mathbf{p}}(\mathbf{x}_{\|\mathbf{p}})\end{array} \end{array}\right]$$
$$= \left[\begin{array}{c|c|c} -\mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) & \begin{array}{c}\partial_1 \eta_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) \\ -\mathbf{x}_{\perp_{\mathbf{q}}}\partial_1 \mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}})\end{array} & \begin{array}{c}\partial_2 \eta_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}}) \\ -\mathbf{x}_{\perp_{\mathbf{q}}}\partial_2 \mathbf{n}_{\mathbf{q}}(\mathbf{x}_{\|\mathbf{q}})\end{array} \end{array}\right] + O_\xi(|\mathbf{p}-\mathbf{q}|),$$

we have

$$\left[\begin{array}{cc} \frac{\partial \mathbf{v}_{\|\mathbf{q},1}}{\partial \mathbf{v}_{\|\mathbf{p},1}} & \frac{\partial \mathbf{v}_{\|\mathbf{q},1}}{\partial \mathbf{v}_{\|\mathbf{p},2}} \\ \frac{\partial \mathbf{v}_{\|\mathbf{q},2}}{\partial \mathbf{v}_{\|\mathbf{p},1}} & \frac{\partial \mathbf{v}_{\|\mathbf{q},2}}{\partial \mathbf{v}_{\|\mathbf{p},2}} \end{array}\right] = \mathbf{Id}_{2,2} + O_\xi(|\mathbf{p}-\mathbf{q}|).$$

□

We are ready to prove Theorem A.3 :

Proof of Theorem A.3. First we consider the case of $t < t_{\mathbf{b}}(x,v)$. In this case

$$(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v)) = (x-(t-s)v, v).$$

Directly

$$\frac{\partial(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s,t,x,v))}{\partial(t,x,v)} = \left[\begin{array}{ccc} -v & \mathbf{Id}_{3,3} & -(t-s)\mathbf{Id}_{3,3} \\ \mathbf{0}_{3,1} & \mathbf{0}_{3,3} & \mathbf{Id}_{3,3} \end{array}\right]_{6\times 7}$$
$$:= \left[\begin{array}{c|ccc|ccc} -v_1 & 1 & 0 & 0 & -(t-s) & 0 & 0 \\ -v_2 & 0 & 1 & 0 & 0 & -(t-s) & 0 \\ -v_3 & 0 & 0 & 1 & 0 & 0 & -(t-s) \\ \hline 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right],$$

where $\mathbf{Id}_{m,m}$ is the m by m identity matrix and $\mathbf{0}_{m,n}$ is the m by n zero matrix.

Now we consider the case of $t \geq t_{\mathbf{b}}(x,v)$. We split our proof into 10 steps.

Step 1. Moving frames and grouping with respect to the scaling $t|v| = L_\xi$, with fixed $0 < L_\xi \ll 1$.

Fix $(t,x,v) \in [0,\infty) \times \bar{\Omega} \times \mathbb{R}^3$. Also we fix small constant $\delta = \delta_\xi > 0$ which depends on the domain. We define, at the boundary,

$$\mathbf{r}^\ell := \frac{|\mathbf{v}_\perp^\ell|}{|v^\ell|} = \frac{|v \cdot n(x^\ell)|}{|v|} = \frac{|V_{\mathbf{cl}}(t^\ell;t,x,v) \cdot n(X_{\mathbf{cl}}(t^\ell;t,x,v))|}{|v|}. \tag{A.73}$$

Bounces ℓ(and (t^ℓ, x^ℓ, v^ℓ)) are categorized as *Type I* or *Type II* :

$$\begin{aligned} &\text{a bounce } \ell \text{ is } \textit{Type I (almost grazing)} \text{ if and only if } \mathbf{r}^\ell \leq \sqrt{\delta}, \\ &\text{a bounce } \ell \text{ is } \textit{Type II (non-grazing)} \text{ if and only if } \mathbf{r}^\ell > \sqrt{\delta}. \end{aligned} \tag{A.74}$$

Let $s_* \in [t^{\ell+1}, t^\ell]$ such that $|\xi(X_{\mathbf{cl}}(s_*;t^\ell,x^\ell,v^\ell))| = \max_{t^{\ell+1}\leq\tau\leq t^\ell} |\xi(X_{\mathbf{cl}}(\tau;t^\ell,x^\ell,v^\ell))|$. Since we have $\frac{d^2}{ds^2}\xi(X_{\mathbf{cl}}(s;t^\ell,x^\ell,v^\ell)) = \frac{d^2}{ds^2}\xi(x^\ell - (t^\ell - s)v^\ell) = v^\ell \cdot \nabla_x^2 \xi(x^\ell - (t^\ell - s)v^\ell) \cdot v^\ell > 0$ there exists a unique s solving $\frac{d}{ds}\xi(X_{\mathbf{cl}}(s;t^\ell,x^\ell,v^\ell)) = v^\ell \cdot \nabla_x \xi(X_{\mathbf{cl}}(s;t^\ell,x^\ell,v^\ell)) = 0$ which is s_*. Note that $v^\ell \cdot \nabla\xi(x^\ell - (t^\ell - s)v^\ell)$ is monotone in either one of the interval $(t^{\ell+1}, s_*)$ or (s_*, t^ℓ). Without of generality we may assume $|t^\ell - s_*| \geq \frac{1}{2}|t^{\ell+1} - t^\ell|$. Then

$$\begin{aligned} |\xi(X_{\mathbf{cl}}(s_*;t^\ell,x^\ell,v^\ell))| &= \Big| \int_{s_*}^{t^\ell} v^\ell \cdot \nabla\xi(x^\ell - (t^\ell - s)v^\ell, v^\ell) \Big| = \Big| \int_{s_*}^{t^\ell} \int_s^{t^\ell} v^\ell \cdot \nabla^2\xi(x^\ell - (t^\ell - \tau)v^\ell, v^\ell) \cdot v^\ell \Big| \\ &\simeq_\xi \frac{|v^\ell|^2 |t^\ell - s_*|^2}{2} \simeq_\xi \Big(\sup_{s\in[t^{\ell+1},t^\ell]} \frac{|v^\ell \cdot n(X_{\mathbf{cl}}(s))|}{|v^\ell|} \Big)^2, \end{aligned}$$

where we used (A.46) and (A.47) and the Velocity lemma (Lemma A.1).

Therefore if a bounce ℓ is *Type I* then $\max_{t^{\ell+1}\leq\tau\leq t^\ell} |\xi(X_{\mathbf{cl}}(\tau;t,x,v))| \leq C\delta$. If a bounce ℓ is *Type II* then $|\xi(X_{\mathbf{cl}}(\tau;t,x,v))| > C\delta$ for some $\tau \in [t^{\ell+1}, t^\ell]$.

Now we assign a coordinate chart for each bounce ℓ (moving frames).

For *Type I* bounce ℓ in (A.74), we assign $\mathbf{p}^\ell \in \partial\Omega \times \mathbb{S}^2$ and $\mathbf{p}^\ell-$spherical coordinates in Lemma A.10 and (A.56) : we choose $\mathbf{p}^\ell := (z^\ell, w^\ell)$ on $\partial\Omega \times \mathbb{S}^2$ with $n(z^\ell) \cdot w^\ell = 0$ such that z^ℓ and w^ℓ do not depends on (t,x,v) and

$$|z^\ell - x^\ell| < \mathbf{r}^\ell, \quad \Big| w^\ell - \frac{v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)}{|v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)|} \Big| < \mathbf{r}^\ell. \tag{A.75}$$

Note that, by the definition of *Type I bounce*, $|v^\ell - (v^\ell \cdot n(z^\ell)n(z^\ell))|^2 = |v|^2 - |\mathbf{v}_\perp^\ell|^2 \gtrsim |v|^2(1-\delta) \gtrsim_\delta |v|^2$ and hence w^ℓ is well-defined.

Moreover

$$|X_{\mathbf{cl}}(s;t,x,v) - \mathcal{L}_{\mathbf{p}^\ell}| \gtrsim C_\delta > 0, \tag{A.76}$$

for $|v||t^\ell - s| \leq \frac{1}{100}\min_{x\in\partial\Omega}|x|$. This is due to the fact that the projection of $V_{\mathbf{cl}}(s)$ on the plane passing z^ℓ and perpendicular to $n(z^\ell) \times w^\ell$ is at most $|v|$ but the distance from z^ℓ to the origin(the projection of poles $\mathcal{N}_{\mathbf{p}^\ell}$ and $\mathcal{S}_{\mathbf{p}^\ell}$) has lower bound $\frac{1}{10}\min_{x\in\partial\Omega}|x|$, $s \sim t^\ell$.

For *Type II* bounce $\ell(t^\ell, x^\ell, v^\ell)$, we choose $\mathbf{p}^\ell = (z^\ell, w^\ell)$ with $|z^\ell - x^\ell| \leq \sqrt{\delta}$ but we choose arbitrary $w^\ell \in \mathbb{S}^2$ satisfying $n(z^\ell) \cdot w^\ell = 0$. We choose $\mathbf{p}^\ell-$spherical coordinate in Lemma A.10 and (A.56) with this $\mathbf{p}^\ell$. Note that unlike *Type I*, this $\mathbf{p}^\ell-$spherical coordinate might not be defined for $s \in [t^{\ell+1}, t^\ell]$ but only defined near the boundary.

Whenever the moving frame is defined (for all $\tau \in (t^{\ell+1}, t^\ell]$ when ℓ is *Type I*, and $\tau \sim t^\ell$ when ℓ is *Type II*) we denote

$$(\mathbf{X}_\ell(\tau), \mathbf{V}_\ell(\tau)) = (\mathbf{x}_{\perp_\ell}(\tau), \mathbf{x}_{\parallel_\ell}(\tau), \mathbf{v}_{\perp_\ell}(\tau), \mathbf{v}_{\parallel_\ell}(\tau)) := \Phi_{\mathbf{p}^\ell}^{-1}(X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau)).$$

Especially at the boundary we denote

$$(\mathbf{x}_{\perp_\ell}^\ell, \mathbf{x}_{\parallel_\ell}^\ell, \mathbf{v}_{\perp_\ell}^\ell, \mathbf{v}_{\parallel_\ell}^\ell) := \lim_{\tau\uparrow t^\ell}(\mathbf{X}_\ell(\tau), \mathbf{V}_\ell(\tau)), \quad \text{with } \mathbf{x}_{\perp_\ell}^\ell = 0,\ \mathbf{v}_{\perp_\ell}^\ell \geq 0.$$

Then we define

$$(\mathbf{x}_{\perp_\ell}^{\ell+1}, \mathbf{x}_{\parallel_\ell}^{\ell+1}, \mathbf{v}_{\parallel_\ell}^{\ell+1}) = \lim_{\tau\downarrow t^{\ell+1}}(\mathbf{x}_{\perp_\ell}(\tau), \mathbf{x}_{\parallel_\ell}(\tau), \mathbf{v}_{\parallel_\ell}(\tau)),$$

and

$$\mathbf{v}_{\perp_\ell}^{\ell+1} := -\lim_{\tau\downarrow t^{\ell+1}} \mathbf{v}_{\perp_\ell}(\tau). \tag{A.77}$$

Now we regroup the indices of the specular cycles, without order changing, as

$$\{0,1,2,\cdots,\ell_*-1,\ell_*\}=\{0\}\cup\mathcal{G}_1\cup\mathcal{G}_2\cup\cdots\cup\mathcal{G}_{[\frac{|t-s||v|}{L_\xi}]}\cup\mathcal{G}_{[\frac{|t-s||v|}{L_\xi}]+1},$$

where $\big[a\big]\in\mathbb{N}$ is the greatest integer less than or equal to a. Each group is

$$\begin{aligned}
\mathcal{G}_1&=\{1,\cdots,\ell_1-1,\ell_1\},\\
\mathcal{G}_2&=\{\ell_1,\ell_1+1,\cdots,\ell_2-1,\ell_2\},\\
&\ \vdots\\
\mathcal{G}_{[\frac{|t-s||v|}{L_\xi}]}&=\{\ell_{[\frac{|t-s||v|}{L_\xi}]-1},\ell_{[\frac{|t-s||v|}{L_\xi}]-1}+1,\cdots,\ell_{[\frac{|t-s||v|}{L_\xi}]}-1,\ell_{[\frac{|t-s||v|}{L_\xi}]}\},\\
\mathcal{G}_{[\frac{|t-s||v|}{L_\xi}]+1}&=\{\ell_{[\frac{|t-s||v|}{L_\xi}]},\ell_{[\frac{|t-s||v|}{L_\xi}]}+1,\cdots,\ell_*\},
\end{aligned}\tag{A.78}$$

where $\ell_1=\inf\{\ell\in\mathbb{N}:|v|\times|t^0-t^{\ell_1}|\geq L_\xi\}$ and inductively

$$\ell_i=\inf\{\ell\in\mathbb{N}:|v|\times|t^{\ell_i}-t^{\ell_{i+1}}|\geq L_\xi\},\tag{A.79}$$

and we have denoted $\ell_*=\ell_{[\frac{|t-s||v|}{L_\xi}]+1}$.

By the chain rule, with the assigned $\mathbf{p}^\ell-$spherical coordinate (moving frame), we have for fixed $0\leq s\leq t$ and $s\in(t^{\ell_*+1},t^{\ell_*})$

$$\begin{aligned}
&\frac{\partial(s,X_{\mathbf{cl}}(s;t,x,v),V_{\mathbf{cl}}(s;t,x,v))}{\partial(t,x,v)}\\
&=\underbrace{\frac{\partial(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))}{\partial(t^{\ell_*},0,\mathbf{x}^{\ell_*}_{\|_{\ell_*}},\mathbf{v}^{\ell_*}_{\perp_{\ell_*}},\mathbf{v}^{\ell_*}_{\|_{\ell_*}})}}_{\text{from the last bounce to the }s-\text{plane}}\\
&\times\underbrace{\prod_{i=1}^{[\frac{|t-s||v|}{L_*}]}\underbrace{\frac{\partial(t^{\ell_{i+1}},0,\mathbf{x}^{\ell_{i+1}}_{\|_{\ell_{i+1}}},\mathbf{v}^{\ell_{i+1}}_{\perp_{\ell_{i+1}}},\mathbf{v}^{\ell_{i+1}}_{\|_{\ell_{i+1}}})}{\partial(t^{\ell_{i+1}-1},0,\mathbf{x}^{\ell_{i+1}-1}_{\|_{\ell_{i+1}-1}},\mathbf{v}^{\ell_{i+1}-1}_{\perp_{\ell_{i+1}-1}},\mathbf{v}^{\ell_{i+1}-1}_{\|_{\ell_{i+1}-1}})}\times\cdots\times\frac{\partial(t^{\ell_i+1},0,\mathbf{x}^{\ell_i+1}_{\|_{\ell_i+1}},\mathbf{v}^{\ell_i+1}_{\perp_{\ell_i+1}},\mathbf{v}^{\ell_i+1}_{\|_{\ell_i+1}})}{\partial(t^{\ell_i},0,\mathbf{x}^{\ell_i}_{\|_{\ell_i}},\mathbf{v}^{\ell_i}_{\perp_{\ell_i}},\mathbf{v}^{\ell_i}_{\|_{\ell_i}})}}_{i-\text{th intermediate group}}}_{\text{whole intermediate groups}}\\
&\times\underbrace{\frac{\partial(t^1,0,\mathbf{x}^1_{\|_1},\mathbf{v}^1_{\perp_1},\mathbf{v}^1_{\|_1})}{\partial(t,x,v)}}_{\text{from the }t-\text{plane to the first bounce}}.
\end{aligned}\tag{A.80}$$

Step 2. From the last bounce ℓ_* to the $s-$plane

We choose $s^{\ell_*}\in(\frac{t^{\ell_*}+s}{2},t^{\ell_*})\subset(s,t^{\ell_*})$ such that $|v||t^{\ell_*}-s^{\ell_*}|\ll1$ and the ℓ_*-spherical coordinate $(\mathbf{X}_{\ell_*}(s^{\ell_*}),\mathbf{V}_{\ell_*}(s^{\ell_*}))$ is well-defined regardless of types of ℓ_* in (A.74). Notice that s^{ℓ_*} is independent of t^{ℓ_*} and s so that $\frac{\partial s^{\ell_*}}{\partial t^{\ell_*}}=0=\frac{\partial s^{\ell_*}}{\partial s}$.

By the chain rule,

$$\begin{aligned}
&\frac{\partial(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))}{\partial(t^{\ell_*},0,\mathbf{x}^{\ell_*}_{\|_{\ell_*}},\mathbf{v}^{\ell_*}_{\perp_{\ell_*}},\mathbf{v}^{\ell_*}_{\|_{\ell_*}})}\\
&=\frac{\partial(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*},\mathbf{X}_{\ell_*}(s^{\ell_*}),\mathbf{V}_{\ell_*}(s^{\ell_*}))}\frac{\partial(s^{\ell_*},\mathbf{x}_{\perp_{\ell_*}}(s^{\ell_*}),\mathbf{x}_{\|_{\ell_*}}(s^{\ell_*}),\mathbf{v}_{\perp_{\ell_*}}(s^{\ell_*}),\mathbf{v}_{\|_{\ell_*}}(s^{\ell_*}))}{\partial(t^{\ell_*},0,\mathbf{x}^{\ell_*}_{\|_{\ell_*}},\mathbf{v}^{\ell_*}_{\perp_{\ell_*}},\mathbf{v}^{\ell_*}_{\|_{\ell_*}})}\\
&=\frac{\partial(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*},X_{\mathbf{cl}}(s^{\ell_*}),V_{\mathbf{cl}}(s^{\ell_*}))}\frac{\partial(s^{\ell_*},X_{\mathbf{cl}}(s^{\ell_*}),V_{\mathbf{cl}}(s^{\ell_*}))}{\partial(s^{\ell_*},\mathbf{X}_{\ell_*}(s^{\ell_*}),\mathbf{V}_{\ell_*}(s^{\ell_*}))}\frac{\partial(s^{\ell_*},\mathbf{x}_{\perp_{\ell_*}}(s^{\ell_*}),\mathbf{x}_{\|_{\ell_*}}(s^{\ell_*}),\mathbf{v}_{\perp_{\ell_*}}(s^{\ell_*}),\mathbf{v}_{\|}(s^{\ell_*}))}{\partial(t^{\ell_*},0,\mathbf{x}^{\ell_*}_{\|_{\ell_*}},\mathbf{v}^{\ell_*}_{\perp_{\ell_*}},\mathbf{v}^{\ell_*}_{\|_{\ell_*}})}.
\end{aligned}$$

Firstly, we claim

$$\frac{\partial(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*},\mathbf{X}_{\ell_*}(s^{\ell_*}),\mathbf{V}_{\ell_*}(s^{\ell_*}))}=\begin{bmatrix}0&\mathbf{0}_{1,3}&\mathbf{0}_{1,3}\\-V_{\mathbf{cl}}(s^{\ell_*})&O_\xi(1)(1+|v||s^{\ell_*}-s|)&O_\xi(1)|s^{\ell_*}-s|\\\mathbf{0}_{3,1}&O_\xi(1)|v|&O_\xi(1)\end{bmatrix}.\tag{A.81}$$

Since

$$X_{\mathbf{cl}}(s) = X_{\mathbf{cl}}(s^{\ell_*}) - (s^{\ell_*} - s)V_{\mathbf{cl}}(s^{\ell_*}), \quad V_{\mathbf{cl}}(s) = V_{\mathbf{cl}}(s^{\ell_*}),$$

and s^{ℓ_*} is independent of s, we have

$$\frac{\partial(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*}, X_{\mathbf{cl}}(s^{\ell_*}), V_{\mathbf{cl}}(s^{\ell_*}))} = \left[\begin{array}{ccc} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ -V_{\mathbf{cl}}(s^{\ell_*}) & \mathbf{Id}_{3,3} & -(s^{\ell_*} - s)\mathbf{Id}_{3,3} \\ \mathbf{0}_{3,1} & \mathbf{0}_{3,3} & \mathbf{Id}_{3,3} \end{array}\right].$$

Due to Lemma A.10,

$$\frac{\partial(s^{\ell_*}, X_{\mathbf{cl}}(s^{\ell_*}), V_{\mathbf{cl}}(s^{\ell_*}))}{\partial(s^{\ell_*}, \mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))}$$
$$= \left[\begin{array}{c|ccc|ccc} 1 & & \mathbf{0}_{1,3} & & & \mathbf{0}_{1,3} & \\ \hline \mathbf{0}_{3,1} & -\mathbf{n}_{\ell_*} & \begin{array}{c}\partial_1\eta_{\ell_*} \\ -\mathbf{x}_{\perp_{\ell_*}}\partial_1\mathbf{n}_{\ell_*}\end{array} & \begin{array}{c}\partial_2\eta_{\ell_*} \\ -\mathbf{x}_{\perp_{\ell_*}}\partial_2\mathbf{n}_{\ell_*}\end{array} & & \mathbf{0}_{3,3} & \\ \hline \mathbf{0}_{3,1} & -\mathbf{v}_{\|_{\ell_*}}\cdot\nabla_{\mathbf{x}_{\|_{\ell_*}}}\mathbf{n}_{\ell_*} & \begin{array}{c}\mathbf{v}_{\|_{\ell_*}}\cdot\nabla\partial_1\eta_{\ell_*} \\ -\mathbf{v}_{\perp_{\ell_*}}\partial_1\mathbf{n}_{\ell_*} \\ -\mathbf{x}_{\perp_{\ell_*}}\mathbf{v}_{\|_{\ell_*}}\cdot\nabla\partial_1\mathbf{n}_{\ell_*}\end{array} & \begin{array}{c}\mathbf{v}_{\|_{\ell_*}}\cdot\nabla\partial_2\eta_{\ell_*} \\ -\mathbf{v}_{\perp_{\ell_*}}\partial_2\mathbf{n}\ell_* \\ -\mathbf{x}_{\perp_{\ell_*}}\mathbf{v}_{\|_{\ell_*}}\cdot\nabla\partial_2\mathbf{n}_{\ell_*}\end{array} & -\mathbf{n}_{\ell_*} & \begin{array}{c}\partial_1\eta_{\ell_*} \\ -\mathbf{x}_{\perp_{\ell_*}}\partial_1\mathbf{n}_{\ell_*}\end{array} & \begin{array}{c}\partial_2\eta_{\ell_*} \\ -\mathbf{x}_{\perp_{\ell_*}}\partial_2\mathbf{n}_{\ell_*}\end{array} \end{array}\right],$$

where all entries are evaluated at $(\mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))$. The multiplication of above two matrices gives (A.81).

Secondly, we claim that whenever $\mathbf{p}^\ell-$spherical coordinate is defined for all $\tau \in [s^\ell, t^\ell]$

$$\frac{\partial(s^\ell, \mathbf{x}_{\perp_\ell}(s^\ell), \mathbf{x}_{\|_\ell}(s^\ell), \mathbf{v}_{\perp_\ell}(s^\ell), \mathbf{v}_{\|_\ell}(s^\ell))}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})}$$
$$= \left[\begin{array}{c|cc|cc} 0 & 0 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\ \hline -\mathbf{v}_\perp(s^\ell) & 0 & O_\xi(1)|v|^2|t^\ell - s^\ell|^2 & O_\xi(1)|t^\ell - s^\ell| & O_\xi(1)|v||t^\ell - s^\ell|^2 \\ -\mathbf{v}_\|(s^\ell) & \mathbf{0}_{2,1} & \mathbf{Id}_{2,2} + O_\xi(1)|v|^2|t^\ell - s^\ell|^2 & O_\xi(1)|v||t^\ell - s^\ell|^2 & O_\xi(1)|t^\ell - s^\ell|(\mathbf{Id}_{2,2} + |v||t^\ell - s^\ell|) \\ \hline O_\xi(1)|v|^2 & 0 & O_\xi(1)|v|^2|t^\ell - s^\ell| & 1 + O_\xi(1)|v||t^\ell - s^\ell| & O_\xi(1)|v||t^\ell - s^\ell| \\ O_\xi(1)|v|^2 & \mathbf{0}_{2,1} & O_\xi(1)|v|^2|t^\ell - s^\ell| & O_\xi(1)|v||t^\ell - s^\ell| & \mathbf{Id}_{2,2} + O_\xi(1)|v||t^\ell - s^\ell| \end{array}\right]. \tag{A.82}$$

In this step we just need (A.82) for $\ell = \ell_*$ but we need (A.82) for general ℓ in Step 8.

Clearly the first raw is identically zero since s^ℓ is chosen to be independent of $(t^\ell, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})$. The first column (temporal derivatives) holds due to the fact that the characteristics ODE (A.57) is autonomous. More explicitly,

$$\begin{aligned}
&\frac{\partial}{\partial t^\ell}(\mathbf{X}_\ell(s^\ell; t^\ell, x^\ell, v^\ell), \mathbf{V}_\ell(s^\ell; t^\ell, x^\ell, v^\ell)) \\
&= \frac{\partial}{\partial t^\ell}(\mathbf{X}_\ell(s^\ell - t^\ell; 0, x^\ell, v^\ell), \mathbf{V}_\ell(s^\ell - t^\ell; 0, x^\ell, v^\ell)) \\
&= -\frac{\partial}{\partial s^\ell}(\mathbf{X}_\ell(s^\ell; t^\ell, x^\ell, v^\ell), \mathbf{V}_\ell(s^\ell; t^\ell, x^\ell, v^\ell)) \\
&= -(\mathbf{V}_\ell(s^\ell; t^\ell, x^\ell, v^\ell), F(\mathbf{X}_\ell(s^\ell; t^\ell, x^\ell, v^\ell), \mathbf{V}_\ell(s^\ell; t^\ell, x^\ell, v^\ell)) \\
&= (-\mathbf{v}_\perp(s^\ell), -\mathbf{v}_\|(s^\ell), O_\xi(1)|v|^2, O_\xi(1)|v|^2).
\end{aligned}$$

Now we prove the the remainder. Firstly we claim that if the $\mathbf{p}^\ell-$spherical coordinate is well-defined for $t^{\ell+1} < \tau < t^\ell$ (τ is independent of t^ℓ) then

$$[\mathbf{X}_\ell(\tau; t, x, v), \mathbf{V}_\ell(\tau; t, x, v)] \equiv [\mathbf{X}_\ell(\tau; t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell}), \mathbf{V}_\ell(\tau; t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})]$$

and

$$\begin{aligned}
|\partial_{\mathbf{x}^\ell_{\|_\ell}}\mathbf{X}_\ell(\tau)| &\lesssim e^{C_\xi|v||\tau - t^\ell|} \lesssim 1, \\
|\partial_{\mathbf{v}^\ell_\ell}\mathbf{X}_\ell(\tau)| &\lesssim |\tau - t^\ell|e^{C_\xi|v||\tau - t^\ell|} \lesssim |\tau - t^\ell|, \\
|\partial_{\mathbf{x}^\ell_{\|_\ell}}\mathbf{V}_\ell(\tau)| &\lesssim |v| \times |v||\tau - t^\ell|e^{C_\xi|v||\tau - t^\ell|} \lesssim |v|^2|\tau - t^\ell|, \\
|\partial_{\mathbf{v}^\ell_\ell}\mathbf{V}_\ell(\tau)| &\lesssim e^{C_\xi|v||\tau - t^\ell|} \lesssim 1,
\end{aligned} \tag{A.83}$$

where $\partial_{\mathbf{v}^\ell_\ell} = [\partial_{\mathbf{v}^\ell_{\perp_\ell}}, \partial_{\mathbf{v}^\ell_{\|_\ell}}]$.

If the $\mathbf{p}^\ell-$spherical coordinate is well-defined for $t^{\ell+1} < \tau < s < t^\ell$ then

$$\begin{aligned}&[\mathbf{X}_\ell(\tau;t,x,v),\mathbf{V}_\ell(\tau;t,x,v)]\\ &\equiv [\mathbf{X}_\ell(\tau;s,\mathbf{X}_\ell(\tau;t,x,v),\mathbf{V}_\ell(\tau;t,x,v)),\mathbf{V}_\ell(\tau;s,\mathbf{X}_\ell(\tau;t,x,v),\mathbf{V}_\ell(\tau;t,x,v))],\end{aligned}$$

and

$$\begin{aligned}|\partial_{\mathbf{X}_\ell(s)}\mathbf{X}_\ell(\tau)| &\lesssim e^{C_\xi|v||\tau-s|} \lesssim 1,\\ |\partial_{\mathbf{V}_\ell(s)}\mathbf{X}_\ell(\tau)| &\lesssim |\tau-s|e^{C_\xi|v||\tau-s|} \lesssim |\tau-s|,\\ |\partial_{\mathbf{X}_\ell(s)}\mathbf{V}_\ell(\tau)| &\lesssim |v|\times|v||\tau-s|e^{C_\xi|v||\tau-s|} \lesssim |v|^2|\tau-s|,\\ |\partial_{\mathbf{V}_\ell(s)}\mathbf{V}_\ell(\tau)| &\lesssim e^{C_\xi|v||\tau-s|} \lesssim 1.\end{aligned} \tag{A.84}$$

Proof of (A.83) and (A.84). From (A.58) and (A.59), $\dot{\mathbf{x}}_{\parallel_\ell} = \mathbf{v}_{\parallel_\ell}$, $\dot{\mathbf{x}}_{\perp_\ell} = \mathbf{v}_{\perp_\ell}$ and $\dot{\mathbf{v}}_{\perp_\ell} = F_{\perp_\ell}$ and $\dot{\mathbf{v}}_{\parallel_\ell} = F_{\parallel_\ell}$. Denote $\partial = [\frac{\partial}{\partial \mathbf{x}^\ell_{\parallel_\ell}}, \frac{\partial}{\partial \mathbf{v}^\ell_{\perp_\ell}}, \frac{\partial}{\partial \mathbf{v}^\ell_{\parallel_\ell}}]$. From (A.58) and (A.59),

$$\begin{aligned}|\partial F_\perp| &\lesssim |v|^2\{|\partial \mathbf{x}_\perp| + |\partial \mathbf{x}_\parallel|\} + |v||\partial \mathbf{v}_\parallel|,\\ |\partial F_\parallel| &\lesssim |v|^2\{|\partial \mathbf{x}_\perp| + |\partial \mathbf{x}_\parallel|\} + |v|\{|\partial \mathbf{v}_\perp| + |\partial \mathbf{v}_\parallel|\}.\end{aligned} \tag{A.85}$$

Now we use a single (rough) bound of $|\partial F_\perp| + |\partial F_\parallel| \lesssim |v|^2\{|\partial \mathbf{x}_\perp| + |\partial \mathbf{x}_\parallel|\} + |v|\{|\partial \mathbf{v}_\perp| + |\partial \mathbf{v}_\parallel|\}$ to have

$$\begin{aligned}\frac{d}{d\tau}\{|\partial \mathbf{v}_{\perp_\ell}(\tau)| + |\partial \mathbf{v}_{\parallel_\ell}(\tau)|\} &\lesssim |\partial F_{\perp_\ell}(\tau)| + |\partial F_{\parallel_\ell}(\tau)|\\ &\lesssim |v|^2\big\{|\partial \mathbf{x}_{\perp_\ell}(\tau)| + |\partial \mathbf{x}_{\parallel_\ell}(\tau)|\big\} + |v|\big\{|\partial \mathbf{v}_{\perp_\ell}(\tau)| + |\partial \mathbf{v}_{\parallel_\ell}(\tau)|\big\}.\end{aligned}$$

Combining with $\frac{d}{d\tau}[\mathbf{x}_{\perp_\ell}(\tau), \mathbf{x}_{\parallel_\ell}(\tau)] = [\mathbf{v}_{\perp_\ell}(\tau), \mathbf{v}_{\parallel_\ell}(\tau)]$,

$$\frac{d}{d\tau}\left[\begin{array}{c} |\partial \mathbf{x}_{\perp_\ell}(\tau)| + |\partial \mathbf{x}_{\parallel_\ell}(\tau)| \\ |\partial \mathbf{v}_{\perp_\ell}(\tau)| + |\partial \mathbf{v}_{\parallel_\ell}(\tau)| \end{array}\right] \lesssim_\xi \left[\begin{array}{cc} 0 & 1 \\ |v|^2 & |v| \end{array}\right]\left[\begin{array}{c} |\partial \mathbf{x}_{\perp_\ell}(\tau)| + |\partial \mathbf{x}_{\parallel_\ell}(\tau)| \\ |\partial \mathbf{v}_{\perp_\ell}(\tau)| + |\partial \mathbf{v}_{\parallel_\ell}(\tau)| \end{array}\right].$$

We diagonalize the matrix as

$$\left[\begin{array}{cc} 0 & 1 \\ |v|^2 & |v| \end{array}\right] = \left[\begin{array}{cc} 1 & 1 \\ \frac{1+\sqrt{5}}{2}|v| & \frac{1-\sqrt{5}}{2}|v| \end{array}\right]\left[\begin{array}{cc} \frac{1+\sqrt{5}}{2}|v| & 0 \\ 0 & \frac{1-\sqrt{5}}{2}|v| \end{array}\right]\left[\begin{array}{cc} -\frac{1-\sqrt{5}}{2\sqrt{5}} & \frac{1}{|v|\sqrt{5}} \\ \frac{1+\sqrt{5}}{2\sqrt{5}} & \frac{-1}{|v|\sqrt{5}} \end{array}\right] := PDP^{-1}.$$

Now

$$\left[\begin{array}{c} |\partial \mathbf{x}_\parallel(\tau)| + |\partial \mathbf{x}_\perp(\tau)| \\ |\partial \mathbf{v}_\parallel(\tau)| + |\partial \mathbf{v}_\perp(\tau)| \end{array}\right] \le P e^{C_\xi|\tau-t^\ell|D}P^{-1}\left[\begin{array}{c} |\partial \mathbf{x}_\parallel(t^\ell)| + |\partial \mathbf{x}_\perp(t^\ell)| \\ |\partial \mathbf{v}_\parallel(t^\ell)| + |\partial \mathbf{v}_\perp(t^\ell)| \end{array}\right],$$

which is further bounded as, by matrix multiplication,

$$\begin{aligned}&\le \left[\begin{array}{cc} -\frac{1-\sqrt{5}}{2\sqrt{5}}e^{C_\xi\frac{1+\sqrt{5}}{2}|v||\tau-t^\ell|} + \frac{1+\sqrt{5}}{2\sqrt{5}}e^{C_\xi\frac{1-\sqrt{5}}{2}|v||\tau-t^\ell|} & \frac{1}{\sqrt{5}|v|}e^{\frac{C_\xi}{2}|v||\tau-t^\ell|}\big\{e^{\frac{C_\xi\sqrt{5}}{2}|v||\tau-t^\ell|} - e^{C_\xi\frac{-\sqrt{5}}{2}|v||\tau-t^\ell|}\big\} \\ \frac{|v|}{\sqrt{5}}e^{C_\xi\frac{|v|}{2}|\tau-t^\ell|}\big\{e^{C_\xi\frac{\sqrt{5}}{2}|v||\tau-t^\ell|} - e^{-C_\xi\frac{\sqrt{5}}{2}|v||\tau-t^\ell|}\big\} & \frac{1+\sqrt{5}}{2\sqrt{5}}e^{C_\xi\frac{1+\sqrt{5}}{2}|v||\tau-t^\ell|} - \frac{1-\sqrt{5}}{2\sqrt{5}}e^{C_\xi\frac{1-\sqrt{5}}{2}|v||\tau-t^\ell|} \end{array}\right]\\ &\quad\times\left[\begin{array}{c} |\partial \mathbf{x}_\parallel(t^\ell)| + |\partial \mathbf{x}_\perp(t^\ell)| \\ |\partial \mathbf{v}_\parallel(t^\ell)| + |\partial \mathbf{v}_\perp(t^\ell)| \end{array}\right]\\ &\le \left[\begin{array}{c} e^{C_\xi|v||\tau-t^\ell|}\big\{|\partial \mathbf{x}_\parallel(t^\ell)| + |\partial \mathbf{x}_\perp(t^\ell)|\big\} + |\tau-t^\ell|e^{C_\xi|v||\tau-t^\ell|}\big\{|\partial \mathbf{v}_\parallel(t^\ell)| + |\partial \mathbf{v}_\perp(t^\ell)|\big\} \\ |v|^2|\tau-t^\ell|e^{C_\xi|v||\tau-t^\ell|}\big\{|\partial \mathbf{x}_\parallel(t^\ell)| + |\partial \mathbf{x}_\perp(t^\ell)|\big\} + e^{C_\xi|v||\tau-t^\ell|}\big\{|\partial \mathbf{v}_\parallel(t^\ell)| + |\partial \mathbf{v}_\perp(t^\ell)|\big\} \end{array}\right].\end{aligned}$$

Since $|v||\tau-t^\ell| \lesssim_\xi 1$, this proves our claim (A.83). The proof of (A.84) is exactly same but we use $\partial = [\partial_{\mathbf{X}_\ell}(s), \partial_{\mathbf{V}_\ell}(s)]$ to conclude the proof.

From the characteristics ODE, (A.57) in the $\mathbf{p}^\ell-$spherical coordinate,

$$\begin{aligned}\mathbf{x}_{\perp_\ell}(s^\ell) &= \mathbf{v}^\ell_{\perp_\ell}(s^\ell-t^\ell) + \int_{t^\ell}^{s^\ell}\int_{t^\ell}^{\tau} F_{\perp_\ell}(s';t^\ell,\mathbf{x}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\perp_\ell})\mathrm{d}s'\mathrm{d}\tau,\\ \mathbf{x}_{\parallel_\ell}(s^\ell) &= \mathbf{x}^\ell_{\parallel_\ell} + \mathbf{v}^\ell_{\parallel_\ell}(s^\ell-t^\ell) + \int_{t^\ell}^{s^\ell}\int_{t^\ell}^{\tau} F_{\parallel}(s';t^\ell,\mathbf{x}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\perp_\ell})\mathrm{d}s'\mathrm{d}\tau,\\ \mathbf{v}_{\perp_\ell}(s^\ell) &= \mathbf{v}^\ell_{\perp_\ell} + \int_{t^\ell}^{s^\ell} F_{\perp_\ell}(\tau;t^n,\mathbf{x}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\perp\ell})\mathrm{d}\tau,\\ \mathbf{v}_{\parallel_\ell}(s^\ell) &= \mathbf{v}^\ell_{\parallel_\ell} + \int_{t^\ell}^{s^\ell} F_{\parallel_\ell}(\tau;t^\ell,\mathbf{x}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\parallel_\ell},\mathbf{v}^\ell_{\perp_\ell})\mathrm{d}\tau.\end{aligned}$$

Plugging (A.83) into (A.58) and (A.59) and collecting terms, we deduce for $|v||s^\ell - t^\ell| \lesssim 1$

$$\begin{aligned}
\frac{\partial \mathbf{x}_{\perp_\ell}(s^\ell)}{\partial \mathbf{x}^\ell_{\|_\ell}} &\leq C_\Omega |v|^2 |s^\ell - t^\ell|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v|^2 |s^\ell - t^\ell|^2, \\
\frac{\partial \mathbf{x}_{\perp_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\perp_\ell}} &\leq |s^\ell - t^\ell| + C_\Omega |v||s^\ell - t^\ell|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |s^\ell - t^\ell|, \\
\frac{\partial \mathbf{x}_{\perp_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\|_\ell}} &\leq C_\Omega |v||s^\ell - t^\ell|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v||s^\ell - t^\ell|, \\
\frac{\partial \mathbf{x}_{\|_\ell}(s^\ell)}{\partial \mathbf{x}^\ell_{\|_\ell}} &\leq \mathbf{Id}_{2,2} + C_\Omega |v|^2 |s^\ell - t^\ell|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \leq \mathbf{Id}_{2,2} + O_\Omega(1) |v|^2 |s^\ell - t^\ell|^2, \\
\frac{\partial \mathbf{x}_{\|_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\perp_\ell}} &\leq C_\Omega |s^\ell - t^\ell|^2 |v| (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v||s^\ell - t^\ell|^2, \\
\frac{\partial \mathbf{x}_{\|_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\|_\ell}} &\leq |s^\ell - t^\ell| \Big\{ \mathbf{Id}_{2,2} + C_\Omega |v||s^\ell - t^\ell| (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \Big\} \\
&\leq |s^\ell - t^\ell| \mathbf{Id}_{2,2} + O_\Omega(1) |v||s^\ell - t^\ell|^2, \\
\frac{\partial \mathbf{v}_{\perp_\ell}(s^\ell)}{\partial \mathbf{x}^\ell_{\|_\ell}} &\leq C_\Omega |s^\ell - t^\ell||v|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v|^2 |s^\ell - t^\ell|, \\
\frac{\partial \mathbf{v}_{\perp_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\perp_\ell}} &\leq 1 + C_\Omega |s^\ell - t^\ell||v| (1 + |v||s^\ell -^\ell|) e^{|v||s^\ell - t^\ell|} \leq 1 + O_\Omega(1) |v||s^\ell - t^\ell|, \\
\frac{\partial \mathbf{v}_{\perp_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\|_\ell}} &\leq C_\Omega |s^\ell - t^\ell||v| (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v||s^\ell - t^\ell|, \\
\frac{\partial \mathbf{v}_{\|_\ell}(s^\ell)}{\partial \mathbf{x}^\ell_{\|_\ell}} &\leq C_\Omega |s^\ell - t^\ell||v|^2 (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v|^2 |s^\ell - t^\ell|, \\
\frac{\partial \mathbf{v}_{\|_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\perp_\ell}} &\leq C_\Omega |s^\ell - t^\ell||v| (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \lesssim_\Omega |v||s^\ell - t^\ell|, \\
\frac{\partial \mathbf{v}_{\|_\ell}(s^\ell)}{\partial \mathbf{v}^\ell_{\|_\ell}} &\leq \mathbf{Id}_{2,2} + C_\Omega |s^\ell - t^\ell||v| (1 + |v||s^\ell - t^\ell|) e^{|v||s^\ell - t^\ell|} \leq \mathbf{Id}_{2,2} + O_\Omega(1) |v||s^\ell - t^\ell|,
\end{aligned}$$

and this proves the claim (A.82).

Step 3. From $t-$plane to the first bounce

We choose $s^1 \in (t^1, \frac{t^1+t}{2}) \subset (t^1, t)$ such that $|v||t^1 - s^1| \ll 1$ and the polar coordinate $(\mathbf{X}_1(s^1), \mathbf{V}_1(s^1))$ is well-defined. More precisely we choose $0 < \Delta$ such that $|v||t - \Delta - t^1| \ll 1$ and define

$$s^1 := t - \Delta. \tag{A.86}$$

Then, by the chain rule,

$$\begin{aligned}
&\frac{\partial(t^1, 0, \mathbf{x}^1_{\|_1}, \mathbf{v}^1_{\perp_1}, \mathbf{v}^1_{\|_1})}{\partial(t, x, v)} \\
&= \frac{\partial(t^1, 0, \mathbf{x}^1_{\|_1}, \mathbf{v}^1_{\perp_1}, \mathbf{v}^1_{\|_1})}{\partial(s^1, X_{\mathbf{cl}}(s^1), V_{\mathbf{cl}}(s^1))} \frac{\partial(s^1, X_{\mathbf{cl}}(s^1), V_{\mathbf{cl}}(s^1))}{\partial(t, x, v)} \\
&= \frac{\partial(t^1, 0, \mathbf{x}^1_{\|_1}, \mathbf{v}^1_{\perp_1}, \mathbf{v}^1_{\|_1})}{\partial(s^1, \mathbf{x}_{\perp_1}(s^1), \mathbf{x}_{\|_1}(s^1), \mathbf{v}_{\perp_1}(s^1), \mathbf{v}_{\|_1}(s^1))} \frac{\partial(s^1, \mathbf{X}_1(s^1), \mathbf{V}_1(s^1))}{\partial(s^1, X_{\mathbf{cl}}(s^1), V_{\mathbf{cl}}(s^1))} \frac{\partial(s^1, X_{\mathbf{cl}}(s^1), V_{\mathbf{cl}}(s^1))}{\partial(t, x, v)}.
\end{aligned}$$

We fix $\mathbf{p}^1-$spherical coordinate and drop the index of the chart.

Firstly, we claim

$$
\begin{aligned}
&\frac{\partial(t^1, 0, \mathbf{x}_{\parallel}^1, \mathbf{v}_{\perp}^1, \mathbf{v}_{\parallel}^1)}{\partial(s^1, \mathbf{x}_{\perp}(s^1), \mathbf{x}_{\parallel}(s^1), \mathbf{v}_{\perp}(s^1), \mathbf{v}_{\parallel}(s^1))} \\
&\lesssim_{\Omega} \left[\begin{array}{c|cc|cc}
1 & \frac{1}{|\mathbf{v}_{\perp}^1|} & \frac{|v|^2|s^1-t^1|^2}{|\mathbf{v}_{\perp}^1|} & \frac{|s^1-t^1|}{|\mathbf{v}_{\perp}^1|} & \frac{|v||s^1-t^1|^2}{|\mathbf{v}_{\perp}^1|} \\
\hline
0 & 0 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\
\mathbf{0}_{2,1} & \frac{|v|}{|\mathbf{v}_{\perp}^1|} + |v|^2|s^1-t^1|^2 & \mathbf{Id}_{2,2} + |v||s^1-t^1| & \frac{|s^1-t^1||v|}{|\mathbf{v}_{\perp}^1|} + |s^1-t^1|^2|v| & |s^1-t^1| \\
\hline
0 & \frac{|v|^2}{|\mathbf{v}_{\perp}^1|} + |v|^2|s^1-t^1| & \frac{|v|^2}{|\mathbf{v}_{\perp}^1|} + |v|^2|s^1-t^1| & 1 + |v||s^1-t^1| & |v||s^1-t^1| \\
\mathbf{0}_{2,1} & \frac{|v|^2}{|\mathbf{v}_{\perp}^1|} + |v|^2|s^1-t^1| & |v|^2|s^1-t^1| & 1 + |v||s^1-t^1| & \mathbf{Id}_2 + |v||s^1-t^1|
\end{array}\right].
\end{aligned} \tag{A.87}
$$

The t^1 is determined via $\mathbf{x}_{\perp}(t^1) = 0$, i.e.

$$
0 = \mathbf{x}_{\perp}(s^1) - \mathbf{v}_{\perp}(s^1)(s^1 - t^1) + \int_{t^1}^{s^1} \int_{s}^{s^1} F_{\perp}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s, \tag{A.88}
$$

where $\mathbf{X_{cl}}(\tau) = \mathbf{X_{cl}}(\tau; s^1, \mathbf{X_{cl}}(s^1; t, x, v), \mathbf{V_{cl}}(s^1; t, x, v)), \mathbf{V_{cl}}(\tau) = \mathbf{V_{cl}}(\tau; s^1, \mathbf{X_{cl}}(s^1; t, x, v), \mathbf{V_{cl}}(s^1; t, x, v))$.

Recall that, from (A.67) and (A.68) and (A.77),

$$
\begin{aligned}
\mathbf{v}_{\perp}^1 &= -\lim_{s \downarrow t^1} \mathbf{v}_{\perp}(s) = -\mathbf{v}_{\perp}(s^1) + \int_{t^1}^{s^1} F_{\perp}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau, \\
\mathbf{x}_{\parallel}^1 &= \mathbf{x}_{\parallel}(s^1) - (s^1 - t^1)\mathbf{v}_{\parallel}(s^1) + \int_{t^1}^{s^1} \int_{\tau}^{s^1} F_{\parallel}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s^1, \\
\mathbf{v}_{\parallel}^1 &= \mathbf{v}_{\parallel}(s^1) - \int_{t^1}^{s^1} F_{\parallel}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau.
\end{aligned}
$$

Note that since ODE is autonomous we have $\frac{\partial t^1}{\partial s} = 1$, $\frac{\partial(\mathbf{x}^1, \mathbf{v}^1)}{\partial s^1} = 0$. From the fact $|s^1 - t^1| \lesssim_{\xi} \min\{\frac{|\mathbf{v}_{\perp}^1|}{|v|^2}, t\}$

and (A.46) and (A.47), and (A.84) and (A.85) to have

$$\begin{aligned}
\frac{\partial t^1}{\partial \mathbf{x}_\perp(s^1)} &= \frac{1}{\mathbf{v}_\perp^1}\left\{1 + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{x}_\perp(s^1)} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\right\}\\
&\lesssim_\xi \frac{1}{|\mathbf{v}_\perp^1|}\left\{1 + \int_{t^1}^{s^1}\int_s^{s^1} \big[1+|v|(s^1-\tau)\big]|v|^2 e^{C_\xi|v|(s^1-\tau)}\mathrm{d}\tau\mathrm{d}s\right\}\\
&\lesssim_\xi \frac{1}{|\mathbf{v}_\perp^1|}\Big\{1 + \big[1+|v||s^1-t^1|\big]|v|^2|s^1-t^1|^2 e^{C_\xi|v||s^1-t^1|}\Big\} \lesssim_{\xi,t} \frac{1}{|\mathbf{v}_\perp^1|},\\
\frac{\partial t^1}{\partial \mathbf{x}_\parallel(s^1)} &= \frac{1}{\mathbf{v}_\perp^1}\int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{x}_\parallel(s^1)} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi \frac{1}{|\mathbf{v}_\perp^1|}\left\{\int_{t^1}^{s^1}\int_s^{s^1} \big[1+|v|(s^1-\tau)\big]|v|^2 e^{C_\xi|v|(s^1-\tau)}\mathrm{d}\tau\mathrm{d}s\right\}\\
&\lesssim_\xi \frac{1}{|\mathbf{v}_\perp^1|}\big[1+|v||s^1-t^1|\big]|v|^2|s^1-t^1|^2 e^{C_\xi|v||s^1-t^1|} \lesssim_{\xi,t} \frac{|v|^2|s^1-t^1|^2}{|\mathbf{v}_\perp^1|},\\
\frac{\partial t^1}{\partial \mathbf{v}_\perp(s^1)} &= \frac{1}{\mathbf{v}_\perp^1}\left\{(t^1-s^1) + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{v}_\perp(s^1)} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\right\}\\
&\lesssim_\xi \frac{|s^1-t^1|}{|\mathbf{v}_\perp^1|} + \frac{1}{|\mathbf{v}_\perp^1|}\int_{t^1}^{s^1}\int_s^{s^1} |v|\big[1+|v||s^1-\tau|\big]e^{C_\xi|v|(s^1-\tau)}\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi \frac{|s^1-t^1|}{|\mathbf{v}_\perp^1|}\Big\{1+|v||s^1-t^1|e^{C_\xi|v||s^1-t^1|}\Big\} \lesssim_{\xi,t} \frac{|s^1-t^1|}{|\mathbf{v}_\perp^1|},\\
\frac{\partial t^1}{\partial \mathbf{v}_\parallel(s_1)} &= \frac{1}{\mathbf{v}_\perp^1}\int_{t^1}^{s_1}\int_s^{s_1} \frac{\partial}{\partial \mathbf{v}_\parallel(s_1)} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi \frac{1}{|\mathbf{v}_\perp^1|}\int_{t^1}^{s^1}\int_s^{s^1} |v|\big[1+|v||s^1-\tau|\big]e^{C_\xi|v|(s^1-\tau)}\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi \frac{|s^1-t^1|}{|\mathbf{v}_\perp^1|}|v||s^1-t^1|e^{C_\xi|v||s^1-t^1|}\\
&\lesssim_{\xi,t} \frac{|v||s^1-t^1|^2}{|\mathbf{v}_\perp^1|}.
\end{aligned}$$

Together with the above estimates and (A.84) and (A.85),

$$\begin{aligned}
\frac{\partial \mathbf{x}_\parallel^1}{\partial \mathbf{x}_\perp(s^1)} &= \frac{\partial t^1}{\partial \mathbf{x}_\perp(s^1)}\mathbf{v}_\parallel^1 + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{x}_\perp(s^1)} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi \frac{|v|}{|\mathbf{v}_\perp^1|} + \big[1+|v||s^1-t^1|\big]|v|^2|s^1-t^1|^2 e^{C_\xi|v||s^1-t^1|} \lesssim_{\xi,t} \frac{|v|}{|\mathbf{v}_\perp^1|} + |v|^2|s^1-t^1|^2,\\
\frac{\partial \mathbf{x}_\parallel^1}{\partial \mathbf{x}_\parallel(s^1)} &= \mathbf{Id}_{2,2} + \mathbf{v}_\parallel^1\frac{\partial t^1}{\partial \mathbf{x}_\parallel(s^1)} + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{x}_\parallel(s^1)} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_{\xi,t} \mathbf{Id}_{2,2} + |v|^2|s^1-t^1|^2 \lesssim_{\xi,t} \mathbf{Id}_{2,2} + |v||s^1-t^1|,\\
\frac{\partial \mathbf{x}_\parallel^1}{\partial \mathbf{v}_\perp(s^1)} &= \frac{\partial t^1}{\partial \mathbf{v}_\perp(s^1)}\mathbf{v}_\parallel^1 + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{v}_\perp(s^1)} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_{\xi,t} \frac{|s^1-t^1||v|}{|\mathbf{v}_\perp^1|} + |s^1-t^1|^2|v|,
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathbf{x}_\parallel^1}{\partial \mathbf{v}_\parallel(s^1)} &= -(s^1-t^1)\mathbf{Id}_{2,2} + \mathbf{v}_\parallel^1\frac{\partial t^1}{\partial \mathbf{v}_\parallel(s^1)} + \int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial}{\partial \mathbf{v}_\parallel(s^1)} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s\\
&\lesssim_\xi -(s^1-t^1)\mathbf{Id}_{2,2} + |v|\frac{|s^1-t^1|}{|\mathbf{v}_\perp^1|}|v||s^1-t^1| + |v||s^1-t^1|^2\big[1+|v||s^1-t^1|\big]\\
&\lesssim_{\xi,t} |s^1-t^1|\Big(1+\frac{|v|^2|s^1-t^1|}{|\mathbf{v}_\perp^1|}\Big) \lesssim_{\xi,t} |s^1-t^1|.
\end{aligned}$$

Moreover by (A.84) and (A.85)

$$
\begin{aligned}
\frac{\partial \mathbf{v}^1_\perp}{\partial \mathbf{x}_\perp(s^1)} &= \frac{-F_\perp(x^1,v)}{\mathbf{v}^1_\perp} - \frac{F_\perp(x^1,v)}{\mathbf{v}^1_\perp}\int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))}{\partial \mathbf{x}_\perp(s^1)}\mathrm{d}\tau\mathrm{d}s + \int_{t^1}^{s^1} \frac{\partial F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))}{\partial \mathbf{x}_\perp(s^1)}\mathrm{d}\tau \\
&\lesssim \frac{F_\perp(x^1,v)}{|\mathbf{v}^1_\perp|} + \Big(|v| + \frac{F_\perp(x^1,v)}{|\mathbf{v}^1_\perp|}|v||s^1-t^1|\Big)\big[1+|v||s^1-t^1|\big]|v||s^1-t^1|e^{C_\xi|v||s^1-t^1|} \\
&\lesssim \frac{|v|^2}{|\mathbf{v}^1_\perp|} + |v|^2|s^1-t^1|, \\
\frac{\partial \mathbf{v}^1_\perp}{\partial \mathbf{x}_\parallel(s^1)} &= \frac{-F_\perp(x^1,v)}{\mathbf{v}^1_\perp} + \int_{t^1}^{s^1} \frac{\partial}{\partial \mathbf{x}_\parallel(s^1)}F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))\mathrm{d}\tau \\
&\lesssim \frac{|F_\perp(x^1,v)|}{|\mathbf{v}^1_\perp|} + |v|^2|s^1-t^1|\big(1+|v||s^1-t^1|\big)e^{C_\xi|v||s^1-t^1|} \lesssim \frac{|v|^2}{|\mathbf{v}^1_\perp|} + |v|^2|s^1-t^1|, \\
\frac{\partial \mathbf{v}^1_\perp}{\partial \mathbf{v}_\perp(s^1)} &= -1 + \frac{(s^1-t^1)F_\perp(x^1,v)}{\mathbf{v}^1_\perp} - \frac{F_\perp(x^1,v)}{\mathbf{v}^1_\perp}\int_{t^1}^{s^1}\int_s^{s^1} \frac{\partial F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))}{\partial \mathbf{v}_\perp(s^1)} \\
&\quad - \int_{s_1}^{t^1} \frac{\partial F_\perp(\mathbf{X_{cl}}(s),\mathbf{V_{cl}}(s))}{\partial \mathbf{v}_\perp(s_1)}\mathrm{d}s \\
&\lesssim -1 + \frac{|s^1-t^1||F_\perp(x^1,v)|}{|\mathbf{v}^1_\perp|}\Big\{1+|v||s^1-t^1|e^{C_\xi|v||s^1-t^1|}\Big\} + |v||s^1-t^1|e^{C_\xi|v||s^1-t^1|} \\
&\lesssim_\xi 1 + |v||s^1-t^1|, \\
\frac{\partial \mathbf{v}^1_\perp}{\partial \mathbf{v}_\parallel(s^1)} &= \frac{-F_\perp(x^1,v)}{\mathbf{v}^1_\perp}\int_{s^1}^{t^1}\int_{s^1}^{s} \frac{\partial F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))}{\partial \mathbf{v}_\parallel(s^1)}\mathrm{d}\tau\mathrm{d}s - \int_{s^1}^{t^1} \frac{\partial F_\perp(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))}{\partial \mathbf{v}_\parallel(s^1)}\mathrm{d}\tau \\
&\lesssim \frac{|v|^2}{|\mathbf{v}^1_\perp|}|s^1-t^1|^2|v| + |s^1-t^1||v| \lesssim |v||s^1-t^1|\Big(1+\frac{|s^1-t^1||v|^2}{|\mathbf{v}^1_\perp|}\Big) \lesssim |v||s^1-t^1|,
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial \mathbf{v}^1_\parallel}{\partial \mathbf{x}_\perp(s^1)} &= \frac{\partial t^1}{\partial \mathbf{x}_\perp(s^1)}F_\parallel(x^1,v) - \int_{t^1}^{s^1} \frac{\partial}{\partial \mathbf{x}_\perp(s^1)}F_\parallel(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))\mathrm{d}\tau \\
&\lesssim_\xi \frac{|F_\parallel(x^1,v)|}{|\mathbf{v}^1_\perp|}\big\{1+[1+|v||s^1-t^1|]|v|^2|s^1-t^1|^2e^{C_\xi|v||s^1-t^1|}\big\} \\
&\quad + |v|^2|s^1-t^1|[1+|v||s^1-t^1|]e^{C_\xi|v||s^1-t^1|} \\
&\lesssim_{\xi,t} \frac{|v|^2}{|\mathbf{v}^1_\perp|} + |v|^2|s^1-t^1|, \\
\frac{\partial \mathbf{v}^1_\parallel}{\partial \mathbf{x}_\parallel(s^1)} &= \frac{\partial t^1}{\partial \mathbf{x}_\parallel(s^1)}F_\parallel(x^1,v) - \int_{t^1}^{s^1} \frac{\partial}{\partial \mathbf{x}_\parallel(s^1)}F_\parallel(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))\mathrm{d}\tau \\
&\lesssim \frac{|F_\parallel(x^1,v)|}{|\mathbf{v}^1_\perp|}\big[1+|v||s^1-t^1|\big]|v|^2|s^1-t^1|^2e^{C_\xi|v||s^1-t^1|} + |v|^2|s^1-t^1|\big[1+|v||s^1-t^1|\big]e^{C_\xi|v||s^1-t^1|} \\
&\lesssim_{\xi,t} |v|^2|s^1-t^1|,
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathbf{v}^1_\parallel}{\partial \mathbf{v}_\perp(s^1)} &= \frac{\partial t^1}{\partial \mathbf{v}_\perp(s^1)}F_\parallel(x^1,v) - \int_{t^1}^{s^1} \frac{\partial}{\partial \mathbf{v}_\perp(s^1)}F_\parallel(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau))\mathrm{d}\tau \\
&\lesssim \frac{|s^1-t^1||v|^2}{|\mathbf{v}^1_\perp|} + |v||s^1-t^1| \lesssim 1 + |v||s^1-t^1|, \\
\frac{\partial \mathbf{v}^1_\parallel}{\partial \mathbf{v}_\parallel(s^1)} &= \mathbf{Id}_{2,2} + \frac{\partial t^1}{\partial \mathbf{v}_\parallel(s^1)}F_\parallel(x^1,v) - \int_{t^1}^{s^1} \frac{\partial}{\partial \mathbf{v}_\parallel(s^1)}F_\parallel(\mathbf{X_{cl}}(\tau),\mathbf{V_{cl}}(\tau)\mathrm{d}\tau \\
&\lesssim \mathbf{Id}_{2,2} + \frac{|v|^3|s^1-t^1|^2}{|\mathbf{v}^1_\perp|} + |s^1-t^1||v|\big[1+|v||s^1-t^1|\big] \lesssim_{\xi,t} \mathbf{Id}_{2,2} + |v||s^1-t^1|.
\end{aligned}
$$

Secondly, we claim

$$
\begin{aligned}
\frac{\partial(s^1,\mathbf{X}_1(s^1),\mathbf{V}_1(s^1))}{\partial(t,x,v)} &= \frac{\partial(s^1,\mathbf{X}_1(s^1),\mathbf{V}_1(s^1))}{\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}\frac{\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}{\partial(t,x,v)} \\
&= \left[\begin{array}{c|c|c}
1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline
 & \frac{(\partial_1\eta\times\partial_2\eta)^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t^1-s^1|) & O_\xi(|t-s^1|) \\
\mathbf{0}_{3,1} & \frac{(\partial_2\eta\times\mathbf{n})^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t^1-s^1|) & O_\xi(|t-s^1|) \\
 & \frac{(\mathbf{n}\times\partial_2\eta)^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t^1-s^1|) & O_\xi(|t-s^1|) \\ \hline
 & O_\xi(|v|) & \frac{(\partial_1\eta\times\partial_2\eta)^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t-s^1|) \\
\mathbf{0}_{3,1} & O_\xi(|v|) & \frac{(\partial_2\eta\times\mathbf{n})^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t-s^1|) \\
 & O_\xi(|v|) & \frac{(\mathbf{n}\times\partial_1\eta)^T}{\mathbf{n}\cdot(\partial_1\eta\times\partial_2\eta)} + O_\xi(|v||t-s^1|)
\end{array}\right],
\end{aligned}
\tag{A.89}
$$

where the entries are evaluated at $(\mathbf{X}_1(s^1),\mathbf{V}_1(s^1))$. Note that $|v||t^1-s^1|\lesssim_\xi 1$.

Clearly

$$
\begin{bmatrix}
\partial s^1/\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1)) \\
\partial\mathbf{X}_{\mathbf{cl}}(s^1)/\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1)) \\
\partial\mathbf{V}_{\mathbf{cl}}(s^1)/\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))
\end{bmatrix}
= \left[\begin{array}{c|c}
1 & \mathbf{0}_{1,6} \\ \hline
\mathbf{0}_{6,1} & \frac{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}
\end{array}\right].
$$

Now we consider the right lower 6 by 6 submatrix. Recall, from (A.65)

$$
\frac{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))} = \frac{\partial\Phi(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s))}{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s))} := \left[\begin{array}{c|c} A & \mathbf{0}_{3,3} \\ \hline B & A\end{array}\right] + \mathbf{x}_\perp\left[\begin{array}{c|c} \mathbf{0}_{3,3} & \mathbf{0}_{3,3} \\ \hline D & \mathbf{0}_{3,3}\end{array}\right].
$$

Note that, from (A.63) and (A.55),

$$
\begin{aligned}
\det(A) &= \det\Big[\ [-\mathbf{n}(\mathbf{x}_\parallel)] \quad \partial_{\mathbf{x}_{\parallel,1}}\eta(\mathbf{x}_\parallel) \quad \partial_{\mathbf{x}_{\parallel,2}}\eta(\mathbf{x}_\parallel)\ \Big] = [-\mathbf{n}(\mathbf{x}_\parallel)]\cdot\big(\partial_{\mathbf{x}_{\parallel,1}}\eta(\mathbf{x}_\parallel)\times\partial_{\mathbf{x}_{\parallel,2}}\eta(x_\parallel)\big)\neq 0, \\
A^{-1} &= \frac{1}{[-\mathbf{n}]\cdot(\partial_{\mathbf{x}_{\parallel,1}}\eta\times\partial_{\mathbf{x}_{\parallel,2}}\eta)}\Big[(\partial_{\mathbf{x}_{\parallel,1}}\eta\times\partial_{\mathbf{x}_{\parallel,2}}\eta)^T, (\partial_{\mathbf{x}_{\parallel,2}}\eta\times[-\mathbf{n}])^T, ([-\mathbf{n}]\times\partial_{\mathbf{x}_{\parallel,1}}\eta)^T\Big].
\end{aligned}
$$

From basic linear algebra

$$
\det\left(\frac{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}\right) = \det\left[\begin{array}{c|c} A & \mathbf{0}_{3,3} \\ \hline B+\mathbf{x}_\perp D & A\end{array}\right] = \{\det(A)\}^2 = \big\{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)\big\}^2,
$$

and $\left(\frac{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}\right)$ is invertible. By the basic linear algebra

$$
\begin{aligned}
\frac{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))} &= \left[\frac{\partial(X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))}{\partial(\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}\right]^{-1} = \left[\begin{array}{c|c} A & \mathbf{0}_{3,3} \\ \hline B+\mathbf{x}_\perp D & A\end{array}\right]^{-1} \\
&= \left[\begin{array}{c|c} A^{-1} & \mathbf{0}_{3,3} \\ \hline -A^{-1}(B+\mathbf{x}_\perp D)A^{-1} & A^{-1}\end{array}\right] = \begin{bmatrix} A^{-1}(\mathbf{x}_\parallel) & \mathbf{0}_{3,3} \\ |v|+O_\xi(\mathbf{x}_\perp) & A^{-1}(\mathbf{x}_\parallel)\end{bmatrix},
\end{aligned}
\tag{A.90}
$$

and we obtain

$$
\frac{\partial(s^1,\mathbf{X}_{\mathbf{cl}}(s^1),\mathbf{V}_{\mathbf{cl}}(s^1))}{\partial(s^1,X_{\mathbf{cl}}(s^1),V_{\mathbf{cl}}(s^1))} = \left[\begin{array}{c|c|c}
1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline
0 & \frac{(\partial_1\eta\times\partial_2\eta)^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)} & \\
0 & \frac{(\partial_2\eta\times[-\mathbf{n}])^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)} & \mathbf{0}_{3,3} \\
0 & \frac{([-\mathbf{n}]\times\partial_1\eta)^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)} & \\ \hline
0 & O_\xi(1)(|v|) & \frac{(\partial_1\eta\times\partial_2\eta)^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)} \\
0 & O_\xi(1)(|v|) & \frac{(\partial_2\eta\times[-\mathbf{n}])^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)} \\
0 & O_\xi(1)(|v|) & \frac{([-\mathbf{n}]\times\partial_1\eta)^T}{[-\mathbf{n}]\cdot(\partial_1\eta\times\partial_2\eta)}
\end{array}\right].
$$

From $X_{\mathbf{cl}}(s_1;t,x,v) = x-(t-s_1)v = x-\Delta\times v$ and $V_{\mathbf{cl}}(s_1;t,x,v)=v$,

$$
\frac{\partial(s_1,X_{\mathbf{cl}}(s_1),V_{\mathbf{cl}}(s_1))}{\partial(t,x,v)} = \begin{bmatrix}
1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\
\mathbf{0}_{3,1} & \mathbf{Id}_{3,3} & -(t-s^1)\mathbf{Id}_{3,3} \\
\mathbf{0}_{3,1} & \mathbf{0}_{3,3} & \mathbf{Id}_{3,3}
\end{bmatrix}.
$$

Finally we multiply above two matrices and use $|\mathbf{x}_\perp(s^1)| \lesssim |v||t^1 - s^1|$ to conclude the second claim (A.89).

Step 4. Estimate of $\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})/\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})$

Recall $\mathbf{r}^\ell$ from (A.73). We show that there exists $M = M_{\xi,t} \gg 1$, which is only depending on Ω, such that for all $\ell \in \mathbb{N}$ and $0 \le t^{\ell+1} \le t^\ell \le t$ and $v \in \mathbb{R}^3$,

$$
\begin{aligned}
J^{\ell+1}_\ell &:= \frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})} \\
&\le \left[\begin{array}{c|c|cc|ccc}
1 & 0 & \frac{M}{|v|}\mathbf{r}^{\ell+1} & \frac{M}{|v|}\mathbf{r}^{\ell+1} & \frac{M}{|v|^2} & \frac{M}{|v|^2}\mathbf{r}^{\ell+1} & \frac{M}{|v|^2}\mathbf{r}^{\ell+1} \\ \hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 + M\mathbf{r}^{\ell+1} & M\mathbf{r}^{\ell+1} & \frac{M}{|v|} & \frac{M}{|v|}\mathbf{r}^{\ell+1} & \frac{M}{|v|}\mathbf{r}^{\ell+1} \\
0 & 0 & M\mathbf{r}^{\ell+1} & 1 + M\mathbf{r}^{\ell+1} & \frac{M}{|v|} & \frac{M}{|v|}\mathbf{r}^{\ell+1} & \frac{M}{|v|}\mathbf{r}^{\ell+1} \\ \hline
0 & 0 & M|v|(\mathbf{r}^{\ell+1})^2 & M|v|(\mathbf{r}^{\ell+1})^2 & 1 + M\mathbf{r}^{\ell+1} & M(\mathbf{r}^{\ell+1})^2 & M(\mathbf{r}^{\ell+1})^2 \\
0 & 0 & M|v|\mathbf{r}^{\ell+1} & M|v|\mathbf{r}^{\ell+1} & M & 1 + M\mathbf{r}^{\ell+1} & M\mathbf{r}^{\ell+1} \\
0 & 0 & M|v|\mathbf{r}^{\ell+1} & M|v|\mathbf{r}^{\ell+1} & M & M\mathbf{r}^{\ell+1} & 1 + M\mathbf{r}^{\ell+1}
\end{array}\right] \\
&:= \underbrace{J(\mathbf{r}^{\ell+1})}_{\text{Definition of } J(\mathbf{r}^{\ell+1})}.
\end{aligned} \tag{A.91}
$$

We also denote the Jacobian matrix within a single $\mathbf{p}^\ell-$ spherical coordinate :

$$
\tilde{J}^{\ell+1}_\ell := \frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_\ell}, \mathbf{v}^{\ell+1}_{\perp_\ell}, \mathbf{v}^{\ell+1}_{\|_\ell})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})}.
$$

Note this bound (A.91) holds for both *Type I* and *Type II* in (A.74). We split the proof for each *Type* :

Proof of (A.91) when $\mathbf{r}^\ell < \sqrt{\delta}$ *and* $\mathbf{r}^{\ell+1} < \sqrt{\delta}$ *:* Note that $\mathbf{p}^\ell-$spherical coordinate is well-defined of all $\tau \in [t^{\ell+1}, t^\ell]$. Due to the chart changing

$$
\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})} = \left[\begin{array}{c|c} 1 & \mathbf{0}_{1,6} \\ \hline \mathbf{0}_{6,1} & \nabla\Phi^{-1}_{\mathbf{p}^\ell}\nabla\Phi_{\mathbf{p}^{\ell+1}} \end{array}\right] \underbrace{\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_\ell}, \mathbf{v}^{\ell+1}_{\perp_\ell}, \mathbf{v}^{\ell+1}_{\|_\ell})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})}}_{=\tilde{J}^{\ell+1}_\ell}.
$$

Note that

$$
\begin{aligned}
|\mathbf{p}^\ell - \mathbf{p}^{\ell+1}| &\le |z^\ell - z^{\ell+1}| + |u^\ell - u^{\ell+1}| \\
&\lesssim |z^\ell - x^\ell| + |x^\ell - x^{\ell+1}| + |z^{\ell+1} - x^{\ell+1}| \\
&\quad + \left| u^\ell - \frac{v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)}{|v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)|} \right| + \left| u^{\ell+1} - \frac{v^{\ell+1} - (v^{\ell+1} \cdot n(z^{\ell+1}))n(z^{\ell+1})}{|v^{\ell+1} - (v^{\ell+1} \cdot n(z^{\ell+1}))n(z^{\ell+1})|} \right| \\
&\quad + \frac{|\mathbf{v}^\ell_\perp| + |\mathbf{v}^{\ell+1}_\perp| + |v||x^\ell - z^\ell| + |v||x^{\ell+1} - z^{\ell+1}|}{|v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)|} \\
&\lesssim_\xi \mathbf{r}^\ell.
\end{aligned}
$$

where we have used $\mathbf{r}^\ell \le C\sqrt{\delta}$ (therefore$|v^\ell - (v^\ell \cdot n(z^\ell))n(z^\ell)| \gtrsim (1 - \sqrt{\delta})|v|$) and $(A.75)$ and (A.46).

In order to show (A.91) it suffices to show that $\tilde{J}^{\ell+1}_\ell$ is bounded as (A.91) :

$$
\tilde{J}^{\ell+1}_\ell \ \le\ J(\mathbf{r}^{\ell+1}). \tag{A.92}
$$

This is due to the following matrix multiplication

$$
\begin{aligned}
&\left[\begin{array}{c|c} 1 & \mathbf{0}_{1,6} \\ \hline \mathbf{0}_{6,1} & \nabla\Phi_{\mathbf{p}^\ell}^{-1}\nabla\Phi_{\mathbf{p}^{\ell+1}} \end{array}\right] \tilde{J}_\ell^{\ell+1} \\
&\leq \left[\begin{array}{c|ccc|ccc}
1 & & \mathbf{0}_{1,3} & & & \mathbf{0}_{1,3} & \\ \hline
 & 1 & 0 & 0 & & & \\
\mathbf{0}_{3,1} & 0 & 1+C\mathbf{r}^{\ell+1} & C\mathbf{r}^{\ell+1} & & \mathbf{0}_{3,3} & \\
 & 0 & C\mathbf{r}^{\ell+1} & 1+C\mathbf{r}^{\ell+1} & & & \\ \hline
 & 0 & 0 & 0 & 1 & 0 & 0 \\
\mathbf{0}_{3,1} & 0 & C\mathbf{r}^{\ell+1}|v| & C\mathbf{r}^{\ell+1}|v| & 0 & 1+C\mathbf{r}^{\ell+1} & C\mathbf{r}^{\ell+1} \\
 & 0 & C\mathbf{r}^{\ell+1}|v| & C\mathbf{r}^{\ell+1}|v| & 0 & C\mathbf{r}^{\ell+1} & 1+C\mathbf{r}^{\ell+1}
\end{array}\right] J(\mathbf{r}^{\ell+1}) \\
&\leq J(C\mathbf{r}^{\ell+1}),
\end{aligned}
$$

where we used (A.60).

Now we prove the claim (A.92). We fix the $\mathbf{p}^\ell-$spherical coordinate and drop the index ℓ for the chart.

If $\mathbf{v}_\perp^\ell = 0$ then $t^{\ell+1} = t^\ell$. Otherwise if $\mathbf{v}_\perp^\ell \neq 0$ then $t^{\ell+1}$ is determined through

$$0 = \mathbf{v}_\perp^\ell (t^{\ell+1} - t^\ell) + \int_{t^{\ell+1}}^{t^\ell} \int_s^{t^\ell} F_\perp(\mathbf{X}_\ell(\tau; t^\ell, x^\ell, v^\ell), \mathbf{V}_\ell(\tau; t^\ell, x^\ell, v^\ell)) \mathrm{d}\tau \mathrm{d}s. \tag{A.93}$$

Since the ODE for $[\mathbf{X}_\ell(\tau; t, x, v), \mathbf{V}_\ell(\tau; t, x, v)]$ is autonomous,

$$0 = \mathbf{v}_\perp^\ell (t^{\ell+1} - t^\ell) + \int_0^{t^\ell - t^{\ell+1}} \int_{t^{\ell+1}-t^\ell+s}^0 F_\perp(\mathbf{X}_\ell(\tau; 0, x^\ell, v^\ell), \mathbf{V}_\ell(\tau; 0, x^\ell, v^\ell)) \mathrm{d}\tau \mathrm{d}s.$$

We take $t^\ell-$derivative to have

$$
\begin{aligned}
0 &= \frac{\partial(t^{\ell+1} - t^\ell)}{\partial t^\ell} \Big\{ \mathbf{v}_\perp^\ell - \int_0^{t^\ell - t^{\ell+1}} F_\perp(\mathbf{X}_\ell(t^{\ell+1} - t^\ell + s; 0, x^\ell, v^\ell), \mathbf{V}_\ell(t^{\ell+1} - t^\ell + s; 0, x^\ell, v^\ell)) \mathrm{d}s \Big\} \\
&= \frac{\partial(t^{\ell+1} - t^\ell)}{\partial t^\ell} \Big\{ \mathbf{v}_\perp^\ell - \int_{t^{\ell+1}}^{t^\ell} F_\perp(\mathbf{X}_\ell(s; t^\ell, x^\ell, v^\ell), \mathbf{V}_\ell(s; t^\ell, x^\ell, v^\ell)) \mathrm{d}s \Big\} \\
&= \frac{\partial(t^{\ell+1} - t^\ell)}{\partial t^\ell} (-\mathbf{v}_\perp^{\ell+1}),
\end{aligned}
$$

where we used the definition

$$\mathbf{v}_\perp^{\ell+1} = -\lim_{s \downarrow t^{\ell+1}} \mathbf{v}_\perp(s) = -\mathbf{v}_\perp^\ell + \int_{t^{\ell+1}}^{t^\ell} F_\perp(\mathbf{X}_{\mathbf{cl}}(\tau; t, x, v), \mathbf{V}_{\mathbf{cl}}(\tau; t, x, v)) \mathrm{d}\tau. \tag{A.94}$$

Therefore we conclude

$$\frac{\partial t^{\ell+1}}{\partial t^\ell} = 1.$$

Then combining with

$$
\begin{aligned}
\mathbf{x}_\parallel^{\ell+1} &= \mathbf{x}_\parallel^\ell + \int_0^{t^{\ell+1} - t^\ell} \mathbf{v}_\parallel(s; 0, x^\ell, v^\ell) \mathrm{d}s, \\
\mathbf{v}^{\ell+1} &= \mathbf{v}^\ell + \int_0^{t^{\ell+1} - t^\ell} F(s; 0, x^\ell, v^\ell) \mathrm{d}s,
\end{aligned}
$$

we conclude

$$\frac{\partial \mathbf{x}_\parallel^{\ell+1}}{\partial t^\ell} = \frac{\partial \mathbf{v}_\parallel^{\ell+1}}{\partial t^\ell} = \frac{\partial \mathbf{v}_\perp^{\ell+1}}{\partial t^\ell} = 0.$$

Now we use $|t^\ell - t^{\ell+1}| \lesssim_{\xi,t} \min\{\frac{|\mathbf{v}_\perp^{\ell+1}|}{|v|^2}, 1\}$, from (A.47), and (A.83) and (A.85) to have

$$
\begin{aligned}
\frac{\partial t^{\ell+1}}{\partial \mathbf{x}_\parallel^\ell} &= \frac{1}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{x}_\parallel^\ell} F_\perp(\mathbf{X}_\ell(\tau), \mathbf{V}_\ell(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\lesssim \frac{|t^\ell - t^{\ell+1}|^2}{|\mathbf{v}_\perp^{\ell+1}|} |v^\ell|^2 [1 + |v^\ell||t^\ell - t^{\ell+1}|] \lesssim \frac{|v^\ell|^2 |t^\ell - t^{\ell+1}|^2}{|\mathbf{v}_\perp^{\ell+1}|} \\
&\lesssim_{\xi,t} |t^\ell - t^{\ell+1}| \lesssim_{\xi,t} \frac{1}{|v|} \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v|}, \\
\frac{\partial t^{\ell+1}}{\partial \mathbf{v}_\perp^\ell} &= \frac{1}{\mathbf{v}_\perp^{\ell+1}} \left\{ (t^{\ell+1} - t^\ell) + \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X}_\ell(\tau), \mathbf{V}_\ell(\tau)) \mathrm{d}\tau \mathrm{d}s \right\} \\
&\lesssim \{1 + |v^\ell||t^\ell - t^{\ell+1}|\} \frac{|t^\ell - t^{\ell+1}|}{|\mathbf{v}_\perp^{\ell+1}|} \lesssim_{\xi,t} \frac{|t^\ell - t^{\ell+1}|}{|\mathbf{v}_\perp^{\ell+1}|} \lesssim_{\xi,t} \frac{1}{|v|^2}, \\
\frac{\partial t^{\ell+1}}{\partial \mathbf{v}_\parallel^\ell} &= \frac{1}{\mathbf{v}_\perp^{\ell+1}} \int_{t^{\ell+1}}^{t^\ell} \int_{s}^{t^\ell} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X}_\ell(\tau), \mathbf{V}_\ell(\tau)) \mathrm{d}\tau \mathrm{d}s \lesssim \frac{|v^\ell||t^\ell - t^{\ell+1}|^2}{|\mathbf{v}_\perp^{\ell+1}|} \lesssim_{\xi,t} \frac{1}{|v|^2} \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v|}.
\end{aligned}
\tag{A.95}
$$

We use (A.95) and (A.83) and (A.85) and (A.47) to have

$$
\begin{aligned}
\frac{\partial \mathbf{x}_\parallel^{\ell+1}}{\partial \mathbf{x}_\parallel^\ell} &= \mathbf{Id}_{2,2} + \frac{\mathbf{v}_\parallel^{\ell+1}}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{x}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s + \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{x}_\parallel^\ell} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\lesssim \mathbf{Id}_{2,2} + \Big(1 + \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|}\Big) |t^{\ell+1} - t^\ell|^2 |v^\ell|^2 \lesssim \mathbf{Id}_{2,2} + \frac{|\mathbf{v}_\perp^\ell|}{|v|}, \\
\frac{\partial \mathbf{x}_\parallel^{\ell+1}}{\partial \mathbf{v}_\perp^\ell} &= \Big\{ \frac{t^{\ell+1} - t^\ell}{\mathbf{v}_\perp^{\ell+1}} + \frac{1}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \Big\} \mathbf{v}_\parallel^{\ell+1} \\
&\quad + \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\lesssim |t^\ell - t^{\ell+1}| \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|} + |t^\ell - t^{\ell+1}|^2 \frac{|v^\ell|^2}{|\mathbf{v}_\perp^{\ell+1}|} + |t^\ell - t^{\ell+1}|^2 |v^\ell| \lesssim \frac{1}{|v|}, \\
\frac{\partial \mathbf{x}_\parallel^{\ell+1}}{\partial \mathbf{v}_\parallel^\ell} &= (t^{\ell+1} - t^\ell) + \frac{\mathbf{v}_\parallel^{\ell+1}}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\quad + \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\lesssim |t^\ell - t^{\ell+1}| + \Big(1 + \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|}\Big) |t^\ell - t^{\ell+1}|^2 |v^\ell| \big[1 + |v^\ell||t^\ell - t^{\ell+1}|\big] \\
&\lesssim |t^\ell - t^{\ell+1}| + \Big(1 + \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|}\Big) |t^\ell - t^{\ell+1}|^2 |v^\ell| \lesssim \frac{1}{|v|} \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v|}.
\end{aligned}
$$

Now we move to $D\mathbf{v}_\perp^{\ell+1}$ estimates. First we claim the crucial estimate of $t^\ell - t^{\ell+1}$:

$$
(t^\ell - t^{\ell+1}) F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell) = 2\mathbf{v}_\perp^{\ell+1} + O_\xi(1) |t^\ell - t^{\ell+1}|^2 |v^\ell|^3. \tag{A.96}
$$

As (A.93), we use the fact $\mathbf{x}_\perp^\ell = 0 = \mathbf{x}_\perp^{\ell+1}$ and the definition $\mathbf{v}_\perp^{\ell+1} = -\lim_{s \downarrow t^{\ell+1}} \mathbf{v}_\perp(s)$ and

$$
\begin{aligned}
\dot{\mathbf{v}}_\perp(s) &= F_\perp(\mathbf{X}_\ell(s; t^\ell, \mathbf{x}^\ell, \mathbf{v}^\ell), \mathbf{V}_\ell(s; t^\ell, \mathbf{x}^\ell, \mathbf{v}^\ell)) \\
&= F_\perp(\mathbf{X}_\ell(s; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1}), \mathbf{V}_\ell(s; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1})),
\end{aligned}
$$

to conclude the similar identity of (A.93)

$$
0 = -\mathbf{v}_\perp^{\ell+1}(t^\ell - t^{\ell+1}) + \int_{t^{\ell+1}}^{t^\ell} \int_{t^{\ell+1}}^{s} F_\perp(\mathbf{X}_\ell(\tau; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1}), \mathbf{V}_\ell(\tau; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1})) \mathrm{d}\tau \mathrm{d}s. \tag{A.97}
$$

For $t^{\ell+1} < \tau < t^{\ell}$, we have

$$\begin{aligned}
&F_{\perp}(\mathbf{X_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}), \mathbf{V_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell})) \\
&= F_{\perp}(\mathbf{x}^{\ell}, \mathbf{v}^{\ell}) + \int_{t^{\ell}}^{\tau} \frac{\partial}{\partial \tau} F_{\perp}(\mathbf{X_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}), \mathbf{V_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}))\mathrm{d}\tau,
\end{aligned}$$

and

$$\begin{aligned}
&F_{\perp}(\mathbf{X_{cl}}(\tau; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1}), \mathbf{V_{cl}}(\tau; t^{\ell+1}, \mathbf{x}^{\ell+1}, \mathbf{v}^{\ell+1})) \\
&= F_{\perp}(\mathbf{x}^{\ell+1}, \mathbf{v}^{\ell}) + \int_{t^{\ell+1}}^{\tau} \frac{\partial}{\partial \tau} F_{\perp}(\mathbf{X_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}), \mathbf{V_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}))\mathrm{d}\tau.
\end{aligned}$$

Therefore

$$F_{\perp}(\mathbf{X_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell}), \mathbf{V_{cl}}(\tau; t^{\ell}, \mathbf{x}^{\ell}, \mathbf{v}^{\ell})) = F_{\perp}(\mathbf{x}^{\ell+1}, \mathbf{v}^{\ell}) + O_{\xi}(1)|t^{\ell+1} - t^{\ell}||v|^3.$$

Plugging this into (A.97) we have

$$0 = -\mathbf{v}_{\perp}^{\ell+1}(t^{\ell} - t^{\ell+1}) + \frac{1}{2}(t^{\ell} - t^{\ell+1})^2 F_{\perp}(\mathbf{x}^{\ell+1}, \mathbf{v}^{\ell}) + O_{\xi}(1)|t^{\ell} - t^{\ell+1}|^3|v|^3,$$

and this proves our claim (A.96).

Using (A.96), we can find an extra cancellation in terms of order of $t^{\ell} - t^{\ell+1}$ to get

$$\begin{aligned}
\frac{\partial \mathbf{v}_{\perp}^{\ell+1}}{\partial \mathbf{x}_{\parallel}^{\ell}} &= \frac{-F_{\perp}(\mathbf{x}^{\ell+1}, \mathbf{v}^{\ell})}{\mathbf{v}_{\perp}^{\ell+1}} \int_{t^{\ell+1}}^{t^{\ell}} \int_{s}^{t^{\ell}} \frac{\partial}{\partial \mathbf{x}_{\parallel}^{\ell}} F_{\perp}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau \mathrm{d}s + \int_{t^{\ell+1}}^{t^{\ell}} \frac{\partial}{\partial \mathbf{x}_{\parallel}^{\ell}} F_{\perp}(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau))\mathrm{d}\tau \\
&= \Big\{ \frac{(t^{\ell} - t^{\ell+1})F_{\perp}(\mathbf{x}^{k+1}, \mathbf{v}^{\ell})}{-2\mathbf{v}_{\perp}^{\ell+1}} + 1 \Big\} (t^{\ell} - t^{\ell+1}) \frac{\partial}{\partial \mathbf{x}_{\parallel}^{\ell}} F_{\perp}(\mathbf{x}^{\ell}, \mathbf{v}^{\ell}) \\
&\quad + O_{\xi}(1) \Big\{ |t^{\ell} - t^{\ell+1}|^2 |v^{\ell}|^3 + \frac{|t^{\ell} - t^{\ell+1}|^3 |v^{\ell}|^3}{|\mathbf{v}_{\perp}^{\ell+1}|} \Big| \frac{\partial}{\partial \mathbf{x}_{\parallel}^{\ell}} F_{\perp}(\mathbf{x}^{\ell}, \mathbf{v}^{\ell}) \Big| \Big\} \\
&\lesssim_{\xi} \Big\{ -1 + O_{\xi}(1) \frac{|t^{\ell} - t^{\ell+1}|^2 |v^{\ell}|^3}{|\mathbf{v}_{\perp}^{\ell+1}|} + 1 \Big\} |t^{\ell} - t^{\ell+1}||v^{\ell}|^2 + |t^{\ell} - t^{\ell+1}|^2 |v^{\ell}|^3 \Big\{ 1 + \frac{|t^{\ell} - t^{\ell+1}||v^{\ell}|^2}{|\mathbf{v}_{\perp}^{\ell+1}|} \Big\} \\
&\lesssim_{\xi} |t^{\ell} - t^{\ell+1}|^2 |v^{\ell}|^3 \Big(1 + \frac{|t^{\ell} - t^{\ell+1}||v^{\ell}|^2}{|\mathbf{v}_{\perp}^{\ell+1}|} \Big) \lesssim_{\xi} |t^{\ell} - t^{\ell+1}|^2 |v^{\ell}|^3, \\
&\lesssim_{\xi,t} \frac{|\mathbf{v}_{\perp}^{\ell+1}|^2}{|v^{\ell}|},
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial \mathbf{v}_\perp^{\ell+1}}{\partial \mathbf{v}_\perp^{\ell}} &= -1 - \frac{\partial t^{\ell+1}}{\partial \mathbf{v}_\perp^{\ell}} F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell) + \int_{t^{\ell+1}}^{t^\ell} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \\
&= -1 + \frac{F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}}(t^\ell - t^{\ell+1}) - \frac{F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\qquad + \int_{t^{\ell+1}}^{t^\ell} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \\
&= -1 + 2 + O_\xi(1) \frac{|t^\ell - t^{\ell+1}|^2 |v^\ell|^3}{\mathbf{v}_\perp^{\ell+1}} \\
&\qquad - \frac{F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} \frac{(t^\ell - t^{\ell+1})^2}{2} \Big\{ \lim_{s \uparrow t^\ell} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) + O_\xi(1) |t^\ell - t^{\ell+1}| |v^\ell|^2 \Big\} \\
&\qquad + (t^\ell - t^{\ell+1}) \Big\{ \lim_{s \uparrow t^\ell} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) + O_\xi(1) |t^\ell - t^{\ell+1}| |v^\ell|^2 \Big\} \\
&= 1 + O_\xi(1) \Big\{ \frac{|t^\ell - t^{\ell+1}|^2 |v^\ell|^3}{|\mathbf{v}_\perp^{\ell+1}|} + \frac{|t^\ell - t^{\ell+1}|^3}{|\mathbf{v}_\perp^{\ell+1}|} |v^\ell|^3 \Big| \lim_{s \uparrow t^\ell} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \Big| + |t^\ell - t^{\ell+1}|^2 |v^\ell|^2 \Big\} \\
&\lesssim 1 + |t^\ell - t^{\ell+1}|^2 |v^\ell|^2 \Big\{ 1 + \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|} + \frac{|t^\ell - t^{\ell+1}| |v^\ell|^2}{|\mathbf{v}_\perp^{\ell+1}|} \Big\} \lesssim_{\xi,t} 1 + \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v^\ell|}, \\
\frac{\partial \mathbf{v}_\perp^{\ell+1}}{\partial \mathbf{v}_\parallel^{\ell}} &= \frac{-F_\perp(\mathbf{x}^{\ell+1}, v^\ell)}{\mathbf{v}_\perp^{\ell+1}} \int_{t^{\ell+1}}^{t^\ell} \int_{s}^{t^\ell} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s - \int_{t^{\ell+1}}^{t^\ell} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \\
&= \Big\{ \frac{(t^\ell - t^{\ell+1}) F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{-2\mathbf{v}_\perp^{\ell+1}} + 1 \Big\} (t^\ell - t^{\ell+1}) \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{x}^\ell, \mathbf{v}^\ell) \\
&\qquad + O_\xi(1) |t^\ell - t^{\ell+1}|^2 |v^\ell|^2 \Big\{ \frac{|F_\perp(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)| |t^\ell - t^{\ell+1}|}{|\mathbf{v}_\perp^{\ell+1}|} + 1 \Big\} \\
&\lesssim_\xi |t^\ell - t^{\ell+1}|^2 |v^\ell|^2 \Big\{ 1 + \frac{|t^\ell - t^{\ell+1}| |v^\ell|^2}{|\mathbf{v}_\perp^{\ell+1}|} \Big\} \lesssim_{\xi,t} \frac{|\mathbf{v}_\perp^{\ell+1}|^2}{|v^\ell|^2}.
\end{aligned}
$$

By (A.83) and (A.47),

$$
\begin{aligned}
\frac{\partial \mathbf{v}_\parallel^{\ell+1}}{\partial \mathbf{x}_\parallel^{\ell}} &= \frac{F_\parallel(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{x}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\qquad + \int_{t^\ell}^{t^{\ell+1}} \frac{\partial}{\partial \mathbf{x}_\parallel^\ell} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \lesssim |t^\ell - t^{\ell+1}| |v^\ell|^2 \Big\{ 1 + \frac{|t^\ell - t^{\ell+1}| |v^\ell|^2}{|\mathbf{v}_\perp^{\ell+1}|} \Big\} \\
&\lesssim_\xi |t^\ell - t^{\ell+1}| |v^\ell|^2 \lesssim_{\xi,t} |\mathbf{v}_\perp^{\ell+1}|, \\
\frac{\partial \mathbf{v}_\parallel^{\ell+1}}{\partial \mathbf{v}_\perp^{\ell}} &= \frac{-(t^\ell - t^{\ell+1}) F_\parallel(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} + \frac{F_\parallel(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s \\
&\qquad + \int_{t^\ell}^{t^{\ell+1}} \frac{\partial}{\partial \mathbf{v}_\perp^\ell} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \\
&\lesssim_{\xi,t} \Big(1 + \frac{|v^\ell|}{|\mathbf{v}_\perp^{\ell+1}|} \Big) \min\{ |v^\ell|, \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v^\ell|} \} \lesssim_{\xi,t} 1 + \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v^\ell|}, \\
\frac{\partial \mathbf{v}_\parallel^{\ell+1}}{\partial \mathbf{v}_\parallel^{\ell}} &= \mathbf{Id}_{2,2} + \frac{F_\parallel(\mathbf{x}^{\ell+1}, \mathbf{v}^\ell)}{\mathbf{v}_\perp^{\ell+1}} \int_{t^\ell}^{t^{\ell+1}} \int_{t^\ell}^{s} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\perp(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \mathrm{d}s + \int_{t^\ell}^{t^{\ell+1}} \frac{\partial}{\partial \mathbf{v}_\parallel^\ell} F_\parallel(\mathbf{X_{cl}}(\tau), \mathbf{V_{cl}}(\tau)) \mathrm{d}\tau \\
&\lesssim_\xi \mathbf{Id}_{2,2} + |t^\ell - t^{\ell+1}| |v^\ell| \{ 1 + \frac{|v^\ell|^2 |t^\ell - t^{\ell+1}|}{|\mathbf{v}_\perp^{\ell+1}|} \} \lesssim_{\xi,t} \mathbf{Id}_{2,2} + \frac{|\mathbf{v}_\perp^{\ell+1}|}{|v^\ell|}.
\end{aligned}
$$

These estimates prove the claim (A.92).

Proof of (A.91) for either $\mathbf{r}^\ell \geq \sqrt{\delta}$ *or* $\mathbf{r}^{\ell+1} \geq \sqrt{\delta}$ *:* Without loss of generality we assume $\mathbf{r}^\ell > C\sqrt{\delta}$ in (A.74). Recall that we chose a $\mathbf{p}^\ell$−spherical coordinate as $\mathbf{p}^\ell = (z^\ell, w^\ell)$ with $|z^\ell - x^\ell| \leq \sqrt{\delta}$ and any $w^\ell \in \mathbb{S}^2$ with $n(z^\ell) \cdot w^\ell = 0$.

Fix ℓ. Let us choose fixed numbers $\Delta_1, \Delta_2 > 0$ such that $|v|\Delta_1 \ll 1$ and $|v||t^{\ell+1} - (t^\ell - \Delta_1 - \Delta_2)| \ll 1$ so that

$$s^\ell \equiv t^\ell - \Delta_1, \quad s^{\ell+1} \equiv s^\ell - \Delta_2 = t^\ell - \Delta_1 - \Delta_2,$$

satisfying $|v||t^{\ell+1} - s^{\ell+1}| = |v||t^{\ell+1} - (t^\ell - \Delta_1 - \Delta_2)| \ll 1$ and $|v||t^\ell - s^\ell| = |v||\Delta_1| \ll 1$ so that the spherical coordinates are well-defined for $s \in [t^{\ell+1}, s^{\ell+1}]$ and $s \in [s^\ell, t^\ell]$.

Notice that

$$\frac{\partial t^{\ell+1}}{\partial s^{\ell+1}} = \frac{\partial(s^{\ell+1} + \Delta_1 + \Delta_2 - t_{\mathbf{b}}(x^\ell, v^\ell))}{\partial s^{\ell+1}} = 1, \quad \frac{\partial s^{\ell+1}}{\partial s^\ell} = \frac{\partial(s^\ell - \Delta_1)}{\partial s^\ell} = 1, \quad \frac{\partial s^\ell}{\partial t^\ell} = \frac{\partial(t^\ell - \Delta_1)}{\partial t^\ell} = 1.$$

By the chain rule,

$$\begin{aligned}
&\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})} \\
=&\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})}{\partial(s^{\ell+1}, \mathbf{x}_{\perp_{\ell+1}}(s^{\ell+1}), \mathbf{x}_{\|_{\ell+1}}(s^{\ell+1}), \mathbf{v}_{\perp_{\ell+1}}(s^{\ell+1}), \mathbf{v}_{\|_{\ell+1}}(s^{\ell+1}))} \frac{\partial(s^{\ell+1}, \mathbf{X}_{\mathbf{p}^{\ell+1}}(s^{\ell+1}), \mathbf{V}_{\mathbf{p}^{\ell+1}}(s^{\ell+1}))}{\partial(s^{\ell+1}, X_{\mathbf{cl}}(s^{\ell+1}), V_{\mathbf{cl}}(s^{\ell+1}))} \\
&\times \frac{\partial(s^{\ell+1}, X_{\mathbf{cl}}(s^{\ell+1}), V_{\mathbf{cl}}(s^{\ell+1}))}{\partial(s^\ell, X_{\mathbf{cl}}(s^\ell), V_{\mathbf{cl}}(s^\ell))} \frac{\partial(s^\ell, X_{\mathbf{cl}}(s^\ell), V_{\mathbf{cl}}(s^\ell))}{\partial(s^\ell, \mathbf{X}_{\mathbf{p}^\ell}(s^\ell), \mathbf{V}_{\mathbf{p}^\ell}(s^\ell))} \frac{\partial(s^\ell, \mathbf{x}_{\perp_\ell}(s^\ell), \mathbf{x}_{\|_\ell}(s^\ell), \mathbf{v}_{\perp_\ell}(s^\ell), \mathbf{v}_{\|_\ell}(s^\ell))}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})}.
\end{aligned}$$

We can express that $t^{\ell+1} = t^\ell - t_{\mathbf{b}}(x^\ell, v^\ell) = s^{\ell+1} + \Delta_1 + \Delta_2 - t_{\mathbf{b}}(x^\ell, v^\ell)$. Let us regard $t^{\ell+1}$ as t^1 and $s^{\ell+1}$ as s^1 and $\Delta_1 + \Delta_2$ as Δ in (A.86). Then we use (A.87) and (A.47) to have

$$\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|}, \mathbf{v}^{\ell+1}_{\perp}, \mathbf{v}^{\ell+1}_{\|})}{\partial(s^{\ell+1}, \mathbf{x}_\perp(s^{\ell+1}), \mathbf{x}_\|(s^{\ell+1}), \mathbf{v}_\perp(s^{\ell+1}), \mathbf{v}_\|(s^{\ell+1}))} \leq \left[\begin{array}{c|c|c} 1 & O_{\delta,\xi}(1)\frac{1}{|v|} & O_{\delta,\xi}(1)\frac{1}{|v|^2} \\ \hline 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \mathbf{0}_{2,1} & O_{\delta,\xi}(1) & O_{\delta,\xi}(1)\frac{1}{|v|} \\ \hline \mathbf{0}_{3,1} & O_{\delta,\xi}(1)|v| & O_{\delta,\xi}(1) \end{array}\right].$$

From (A.90)

$$\frac{\partial(s^{\ell+1}, \mathbf{X}_{\mathbf{p}^{\ell+1}}(s^{\ell+1}), \mathbf{V}_{\mathbf{p}^{\ell+1}}(s^{\ell+1}))}{\partial(s^{\ell+1}, X_{\mathbf{cl}}(s^{\ell+1}), V_{\mathbf{cl}}(s^{\ell+1}))} \lesssim_\xi \left[\begin{array}{c|c|c} 1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline \mathbf{0}_{3,1} & O_\xi(1) & \mathbf{0}_{3,3} \\ \hline \mathbf{0}_{3,1} & O_\xi(1)|v| & O_\xi(1) \end{array}\right],$$

and from $s^{\ell+1} = s^\ell - \Delta_2,\ X_{\mathbf{cl}}(s^{\ell+1}) = X_{\mathbf{cl}}(s^\ell) - (s^{\ell+1} - s^\ell)V_{\mathbf{cl}}(s^\ell),\ V_{\mathbf{cl}}(s^{\ell+1}) = V_{\mathbf{cl}}(s^\ell)$,

$$\frac{\partial(s^{\ell+1}, X_{\mathbf{cl}}(s^{\ell+1}), V_{\mathbf{cl}}(s^{\ell+1}))}{\partial(s^\ell, X_{\mathbf{cl}}(s^\ell), V_{\mathbf{cl}}(s^\ell))} \lesssim_\xi \begin{bmatrix} 1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \mathbf{0}_{3,1} & \mathbf{Id}_{3,3} & |s_1 - s_2|\mathbf{Id}_{3,3} \\ \mathbf{0}_{3,1} & \mathbf{0}_{3,3} & \mathbf{Id}_{3,3} \end{bmatrix},$$

and from (A.65)

$$\frac{\partial(s^\ell, X_{\mathbf{cl}}(s^\ell), V_{\mathbf{cl}}(s^\ell))}{\partial(s^\ell, \mathbf{X}_{\mathbf{p}^\ell}(s^\ell), \mathbf{V}_{\mathbf{p}^\ell}(s^\ell))} \lesssim_\xi \begin{bmatrix} 1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \mathbf{0}_{3,1} & O_\xi(1) & \mathbf{0}_{3,3} \\ \mathbf{0}_{3,1} & |v| & O_\xi(1) \end{bmatrix}.$$

Recall (A.82) to have

$$\frac{\partial(s^\ell, \mathbf{x}_{\perp_\ell}(s^\ell), \mathbf{x}_{\|_\ell}(s^\ell), \mathbf{v}_{\perp_\ell}(s^\ell), \mathbf{v}_{\|_\ell}(s^\ell))}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})} \lesssim_\xi \left[\begin{array}{c|cc|c} 1 & 0 & \mathbf{0}_{1,2} & \mathbf{0}_{1,3} \\ \hline O_\xi(1)|v| & 0 & O_\xi(1) & O_\xi(1)|t^\ell - s_1| \\ \hline O_\xi(1)|v|^2 & 0 & O_\xi(1)|v| & O_\xi(1) \end{array}\right].$$

By direct matrix multiplication

$$\frac{\partial(t^{\ell+1}, 0, \mathbf{x}^{\ell+1}_{\|_{\ell+1}}, \mathbf{v}^{\ell+1}_{\perp_{\ell+1}}, \mathbf{v}^{\ell+1}_{\|_{\ell+1}})}{\partial(t^\ell, 0, \mathbf{x}^\ell_{\|_\ell}, \mathbf{v}^\ell_{\perp_\ell}, \mathbf{v}^\ell_{\|_\ell})} \lesssim_{t,\xi} \left[\begin{array}{c|c|c|c} 1 & 0 & \frac{1}{|v|} & \frac{1}{|v|^2} \\ \hline 0 & 0 & \mathbf{0}_{1,2} & \mathbf{0}_{1,3} \\ \mathbf{0}_{2,1} & \mathbf{0}_{2,1} & 1 & \frac{1}{|v|} \\ \hline \mathbf{0}_{3,1} & \mathbf{0}_{3,1} & |v| & 1 \end{array}\right].$$

Note that for *Type II* we have $\mathbf{r}^{\ell+1} \gtrsim \sqrt{\delta}$ so that from (A.91)

$$J(\mathbf{r}^{\ell+1}) \gtrsim \left[\begin{array}{c|c|c|c} 1 & 0 & \frac{M}{|v|}\sqrt{\delta} & \frac{M}{|v|^2}\min\{1,\sqrt{\delta}\} \\ \hline 0 & 0 & \mathbf{0}_{1,2} & \mathbf{0}_{1,3} \\ \mathbf{0}_{2,1} & \mathbf{0}_{2,1} & M\sqrt{\delta} & \frac{M}{|v|}\min\{1,\sqrt{\delta}\} \\ \hline \mathbf{0}_{3,1} & \mathbf{0}_{3,1} & M|v|\min\{\delta,\sqrt{\delta}\} & M\min\{\delta,\sqrt{\delta}\} \end{array}\right] \gtrsim_{\delta,t,\xi} \frac{\partial(t^{\ell+1},0,\mathbf{x}^{\ell+1}_{\parallel_{\ell+1}},\mathbf{v}^{\ell+1}_{\perp_{\ell+1}},\mathbf{v}^{\ell+1}_{\parallel_{\ell+1}})}{\partial(t^{\ell},0,\mathbf{x}^{\ell}_{\parallel_{\ell}},\mathbf{v}^{\ell}_{\perp_{\ell}},\mathbf{v}^{\ell}_{\parallel_{\ell}})}.$$

This proves our claim (A.91) for *Type II.*

Step 5. Eigenvalues and diagonalization of of (A.91)

By a basic linear algebra (row and column operations), the characteristic polynomial of (A.91) equals, with $\mathbf{r} = \mathbf{r}^{\ell+1}$,

$$\det \begin{bmatrix} 1-\lambda & 0 & \frac{M}{|v|}\mathbf{r} & \frac{M}{|v|}\mathbf{r} & \frac{M}{|v|^2} & \frac{M}{|v|^2}\mathbf{r} & \frac{M}{|v|^2}\mathbf{r} \\ 0 & -\lambda & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1+M\mathbf{r}-\lambda & M\mathbf{r} & \frac{M}{|v|} & \frac{M}{|v|}\mathbf{r} & \frac{M}{|v|}\mathbf{r} \\ 0 & 0 & M\mathbf{r} & 1+M\mathbf{r}-\lambda & \frac{M}{|v|} & \frac{M}{|v|}\mathbf{r} & \frac{M}{|v|}\mathbf{r} \\ 0 & 0 & M|v|\mathbf{r}^2 & M|v|\mathbf{r}^2 & 1+M\mathbf{r}-\lambda & M\mathbf{r}^2 & M\mathbf{r}^2 \\ 0 & 0 & M|v|\mathbf{r} & M|v|\mathbf{r} & M & 1+M\mathbf{r}-\lambda & M\mathbf{r} \\ 0 & 0 & M|v|\mathbf{r} & M|v|\mathbf{r} & M & M\mathbf{r} & 1+M\mathbf{r}-\lambda \end{bmatrix}$$
$$= -\lambda(\lambda-1)^5[\lambda-(1+5M\mathbf{r})].$$

Therefore eigenvalues are

$$\begin{aligned} &\lambda_0 = 0, \quad \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = 1, \\ &\lambda_7 = 1 + 5M\mathbf{r}^{\ell+1} = 1 + 5M\frac{|\mathbf{v}_{\perp}^{\ell+1}|}{|v^{\ell+1}|}. \end{aligned} \tag{A.97}$$

Corresponding eigenvectors are

$$\begin{pmatrix} 0\\1\\0\\0\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 1\\0\\0\\0\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\1\\-1\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\1\\0\\-|v|\mathbf{r}\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\1\\0\\0\\-|v|\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\1\\0\\0\\0\\-|v| \end{pmatrix}, \begin{pmatrix} 1\\0\\|v|\\|v|\\|v|^2\mathbf{r}\\|v|^2\\|v|^2 \end{pmatrix}.$$

Write $P = P(\mathbf{r}^\ell)$ as a block matrix of above column eigenvectors. Then

$$\mathcal{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & |v| \\ 0 & 0 & -1 & 0 & 0 & 0 & |v| \\ 0 & 0 & 0 & -|v|\mathbf{r} & 0 & 0 & |v|^2\mathbf{r} \\ 0 & 0 & 0 & 0 & -|v| & 0 & |v|^2 \\ 0 & 0 & 0 & 0 & 0 & -|v| & |v|^2 \end{bmatrix}, \ \mathcal{P}^{-1} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \frac{-1}{5|v|} & \frac{-1}{5|v|} & \frac{-1}{5|v|^2\mathbf{r}} & \frac{-1}{5|v|^2} & \frac{-1}{5|v|^2} \\ 0 & 0 & \frac{1}{5} & \frac{-4}{5} & \frac{1}{5|v|\mathbf{r}} & \frac{1}{5|v|} & \frac{1}{5|v|} \\ 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-4}{5|v|\mathbf{r}} & \frac{1}{5|v|} & \frac{1}{5|v|} \\ 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{1}{5|v|\mathbf{r}} & \frac{-4}{5|v|} & \frac{1}{5|v|} \\ 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{1}{5|v|\mathbf{r}} & \frac{1}{5|v|} & \frac{-4}{5|v|} \\ 0 & 0 & \frac{1}{5|v|} & \frac{1}{5|v|} & \frac{1}{5|v|^2\mathbf{r}} & \frac{1}{5|v|^2} & \frac{1}{5|v|^2} \end{bmatrix}. \tag{A.98}$$

Therefore

$$J(\mathbf{r}) = \mathcal{P}(\mathbf{r})\Lambda(\mathbf{r})\mathcal{P}^{-1}(\mathbf{r}),$$

and

$$\Lambda(\mathbf{r}) := \mathrm{diag}\Big[0,1,1,1,1,1,1+5M\mathbf{r}\Big],$$

where the notation $\mathrm{diag}[a_1,\cdots,a_m]$ is a $m\times m-$matrix with $a_{ii} = a_i$ and $a_{ij} = 0$ for all $i \neq j$.

Step 6. The $i-$th intermediate group

We claim that, for $i = 1, 2, \cdots, [\frac{|t-s||v|}{L_\xi}]$,

$$\begin{aligned}
&J^{\ell_{i+1}}_{\ell_{i+1}-1} \times \cdots \times J^{\ell_i+1}_{\ell_i} \\
&= \frac{\partial(t^{\ell_{i+1}}, 0, \mathbf{x}^{\ell_{i+1}}_{\|_{\ell_{i+1}}}, \mathbf{v}^{\ell_{i+1}}_{\perp_{\ell_{i+1}}}, \mathbf{v}^{\ell_{i+1}}_{\|_{\ell_{i+1}}})}{\partial(t^{\ell_{i+1}-1}, 0, \mathbf{x}^{\ell_{i+1}-1}_{\|_{\ell_{i+1}-1}}, \mathbf{v}^{\ell_{i+1}-1}_{\perp_{\ell_{i+1}-1}}, \mathbf{v}^{\ell_{i+1}-1}_{\|_{\ell_{i+1}-1}})} \times \cdots \times \frac{\partial(t^{\ell_i+1}, 0, \mathbf{x}^{\ell_i+1}_{\|_{\ell_{i+1}}}, \mathbf{v}^{\ell_i+1}_{\perp_{\ell_{i+1}}}, \mathbf{v}^{\ell_i+1}_{\|_{\ell_{i+1}}})}{\partial(t^{\ell_i}, 0, \mathbf{x}^{\ell_i}_{\|_{\ell_i}}, \mathbf{v}^{\ell_i}_{\perp_{\ell_i}}, \mathbf{v}^{\ell_i}_{\|_{\ell_i}})} \\
&\leq \mathcal{P}(\mathbf{r}_i)(\Lambda(\mathbf{r}_i))^{\frac{C_\xi}{\mathbf{r}_i}} \mathcal{P}^{-1}(\mathbf{r}_i).
\end{aligned} \tag{A.99}$$

By the definition of the group, $L_\xi \leq |v||t^{\ell_i} - t^{\ell_{i+1}}| \leq C_1 < +\infty$ for all i. By the Velocity lemma(Lemma A.1),

$$\frac{1}{\mathcal{C}_1} e^{-\frac{\mathcal{C}}{2}C_1} \mathbf{r}^{\ell_i} \leq \mathbf{r}^{\ell_{i+1}} \equiv \frac{|\mathbf{v}^{\ell_{i+1}}_\perp|}{|v|}, \mathbf{r}^{\ell_{i+1}-1} \equiv \frac{|\mathbf{v}^{\ell_{i+1}-1}_\perp|}{|v|}, \cdots, \mathbf{r}^{\ell_i+1} \equiv \frac{|\mathbf{v}^{\ell_i+1}_\perp|}{|v|}, \mathbf{r}^{\ell_i} \equiv \frac{|\mathbf{v}^{\ell_i}_\perp|}{|v|} \leq \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}C_1} \mathbf{r}^{\ell_i},$$

and define

$$\mathbf{r}_i \equiv \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}C_1} \mathbf{r}^{\ell_i}.$$

Then we have

$$\frac{1}{(\mathcal{C}_1)^2} e^{-\mathcal{C}C_1} \mathbf{r}_i \ \leq\ \mathbf{r}^j \ \leq\ \mathbf{r}_i \quad \text{for all} \quad \ell_{i+1} \leq j \leq \ell_i. \tag{A.100}$$

From (A.91), we have a uniform bound for all $\ell_{i+1} \leq j \leq \ell_i$

$$J^{j+1}_j \lesssim J(\mathbf{r}_i) = \mathcal{P}(\mathbf{r}_i)\Lambda(\mathbf{r}_i)\mathcal{P}^{-1}(\mathbf{r}_i).$$

Therefore

$$J^{\ell_{i+1}}_{\ell_{i+1}-1} \times \cdots \times J^{\ell_i+1}_{\ell_i} \leq \mathcal{P}(\mathbf{r}_i)[\Lambda(\mathbf{r}_i)]^{|\ell_{i+1}-\ell_i|}\mathcal{P}^{-1}(\mathbf{r}_i).$$

Now we only left to prove $|\ell_{i+1} - \ell_i| \lesssim_\Omega \frac{1}{\mathbf{r}_i}$: For any $\ell_{i+1} \leq j \leq \ell_i$, we have $\xi(x^j) = 0 = \xi(x^{j+1}) = \xi(x^j - (t^j - t^{j+1})v^j)$. We expand $\xi(x^j - (t^j - t^{j+1})v^j)$ in time to have

$$\begin{aligned}
\xi(x^{j+1}) &= \xi(x^j) + \int_{t^j}^{t^{j+1}} \frac{d}{ds}\xi(X_{\mathbf{cl}}(s))\mathrm{d}s \\
&= \xi(x^j) + (v^j \cdot \nabla\xi(x^j))(t^{j+1} - t^j) + \int_{t^j}^{t^{j+1}} \int_{t^j}^{s} \frac{d^2}{d\tau^2}\xi(X_{\mathbf{cl}}(\tau))\mathrm{d}\tau\mathrm{d}s,
\end{aligned}$$

and

$$0 = (v^j \cdot \nabla\xi(x^j))(t^{j+1} - t^j) + \frac{(t^j - t^{j+1})^2}{2}(v^j \cdot \nabla^2\xi(X_{\mathbf{cl}}(\tau_*)) \cdot v^j), \quad \text{for some } \tau_* \in [t^{j+1}, t^j].$$

Therefore

$$\frac{v^j \cdot \nabla\xi(x^j)}{|v|} = (t^j - t^{j+1})|v| \frac{v^j \cdot \nabla^2\xi(X_{\mathbf{cl}}(\tau_*)) \cdot v^j}{2|v|^2}.$$

From the convexity (A.3), there exists $C_2 \gg 1$

$$\frac{1}{C_2}|t^j - t^{j+1}||v| \leq |\mathbf{r}^j| = \frac{|\mathbf{v}^j_\perp|}{|v|} = \frac{|v^j \cdot \nabla\xi(x^j)|}{|v|} \leq C_2|t^j - t^{j+1}||v|. \tag{A.101}$$

Therefore we have a lower bound of $|v||t^j - t^{j+1}| : |v||t^j - t^{j+1}| \geq \frac{1}{C_2}|\mathbf{r}^j| \geq \frac{1}{(\mathcal{C}_1)^2C_2}e^{-\mathcal{C}C_1}\mathbf{r}_i$, where we have used (A.100). Finally, using the definition of one group($1 \leq |v||t^{\ell_i} - t^{\ell_{i+1}}| \leq C_1$), we have the following upper bound of the number of bounces in this one group($i-$th intermediate group)

$$|\ell_i - \ell_{i+1}| \leq \frac{|v||t^{\ell_i} - t^{\ell_{i+1}}|}{\min_{\ell_i \leq j \leq \ell_{i+1}} |v||t^j - t^{j+1}|} \leq \frac{C_1}{\frac{1}{(\mathcal{C}_1)^2C_2}e^{-\mathcal{C}C_1}\mathbf{r}_i} \lesssim_\xi \frac{1}{\mathbf{r}_i},$$

and this complete our claim (A.99).

Step 7. Whole intermediate groups

Recall $\mathcal{P}$ and $\mathcal{P}^{-1}$ from (A.98). We claim that, there exists $C_3 > 0$ such that

$$\prod_{i=1}^{[\frac{|t-s||v|}{L_\xi}]} J^{\ell_{i+1}}_{\ell_{i+1}-1} \times \cdots \times J^{\ell_i+1}_{\ell_i} \leq (C_3)^{|t-s||v|} \mathcal{P}(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}) \mathcal{P}^{-1}(\mathbf{r}_1). \tag{A.102}$$

From the one group estimate (A.99),

$$\begin{aligned}
&\prod_{i=1}^{[\frac{|t-s||v|}{L_\xi}]} J^{\ell_{i+1}}_{\ell_{i+1}-1} \times \cdots \times J^{\ell_i+1}_{\ell_i} \\
&\lesssim \mathcal{P}(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}) (\Lambda(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}))^{\frac{C_\xi}{\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}) \times \mathcal{P}(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]-1})} \\
&\quad \times (\Lambda(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]-1}))^{\frac{C_\xi}{\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]-1}}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]-1}) \times \quad \cdots} \\
&\quad \times \cdots \underbrace{\quad \times \mathcal{P}(\mathbf{r}_{i+1})} (\Lambda(\mathbf{r}_{i+1}))^{\frac{C_\xi}{\mathbf{r}_{i+1}}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_{i+1}) \times \mathcal{P}(\mathbf{r}_i)} (\Lambda(\mathbf{r}_i))^{\frac{C_\xi}{\mathbf{r}_i}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_i) \times \mathcal{P}(\mathbf{r}_{i-1})} \\
&\quad \times (\Lambda(\mathbf{r}_{i-1}))^{\frac{C_\xi}{\mathbf{r}_{i-1}}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_{i-1}) \times \quad \cdots} \\
&\quad \times \cdots \underbrace{\quad \times \mathcal{P}(\mathbf{r}_2)} (\Lambda(\mathbf{r}_2))^{\frac{C_\xi}{\mathbf{r}_2}} \underbrace{\mathcal{P}^{-1}(\mathbf{r}_2) \times \mathcal{P}(\mathbf{r}_1)} (\Lambda(\mathbf{r}_1))^{\frac{C_\xi}{\mathbf{r}_1}} \mathcal{P}^{-1}(\mathbf{r}_1).
\end{aligned}$$

Now we focus on the underbraced matrix multiplication. Directly

$$\mathcal{P}^{-1}(\mathbf{r}_{i+1})\mathcal{P}(\mathbf{r}_i) = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \frac{-1+\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5|v|} & 0 & 0 & \frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} \\
0 & 0 & 1 & \frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} & 0 & 0 & |v|\frac{-1+\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} \\
0 & 0 & 0 & \frac{1+4\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} & 0 & 0 & 4|v|\frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} \\
0 & 0 & 0 & \frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} & 1 & 0 & |v|\frac{-1+\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} \\
0 & 0 & 0 & \frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} & 0 & 1 & |v|\frac{-1+\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5} \\
0 & 0 & 0 & \frac{1-\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5|v|} & 0 & 0 & \frac{4+\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}}{5}
\end{bmatrix}.$$

Due to the choice of $\mathbf{r}_i \equiv \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}C_1}\mathbf{r}^{\ell_i}$ in (A.100) we have $\left|\frac{\mathbf{r}_i}{\mathbf{r}_{i+1}}\right| = \left|\frac{\mathbf{r}^{\ell_i}}{\mathbf{r}^{\ell_{i+1}}}\right| \leq C_\xi$, where we have used the Velocity lemma and (A.46) and (A.47) : $\frac{1}{\mathcal{C}_1}e^{-\frac{\mathcal{C}}{2}C_1}\mathbf{r}^{\ell_{i+1}} \leq \frac{1}{\mathcal{C}_1}e^{-\frac{\mathcal{C}}{2}|t^{\ell_i}-t^{\ell_{i+1}}|}\mathbf{r}^{\ell_{i+1}} \leq \mathbf{r}^{\ell_i} \leq \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}|t^{\ell_i}-t^{\ell_{i+1}}|}\mathbf{r}^{\ell_{i+1}} \leq \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}C_1}\mathbf{r}^{\ell_{i+1}}$.

Therefore for sufficiently large $C_\xi > 0$, for all i

$$\mathcal{P}^{-1}\widetilde{(\mathbf{r}_{i+1})\mathcal{P}}(\mathbf{r}_i) \ \leq \ \mathcal{Q} := \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \frac{C_\xi}{|v|} & 0 & 0 & C_\xi \\
0 & 0 & 1 & C_\xi & 0 & 0 & C_\xi|v| \\
0 & 0 & 0 & C_\xi & 0 & 0 & C_\xi|v| \\
0 & 0 & 0 & C_\xi & 1 & 0 & C_\xi|v| \\
0 & 0 & 0 & C_\xi & 0 & 1 & C_\xi|v| \\
0 & 0 & 0 & \frac{C_\xi}{|v|} & 0 & 0 & C_\xi
\end{bmatrix}, \tag{A.103}$$

where we use a notation : For a matrix A, the entries of a matrix $\widetilde{A}$ is an absolute value of the entries of A, i.e. $(\widetilde{A})_{ij} = |(A)_{ij}|$.

Again we diagonalize $\mathcal{Q}$ as

$$
\mathcal{Q} = \mathcal{F}\mathcal{A}\mathcal{F}^{-1}
$$
$$
:= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & \frac{2C_\xi}{2C_\xi - 1} \\ 0 & 0 & 1 & 0 & 0 & 0 & \frac{2C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & 0 & 0 & -|v| & |v| \\ 0 & 0 & 0 & 1 & 0 & 0 & \frac{2C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & 0 & 1 & 0 & \frac{2C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & 0 & \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & 0 & & & & 0 & \\ & & & & & & 2C_\xi \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{-C_\xi}{2C_\xi - 1} \frac{1}{|v|} & 0 & 0 & \frac{-C_\xi}{2C_\xi - 1} \\ 0 & 0 & 1 & \frac{-C_\xi}{2C_\xi - 1} & 0 & 0 & \frac{-C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & \frac{-C_\xi}{2C_\xi - 1} & 1 & 0 & \frac{-C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & \frac{-C_\xi}{2C_\xi - 1} & 0 & 1 & \frac{-C_\xi |v|}{2C_\xi - 1} \\ 0 & 0 & 0 & \frac{-1}{2|v|} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2|v|} & 0 & 0 & \frac{1}{2} \end{bmatrix},
$$

and directly

$$
\begin{aligned}
&\mathcal{Q}^{[\frac{|t-s||v|}{L_\xi}]} = \mathcal{F}\mathcal{A}^{[\frac{|t-s||v|}{L_\xi}]}\mathcal{F}^{-1} \\
&= \mathcal{F} \ \mathrm{diag}\Big[1,1,1,1,1,0,(2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}\Big] \ \mathcal{F}^{-1} \\
&= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{|v|}\frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) & 0 & 0 & \frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) \\ 0 & 0 & 1 & \frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) & 0 & 0 & |v|\frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) \\ 0 & 0 & 0 & \frac{(2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}}{2} & 0 & 0 & |v|\frac{(2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}}{2} \\ 0 & 0 & 0 & \frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) & 1 & 0 & |v|\frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) \\ 0 & 0 & 0 & \frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) & 0 & 1 & |v|\frac{C_\xi}{2C_\xi-1}((2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}-1) \\ 0 & 0 & 0 & \frac{1}{|v|}\frac{(2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}}{2} & 0 & 0 & \frac{(2C_\xi)^{[\frac{|t-s||v|}{L_\xi}]}}{2} \end{bmatrix}.
\end{aligned} \tag{A.104}
$$

Notice that from (A.97)

$$
\Big[\Lambda(\mathbf{r}_i)\Big]^{\frac{C_\xi}{\mathbf{r}_i}} \leq (1+5M\mathbf{r}_i)^{\frac{C_\xi}{\mathbf{r}_i}} \ \mathbf{Id}_{7,7} \leq C'_\xi \ \mathbf{Id}_{7,7}.
$$

Now we use (A.99) and take the absolute value of the entries and then use (A.103) and (A.104), for $\tilde{t} := t - s$,

$$
\begin{aligned}
&\prod_{i=1}^{[\frac{\tilde{t}|v|}{L_\xi}]} J^{\ell_{i+1}}_{\ell_{i+1}-1} \times \cdots \times J^{\ell_i+1}_{\ell_i} \\
&\leq \widetilde{\mathcal{P}(\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]}})(1+5M\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]})^{\frac{C_\xi}{\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]}}}\mathcal{Q}(1+5M\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]-1})^{\frac{C_\xi}{\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]-1}}}\mathcal{Q}\times\cdots \\
&\quad \times \cdots \times \mathcal{Q}(1+5M\mathbf{r}_{i+1})^{\frac{C_\xi}{\mathbf{r}_{i+1}}}\mathcal{Q}(1+5M\mathbf{r}_i)^{\frac{C_\xi}{\mathbf{r}_i}}\mathcal{Q}(1+5M\mathbf{r}_{i-1})^{\frac{C_\xi}{\mathbf{r}_{i-1}}}\mathcal{Q}\times\cdots \\
&\quad \times \cdots \times \mathcal{Q}(1+5M\mathbf{r}_2)^{\frac{C_\xi}{\mathbf{r}_2}}\mathcal{Q}(1+5M\mathbf{r}_1)^{\frac{C_\xi}{\mathbf{r}_1}}\widetilde{\mathcal{P}^{-1}(\mathbf{r}_1)} \\
&\leq (C'_\xi)^{[\frac{\tilde{t}|v|}{L_\xi}]} \times \widetilde{\mathcal{P}(\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]}})\mathcal{Q}^{[\frac{\tilde{t}|v|}{L_\xi}]-1}\widetilde{\mathcal{P}^{-1}(\mathbf{r}_1)} \\
&\leq (C'_\xi)^{[\frac{\tilde{t}|v|}{L_\xi}]} \times \widetilde{\mathcal{P}(\mathbf{r}_{[\frac{\tilde{t}|v|}{L_\xi}]}})\mathcal{F}\mathcal{A}^{[\frac{\tilde{t}|v|}{L_\xi}]}\mathcal{F}^{-1}\widetilde{\mathcal{P}^{-1}(\mathbf{r}_1)}.
\end{aligned}
$$

Now we use the explicit form of (A.104) to bound

$$
\begin{aligned}
&C^{C\tilde{t}|v|}\left[\begin{array}{cc|cc|c|cc}
1 & 0 & \frac{(C_\xi)^{\tilde t|v|}}{|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|^2}\frac{1}{|\mathbf{r}_1|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|^2} & \frac{(C_\xi)^{\tilde t|v|}}{|v|^2} \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & 0 & (C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|}\frac{1}{|\mathbf{r}_1|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|} \\
0 & 0 & (C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|}\frac{1}{|\mathbf{r}_1|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|} & \frac{(C_\xi)^{\tilde t|v|}}{|v|} \\ \hline
0 & 0 & |v|(C_\xi)^{\tilde t|v|}|\mathbf{r}_{[\frac{\tilde t|v|}{L_\xi}]}| & |v|(C_\xi)^{\tilde t|v|}|\mathbf{r}_{[\frac{\tilde t|v|}{L_\xi}]}| & (C_\xi)^{\tilde t|v|}\frac{|\mathbf{r}_{[\frac{\tilde t|v|}{L_\xi}]}|}{|\mathbf{r}_1|} & (C_\xi)^{\tilde t|v|}|\mathbf{r}_{[\frac{\tilde t|v|}{L_\xi}]}| & (C_\xi)^{\tilde t|v|}|\mathbf{r}_{[\frac{\tilde t|v|}{L_\xi}]}| \\ \hline
0 & 0 & |v|(C_\xi)^{\tilde t|v|} & |v|(C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|}\frac{1}{|\mathbf{r}_1|} & (C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|} \\
0 & 0 & |v|(C_\xi)^{\tilde t|v|} & |v|(C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|}\frac{1}{|\mathbf{r}_1|} & (C_\xi)^{\tilde t|v|} & (C_\xi)^{\tilde t|v|}
\end{array}\right] \\
&\lesssim C^{C|t-s||v|}\left[\begin{array}{cc|c|c|c}
1 & 0 & \frac{1}{|v|} & \frac{1}{|v||\mathbf{v}^1_\perp|} & \frac{1}{|v|^2} \\
0 & 1 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\ \hline
\mathbf{0}_{2,1} & \mathbf{0}_{2,1} & O_\xi(1) & \frac{1}{|\mathbf{v}^1_\perp|} & \frac{1}{|v|} \\ \hline
0 & 0 & |\mathbf{v}^1_\perp| & O_\xi(1) & \frac{|\mathbf{v}^1_\perp|}{|v|} \\ \hline
\mathbf{0}_{2,1} & \mathbf{0}_{2,1} & |v| & \frac{|v|}{|\mathbf{v}^1_\perp|} & O_\xi(1)
\end{array}\right]_{7\times 7},
\end{aligned}
\tag{A.105}
$$

where we have used (A.101) and the Velocity lemma (Lemma A.1) and (A.46), (A.47) and

$$
\mathbf{r}_i = \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}C_1}\mathbf{r}^i \lesssim e^{C|t-s||v|}\frac{|\mathbf{v}^1_\perp|}{|v|}, \quad \text{and} \quad \frac{\mathbf{r}_{[\frac{|t-s||v|}{L_\xi}]}}{\mathbf{r}_1} = \frac{\mathbf{r}^{[\frac{|t-s||v|}{L_\xi}]}}{\mathbf{r}^1} = \frac{\left|\mathbf{v}_\perp^{[\frac{|t-s||v|}{L_\xi}]}\right|}{|\mathbf{v}^1_\perp|} \leq \mathcal{C}_1 e^{\frac{\mathcal{C}}{2}|v||t-s|}.
$$

Step 8. Intermediate summary for the matrix method and the final estimate for Type II

Recall from (A.80) and (A.82), (A.105), (A.87),

$$
\begin{aligned}
&\frac{\partial(s^{\ell_*}, \mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))}{\partial(s^1, \mathbf{X}_1(s^1), \mathbf{V}_1(s^1))} \equiv \frac{\partial(s^{\ell_*}, \mathbf{x}_{\perp_{\ell_*}}(s^{\ell_*}), \mathbf{x}_{\parallel_{\ell_*}}(s^{\ell_*}), \mathbf{v}_{\perp_{\ell_*}}(s^{\ell_*}), \mathbf{v}_{\parallel_{\ell_*}}(s^{\ell_*}))}{\partial(s^1, \mathbf{x}_{\perp_1}(s^1), \mathbf{x}_{\parallel_1}(s^1), \mathbf{v}_{\perp_1}(s^1), \mathbf{v}_{\parallel_1}(s^1))} \\
&= \frac{\partial(s^{\ell_*}, \mathbf{x}_{\perp_{\ell_*}}(s^{\ell_*}), \mathbf{x}_{\parallel_{\ell_*}}(s^{\ell_*}), \mathbf{v}_{\perp_{\ell_*}}(s^{\ell_*}), \mathbf{v}_{\parallel_{\ell_*}}(s^{\ell_*}))}{\partial(t^{\ell_*}, 0, \mathbf{x}^{\ell_*}_{\parallel_{\ell_*}}, \mathbf{v}^{\ell_*}_{\perp_{\ell_*}}, \mathbf{v}^{\ell_*}_{\parallel_{\ell_*}})} \\
&\quad\times \prod_{i=1}^{[\frac{|t-s||v|}{L_\xi}]} \frac{\partial(t^{\ell_{i+1}}, 0, \mathbf{x}^{\ell_{i+1}}_{\parallel_{\ell_{i+1}}}, \mathbf{v}^{\ell_{i+1}}_{\perp_{\ell_{i+1}}}, \mathbf{v}^{\ell_{i+1}}_{\parallel_{\ell_{i+1}}})}{\partial(t^{\ell_{i+1}-1}, 0, \mathbf{x}^{\ell_{i+1}-1}_{\parallel_{\ell_{i+1}-1}}, \mathbf{v}^{\ell_{i+1}-1}_{\perp_{\ell_{i+1}-1}}, \mathbf{v}^{\ell_{i+1}-1}_{\parallel_{\ell_{i+1}-1}})} \times \cdots \times \frac{\partial(t^{\ell_i+1}, 0, \mathbf{x}^{\ell_i+1}_{\parallel_{\ell_i+1}}, \mathbf{v}^{\ell_i+1}_{\perp_{\ell_i+1}}, \mathbf{v}^{\ell_i+1}_{\parallel_{\ell_i+1}})}{\partial(t^{\ell_i}, 0, \mathbf{x}^{\ell_i}_{\parallel_{\ell_i}}, \mathbf{v}^{\ell_i}_{\perp_{\ell_i}}, \mathbf{v}^{\ell_i}_{\parallel_{\ell_i}})} \\
&\quad\times \frac{\partial(t^1, 0, \mathbf{x}^1_{\parallel_1}, \mathbf{v}^1_{\perp_1}, \mathbf{v}^1_{\parallel_1})}{\partial(s^1, \mathbf{x}_{\perp_1}(s^1), \mathbf{x}_{\parallel_1}(s^1), \mathbf{v}_{\perp_1}(s^1), \mathbf{v}_{\parallel_1}(s^1))} \\
&\leq (A.82) \times (A.105) \times (A.87).
\end{aligned}
$$

Then directly we bound

$$
\begin{aligned}
&\leq (A.82) \times C^{C|t-s||v|} \\
&\times \left[\begin{array}{c|cc|cc}
1 & \frac{1}{|\mathbf{v}^1_\perp|} + \frac{|v|}{|\mathbf{v}^1_\perp|^2} + |t^1 - s^1| & \frac{1}{|v|} + \frac{|v|}{|\mathbf{v}^1_\perp|^2} + |s^1 - t^1| & \frac{1}{|v||\mathbf{v}^1_\perp|} + |s^1 - t^1|^2 & \frac{1}{|v|^2} + \frac{|s^1 - t^1|}{|v|} \\ \hline
0 & 0 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\
\mathbf{0}_{2,1} & \frac{|v|^2}{|\mathbf{v}^1_\perp|^2} + \frac{|v|}{|\mathbf{v}^1_\perp|} + |v||s^1 - t^1| & 1 + \frac{|v|^2}{|\mathbf{v}^1_\perp|^2} & \frac{1}{|\mathbf{v}^1_\perp|} + |s^1 - t^1| & \frac{1}{|v|} \\ \hline
0 & \frac{|v|^2}{|\mathbf{v}^1_\perp|} + |v| & |\mathbf{v}^1_\perp| + \frac{|v|^2}{|\mathbf{v}^1_\perp|} & O_\xi(1) & \frac{|\mathbf{v}^1_\perp|}{|v|} \\
\mathbf{0}_{2,1} & \frac{|v|^3}{|\mathbf{v}^1_\perp|^2} + \frac{|v|^2}{|\mathbf{v}^1_\perp|} + |v|^2|s_1 - t^1| & |v| + \frac{|v|^3}{|\mathbf{v}^1_\perp|^2} & \frac{|v|}{|\mathbf{v}^1_\perp|} + |v||s_1 - t^1| & O_\xi(1)
\end{array}\right],
\end{aligned}
\tag{A.106}
$$

where we have used the Velocity lemma (Lemma A.1) and (A.101), (A.46), (A.47) and

$$
|v||t^1 - s^1| \leq \min\{|v|(t_{\mathbf{b}}(x,v) + t_{\mathbf{b}}(x,-v)), (t-s)|v|\} \lesssim_\Omega \min\{\frac{|\mathbf{v}^1_\perp|}{|v|}, (t-s)|v|\} \lesssim_\Omega C^{C|t-s||v|}\min\{\frac{|\mathbf{v}^1_\perp|}{|v|}, 1\}.
$$

Again we use the Velocity lemma (Lemma A.1) and (A.101), (A.46), (A.47) and

$$
|v||t^{\ell_*} - s^{\ell_*}| \leq \min\{|v||t^{\ell_*} - t^{\ell_*+1}|, |t-s||v|\} \lesssim_\Omega \min\{\frac{|\mathbf{v}^{\ell_*}_\perp|}{|v|}, |t-s||v|\} \lesssim_\Omega C^{C|t-s||v|}\min\{\frac{|\mathbf{v}^1_\perp|}{|v|}, 1\},
$$

and $|\mathbf{v}_\perp(s^{\ell_*})| \lesssim_\Omega C^{C|v|(t-s)}|\mathbf{v}_\perp^1|$ to have, from (A.106)

$$\frac{\partial(s^{\ell_*}, \mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))}{\partial(s^1, \mathbf{X}_1(s^1), \mathbf{V}_1(s^1))} \lesssim C^{C|t-s||v|} \left[\begin{array}{c|c|cc} 0 & \mathbf{0}_{1,3} & 0 & \mathbf{0}_{1,2} \\ \hline |\mathbf{v}_\perp^1| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|} \\ |v| & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{1}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) \end{array}\right]_{7\times 7}. \tag{A.107}$$

We consider the following case :

$$\text{There exists } \ell \in [\ell_*(s;t,x,v), 0] \text{ such that } \mathbf{r}^\ell \geq \sqrt{\delta}. \tag{A.108}$$

Therefore ℓ is *Type II* in (A.74). Equivalently $\tau \in [t^{\ell+1}, t^\ell]$ for some $\ell_* \leq \ell \leq 0$ and $|\xi(X_{\mathbf{cl}}(\tau;t,x,v))| \geq C\delta$. By the Velocity lemma (Lemma A.1), for all $1 \leq i \leq \ell_*(s;t,x,v)$,

$$|\mathbf{r}^i| \;=\; \frac{|\mathbf{v}_\perp^i|}{|v|} \;\gtrsim_\xi\; e^{-C_\xi|v||t^i-t^\ell|}|\mathbf{r}^\ell| \;\gtrsim_\xi\; e^{-C_\xi|v|(t-s)}\sqrt{\delta}.$$

Especially, for all $1 \leq i \leq \ell_*(s;t,x,v)$,

$$|\mathbf{r}^1| \gtrsim_\xi e^{-C_\xi|v|(t-s)}\sqrt{\delta}, \quad \frac{1}{|\mathbf{r}^i|} = \frac{|v|}{|\mathbf{v}_\perp^i|} \lesssim_\xi \frac{e^{C_\xi|v|(t-s)}}{\sqrt{\delta}}.$$

Note that $\ell_*(s;t,x,v) \lesssim \max_i \frac{|v||t-s|}{\mathbf{r}^i} \lesssim_\delta C^{C|v||t-s|}$.

Therefore in the case of (A.108), from (A.107),

$$\begin{aligned} \frac{\partial(s^{\ell_*}, \mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))}{\partial(s^1, \mathbf{X}_1(s^1), \mathbf{V}_1(s^1))} &\lesssim C^{C(t-s)|v|} \left[\begin{array}{c|cc|cc} 0 & 0 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\ \hline |\mathbf{v}_\perp^1| & \frac{1}{\sqrt{\delta}} & \frac{1}{\sqrt{\delta}} & \frac{1}{|v|} & \frac{1}{|v|} \\ |v| & \frac{1}{\delta} & \frac{1}{\delta} & \frac{1}{|v|}\frac{1}{\sqrt{\delta}} & \frac{1}{|v|} \\ \hline |v|^2 & |v|\frac{1}{\delta} & |v|\frac{1}{\delta} & \frac{1}{\sqrt{\delta}} & 1 \end{array}\right] \\ &\lesssim_\delta C^{C|v|(t-s)} \left[\begin{array}{c|c|c} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline |v| & 1 & \frac{1}{|v|} \\ \hline |v|^2 & |v| & 1 \end{array}\right]. \end{aligned}$$

Using (A.81) and (A.89) we conclude

$$\begin{aligned} &\frac{\partial(s, X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v))}{\partial(t,x,v)} \\ &\lesssim_{\delta,\xi} \; C^{C|v|(t-s)} \; \frac{\partial(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*}, \mathbf{X}_{\ell_*}(s^{\ell_*}), \mathbf{V}_{\ell_*}(s^{\ell_*}))} \left[\begin{array}{c|c|c} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline |v| & 1 & \frac{1}{|v|} \\ \hline |v|^2 & |v| & 1 \end{array}\right] \frac{\partial(s^1, \mathbf{x}_{\perp_1}(s^1), \mathbf{x}_{\parallel_1}(s^1), \mathbf{v}_{\perp_1}(s^1), \mathbf{v}_{\parallel_1}(s^1))}{\partial(t,x,v)} \\ &\lesssim_{\delta,\xi} \; C^{C|v|(t-s)} \begin{bmatrix} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ |v| & 1 & |s^{\ell_*} - s| \\ \mathbf{0}_{3,1} & |v| & 1 \end{bmatrix} \begin{bmatrix} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ |v| & 1 & \frac{1}{|v|} \\ |v|^2 & |v| & 1 \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \mathbf{0}_{3,1} & 1 & |t - s^1| \\ \mathbf{0}_{3,1} & |v| & 1 \end{bmatrix} \\ &\lesssim_{\delta,\xi} \; C^{C|v|(t-s)} \begin{bmatrix} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ |v| & 1 & \frac{1}{|v|} \\ |v|^2 & |v| & 1 \end{bmatrix}. \end{aligned} \tag{A.109}$$

Now we only need to consider the remainder case of (A.108), i.e.

$$\text{For all } \ell \in [\ell_*(s;t,x,v), 0], \text{ we have } \mathbf{r}_\ell \leq \sqrt{\delta}. \tag{A.110}$$

Note that in this case the moving frame($\mathbf{p}^{\ell}-$spherical coordinate) is well-defined for all $\tau \in [s,t]$. In next two step we use the ODE method to refine the submatrix of (A.107) :

$$\frac{\partial(\mathbf{x}_{\|_{\ell_*}}(s^{\ell_*}),\mathbf{v}_{\|_{\ell_*}}(s^{\ell_*}))}{\partial(\mathbf{x}_{\perp_1}(s^1),\mathbf{x}_{\|_1}(s^1),\mathbf{v}_{\perp_1}(s^1),\mathbf{v}_{\|_1}(s^1))} = \begin{bmatrix} \frac{\partial \mathbf{x}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{x}_{\perp_1}(s^1)} & \frac{\partial \mathbf{x}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{x}_{\|_1}(s^1)} & \frac{\partial \mathbf{x}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{v}_{\perp_1}(s^1)} & \frac{\partial \mathbf{x}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{v}_{\|_1}(s^1)} \\ \frac{\partial \mathbf{v}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{x}_{\perp_1}(s^1)} & \frac{\partial \mathbf{v}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{x}_{\|_1}(s^1)} & \frac{\partial \mathbf{v}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{v}_{\perp_1}(s^1)} & \frac{\partial \mathbf{v}_{\|_{\ell_*}}(s^{\ell_*})}{\partial \mathbf{v}_{\|_1}(s^1)} \end{bmatrix}_{4\times 6}.$$

Step 9. ODE method within the time scale $|t-s||v| \sim L_\xi$

Recall the end points (time) of intermediate groups from (A.78) :

$$s < \underbrace{t^{\ell_*} < t^{\ell_{[\frac{|t-s||v|}{L_\xi}]}+1}}_{[\frac{|t-s||v|}{L_\xi}]+1} < \underbrace{t^{\ell_{[\frac{|t-s||v|}{L_\xi}]}} < t^{\ell_{[\frac{|t-s||v|}{L_\xi}]-1}+1}}_{[\frac{|t-s||v|}{L_\xi}]} < \cdots < \underbrace{t^{\ell_i} < t^{\ell_{i-1}+1}}_{i} < \cdots < \underbrace{t^{\ell_2} < t^{\ell_1+1}}_{2} < \underbrace{t^{\ell_1} < t^1}_{1} < t,$$

where the underbraced numbering indicates the index of the intermediate group. We further choose points independently on (t,x,v) for all $i = 1,2,\cdots,[\frac{|t-s||v|}{L_\xi}]$:

$$\begin{aligned} t^{\ell_1+1} &< s^2 < t^{\ell_1}, \\ t^{\ell_2+1} &< s^3 < t^{\ell_2}, \\ &\vdots \\ t^{\ell_i+1} < s^{i+1} &< \underbrace{t^{\ell_i} < \cdots\cdots < t^{\ell_{i-1}+1}}_{i-\text{intermediate group}} < s^i < t^{\ell_{i-1}}, \\ &\vdots \\ t^{\ell_{[\frac{|t-s||v|}{L_\xi}]}+1} &< s^{\ell_{[\frac{|t-s||v|}{L_\xi}]}+1} < t^{\ell_{[\frac{|t-s||v|}{L_\xi}]}}. \end{aligned}$$

We claim the following estimate at s^{i+1} via s^i :

$$\begin{aligned} &\begin{bmatrix} |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{x}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{x}_{\|_1}(s^1)}| \\ |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{x}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{x}_{\|_1}(s^1)}| \end{bmatrix} \\ &\lesssim_{\delta,\xi} \begin{bmatrix} 1 & \frac{1}{|v|} \\ |v| & 1 \end{bmatrix} \begin{bmatrix} |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{x}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{x}_{\|_1}(s^1)}| \\ |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{x}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{x}_{\|_1}(s^1)}| \end{bmatrix} + e^{C|v||t-s^i|} \begin{bmatrix} 1 & \frac{1}{|v|} \\ |v| & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ |v|\Big(1+\frac{|v|}{|\mathbf{v}_\perp^1|}\Big) & |v|\Big(1+\frac{|v|}{|\mathbf{v}_\perp^1|}\Big) \end{bmatrix}, \\ &\begin{bmatrix} |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{v}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{v}_{\|_1}(s^1)}| \\ |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{v}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i+1})}{\partial \mathbf{v}_{\|_1}(s^1)}| \end{bmatrix} \\ &\lesssim_{\delta,\xi} \begin{bmatrix} 1 & \frac{1}{|v|} \\ |v| & 1 \end{bmatrix} \begin{bmatrix} |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{v}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{x}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{v}_{\|_1}(s^1)}| \\ |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{v}_{\perp_1}(s^1)}| & |\frac{\partial \mathbf{v}_{\|_{\ell_i}}(s^{i})}{\partial \mathbf{v}_{\|_1}(s^1)}| \end{bmatrix} + e^{C|v||t-s^i|} \begin{bmatrix} 1 & \frac{1}{|v|} \\ |v| & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}. \end{aligned} \tag{A.111}$$

Within the $i-$th intermediate group, we fix $\mathbf{p}^{\ell_i}-$spherical coordinate in *Step 9*. For the sake of simplicity we drop the index ℓ_i.

Denote, from (A.59),

$$F_\|(\mathbf{x}_\perp,\mathbf{x}_\|,\mathbf{v}_\perp,\mathbf{v}_\|) := D(\mathbf{x}_\perp,\mathbf{x}_\|,\mathbf{v}_\|) + E(\mathbf{x}_\perp,\mathbf{x}_\|,\mathbf{v}_\|)\mathbf{v}_\perp, \tag{A.112}$$

where D is a $\mathbf{r}^3$-vector-valued function and E is a 3×3 matrix-valued function :

$$\begin{aligned} D(\mathbf{x}_\perp,\mathbf{x}_\|,\mathbf{v}_\|) = &\sum_i G_{ij}(\mathbf{x}_\perp,\mathbf{x}_\|) \frac{(-1)^{i+1}}{-\mathbf{n}(\mathbf{x}_\|)\cdot(\partial_1\eta(\mathbf{x}_\|)\times\partial_2\eta(\mathbf{x}_\|))} \\ &\times \Big\{ \mathbf{v}_\| \cdot \nabla^2\eta(\mathbf{x}_\|)\cdot\mathbf{v}_\| - \mathbf{x}_\perp\mathbf{v}_\| \cdot \nabla^2\mathbf{n}(\mathbf{x}_\|)\cdot\mathbf{v}_\| \Big\} \cdot (-\mathbf{n}(\mathbf{x}_\|)\times\partial_{i+1}\eta(\mathbf{x}_\|)), \end{aligned}$$

and

$$E(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\parallel) = \sum_i G_{ij}(\mathbf{x}_\perp, \mathbf{x}_\parallel) \frac{(-1)^{i+1}}{-\mathbf{n}(\mathbf{x}_\parallel)\cdot(\partial_1\eta(\mathbf{x}_\parallel)\times\partial_2\eta(\mathbf{x}_\parallel))} 2\mathbf{v}_\perp\mathbf{v}_\parallel\cdot\nabla\mathbf{n}(\mathbf{x}_\parallel)\cdot(-\mathbf{n}(\mathbf{x}_\parallel)\times\partial_{i+1}\eta(\mathbf{x}_\parallel)).$$

Here $G_{ij}(\cdot,\cdot)$ is a smooth bounded function defined in (A.69) and we used the notational convention $i \equiv i \bmod 2$.

From Lemma A.10 we take the time integration of (A.57) along the characteristics to have

$$\begin{aligned}
\mathbf{x}_\parallel(s^{i+1}) &= \mathbf{x}_\parallel(s^i) - \int_{s^{i+1}}^{s^i} \mathbf{v}_\parallel(\tau)\mathrm{d}\tau, \\
\mathbf{v}_\parallel(s^{i+1}) &= \mathbf{v}_\parallel(s^i) - \int_{s^{i+1}}^{s^i} \left\{E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\mathbf{v}_\perp(\tau) + D(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\right\} \mathrm{d}\tau.
\end{aligned}$$

Note that $\mathbf{v}_\perp(\tau)$ is not continuous with respect to the time τ. Using (A.57) we rewrite this time integration as

$$\int_{s^{i+1}}^{s^i} E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\mathbf{v}_\perp(\tau)\mathrm{d}\tau = \int_{t^{\ell_{i-1}+1}}^{s^i} + \sum_{\ell=\ell_i-1}^{\ell_{i-1}+1} \int_{t^{\ell+1}}^{t^\ell} + \int_{s^{i+1}}^{t^{\ell_i}},$$

then we use $\mathbf{v}_\perp(\tau) = \dot{\mathbf{x}}_\perp(\tau)$ and the integration by parts to have

$$\begin{aligned}
&\int_{t^{\ell_{i-1}+1}}^{s^i} E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\dot{\mathbf{x}}_\perp(\tau)\mathrm{d}\tau + \sum_{\ell=\ell_i-1}^{\ell_{i-1}+1} \int_{t^{\ell+1}}^{t^\ell} E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\dot{\mathbf{x}}_\perp(\tau)\mathrm{d}\tau \\
&\quad + \int_{s^{i+1}}^{t^{\ell_i}} E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau))\dot{\mathbf{x}}_\perp(\tau)\mathrm{d}\tau \\
&= E(s^i)\mathbf{x}_\perp(s^i) - E(t^{\ell_{i-1}+1})\underbrace{\mathbf{x}_\perp(t^{\ell_{i-1}+1})}_{=0} - \int_{t^{\ell_{i-1}+1}}^{s^i} \left[\mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau), F_\parallel(\tau)\right]\cdot\nabla E(\tau)\mathbf{x}_\perp(\tau)\mathrm{d}\tau \\
&\quad + \sum_{\ell=\ell_i-1}^{\ell_{i-1}+1} \left\{E(t^\ell)\underbrace{\mathbf{x}_\perp(t^\ell)}_{=0} - E(t^{\ell+1})\underbrace{\mathbf{x}_\perp(t^{\ell+1})}_{=0} - \int_{t^{\ell+1}}^{t^\ell} \left[\mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau), F_\parallel(\tau)\right]\cdot\nabla E(\tau)\mathbf{x}_\perp(\tau)\mathrm{d}\tau\right\} \\
&\quad + E(t^{\ell_i})\underbrace{\mathbf{x}_\perp(t^{\ell_i})}_{=0} - E(s^{i+1})\mathbf{x}_\perp(s^{i+1}) - \int_{s^{i+1}}^{t^{\ell_i}} \left[\mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau), F_\parallel(\tau)\right]\cdot\nabla E(\tau)\mathbf{x}_\perp(\tau)\mathrm{d}\tau \\
&= E(\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\parallel)(s^i)\mathbf{x}_\perp(s^i) - E(s^{i+1})\mathbf{x}_\perp(s^{i+1}) - \int_{s^i}^{s^{i+1}} \left[\mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau), F_\parallel(\tau)\right]\cdot\nabla E(\tau)\mathbf{x}_\perp(\tau)\mathrm{d}\tau,
\end{aligned}$$

where we have used the fact $X_{\mathbf{cl}}(t^\ell) \in \partial\Omega$ (therefore $\mathbf{x}_\perp(t^\ell) = 0$) and the notations

$$E(\tau) = E(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau)),\ D(\tau) = D(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\parallel(\tau)),\ F_\parallel(\tau) = F_\parallel(\mathbf{x}_\perp(\tau), \mathbf{x}_\parallel(\tau), \mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau)).$$

Overall we have

$$\begin{aligned}
\mathbf{x}_\parallel(s^{i+1}) &= \mathbf{x}_\parallel(s^i) - \int_{s^{i+1}}^{s^i} \mathbf{v}_\parallel(\tau)\mathrm{d}\tau, \\
\mathbf{v}_\parallel(s^{i+1}) &= \mathbf{v}_\parallel(s^i) - E(s^i)\mathbf{x}_\perp(s^i) + E(s^{i+1})\mathbf{x}_\perp(s^{i+1}) \\
&\quad + \int_{s^{i+1}}^{s^i} \left[\mathbf{v}_\perp(\tau), \mathbf{v}_\parallel(\tau), F_\parallel(\tau)\right]\cdot\nabla E(\tau)\mathbf{x}_\perp(\tau)\mathrm{d}\tau - \int_{s^{i+1}}^{s^i} D(\tau)\mathrm{d}\tau.
\end{aligned} \tag{A.113}$$

Denote

$$\partial = [\partial_{\mathbf{x}_\perp(s^1)}, \partial_{\mathbf{x}_\parallel(s^1)}, \partial_{\mathbf{v}_\perp(s^1)}, \partial_{\mathbf{v}_\parallel(s^1)}] = [\frac{\partial}{\partial\mathbf{x}_\perp(s^1)}, \frac{\partial}{\partial\mathbf{x}_\parallel(s^1)}, \frac{\partial}{\partial\mathbf{v}_\perp(s^1)}, \frac{\partial}{\partial\mathbf{v}_\parallel(s^1)}].$$

We claim that, in a sense of distribution on $(s^1, \mathbf{x}_\perp(s^1), \mathbf{x}_\parallel(s^1), \mathbf{v}_\perp(s^1), \mathbf{v}_\parallel(s^1)) \in [0,\infty) \times (0, C_\xi) \times (0, 2\pi] \times (\delta, \pi - \delta) \times \mathbb{R} \times \mathbb{R}^2$,

$$\begin{aligned}
&\big[\partial \mathbf{x}_\perp(s^{i+1}; s^1, \mathbf{x}(s^1), \mathbf{v}(s^1)), \partial \mathbf{x}_\parallel(s^{i+1}; s^1, \mathbf{x}(s^1), \mathbf{v}(s^1)),\ \partial \mathbf{v}_\parallel(s^{i+1}; s^1, \mathbf{x}(s^1), \mathbf{v}(s^1))\big] \\
&= \sum_\ell \mathbf{1}_{[t^{\ell+1}, t^\ell)}(s^{i+1}) \big[\partial \mathbf{x}_\perp, \partial \mathbf{x}_\parallel, \partial \mathbf{v}_\parallel\big], \\
&\partial\big[\mathbf{v}_\perp(s^{i+1}; s^1, \mathbf{x}(s^1), \mathbf{v}(s^1)) \mathbf{x}_\perp(s^{i+1}; s^1, \mathbf{x}(s^1), \mathbf{v}(s^1))\big] = \sum_\ell \mathbf{1}_{[t^{\ell+1}, t^\ell)}(s^{i+1}) \big\{\partial \mathbf{v}_\perp \mathbf{x}_\perp + \mathbf{v}_\perp \partial \mathbf{x}_\perp\big\},
\end{aligned} \tag{A.114}$$

i.e. the distributional derivatives of $[\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\parallel]$ and $\mathbf{v}_\perp \mathbf{x}_\perp$ equal the piecewise derivatives. Let us take $\phi(\tau', \mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel) \in C_c^\infty([0,\infty) \times (0, C_\xi) \times \mathbb{S}^2 \times \mathbb{R} \times \mathbb{R}^2)$. Therefore $\phi \equiv 0$ when $\mathbf{x}_\perp < \delta$. For $\mathbf{x}_\perp \geq \delta$ we use the proof of Lemma A.10 : For $x = \eta(\mathbf{x}_\parallel) + \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)]$,

$$|\mathbf{x}_\perp| \ \lesssim_\xi\ \xi(x) = \xi(\eta(\mathbf{x}_\parallel) + \mathbf{x}_\perp[-\mathbf{n}(\mathbf{x}_\parallel)]) \ \lesssim_\xi\ |\mathbf{x}_\perp|,$$

and therefore $\xi(x) \gtrsim_\xi \delta$ and $\alpha(x,v) \gtrsim_\xi |\xi(x)||v|^2 \gtrsim_\xi |v|^2\delta$. Since we are considering the case $t - s > t_{\mathbf{b}}(x,v)$, from $|v| t_{\mathbf{b}}(x,v) \gtrsim \mathbf{x}_\perp \geq \delta$ we have $|v| \gtrsim_\xi \frac{\delta}{t-s}$ and finally we obtain the lower bound $\alpha(x,v) \gtrsim_\xi \frac{\delta^3}{|t-s|^2} > 0$. By the Velocity lemma, for $(x,v) \in \mathrm{supp}(\phi)$

$$\alpha(x^\ell, v^\ell) \gtrsim_\xi e^{-C|v||t^1 - t^\ell|} \alpha(x,v) \gtrsim_\xi e^{-C|v|(t-s)} \frac{\delta^3}{|t-s|^2} \gtrsim_{\xi, |t-s|, \delta, \phi} 1 > 0,$$

where we used the fact that ϕ vanishes away from a compact subset $\mathrm{supp}(\phi)$. Therefore $t^\ell(t,x,v) = t^\ell(t, \mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel)$ is smooth with respect to $\mathbf{x}_\perp, \mathbf{x}_\parallel, \mathbf{v}_\perp, \mathbf{v}_\parallel$ locally on $\mathrm{supp}(\phi)$ and therefore $\mathcal{M} = \{(\tau', \mathbf{x}, \mathbf{v}) \in \mathrm{supp}(\phi) : \tau' = t^\ell(t, \mathbf{x}, \mathbf{v})\}$ is a smooth manifold.

It suffices to consider the case $\tau' \sim t^\ell(t,x,v)$. Denote $\partial_{\mathbf{e}} = [\partial_{\mathbf{x}_\perp}, \partial_{\mathbf{x}_{\parallel,1}}, \partial_{\mathbf{x}_{\parallel,2}}, \partial_{\mathbf{v}_\perp}, \partial_{\mathbf{v}_{\parallel,1}}, \partial_{\mathbf{v}_{\parallel,2}}]$ and $n_{\mathcal{M}} = \mathbf{e}_1$ to have

$$\begin{aligned}
&\int_{\{(\tau', \mathbf{x}, \mathbf{v}) \in \mathrm{supp}(\phi)\}} [\partial_{\mathbf{e}} \mathbf{x}_\perp(\tau'; t, \mathbf{x}, \mathbf{v}), \partial_{\mathbf{e}} \mathbf{x}_\parallel(\tau'; t, \mathbf{x}, \mathbf{v}), \partial_{\mathbf{e}} \mathbf{v}_\parallel(\tau'; t, \mathbf{x}, \mathbf{v})] \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v} \mathrm{d}\tau' \\
&= \int_{\tau' < t^\ell} + \int_{\tau' \geq t^\ell} \\
&= \int_{\mathcal{M}} \Big(\lim_{\tau' \uparrow t^\ell} [\mathbf{x}_\perp(\tau'), \mathbf{x}_\parallel(\tau'), \mathbf{v}_\parallel(\tau')] - \lim_{\tau' \downarrow t^\ell} [\mathbf{x}_\perp(\tau'), \mathbf{x}_\parallel(\tau'), \mathbf{v}_\parallel(\tau')] \Big) \phi(\tau', \mathbf{x}, \mathbf{v}) \{\mathbf{e} \cdot n_{\mathcal{M}}\} \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v} \\
&\quad - \int_{\{\tau' \neq t^\ell(t, \mathbf{x}, \mathbf{v})\}} [\mathbf{x}_\perp(\tau'), \mathbf{x}_\parallel(\tau'), \mathbf{v}_\parallel(\tau')] \partial_{\mathbf{e}} \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\tau' \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{x} \\
&= - \int_{\{\tau' \neq t^\ell(t, \mathbf{x}, \mathbf{v})\}} [\mathbf{x}_\perp(\tau'), \mathbf{x}_\parallel(\tau'), \mathbf{v}_\parallel(\tau')] \partial_{\mathbf{e}} \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\tau' \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{x},
\end{aligned}$$

where we used the continuity of $[\mathbf{x}_\perp(\tau'; t, \mathbf{x}, \mathbf{v}), \mathbf{x}_\parallel(\tau'; t, \mathbf{x}, \mathbf{v}), \mathbf{v}_\parallel(\tau'; t, \mathbf{x}, \mathbf{v})]$ in terms of τ' near $t^\ell(t, \mathbf{x}, \mathbf{v})$.

Note that $\mathbf{v}_\perp(\tau'; t, \mathbf{x}, \mathbf{v})$ is discontinuous around $\tau' \sim t^\ell$.($\lim_{\tau' \downarrow t^\ell} \mathbf{v}_\perp(\tau') = -\lim_{\tau' \uparrow t^\ell} \mathbf{v}_\perp(\tau')$) However with crucial $\mathbf{x}_\perp(\tau')-$multiplication we have $\mathbf{x}_\perp(t^\ell) \mathbf{v}_\perp(t^\ell) = 0$ and therefore

$$\begin{aligned}
&\int_{\{(\tau', \mathbf{x}, \mathbf{v}) \in \mathrm{supp}(\phi)\}} \partial_{\mathbf{e}} [\mathbf{x}_\perp(\tau'; t, \mathbf{x}, \mathbf{v}) \mathbf{v}_\perp(\tau'; t, \mathbf{x}, \mathbf{v})] \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v} \mathrm{d}\tau' \\
&= \int_{\tau' < t^\ell} + \int_{\tau' \geq t^\ell} \\
&= \int_{\mathcal{M}} \Big(\lim_{\tau' \uparrow t^\ell} [\mathbf{x}_\perp(\tau') \mathbf{v}_\perp(\tau')] - \lim_{\tau' \downarrow t^\ell} [\mathbf{x}_\perp(\tau') \mathbf{v}_\perp(\tau')] \Big) \phi(\tau', \mathbf{x}, \mathbf{v}) \{\mathbf{e} \cdot n_{\mathcal{M}}\} \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v} \\
&\quad - \int_{\{\tau' \neq t^\ell(t, \mathbf{x}, \mathbf{v})\}} [\mathbf{x}_\perp(\tau') \mathbf{v}_\perp(\tau')] \partial_{\mathbf{e}} \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\tau' \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{x} \\
&= - \int_{\{\tau' \neq t^\ell(t, \mathbf{x}, \mathbf{v})\}} [\mathbf{x}_\perp(\tau'; t, \mathbf{x}, \mathbf{v}) \mathbf{v}_\perp(\tau'; t, \mathbf{x}, \mathbf{v})] \partial_{\mathbf{e}} \phi(\tau', \mathbf{x}, \mathbf{v}) \mathrm{d}\tau' \mathrm{d}\mathbf{v} \mathrm{d}\mathbf{x}.
\end{aligned}$$

We apply (A.114) to (A.113)

$$
\begin{aligned}
&\partial \mathbf{x}_{\|}(s^{i+1}) = \partial \mathbf{x}_{\|}(s^{i}) - \int_{s^{i+1}}^{s^{i}} \partial \mathbf{v}_{\|}(\tau)\mathrm{d}\tau,\\
&\partial \mathbf{v}_{\|}(s^{i+1}) = \partial E(s^{i+1})\mathbf{x}_{\perp}(s^{i+1}) + E(s^{i+1})\partial \mathbf{x}_{\perp}(s^{i+1}) + \partial \mathbf{v}_{\|}(s^{i}) - \partial[E(\mathbf{x}_{\perp},\mathbf{x}_{\|},\mathbf{v}_{\|})\mathbf{x}_{\perp}](s^{i+1})\\
&\quad + \int_{s^{i+1}}^{s^{i}} \partial \mathbf{v}_{\perp}(\tau)\partial_{\mathbf{x}_{\perp}}E(\tau)\mathbf{x}_{\perp}(\tau) + \partial \mathbf{v}_{\|}(\tau)\cdot\nabla_{\mathbf{x}_{\|}}E(\tau)\mathbf{x}_{\perp}(\tau)\mathrm{d}\tau\\
&\quad + \int_{s^{i+1}}^{s^{i}} \Big\{ \Big[\partial \mathbf{x}_{\perp}(\tau)\partial_{\mathbf{x}_{\perp}}E(\tau) + \partial \mathbf{x}_{\|}(\tau)\cdot\nabla_{\mathbf{x}_{\|}}E(\tau) + \partial \mathbf{v}_{\|}(\tau)\cdot\nabla_{\mathbf{v}_{\|}}E(\tau)\Big]\mathbf{v}_{\perp}(\tau)\\
&\qquad + E(\tau)\partial \mathbf{v}_{\perp}(\tau) + \partial \mathbf{x}_{\perp}(\tau)\partial_{\mathbf{x}_{\perp}}D(\tau) + \partial \mathbf{x}_{\|}(\tau)\cdot\nabla_{\mathbf{x}_{\|}}D(\tau) + \partial \mathbf{v}_{\|}(\tau)\nabla_{\mathbf{v}_{\|}}D(\tau)\Big\}\cdot\nabla_{\mathbf{v}_{\|}}E(\tau)\mathbf{x}_{\perp}(\tau)\mathrm{d}\tau\\
&\quad + \int_{s^{i+1}}^{s^{i}} \Big\{ \mathbf{v}_{\perp}(\tau)[\partial \mathbf{x}_{\perp}(\tau),\partial \mathbf{x}_{\|}(\tau),\partial \mathbf{v}_{\|}(\tau)]\cdot\nabla\partial_{\mathbf{x}_{\perp}}E(\tau) + \mathbf{v}_{\|}(\tau)\cdot[\partial \mathbf{x}_{\perp}(\tau),\partial \mathbf{x}_{\|}(\tau),\partial \mathbf{v}_{\|}(\tau)]\cdot\nabla\nabla_{\mathbf{x}_{\|}}E(\tau)\\
&\qquad\quad + F_{\|}(\tau)\cdot[\partial \mathbf{x}_{\perp}(\tau),\partial \mathbf{x}_{\|}(\tau),\partial \mathbf{v}_{\|}(\tau)]\cdot\nabla\nabla_{\mathbf{v}_{\|}}E(\tau)\Big\}\mathbf{x}_{\perp}(\tau)\mathrm{d}\tau\\
&\quad + \int_{s^{i+1}}^{s^{i}} \big\{\mathbf{v}_{\perp}(\tau)\partial_{\mathbf{x}_{\perp}}E(\tau) + \mathbf{v}_{\|}(\tau)\cdot\nabla_{\mathbf{x}_{\|}}E(\tau) + F_{\|}(\tau)\cdot\nabla_{\mathbf{v}_{\|}}E(\tau)\big\}\partial \mathbf{x}_{\perp}(\tau)\mathrm{d}\tau\\
&\quad - \int_{s^{i+1}}^{s^{i}} \big[\partial \mathbf{x}_{\perp}(\tau),\partial \mathbf{x}_{\|}(\tau),\partial \mathbf{v}_{\|}(\tau)\big]\cdot\nabla D(\tau)\mathrm{d}\tau.
\end{aligned}
\tag{A.115}
$$

Now we use (A.107) to control $[\partial\mathbf{x}_{\perp},\partial\mathbf{v}_{\perp}]$. Notice that we cannot directly use (A.107) since now we fix the chart for whole $i-$th intermediate group but the estimate (A.107) is for the moving frame. (For clarity, we write the index for the chart for this part.) Note the time of bounces within the $i-$th intermediate group ($|t^{\ell_{i-1}} - t^{\ell_i}||v| \sim L_\xi$) are

$$
t^{\ell_i+1} < s^{i+1} < t^{\ell_i} < t^{\ell_i-1} < \cdots\cdots < t^{\ell_{i-1}+2} < t^{\ell_{i-1}+1} < s^{i} < t^{\ell_{i-1}}.
$$

Now we apply (A.60) and (A.107) to bound, for $\tau \in (s^{i+1}, s^i)$ and $\ell \in \{\ell_i, \ell_i - 1, \cdots, \ell_{i-1}+2, \ell_{i-1}+1, \ell_{i-1}\}$

$$
\begin{aligned}
&\frac{\partial(\mathbf{x}_{\perp_\ell}(\tau),\mathbf{x}_{\|_\ell}(\tau),\mathbf{v}_{\perp_\ell}(\tau),\mathbf{v}_{\|_\ell}(\tau))}{\partial(\mathbf{x}_{\perp_1}(s^1),\mathbf{x}_{\|_1}(s^1),\mathbf{v}_{\perp_1}(s^1),\mathbf{v}_{\|_1}(s^1))}\\
=&\frac{\partial(\mathbf{x}_{\perp_\ell}(\tau),\mathbf{x}_{\|_\ell}(\tau),\mathbf{v}_{\perp_\ell}(\tau),\mathbf{v}_{\|_\ell}(\tau))}{\partial(\mathbf{x}_{\perp_{\ell_i}}(\tau),\mathbf{x}_{\|_{\ell_i}}(\tau),\mathbf{v}_{\perp_{\ell_i}}(\tau),\mathbf{v}_{\|_{\ell_i}}(\tau))}\frac{\partial(\mathbf{x}_{\perp_{\ell_i}}(\tau),\mathbf{x}_{\|_{\ell_i}}(\tau),\mathbf{v}_{\perp_{\ell_i}}(\tau),\mathbf{v}_{\|_{\ell_i}}(\tau))}{\partial(\mathbf{x}_{\perp_1}(s^1),\mathbf{x}_{\|_1}(s^1),\mathbf{v}_{\perp_1}(s^1),\mathbf{v}_{\|_1}(s^1))}\\
\lesssim& e^{C|t-s||v|}\left\{\mathbf{Id}_{6,6} + O_\xi(|\mathbf{p}^\ell - \mathbf{p}^{\ell_i}|)\left[\begin{array}{ccc|ccc} 0 & 0 & 0 & & & \\ 0 & 1 & 1 & & \mathbf{0}_{3,3} & \\ 0 & 1 & 1 & & & \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & |v| & |v| & 0 & 1 & 1 \\ 0 & |v| & |v| & 0 & 1 & 1 \end{array}\right]\right\}
\begin{bmatrix}
\frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{1}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{1}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)
\end{bmatrix}\\
\lesssim& e^{C|t-s||v|}
\begin{bmatrix}
\frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{1}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^2}{|\mathbf{v}_\perp^1|^2} & \frac{1}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|}\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)\\
\frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1)
\end{bmatrix},
\end{aligned}
\tag{A.116}
$$

where we have used $|\mathbf{p}^\ell - \mathbf{p}^{\ell_i}| \lesssim 1$.

Together with (A.107), we have (for clarity, we write estimates for each derivative $\partial = [\partial_{\mathbf{x}_\perp}, \partial_{\mathbf{x}_\parallel}, \partial_{\mathbf{v}_\perp}, \partial_{\mathbf{v}_\parallel}]$) :

$$
\begin{aligned}
&|\partial_{\mathbf{x}_\perp}\mathbf{x}_\parallel(s^{i+1})| \lesssim_\xi \int_{s^{i+1}}^{s^i} |\partial_{\mathbf{x}_\perp}\mathbf{v}_\parallel(\tau)|\mathrm{d}\tau,\\
&|\partial_{\mathbf{x}_\perp}\mathbf{v}_\parallel(s^{i+1})| \lesssim_\xi |v||\mathbf{x}_\perp(\tau_i)||\partial_{\mathbf{x}_\perp}\mathbf{x}_\parallel(s^{i+1})| + |\mathbf{x}_\perp(s^{i+1})||\partial_{\mathbf{x}_\perp}\mathbf{v}_\parallel(s^{i+1})| + e^{C|v||t-s|}\Big[\frac{|v|^2}{|\mathbf{v}_\perp^{\ell_{i-1}}|} + |v|\Big]\\
&\qquad + \int_{s^{i+1}}^{s^i} \Big\{|v|^2|\partial_{\mathbf{x}_\perp}\mathbf{x}_\parallel(\tau)| + |v||\partial_{\mathbf{x}_\perp}\mathbf{v}_\parallel(\tau)| + e^{C|v||t-s|}\Big[\frac{|v|^4|\mathbf{x}_\perp(\tau)|}{|\mathbf{v}_\perp^{\ell_{i-1}}|^2} + \frac{|v|^3}{|\mathbf{v}_\perp^{\ell_{i-1}}|}\Big]\Big\}\mathrm{d}\tau.
\end{aligned}
$$

We use (A.46), (A.47) and (A.64) and the condition $|\xi(X_{\mathbf{cl}}(\tau))| < \delta$ for all $\tau \in [s,t]$ to have, $\mathbf{x}_\perp(\tau;t,\mathbf{x},\mathbf{v}) \lesssim_\xi |\xi(X_{\mathbf{cl}}(\tau;t,x,v))|$ for all $\tau \in [s,t]$, and therefore

$$
\begin{aligned}
|v|^2|\mathbf{x}_\perp(\tau;t,\mathbf{x},\mathbf{v})| &\lesssim_\xi 2\xi(X_{\mathbf{cl}}(\tau;t,x,v))\{V_{\mathbf{cl}}(\tau;t,x,v)\cdot\nabla^2\xi(X_{\mathbf{cl}}(\tau;t,x,v))\cdot V_{\mathbf{cl}}(\tau;t,x,v)\}\\
&\lesssim_\xi \alpha(\tau;t,\mathbf{x},\mathbf{v}) \lesssim_\xi e^{C|v||t-\tau|}|\mathbf{v}_\perp^1|^2,
\end{aligned}
$$

where we used the convexity of ξ in (A.3) and the Velocity lemma(Lemma A.1).

Hence we rewrite as, for $0<\delta\ll 1$,

$$
\begin{aligned}
|\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{x}_\perp}| &\lesssim_\xi |\frac{\partial\mathbf{x}_\parallel(s^{i})}{\partial\mathbf{x}_\perp}| + \int_{s^{i+1}}^{s^i}|\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{x}_\perp}|\mathrm{d}\tau',\\
|\frac{\partial\mathbf{v}_\parallel(s^{i+1})}{\partial\mathbf{x}_\perp}| - \delta|v||\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{x}_\perp}| &\lesssim_{\xi,\delta} |\frac{\partial\mathbf{v}_\parallel(s^{i})}{\partial\mathbf{x}_\perp}| + \int_{s^{i+1}}^{s^i}\Big\{|v|^2|\frac{\partial\mathbf{x}_\parallel(\tau')}{\partial\mathbf{x}_\perp}| + |v||\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{x}_\perp}|\Big\}\mathrm{d}\tau'\\
&\quad + |v|e^{C|v||t-s|}(1+\frac{|v|}{|\mathbf{v}_\perp^1|}).
\end{aligned}
\tag{A.117}
$$

Similarly, from (A.115) and (A.116)

$$
\begin{aligned}
|\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{x}_\parallel}| &\lesssim_\xi |\frac{\partial\mathbf{x}_\parallel(s^{i})}{\partial\mathbf{x}_\parallel}| + \int_{s^{i+1}}^{s^i}|\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{x}_\parallel}|\mathrm{d}\tau',\\
|\frac{\partial\mathbf{v}_\parallel(s^{i+1})}{\partial\mathbf{x}_\parallel}| - \delta|v||\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{x}_\parallel}| &\lesssim_{\xi,\delta} |\frac{\partial\mathbf{v}_\parallel(s^{i})}{\partial\mathbf{x}_\parallel}|\\
&\quad + |v|\Big(1+\frac{|v|}{|\mathbf{v}_\perp^1|}\Big)e^{C|v||t-s|} + \int_{s^{i+1}}^{s^i}\Big\{|v|^2|\frac{\partial\mathbf{x}_\parallel(\tau')}{\partial\mathbf{x}_\parallel}| + |v||\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{x}_\parallel}|\Big\}\mathrm{d}\tau',\\
|\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{v}_\perp}| &\lesssim_\xi |\frac{\partial\mathbf{x}_\parallel(s^{i})}{\partial\mathbf{v}_\perp}| + \int_{s^{i+1}}^{s^i}|\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{v}_\perp}|\mathrm{d}\tau',\\
|\frac{\partial\mathbf{v}_\parallel(s^{i+1})}{\partial\mathbf{v}_\perp}| - \delta|v||\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{v}_\perp}| &\lesssim_{\xi,\delta} |\frac{\partial\mathbf{v}_\parallel(s^{i})}{\partial\mathbf{v}_\perp}| + e^{C|v||t-s|} + \int_{s^{i+1}}^{s^i}\Big\{|v|^2|\frac{\partial\mathbf{x}_\parallel(\tau')}{\partial\mathbf{v}_\perp}| + |v||\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{v}_\perp}|\Big\}\mathrm{d}\tau',\\
|\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{v}_\parallel}| &\lesssim_\xi |\frac{\partial\mathbf{x}_\parallel(s^{i})}{\partial\mathbf{v}_\parallel}| + \int_{s^{i+1}}^{s^i}|\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{v}_\parallel}|\mathrm{d}\tau',\\
|\frac{\partial\mathbf{v}_\parallel(s^{i+1})}{\partial\mathbf{v}_\parallel}| - \delta|v||\frac{\partial\mathbf{x}_\parallel(s^{i+1})}{\partial\mathbf{v}_\parallel}| &\lesssim_{\xi,\delta} |\frac{\partial\mathbf{v}_\parallel(s^{i})}{\partial\mathbf{v}_\parallel}| + e^{C|v||t-s|} + \int_{s^{i+1}}^{s^i}\Big\{|v|^2|\frac{\partial\mathbf{x}_\parallel(\tau')}{\partial\mathbf{v}_\parallel}| + |v||\frac{\partial\mathbf{v}_\parallel(\tau')}{\partial\mathbf{v}_\parallel}|\Big\}\mathrm{d}\tau'.
\end{aligned}
$$

Now we claim a version of Gronwall's estimate : If $a(\tau), b(\tau), f(\tau), g(\tau) \geq 0$ for all $0 \leq \tau \leq t$, and satisfy, for $0<\delta\ll 1$

$$
\begin{bmatrix} 1 & 0\\ -\delta|v| & 1\end{bmatrix}\begin{bmatrix} a(\tau)\\ b(\tau)\end{bmatrix} \lesssim_\xi \begin{bmatrix} 0 & 1\\ |v|^2 & |v|\end{bmatrix}\begin{bmatrix} \int_\tau^t a(\tau')\mathrm{d}\tau'\\ \int_\tau^t b(\tau')\mathrm{d}\tau'\end{bmatrix} + \begin{bmatrix} g(t-\tau)\\ h(t-\tau)\end{bmatrix}
$$

then

$$
\begin{bmatrix} a(\tau)\\ b(\tau)\end{bmatrix} \lesssim_{\delta,\xi} \int_\tau^t e^{|v|(\tau'-\tau)}\{g(\tau') + \frac{h(\tau')}{|v|}\}\mathrm{d}\tau'\begin{bmatrix} |v|\\ |v|^2\end{bmatrix} + \begin{bmatrix} g(t-\tau)\\ \delta|v|g(t-\tau)+h(t-\tau)\end{bmatrix}. \tag{A.118}
$$

Define $\tilde{a}(\tau) := a(t-\tau), \tilde{b}(\tau) := b(t-\tau)$ and $A(\tau) := \int_0^\tau \tilde{a}(\tau')\mathrm{d}\tau', B(\tau) := \int_0^\tau \tilde{b}(\tau')\mathrm{d}\tau'$. Then

$$\frac{d}{d\tau}\begin{bmatrix} 1 & 0 \\ -\delta|v| & 1 \end{bmatrix}\begin{bmatrix} A(\tau) \\ B(\tau) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -\delta|v| & 1 \end{bmatrix}\begin{bmatrix} \tilde{a}(\tau) \\ b(\tilde{\tau}) \end{bmatrix} \lesssim_\xi \begin{bmatrix} 0 & 1 \\ |v|^2 & |v| \end{bmatrix}\begin{bmatrix} A(\tau) \\ B(\tau) \end{bmatrix} + \begin{bmatrix} \tilde{g}(\tau) \\ \tilde{h}(\tau) \end{bmatrix}$$
$$\lesssim_\xi \begin{bmatrix} \delta|v| & 1 \\ (1+\delta)|v|^2 & |v| \end{bmatrix}\begin{bmatrix} 1 & 0 \\ -\delta|v| & 1 \end{bmatrix}\begin{bmatrix} A(\tau) \\ B(\tau) \end{bmatrix} + \begin{bmatrix} \tilde{g}(\tau) \\ \tilde{h}(\tau) \end{bmatrix}.$$

Using $\begin{bmatrix} 0 & 1 \\ |v|^2 & |v| \end{bmatrix}\begin{bmatrix} 1 & 0 \\ \delta|v| & 1 \end{bmatrix} = \begin{bmatrix} \delta|v| & 1 \\ (1+\delta)|v|^2 & |v| \end{bmatrix}$ and the notation

$$\begin{bmatrix} \tilde{A}(\tau) \\ \tilde{B}(\tau) \end{bmatrix} := \begin{bmatrix} 1 & 0 \\ -\delta|v| & 1 \end{bmatrix}\begin{bmatrix} A(\tau) \\ B(\tau) \end{bmatrix},$$

we have

$$\frac{d}{d\tau}\begin{bmatrix} \tilde{A}(\tau) \\ \tilde{B}(\tau) \end{bmatrix} \lesssim_\xi \begin{bmatrix} \delta|v| & 1 \\ (1+\delta)|v|^2 & |v| \end{bmatrix}\begin{bmatrix} \tilde{A}(\tau) \\ \tilde{B}(\tau) \end{bmatrix} + \begin{bmatrix} \tilde{g}(\tau) \\ \tilde{h}(\tau) \end{bmatrix},$$

We diagonalize $\begin{bmatrix} \delta|v| & 1 \\ (1+\delta)|v|^2 & |v| \end{bmatrix}$ as

$$= \begin{bmatrix} 1 & 1 \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2}|v| & \frac{(1-\delta)-\sqrt{(1+\delta)^2+4}}{2}|v| \end{bmatrix}\begin{bmatrix} \frac{(1+\delta)+\sqrt{(1+\delta)^2+4}}{2}|v| & 0 \\ 0 & \frac{(1+\delta)-\sqrt{(1+\delta)^2+4}}{2}|v| \end{bmatrix}$$
$$\times \begin{bmatrix} \frac{-(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{-1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \end{bmatrix}.$$

Denote $\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix} := \begin{bmatrix} \frac{-(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{-1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \end{bmatrix}\begin{bmatrix} \tilde{A}(\tau) \\ \tilde{B}(\tau) \end{bmatrix}$ to rewrite

$$\frac{d}{d\tau}\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix} \lesssim_\xi \begin{bmatrix} \frac{(1+\delta)+\sqrt{(1+\delta)^2+4}}{2}|v| & 0 \\ 0 & \frac{(1+\delta)-\sqrt{(1+\delta)^2+4}}{2}|v| \end{bmatrix}\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix}$$
$$+ \begin{bmatrix} \frac{-(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{-1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \end{bmatrix}\begin{bmatrix} \tilde{g}(\tau) \\ \tilde{h}(\tau) \end{bmatrix}.$$

Therefore, writing $\rho_\pm = \frac{(1+\delta)\pm\sqrt{(1+\delta)^2+4}}{2}$, we have

$$\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix} \lesssim_\xi \begin{bmatrix} e^{C_{\xi,\delta}\rho_+|v|\tau}\mathcal{A}(0) \\ e^{C_{\xi,\delta}\rho_-|v|\tau}\mathcal{B}(0) \end{bmatrix}$$
$$+ \int_0^\tau \begin{bmatrix} e^{\rho_+|v|(\tau-\tau')} & 0 \\ 0 & e^{\rho_-|v|(\tau-\tau')} \end{bmatrix}\begin{bmatrix} \frac{-(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2\sqrt{(1+\delta)^2+4}} & \frac{-1}{\sqrt{(1+\delta)^2+4}}\frac{1}{|v|} \end{bmatrix}\begin{bmatrix} \tilde{g}(\tau') \\ \tilde{h}(\tau') \end{bmatrix}\mathrm{d}\tau',$$

and then

$$\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \delta|v| & 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ \frac{(1-\delta)+\sqrt{(1+\delta)^2+4}}{2}|v| & \frac{(1-\delta)-\sqrt{(1+\delta)^2+4}}{2}|v| \end{bmatrix}\begin{bmatrix} \mathcal{A}(\tau) \\ \mathcal{B}(\tau) \end{bmatrix}$$
$$\lesssim_{\xi,\delta} \int_0^\tau e^{C_{\xi,\delta}|v|(\tau-\tau')}\{\tilde{g}(\tau') + \frac{\tilde{h}(\tau')}{|v|}\}\mathrm{d}\tau'\begin{bmatrix} 1 \\ |v| \end{bmatrix}.$$

Together with the first inequality (the condition of the claim)

$$\begin{aligned}
\begin{bmatrix} a(\tau) \\ b(\tau) \end{bmatrix} &\lesssim_\xi \begin{bmatrix} 0 & 1 \\ |v|^2 & (1+\delta)|v| \end{bmatrix} \begin{bmatrix} A(t-\tau) \\ B(t-\tau) \end{bmatrix} + \begin{bmatrix} g(t-\tau) \\ \delta|v|g(t-\tau)+h(t-\tau) \end{bmatrix} \\
&\lesssim_{\xi,\delta} \int_\tau^t e^{|v|(\tau'-\tau)}\{g(\tau')+\frac{h(\tau')}{|v|}\}\mathrm{d}\tau' \begin{bmatrix} |v| \\ |v|^2 \end{bmatrix} + \begin{bmatrix} g(t-\tau) \\ \delta|v|g(t-\tau)+h(t-\tau) \end{bmatrix} \\
&\lesssim_{\xi,\delta} e^{C|v||t-\tau|} \begin{bmatrix} 1 & \frac{1}{|v|} \\ |v| & 1 \end{bmatrix} \begin{bmatrix} \sup|g| \\ \sup|h| \end{bmatrix},
\end{aligned}$$

and this proves the claim (A.118). We apply (A.118) to (A.117) and we prove the claim (A.111).

Step 10. ODE method within the time scale $|t-s|\sim 1$: Refinement of the estimate (A.107) We claim that

$$\begin{bmatrix} |\frac{\partial \mathbf{x}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{x}_{\perp_1}}| & |\frac{\partial \mathbf{x}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{x}_{\|_1}}| & |\frac{\partial \mathbf{x}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{v}_{\perp_1}}| & |\frac{\partial \mathbf{x}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{v}_{\|_1}}| \\ |\frac{\partial \mathbf{v}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{x}_{\perp_1}}| & |\frac{\partial \mathbf{v}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{x}_{\|_1}}| & |\frac{\partial \mathbf{v}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{v}_{\perp_1}}| & |\frac{\partial \mathbf{v}_{\|_{\tilde\ell}}(s)}{\partial \mathbf{v}_{\|_1}}| \end{bmatrix} \lesssim C^{C|v||t-s|} \begin{bmatrix} \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|} \\ \frac{|v|^2}{|\mathbf{v}_\perp^1|} & \frac{|v|^2}{|\mathbf{v}_\perp^1|} & 1 & 1 \end{bmatrix}, \tag{A.119}$$

where $\tilde\ell = [\frac{|t-s||v|}{L_\xi}]$.

Proof of the claim (A.119). By the chain rule

$$\begin{bmatrix} D_\mathbf{x}\mathbf{x}_{\|_i} & D_\mathbf{v}\mathbf{x}_{\|_i} \\ D_\mathbf{x}\mathbf{v}_{\|_i} & D_\mathbf{v}\mathbf{v}_{\|_i} \end{bmatrix} = \frac{\partial(\mathbf{x}_{\|_i},\mathbf{v}_{\|_i})}{\partial(\mathbf{x}_{\|_{i-1}},\mathbf{v}_{\|_{i-1}})} \begin{bmatrix} D_\mathbf{x}\mathbf{x}_{\|_{i-1}} & D_\mathbf{v}\mathbf{x}_{\|_{i-1}} \\ D_\mathbf{x}\mathbf{v}_{\|_{i-1}} & D_\mathbf{v}\mathbf{v}_{\|_{i-1}} \end{bmatrix}.$$

Note, from (A.60)

$$\frac{\partial(\mathbf{x}_{\|_i},\mathbf{v}_{\|_i})}{\partial(\mathbf{x}_{\|_{i-1}},\mathbf{v}_{\|_{i-1}})} \leq C\left[\begin{array}{c|c} 1 & \mathbf{0} \\ \hline |v| & 1 \end{array}\right] \leq C\left[\begin{array}{c|c} 1 & \frac{1}{|v|} \\ \hline |v| & 1 \end{array}\right] := C\mathbf{B}.$$

Denote

$$\mathbf{D}_i(s) = \begin{bmatrix} |D_\mathbf{x}\mathbf{x}_{\|_i}(s)| & |D_\mathbf{v}\mathbf{x}_{\|_i}(s)| \\ |D_\mathbf{x}\mathbf{v}_{\|_i}(s)| & |D_\mathbf{v}\mathbf{v}_{\|_i}(s)| \end{bmatrix}, \quad \mathbf{G} := \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \frac{|v|^2}{|\mathbf{v}_\perp^1|} & 1 \end{bmatrix}.$$

Note that from (A.111)

$$\mathbf{D}_i(s^{i+1}) \leq C\mathbf{B}\mathbf{D}_i(s^i) + C\mathbf{B}\mathbf{G}.$$

Therefore, by induction,

$$\begin{aligned}
\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]}(s) &\leq C\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]}(\tau_{[\frac{|t-s||v|}{L_\xi}]}) + C\mathbf{B}\mathbf{G} \\
&\leq C^2\mathbf{B}\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]-1}(\tau_{[\frac{|t-s||v|}{L_\xi}]}) + C\mathbf{B}\mathbf{G} \\
&\leq C^2\mathbf{B}\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]-1}(\tau_{[\frac{|t-s||v|}{L_\xi}]-1}) + C^3\mathbf{B}\mathbf{G} + C\mathbf{B}\mathbf{G} \\
&\leq C^3\mathbf{B}^2\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]-1}(\tau_{[\frac{|t-s||v|}{L_\xi}]-2}) + \{C^2\mathbf{B}+\mathbf{Id}\}C\mathbf{B}\mathbf{G} \\
&\leq C^4\mathbf{B}^3\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]-2}(\tau_{[\frac{|t-s||v|}{L_\xi}]-2}) + \{C^3\mathbf{B}^2+C^2\mathbf{B}+\mathbf{Id}\}C\mathbf{B}\mathbf{G} \\
&\ \vdots \\
&\lesssim C^{C|t-s||v|}\mathbf{B}^{C[|t-s||v|]}\mathbf{D}_1(\tau_1) + \sum_{i=0}^{C[|t-s||v|]} C^{i+1}\mathbf{B}^i\mathbf{B}\mathbf{G}.
\end{aligned}$$

But direct computation yields $\mathbf{B}^j \leq 2^j\mathbf{B}$. Therefore

$$\mathbf{D}_{[\frac{|t-s||v|}{L_\xi}]}(s) \lesssim C^{C|t-s||v|}\mathbf{B}\{\mathbf{D}_1(\tau_1)+\mathbf{B}\mathbf{G}\}.$$

From (A.83) we have $\mathbf{D}_1(\tau_1) \lesssim \left[\begin{array}{c|c} 1 & \frac{1}{|v|} \\ \hline |v| & 1 \end{array}\right]$ and we conclude our claim (A.119).

With these estimates, we refine (A.107) to give a final estimate for the case that $|\xi(X_{\mathbf{cl}}(\tau;t,x,v))| < \delta$ for all $\tau \in [s,t]$:

$$\frac{\partial(s^{\ell_*}, \mathbf{x}_\perp(s^{\ell_*}), \mathbf{x}_\parallel(s^{\ell_*}), \mathbf{v}_\perp(s^{\ell_*}), \mathbf{v}_\parallel(s^{\ell_*}))}{\partial(s^1, \mathbf{x}_\perp(s^1), \mathbf{x}_\parallel(s^1), \mathbf{v}_\perp(s^1), \mathbf{v}_\parallel(s^1))} \lesssim C^{C|v|(t-s)} \left[\begin{array}{c|cc|cc} 0 & 0 & \mathbf{0}_{1,2} & 0 & \mathbf{0}_{1,2} \\ \hline |\mathbf{v}_\perp^1| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} & \frac{1}{|v|} \\ |v| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{|v|}{|\mathbf{v}_\perp^1|} & |t-s| & |t-s| \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} & O_\xi(1) \\ |v|^2 & \frac{|v|^2}{|\mathbf{v}_\perp^1|} & \frac{|v|^2}{|\mathbf{v}_\perp^1|} & O_\xi(1) & O_\xi(1) \end{array}\right], \tag{A.120}$$

and from (A.81) and (A.89)

$$\begin{aligned}
&\frac{\partial(s, X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v))}{\partial(t,x,v)} \\
&\lesssim C^{C|v|(t-s)} \frac{\partial(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))}{\partial(s^{\ell_*}, \mathbf{X}_{\mathbf{cl}}(s^{\ell_*}), \mathbf{V}_{\mathbf{cl}}(s^{\ell_*}))} \left[\begin{array}{c|c|c} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline |v| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} \end{array}\right] \frac{\partial(s^1, \mathbf{x}_\perp(s^1), \mathbf{x}_\parallel(s^1), \mathbf{v}_\perp(s^1), \mathbf{v}_\parallel(s^1))}{\partial(t,x,v)} \\
&\lesssim C^{C|v|(t-s)} \begin{bmatrix} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ |v| & 1 & |s^{\ell_*}-s| \\ \mathbf{0}_{3,1} & |v| & 1 \end{bmatrix} \left[\begin{array}{c|c|c} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline |v| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} \end{array}\right] \begin{bmatrix} 1 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \mathbf{0}_{3,1} & 1 & |t-s^1| \\ \mathbf{0}_{3,1} & |v| & 1 \end{bmatrix} \\
&\lesssim C^{C|v|(t-s)} \left[\begin{array}{c|c|c} 0 & \mathbf{0}_{1,3} & \mathbf{0}_{1,3} \\ \hline |v| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} \end{array}\right].
\end{aligned} \tag{A.121}$$

Finally from (A.109) and (A.121) we conclude, for all $\tau \in [s,t]$

$$\frac{\partial(X_{\mathbf{cl}}(s;t,x,v), V_{\mathbf{cl}}(s;t,x,v))}{\partial(t,x,v)} \leq Ce^{C|v|(t-s)} \left[\begin{array}{c|c|c} |v| & \frac{|v|}{|\mathbf{v}_\perp^1|} & \frac{1}{|v|} \\ \hline |v|^2 & \frac{|v|^3}{|\mathbf{v}_\perp^1|^2} & \frac{|v|}{|\mathbf{v}_\perp^1|} \end{array}\right]_{6\times 7}$$

From the Velocity lemma(Lemma A.1),

$$\begin{aligned} |\mathbf{v}_\perp^1| &= |v^1 \cdot [-n(x^1)]| = |V_{\mathbf{cl}}(t^1;t,x,v) \cdot n(X_{\mathbf{cl}}(t^1;t,x,v))| \\ &= \sqrt{\alpha(X_{\mathbf{cl}}(t^1), V_{\mathbf{cl}}(t^1))} \geq e^{\mathcal{C}|v||t-t^1|}\alpha(x,v) \gtrsim \alpha(x,v), \end{aligned}$$

and this completes the proof for the case (A.108).

□

Proof of Theorem A.2. We use the approximation sequence (A.30) with (A.32). Due to Lemma A.6 we have $\sup_m \sup_{0\leq t\leq T} ||e^{\theta|v|^2} f^m(t)||_\infty \lesssim_{\xi,T} P(||e^{\theta'|v|^2} f_0||_\infty)$.

Now we claim that the distributional derivatives coincide with the piecewise derivatives. This is due to Proposition A.1 and Proposition A.2 together with an invariant property of $\Gamma(f,f) = \Gamma_{\text{gain}}(f,f) - \nu(\sqrt{\mu}f)f$: *Assume* $f^m(v) = f^{m-1}(\mathcal{O}v)$ *holds for some orthonormal matrix. Then*

$$\Gamma(f^m, f^m)(v) = \Gamma(f^{m-1}, f^{m-1})(\mathcal{O}v). \tag{A.122}$$

We apply Proposition 1 to have

$$\begin{aligned} &f^m(t,x,v) \\ &= e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\nu(\sqrt{\mu}f^{m-\ell})(s)\mathrm{d}s} f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \\ &+ \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) e^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\mathrm{d}s. \end{aligned}$$

Now we consider the spatial and velocity derivatives. In the sense of distributions, we have for $\partial_{\mathbf{e}} = [\partial_x, \partial_v]$ with $\mathbf{e} \in \{x, v\}$,

$$\partial_{\mathbf{e}} f^m(t,x,v) = \mathrm{I}_{\mathbf{e}} + \mathrm{II}_{\mathbf{e}} + \mathrm{III}_{\mathbf{e}}. \tag{A.123}$$

Here

$$\mathrm{I}_{\mathbf{e}} \;=\; e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\nu(F^{m-\ell})(s)\mathrm{d}s}\; \partial_{\mathbf{e}}[X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)] \cdot \nabla_{x,v} f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)),$$

and

$$\begin{aligned}
\mathrm{II}_{\mathbf{e}} = &\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) e^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \partial_{\mathbf{e}}\big[\Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\big]\mathrm{d}s \\
&- \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) e^{-\int_s^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\partial_{\mathbf{e}}[\nu(F^{m-j})(\tau, X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))]\mathrm{d}\tau \\
&\quad \times \Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\mathrm{d}s \\
&- e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\nu(F^{m-\ell})(s)\mathrm{d}s}\; f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\partial_{\mathbf{e}}\big[\nu(F^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\big]\mathrm{d}s,
\end{aligned}$$

and

$$\begin{aligned}
\mathbf{III}_{\mathbf{e}} = &\sum_{\ell=0}^{\ell_*(0)} \big[-\partial_{\mathbf{e}} t^\ell \lim_{s\uparrow t^\ell} \nu(\sqrt{\mu} f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)) + \partial_{\mathbf{e}} t^{\ell+1} \lim_{s\downarrow t^{\ell+1}} \mu(\sqrt{\mu} f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\big] \\
&\quad \times e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\nu(\sqrt{\mu} f^{m-\ell})(s)} \\
&+ \sum_{\ell=0}^{\ell_*(0)} \Big[\lim_{s\uparrow t^\ell} e^{-\int_s^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)) \\
&\qquad - \lim_{s\downarrow t^{\ell+1}} e^{-\int_s^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)) \\
&+ \int_0^t \sum_\ell \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) \sum_{j=0}^{\ell_*(s)} \big[-\lim_{\tau\downarrow t^j} \nu(F^{m-j})(\tau, X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau)) + \lim_{\tau\uparrow t^{j+1}} \nu(F^{m-j})(\tau, X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))\big] \\
&\qquad \times e^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)).
\end{aligned}$$

For $\mathbf{III}_{\mathbf{e}}$ we rearrange the summation and use (A.77) and apply (A.122)

$$\begin{aligned}
\mathbf{III}_{\mathbf{e}} = &\sum_{\ell=0}^{\ell_*(0)} \Big[-\nu(\sqrt{\mu} f^{m-\ell})(t^\ell, x^\ell, v^\ell) + \nu(\sqrt{\mu} f^{m-\ell+1})(t^\ell, x^\ell, R_{x^\ell} v^\ell)\Big] \partial_{\mathbf{e}} t^\ell e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\nu(\sqrt{\mu} f^{m-\ell})(s)} \\
&+ \sum_{\ell=0}^{\ell_*(0)} e^{-\int_{t^\ell}^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(\sqrt{\mu} f^{m-j})(\tau)\mathrm{d}\tau} \\
&\quad \times \Big[\Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(t^\ell, x^\ell, v^\ell) - \Gamma_{\mathrm{gain}}(f^{m-\ell+1}, f^{m-\ell+1})(t^\ell, x^\ell, R_{x^\ell} v^\ell)\Big] \\
&+ \int_0^t \sum_\ell \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\mathrm{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)) \\
&\quad \times \sum_{\ell=0}^{\ell_*(s)} \Big[-\nu(\sqrt{\mu} f^{m-\ell})(t^\ell, x^\ell, v^\ell) + \nu(\sqrt{\mu} f^{m-\ell+1})(t^\ell, x^\ell, R_{x^\ell} v^\ell)\Big] \\
&= 0.
\end{aligned}$$

Proof of (A.122). The proof is due to the change of variables

$$\tilde{u} = \mathcal{O}u, \quad \tilde{\omega} = \mathcal{O}\omega, \quad \mathrm{d}\tilde{u} = \mathrm{d}u, \quad \mathrm{d}\tilde{\omega} = \mathrm{d}\omega.$$

Note

$$
\begin{aligned}
&\Gamma(f^m, f^m)(v)\\
&= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} |v-u|^\kappa q_0(\frac{v-u}{|v-u|}\cdot\omega)\sqrt{\mu(u)}\Big\{f^m(u-[(u-v)\cdot\omega]\omega)f^m(v+[(u-v)\cdot\omega]\omega) - f^m(u)f^m(v)\Big\}\mathrm{d}\omega\mathrm{d}u\\
&= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} |\mathcal{O}v-\mathcal{O}u|^\kappa q_0(\frac{\mathcal{O}v-\mathcal{O}u}{|\mathcal{O}v-\mathcal{O}u|}\cdot\mathcal{O}\omega)\sqrt{\mu(\mathcal{O}u)}\\
&\quad\times\Big\{f^{m-1}(\mathcal{O}u-[(\mathcal{O}u-\mathcal{O}v)\cdot\mathcal{O}\omega]\mathcal{O}\omega)f^{m-1}(\mathcal{O}v+[(\mathcal{O}u-\mathcal{O}v)\cdot\mathcal{O}\omega]\mathcal{O}\omega) - f^{m-1}(\mathcal{O}u)f^{m-1}(\mathcal{O}v)\Big\}\mathrm{d}\omega\mathrm{d}u\\
&= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} |\mathcal{O}v-\tilde{u}|^\kappa q_0(\frac{\mathcal{O}v-\tilde{u}}{|\mathcal{O}v-\tilde{u}|}\cdot\tilde{\omega})\sqrt{\mu(\tilde{u})}\\
&\quad\times\Big\{f^{m-1}(\tilde{u}-[(\tilde{u}-\mathcal{O}v)\cdot\tilde{\omega}]\tilde{\omega})f^{m-1}(\mathcal{O}v+[(\tilde{u}-\mathcal{O}v)]\cdot\tilde{\omega})\tilde{\omega} - f^{m-1}(\tilde{u})f^{m-1}(\mathcal{O}v)\Big\}\mathrm{d}\tilde{\omega}\mathrm{d}\tilde{u}\\
&= \Gamma(f^{m-1}, f^{m-1})(\mathcal{O}v).
\end{aligned}
$$

This proves (A.122). Especially we can apply (A.122) for the specular reflection BC (A.32) with $\mathcal{O}v = R_x v$ as well as the bounce-back reflection BC (A.33) with $\mathcal{O}v = -v$.

Using Lemma A.5,

$$
\begin{aligned}
\mathrm{II}_{\mathbf{e}} \lesssim\ & P(||e^{\theta|v|^2}f_0||_\infty)\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)|\partial_{\mathbf{e}}X_{\mathbf{cl}}(s)|\int_{\mathbb{R}^3}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}|\nabla_x f^{m-\ell}(s,X_{\mathbf{cl}}(s),u)|\mathrm{d}u\mathrm{d}s\\
&+ P(||e^{\theta|v|^2}f_0||_\infty)\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)|\partial_{\mathbf{e}}V_{\mathbf{cl}}(s)|\int_{\mathbb{R}^3}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}|\nabla_v f^{m-\ell}(s,X_{\mathbf{cl}}(s),u)|\mathrm{d}u\mathrm{d}s\\
&+ tP(||e^{\theta|v|^2}f_0||_\infty)\langle v\rangle^\kappa e^{-\theta|v|^2}\sup_{0\le s\le t}|\partial_{\mathbf{e}}V(s;t,x,v)|.
\end{aligned}
$$

We shall estimate the followings :

$$
e^{-\varpi\langle v\rangle t}\frac{[\alpha(x,v)]^\beta}{\langle v\rangle^{b+1}}|\partial_x f(t,x,v)|, \quad e^{-\varpi\langle v\rangle t}\frac{|v|[\alpha(x,v)]^{\beta-\frac12}}{\langle v\rangle^b}|\partial_v f(t,x,v)|.
$$

From (A.20), the Velocity lemma (Lemma A.1), Lemma A.6, and $F^m \ge 0$ for all m, with $\varpi \gg 1$

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{1}{\langle v\rangle^{b+1}}[\alpha(x,v)]^\beta\ \mathrm{I}_{\mathbf{x}}\\
&\lesssim_{\xi,t} e^{-\varpi\langle v\rangle t}\frac{1}{\langle v\rangle^{b+1}}[\alpha(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))]^\beta e^{2\mathcal{C}|v|t}\\
&\quad\times\Big\{\frac{|v|}{\sqrt{\alpha(x,v)}}|\partial_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))| + \frac{|v|^3}{\alpha(x,v)}|\partial_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|\Big\}\\
&\lesssim_{\xi,t} \Big|\Big|\ \frac{|v|}{\langle v\rangle^{b+1}}\alpha^{\beta-\frac12}\partial_x f_0\ \Big|\Big|_\infty + \Big|\Big|\ \frac{|v|^3}{\langle v\rangle^{b+1}}\alpha^{\beta-1}\partial_v f_0\ \Big|\Big|_\infty\\
&\lesssim_{\xi,t} \Big|\Big|\ \frac{\alpha^{\beta-\frac12}}{\langle v\rangle^b}\partial_x f_0\ \Big|\Big|_\infty + \Big|\Big|\ \frac{|v|^2\alpha^{\beta-1}}{\langle v\rangle^b}\partial_v f_0\ \Big|\Big|_\infty,
\end{aligned}
$$

and

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^b}[\alpha(x,v)]^{\beta-\frac12}\ \mathrm{I}_{\mathbf{v}}\\
&\lesssim_{\xi,t} e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^b}[\alpha(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))]^{\beta-\frac12}e^{2\mathcal{C}|v|t}\\
&\quad\times\Big\{\frac{1}{|v|}|\partial_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))| + \frac{|v|}{\sqrt{\alpha(x,v)}}|\partial_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|\Big\}\\
&\lesssim_{\xi,t} \Big|\Big|\ \frac{\alpha^{\beta-\frac12}}{\langle v\rangle^b}\partial_x f_0\ \Big|\Big|_\infty + \Big|\Big|\ \frac{|v|^2}{\langle v\rangle^b}\alpha^{\beta-1}\partial_v f_0\ \Big|\Big|_\infty,
\end{aligned}
$$

where we have used $\alpha(x,v) \lesssim_\xi |v|^2$ and the choice of $\varpi \gg 1$.

From Lemma A.4, Lemma A.5, and Lemma A.6,

$$
\begin{aligned}
\mathrm{II}_{\mathbf{e}} \lesssim_t\ & P(\|e^{\theta|v|^2} f_0\|_\infty) \int_0^t \mathrm{d}s \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1}, t^\ell)}(s) \int_{\mathbb{R}^3} \mathrm{d}u \frac{e^{-C_\theta|u-V_{\mathbf{cl}}(s)|^2}}{|u-V_{\mathbf{cl}}(s)|^{2-\kappa}} \\
& \times \Big\{ |\partial_{\mathbf{e}} X_{\mathbf{cl}}(s)| |\partial_x f^{m-j}(s, X_{\mathbf{cl}}(s), u)| + |\partial_{\mathbf{e}} V_{\mathbf{cl}}(s)| \big(1 + |\partial_v f^{m-j}(s, X_{\mathbf{cl}}(s), u)|\big) \Big\}.
\end{aligned}
$$

Now we use (A.20) to have

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t} \frac{[\alpha(x,v)]^\beta}{\langle v\rangle^{b+1}} \mathrm{II}_{\mathbf{x}} \lesssim_{t,\xi} P(\|e^{\theta|v|^2} f_0\|_\infty) \\
& \times \Big\{ \int_0^t \int_{\mathbb{R}^3} \frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|u-V_{\mathbf{cl}}(s)|^{2-\kappa}} e^{-\varpi\langle v\rangle t} e^{\varpi\langle u\rangle s} e^{C|v||t-s|} \frac{|v|[\alpha(x,v)]^{\beta-\frac12}}{[\alpha(X_{\mathbf{cl}}(s),u)]^\beta} \frac{\langle u\rangle^{b+1}}{\langle v\rangle^{b+1}} \mathrm{d}u\mathrm{d}s \\
& \qquad \times \sup_m \sup_{0\le s\le t} \Big\| e^{-\varpi\langle u\rangle s} \frac{[\alpha(X_{\mathbf{cl}}(s),u)]^\beta}{\langle u\rangle^{b+1}} \partial_x f^{m-j}(s, X_{\mathbf{cl}}(s), u) \Big\|_\infty \\
& \quad + \int_0^t \int_{\mathbb{R}^3} \frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|u-V_{\mathbf{cl}}(s)|^{2-\kappa}} e^{-\varpi\langle v\rangle t} e^{\varpi\langle u\rangle s} e^{C|v||t-s|} \frac{\langle u\rangle^b}{\langle v\rangle^b} \frac{|v|^2[\alpha(x,v)]^{\beta-1}}{|u|[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta-\frac12}} \\
& \qquad \times \sup_m \sup_{0\le s\le t} \Big\| e^{-\varpi\langle u\rangle s} \frac{|u|[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta-\frac12}}{\langle u\rangle^b} \partial_v f^{m-j}(s, X_{\mathbf{cl}}(s), u) \Big\|_\infty \Big\}.
\end{aligned}
$$

We first claim that

$$
e^{-\varpi\langle v\rangle t} e^{\varpi\langle u\rangle s} e^{C|v|(t-s)} e^{-C'|v-u|^2} \lesssim e^{-\frac{\varpi\langle v\rangle}{2}(t-s)} e^{C''(s+s^2)} e^{-C''|v-u|^2}. \tag{A.124}
$$

Using $\langle u\rangle \le 1+|u| \le 1+|v|+|u-v| \le 1+\langle v\rangle+|v-u|$, we bound the first three exponents as

$$
-(\varpi - C)\langle v\rangle(t-s) - \varpi(\langle v\rangle - \langle u\rangle)s \le -(\varpi - C)\langle v\rangle(t-s) + \varpi|v-u|s + \varpi s.
$$

Then we use a complete square trick, for $0<\sigma\ll 1$

$$
\varpi|v-u|s = \frac{\sigma\varpi^2}{2}|v-u|^2 + \frac{s^2}{2\sigma} - \frac{1}{2\sigma}\big[s - \sigma\varpi|v-u|\big]^2 \le \frac{\sigma\varpi^2}{2}|v-u|^2 + \frac{s^2}{2\sigma},
$$

to bound the whole exponents of (A.124) by

$$
\begin{aligned}
& -(\varpi - C)\langle v\rangle(t-s) + \varpi|v-u|s - C'|v-u|^2 + \varpi s \\
& \le -(\varpi - C)\langle v\rangle(t-s) - (C - \frac{\sigma\varpi^2}{2})|v-u|^2 + \frac{s^2}{2\sigma} + \varpi s \\
& \le -(\varpi - C)\langle v\rangle(t-s) - C_{\sigma,\varpi}|v-u|^2 + C'_{\sigma,\varpi}\{s^2+s\}.
\end{aligned}
$$

Hence we prove the claim (A.124) for $\varpi \gg 1$.

Now we use (A.124) to bound

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t} \frac{1}{\langle v\rangle^{b+1}} [\alpha(x,v)]^\beta \, \mathrm{II}_{\mathbf{x}} \\
& \lesssim_{t,\xi} P(\|e^{\theta|v|^2} f_0\|_\infty) \times \\
& \times \Big\{ \underbrace{\int_0^t \int_{\mathbb{R}^3} e^{-\frac{\varpi\langle v\rangle}{2}(t-s)} \frac{e^{-C'_\theta|v-u|^2}}{|v-u|^{2-\kappa}} \frac{\langle u\rangle^{b+1}}{\langle v\rangle^{b+1}} \frac{\langle v\rangle[\alpha(x,v)]^{\beta-\frac12}}{[\alpha(X_{\mathbf{cl}}(s),u)]^\beta} \mathrm{d}u\mathrm{d}s}_{(\mathbf{A})} \sup_m \sup_{0\le s\le t} \Big\| e^{-\varpi\langle v\rangle s} \frac{\alpha^\beta}{\langle v\rangle^{b+1}} \partial_x f^m(s) \Big\|_\infty \\
& \quad + \underbrace{\int_0^t \int_{\mathbb{R}^3} e^{-\frac{\varpi\langle v\rangle}{2}(t-s)} \frac{e^{-C'_\theta|v-u|^2}}{|v-u|^{2-\kappa}} \frac{\langle u\rangle^b}{\langle v\rangle^b} \frac{|v|^2[\alpha(x,v)]^{\beta-1}}{|u|[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta-\frac12}} \mathrm{d}u\mathrm{d}s}_{(\mathbf{B})} \sup_m \sup_{0\le s\le t} \Big\| e^{-\varpi\langle v\rangle s} \frac{|v|\alpha^{\beta-\frac12}}{\langle v\rangle^b} \partial_v f^m(s) \Big\|_\infty \Big\}.
\end{aligned}
\tag{A.125}
$$

For $(\mathbf{A})$ we use (A.16) with $Z = \langle v\rangle\big[\alpha(x,v)\big]^{\beta-\frac12}$ and $l = \frac{\varpi}{2}$ and $r = b+1$. For $(\mathbf{B})$ we use (A.51) with $\beta \mapsto \beta - \frac12$ and $Z = \langle v\rangle\big[\alpha(x,v)\big]^{\beta-1}$ and $l = \frac{\varpi}{2}$ and $r = b$. Then

$$
(\mathbf{A}),\ (\mathbf{B}) \ \ll\ 1.
$$

Similarly, but with different weight $e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^b}[\alpha(x,v)]^{\beta-\frac{1}{2}}$, we use (A.20) to have

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^b}[\alpha(x,v)]^{\beta-\frac{1}{2}}\ \mathrm{II}_{\mathbf{v}}\\
&\lesssim_{t,\xi} P(||e^{\theta|v|^2}f_0||_\infty)\times\\
&\quad\times\Big\{\int_0^t\int_{\mathbb{R}^3}\frac{e^{-C|V_{\mathbf{cl}}(s)-u|^2}}{|u-V_{\mathbf{cl}}(s)|^{2-\kappa}}e^{-\varpi\langle v\rangle t}e^{\varpi\langle u\rangle s}e^{C|v||t-s|}\frac{\langle v\rangle[\alpha(x,v)]^{\beta-\frac{1}{2}}}{[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta}}\frac{\langle u\rangle^{b+1}}{\langle v\rangle^{b+1}}\mathrm{d}u\mathrm{d}s\\
&\qquad\qquad\times\sup_m\sup_{0\le s\le t}\big|\big|e^{-\varpi\langle u\rangle s}\frac{[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta}}{\langle u\rangle^{b+1}}\partial_x f^m(s,X_{\mathbf{cl}}(s),u)\big|\big|_\infty\\
&\qquad+\int_0^t\int_{\mathbb{R}^3}\frac{e^{-C|V_{\mathbf{cl}}(s)-u|^2}}{|u-V_{\mathbf{cl}}(s)|^{2-\kappa}}e^{-\varpi\langle v\rangle t}e^{\varpi\langle u\rangle s}e^{C|v||t-s|}\frac{\langle u\rangle^b}{\langle v\rangle^b}\frac{|v|^2[\alpha(x,v)]^{\beta-1}}{|u|[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta-\frac{1}{2}}}\\
&\qquad\qquad\times\sup_m\sup_{0\le s\le t}\big|\big|e^{-\varpi\langle u\rangle s}\frac{|u|[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta-\frac{1}{2}}}{\langle u\rangle^{b}}\partial_v f^m(s,X_{\mathbf{cl}}(s),u)\big|\big|_\infty\Big\}.
\end{aligned}$$

Again we use (A.124) and (A.16) and (A.51) exactly as (A.125). Therefore for $0<\delta=\delta(||e^{\theta|v|^2}f_0||_\infty)\ll 1$

$$\begin{aligned}
&e^{-\varpi\langle v\rangle t}\frac{1}{\langle v\rangle^{b+1}}[\alpha(x,v)]^{\beta}\mathrm{II}_{\mathbf{x}}+e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^b}[\alpha(x,v)]^{\beta-\frac{1}{2}}\mathrm{II}_{\mathbf{v}}\\
&\lesssim\delta\,\big\{\sup_m\sup_{0\le s\le t}\big|\big|e^{-\varpi\langle v\rangle s}\frac{\alpha^\beta}{\langle v\rangle^{b+1}}\partial_x f^m(s)\big|\big|_\infty+\sup_m\sup_{0\le s\le t}\big|\big|e^{-\varpi\langle v\rangle s}\frac{|v|\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_v f^m(s)\big|\big|_\infty\big\}.
\end{aligned}$$

Collecting all the terms, for $1<\beta<\frac{3}{2}$ and $b\in\mathbb{R}$ with $\varpi\gg 1$ and $0<\delta\ll 1$

$$\begin{aligned}
&\sup_m\sup_{0\le s\le t}||e^{-\varpi\langle v\rangle t}\frac{\alpha^\beta}{\langle v\rangle^{b+1}}\partial_x f^m(t)||_\infty+\sup_m\sup_{0\le s\le t}||e^{-\varpi\langle v\rangle t}\frac{|v|\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_v f^m(t)||_\infty\\
&\lesssim||\frac{\alpha^{\beta-\frac{1}{2}}}{\langle v\rangle^b}\partial_x f_0||_\infty+||\frac{|v|^2\alpha^{\beta-1}}{\langle v\rangle^b}\partial_v f_0||_\infty+P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}$$

We remark that this sequence f^m is Cauchy in $L^\infty([0,T]\times\bar{\Omega}\times\mathbb{R}^3)$ for $0<T\ll 1$. Therefore the limit function f is a solution of the Boltzmann equation satisfying the specular reflection BC. On the other hand, due to the weak lower semi-continuity of L^p, $p>1$, we pass a limit $\partial f^m\rightharpoonup\partial f$ weakly in the weighted $L^\infty-$norm.

Now we consider the continuity of $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f$. Remark that both $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f^m$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f^m$ satisfy all the conditions of Proposition A.2. Therefore we conclude

$$e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f^m\in C^0([0,T^*]\times\bar{\Omega}\times\mathbb{R}^3),\ e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f^m\in C^0([0,T^*]\times\bar{\Omega}\times\mathbb{R}^3).$$

Now we follow $W^{1,\infty}$ estimate proof for $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta[\partial_x f^{m+1}-\partial_x f^m]$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}[\partial_v f^{m+1}-\partial f^m]$ to show that $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f^m$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f^m$ are Cauchy in L^∞. Then we pass a limit $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f^m\to e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f^m\to e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f$ strongly in L^∞ so that $e^{-\varpi\langle v\rangle t}\langle v\rangle^{-1}\alpha^\beta\partial_x f\in C^0([0,T^*]\times\bar{\Omega}\times\mathbb{R}^3)$ and $e^{-\varpi\langle v\rangle t}|v|\alpha^{\beta-\frac{1}{2}}\partial_v f\in C^0([0,T^*]\times\bar{\Omega}\times\mathbb{R}^3)$. □

A.6 Bounce-Back Reflection BC

We recall the bounce-back cycles from *(iv)* of Definition A.1 : $(t^0,x^0,v^0)=(t,x,v)$ and for $\ell\ge 1$,

$$t^\ell=t^1-(\ell-1)t_{\mathbf{b}}(x^1,v^1),\quad x^\ell=\frac{1-(-1)^\ell}{2}x^1+\frac{1+(-1)^\ell}{2}x^2,\quad v^{\ell+1}=(-1)^{\ell+1}v,$$

where $t_{\mathbf{b}}(x,v)$ is defined in (A.4).

Lemma A.11. *For all* $0 \leq s \leq t$,

$$\min\{\alpha(x^1,v^1),\alpha(x^2,v^2)\} \lesssim_\Omega \alpha(X_{\mathbf{cl}}(s;t,x,v),V_{\mathbf{cl}}(s;t,x,v)) \lesssim_\Omega \max\{\alpha(x^1,v^1),\alpha(x^2,v^2)\}.$$

For $\ell_*(s;t,x,v) \in \mathbb{N}$ *(therefore* $t^{\ell_*+1}(t,x,v) \leq s \leq t^{\ell_*}(t,x,v)$*)*

$$\ell_*(s;t,x,v) \ \leq \ \frac{|t-s|}{t_{\mathbf{b}}(x_1,v_1)} \ \lesssim_\Omega \ \frac{|t-s||v|^2}{\sqrt{\alpha(x,v)}}.$$

For all $0 \leq s \leq t$ *uniformly*

$$\begin{aligned}
|\partial_{x_i} t^\ell(t,x,v)| &= \ \Big| -\ell \frac{\partial_{x_i}\xi(x^1)}{v\cdot\nabla\xi(x^1)} - (\ell-1)\frac{\partial_{x_i}\xi(x^2)}{-v\cdot\nabla\xi(x^2)}\Big| \ \lesssim_\Omega \frac{t|v|^2}{\alpha(x,v)},\\
|\partial_{v_i} t^\ell(t,x,v)| &= \ \Big|\ell t_{\mathbf{b}}(x,v)\frac{\partial_{x_i}\xi(x^1)}{v\cdot\nabla\xi(x^1)} + (\ell-1)t_{\mathbf{b}}(x,-v)\frac{\partial_{x_i}\xi(x^2)}{-v\cdot\nabla\xi(x^2)}\Big| \ \lesssim_\Omega \frac{t}{\sqrt{\alpha(x,v)}},\\
|\partial_{x_i} x_j^\ell(x,v)| &= \ \Big|\frac{1-(-1)^\ell}{2}\Big\{\delta_{ij} - \frac{v_j\partial_{x_i}\xi(x_1)}{v\cdot\nabla\xi(x_1)}\Big\} + \frac{1+(-1)^\ell}{2}\Big\{\delta_{ij} - \frac{v_j\partial_{x_i}\xi(x_2)}{v\cdot\nabla\xi(x_2)}\Big\}\Big| \ \lesssim_\Omega 1 + \frac{|v|}{\sqrt{\alpha(x,v)}},\\
|\partial_{v_i} x_j^\ell(x,v)| &= \ \Big|\frac{1-(-1)^\ell}{2}(-t_{\mathbf{b}}(x,v))\Big\{\delta_{ij} - \frac{v_j\partial_{x_i}\xi(x_1)}{v\cdot\nabla\xi(x_1)}\Big\} + \frac{1+(-1)^\ell}{2}(-t_{\mathbf{b}}(x,-v))\Big\{\delta_{ij} - \frac{v_j\partial_{x_i}\xi(x_2)}{v\cdot\nabla\xi(x_2)}\Big\}\Big|,\\
&\lesssim_\Omega \frac{1}{|v|},\\
\partial_{x_i} v^\ell &= \ 0, \quad |\partial_{v_i} v_j^\ell| = |(-1)^\ell\delta_{ij}| \ \lesssim_\Omega 1,\\
|\partial_{x_i}(t^\ell - t^{\ell+1})| &= \ \Big|\frac{\partial_{x_i}\xi(x_1)}{v\cdot\nabla\xi(x_1)} + \frac{\partial_{x_i}\xi(x_2)}{-v\cdot\nabla\xi(x_2)}\Big| \ \lesssim_\Omega \frac{1}{\sqrt{\alpha(x,v)}},\\
|\partial_{v_i}(t^\ell - t^{\ell+1})| &= \ \Big|t_{\mathbf{b}}(x,v)\frac{-\partial_{x_i}\xi(x_1)}{v\cdot\nabla\xi(x_1)} + t_{\mathbf{b}}(x,-v)\frac{\partial_{x_i}\xi(x_2)}{v\cdot\nabla\xi(x_2)}\Big| \ \lesssim_\Omega \frac{1}{|v|^2}.
\end{aligned}$$

Proof. These are direct consequence of the Velocity Lemma (Lemma A.1) and the following derivatives of $x_{\mathbf{b}}$ and $t_{\mathbf{b}}$ (from Lemma 2 in [75]) :

$$\begin{aligned}
\nabla_x t_{\mathbf{b}} &= \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}, \quad \nabla_v t_{\mathbf{b}} = -\frac{t_{\mathbf{b}} n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})},\\
\nabla_x x_{\mathbf{b}} &= I - \frac{n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\otimes v, \quad \nabla_v x_{\mathbf{b}} = -t_{\mathbf{b}} I + \frac{t_{\mathbf{b}} n(x_{\mathbf{b}})}{v\cdot n(x_{\mathbf{b}})}\otimes v.
\end{aligned} \tag{A.126}$$

. $\square$

Now we state the key ingredient in the case of the bounce-back BC which is the general version of Lemma A.3 : In the sense of distribution,

$$\begin{aligned}
&\partial_{\mathbf{e}}\Big[\sum_{\ell=0}^{\ell_*(s)}\int_{\max\{s,t^{j+1}\}}^{t^j} A^{m-j}(\tau, x^j-(t^j-\tau)v^j, v^j)\mathrm{d}\tau\Big]\\
&= \sum_{j=0}^{\ell_*(s)}\int_{\max\{s,t^{j+1}\}}^{t^j}\big[\partial_{\mathbf{e}}t^j, \partial_{\mathbf{e}}x^j + \tau\partial_{\mathbf{e}}v^j, \partial_{\mathbf{e}}v^j\big]\cdot\nabla_{t,x,v}A^{m-j}(\tau, x^j-(t^j-\tau)v^j, v^j)\mathrm{d}\tau\\
&\quad + \sum_{j=0}^{\ell_*(s)-1}\partial_{\mathbf{e}}[t^j - t^{j+1}]\lim_{\tau\downarrow-(t^j-t^{j+1})} A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j)\\
&\quad + \partial_{\mathbf{e}}t^{\ell_*(s)}\lim_{\tau\downarrow-(t^{\ell_*(s)}-s)} A^{m-\ell_*(s)}(\tau+t^{\ell_*(s)}, x^{\ell_*(s)}+\tau v^{\ell_*(s)}, v^{\ell_*(s)}).
\end{aligned} \tag{A.127}$$

Note that (A.127) is more general than Lemma A.3.

Proof of (A.127) and Lemma A.3. Once we prove (A.127) then Lemma A.3 holds clearly. Now we prove (A.127) : For each time intervals $[t^{j+1},t^j]$, we apply the change of variables

$$\begin{aligned}
x^j-(t^j-\tau)v^j,\ \tau\in[t^{j+1},t^j] \ &\mapsto \ x^j+\tau v^j,\ \tau\in[-(t^j-t^{j+1}),0],\\
&\qquad\qquad \text{for } j=0,1,\cdots,\ell_*(s)-1,\\
x^{\ell_*(s)}-(t^{\ell_*(s)}-\tau)v^{\ell_*(s)},\ \tau\in[s,t^{\ell_*(s)}] \ &\mapsto \ x^{\ell_*(s)}+\tau v^{\ell_*(s)},\ \tau\in[-(t^{\ell_*(s)}-s),0].
\end{aligned} \tag{A.128}$$

From (7.51) in Chapter 7 the piecewise derivatives equal distributional derivatives almost everywhere. Therefore we prove Lemma A.3. Moreover

$$
\begin{aligned}
&\partial_{\mathbf{e}}\Big[\sum_{j=0}^{\ell_*(s)}\int_{\max\{s,t^{j+1}\}}^{t^j} A^{m-j}(\tau, x^j-(t^j-\tau)v^j, v^j)\mathrm{d}\tau\Big]\\
&= \partial_{\mathbf{e}}\Big[\sum_{j=0}^{\ell_*(s)-1}\int_{t^{j+1}}^{t^j}\cdots\Big] + \partial_{\mathbf{e}}\Big[\int_s^{t^{\ell_*(s)}}\cdots\Big]\\
&= \partial_{\mathbf{e}}\Big[\sum_{j=0}^{\ell_*(s)-1}\int_{-(t^j-t^{j+1})}^{0} A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j)\mathrm{d}\tau\Big]\\
&\quad + \partial_{\mathbf{e}}\Big[\int_{-(t^{\ell_*(s)}-s)}^{0} A^{m-\ell_*(s)}(\tau+t^{\ell_*(s)}, x^{\ell_*(s)}+\tau v^{\ell_*(s)}, v^{\ell_*(s)})\Big]\\
&= \sum_{j=0}^{\ell_*(s)-1}\int_{-(t^j-t^{j+1})}^{0} \partial_{\mathbf{e}}\big[A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j)\big]\mathrm{d}\tau\\
&\quad + \sum_{j=0}^{\ell_*(s)-1}\partial_{\mathbf{e}}[t^j-t^{j+1}]\lim_{\tau\downarrow -(t^j-t^{j+1})} A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j)\\
&\quad + \int_{-(t^{\ell_*(s)}-s)}^{0}\partial_{\mathbf{e}}\big[A^{m-\ell_*(s)}(\tau+t^{\ell_*(s)}, x^{\ell_*(s)}+\tau v^{\ell_*(s)}, v^{\ell_*(s)})\big]\\
&\quad + \partial_{\mathbf{e}}t^{\ell_*(s)}\lim_{\tau\downarrow -(t^{\ell_*(s)}-s)} A^{m-\ell_*(s)}(\tau+t^{\ell_*(s)}, x^{\ell_*(s)}+\tau v^{\ell_*(s)}, v^{\ell_*(s)}).
\end{aligned}
$$

Directly we have

$$
\partial_{\mathbf{e}}\big[A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j)\big] = \big[\partial_{\mathbf{e}}t^j, \partial_{\mathbf{e}}x^j+\tau\partial_{\mathbf{e}}v^j, \partial_{\mathbf{e}}v^j\big]\cdot\nabla_{t,x,v}A^{m-j}(\tau+t^j, x^j+\tau v^j, v^j).
$$

Then we apply the inverse of the change of variables in (A.128) to the time integration terms :

$$
\sum_{j=0}^{\ell_*(s)}\int_{\max\{s,t^{j+1}\}}^{t^j}\big[\partial_{\mathbf{e}}t^j, \partial_{\mathbf{e}}x^j+\tau\partial_{\mathbf{e}}v^j, \partial_{\mathbf{e}}v^j\big]\cdot\nabla_{t,x,v}A^{m-j}(\tau, x^j-(t^j-\tau)v^j, v^j)\mathrm{d}\tau.
$$

We collect the terms and conclude (A.127). □

Now we are ready to proof the main theorem :

Proof of Theorem A.4. We use the approximation sequence (A.30) with (A.33). Due to Lemma A.6 we have (A.27) and (A.28).

Now we consider the spatial and velocity derivatives. From the iteration (A.29) and (A.33), for $\ell_*(0;t,x,v)=\ell_*$ with $t^{\ell_*+1}\le 0<t^{\ell_*}$,

$$
\begin{aligned}
&f^{m+1}(t,x,v)\\
&= e^{-\sum_{j=0}^{\ell_*(0)}\int_{\max\{0,t^{j+1}\}}^{t^j}\nu(F^{m-j})(\tau)\mathrm{d}\tau}\, f_0(x^{\ell_*(0)}-t^{\ell_*(0)}v^{\ell_*(0)}, v^{\ell_*(0)})\\
&+\sum_{\ell=0}^{\ell_*(0)}\int_{\max\{0,t^{\ell+1}\}}^{t^\ell} e^{-\sum_{j=0}^{\ell_*(s)}\int_{\max\{0,t^{j+1}\}}^{t^j}\nu(F^{m-j})(\tau)\mathrm{d}\tau}\,\Gamma_{\text{gain}}(f^{m-\ell},f^{m-\ell})(s,x^\ell-(t^\ell-s)v^\ell,v^\ell)\mathrm{d}s,
\end{aligned}
$$

where $\nu(F^{m-j})(\tau)=\mu(\sqrt{\mu}f^{m-j})(\tau)=\nu(\sqrt{\mu}f^{m-j})(\tau,x^j-(t^j-\tau)v^j,v^j)$.

From Lemma A.3 and (A.127) and (A.122), in the sense of distribution, for $\partial_{\mathbf{e}}=[\partial_x,\partial_v]$ with

$\mathbf{e} \in \{x, v\}$,

$$
\begin{aligned}
&\partial_{\mathbf{e}} f^m(t,x,v) \\
&= \mathbf{I_e} + \mathbf{II_e} \\
&= e^{-\int_0^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau, X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))\mathrm{d}\tau} f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \\
&\quad \times \Big\{ - \sum_{j=0}^{\ell_*(0)} \underline{\int_{\max\{0,t^{j+1}\}}^{t^j} \big[\partial_{\mathbf{e}} t^j, \partial_{\mathbf{e}} x^j + \tau \partial_{\mathbf{e}} v^j, \partial_{\mathbf{e}} v^j\big] \cdot \nabla_{t,x,v} \nu(F^{m-j})(\tau, x^j - (t^j-\tau)v^j, v^j)\mathrm{d}\tau}_{\mathbf{II_e}} \\
&\qquad - \sum_{j=0}^{\ell_*(0)-1} \underline{\partial_{\mathbf{e}}[t^j - t^{j+1}]\nu(F^{m-j})(t^{j+1}, x^{j+1}, v^j)}_{\mathbf{I_e}} - \underline{\partial_{\mathbf{e}} t^{\ell_*(0)} \nu(F^{m-\ell_*(0)})(0, x^j - t^j v^j, v^j)}_{\mathbf{I_e}} \Big\} \\
&+ \underline{e^{-\int_0^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau, X_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))\mathrm{d}\tau} \partial_{\mathbf{e}} \big[x^{\ell_*(0)} - t^{\ell_*(0)} v^{\ell_*(0)}, v^{\ell_*(0)}\big] \cdot \nabla_{x,v} f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0))}_{\mathbf{I_e}} \\
&+ \sum_{\ell=0}^{\ell_*(0)-1} \partial_{\mathbf{e}}[t^\ell - t^{\ell+1}] e^{-\sum_{j=0}^{\ell_*(t^\ell - t^{\ell+1})} \int^0_{\max\{t^\ell - t^{\ell+1} - t^j, -(t^j - t^{j+1})\}} \nu(F^{m-j})(\tau + t^j, x^j + \tau v^j, v^j)\mathrm{d}\tau} \\
&\quad \times \underline{\Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})(t^{\ell+1}, x^{\ell+1}, v^\ell)}_{\mathbf{I_e}} \\
&+ \underline{\partial_{\mathbf{e}} t^{\ell_*(0)} e^{-\int_0^t \mathbf{1}_{[t^{j+1},t^j)}(s)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\text{gain}}(f^{m-\ell_*(0)}, f^{m-\ell_*(0)})(0, x^{\ell_*(0)} - t^{\ell_*(0)} v^{\ell_*(0)}, v^{\ell_*(0)})}_{\mathbf{I_e}} \\
&+ \int_0^t \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) e^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(s)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \\
&\quad \times \underline{[\partial_{\mathbf{e}} t^\ell, \partial_{\mathbf{e}} x^\ell + s \partial_{\mathbf{e}} v^\ell, \partial_{\mathbf{e}} v^\ell] \cdot \nabla_{t,x,v} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})](s, x^\ell - (t^\ell - s)v^\ell, v^\ell)\mathrm{d}s}_{\mathbf{II_e}} \\
&+ \int_0^t \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\mathrm{d}s \\
&\quad \times \Big\{ - \sum_{j=0}^{\ell_*(s)-1} \underline{\partial_{\mathbf{e}}[t^j - t^{j+1}]\nu(F^{m-j})(t^{j+1}, x^{j+1}, v^j)}_{\mathbf{I_e}} - \underline{\partial_{\mathbf{e}} t^{\ell_*(s)} \nu(F^{m-\ell_*(s)})(s, X_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))}_{\mathbf{I_e}} \\
&\qquad - \sum_{j=0}^{\ell_*(s)} \underline{\int_{\max\{s,t^{j+1}\}}^{t^j} [\partial_{\mathbf{e}} t^j, \partial_{\mathbf{e}} x^j + \tau \partial_{\mathbf{e}} v^j, \partial_{\mathbf{e}} v^j] \cdot \nabla_{t,x,v} \nu(F^{m-j})(\tau, x^j - (t^j - \tau)v^j, v^j)\mathrm{d}\tau}_{\mathbf{II_e}} \Big\}.
\end{aligned}
\tag{A.129}
$$

We shall estimate the followings :

$$
e^{-\varpi \langle v \rangle t} \frac{\alpha(x,v)}{\langle v \rangle^2} \partial_x f(t,x,v), \qquad e^{-\varpi \langle v \rangle t} \frac{|v|\alpha(x,v)^{1/2}}{\langle v \rangle^2} \partial_v f(t,x,v).
$$

Firstly, we estimate $\mathbf{I_e}$. Using Lemma A.11 and Lemma A.5 and $F^m \geq 0$ from (A.29) and Lemma A.6, for some polynomial P,

$$
\begin{aligned}
&e^{-\varpi \langle v \rangle t} \langle v \rangle^{-2} \alpha(x,v) \mathbf{I_x} \\
&\lesssim e^{-\varpi \langle v \rangle t} \langle v \rangle^{-2} \alpha(x,v) P(||e^{\theta|v|^2} f||_\infty) \\
&\quad \times \Big\{ e^{-\theta|v|^2} \frac{t|v|^2}{\alpha(x,v)} \langle v \rangle^\kappa + \big[(1 + \frac{|v|}{\alpha(x,v)}) + \frac{t|v|^3}{\alpha(x,v)}\big] |\partial_x f_0| + \frac{t|v|^2}{\alpha(x,v)} e^{-\frac{\theta}{2}|v|^2} + t e^{-\frac{\theta}{2}|v|^2} \langle v \rangle^\kappa \frac{t|v|^2}{\alpha(x,v)} \Big\} \\
&\lesssim ||\langle v \rangle^{-2} \alpha (1 + \frac{|v| + |v|^3}{\alpha(x,v)}) \partial_x f_0||_\infty + \langle v \rangle^{-2} e^{-C_\theta |v|^2} P(||e^{\theta|v|^2} f_0||_\infty) \\
&\lesssim (1 + ||\langle v \rangle \partial_x f_0||_\infty) \times P(||e^{\theta|v|^2} f_0||_\infty).
\end{aligned}
$$

Similarly

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}|v|\langle v\rangle^{-2}\alpha^{1/2}\mathbf{I_v} \\
\lesssim\; & e^{-\varpi\langle v\rangle t}|v|\langle v\rangle^{-2}[\alpha(x,v)]^{1/2}P(||e^{\theta|v|^2}f||_\infty) \\
& \times\Big\{e^{-\frac{\theta}{2}|v|^2}\frac{t}{\alpha(x,v)^{1/2}}\langle v\rangle^\kappa+\big[(\frac{1}{|v|}+\frac{\alpha(x,v)^{1/2}}{|v|^2})+\frac{t|v|}{\alpha(x,v)^{1/2}}+t\big]|\partial_x f_0|+|\nabla_v f_0| \\
& \quad+\frac{t}{\alpha(x,v)^{1/2}}e^{-\frac{\theta}{2}|v|^2}+te^{-\frac{\theta}{2}|v|^2}\langle v\rangle^\kappa\frac{t}{\alpha(x,v)^{1/2}}\Big\} \\
\lesssim\; & (1+||\langle v\rangle\partial_x f_0||_\infty+||\partial_v f_0||_\infty)P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}
$$

Secondly, we estimate $\mathbf{II_e}$. Let $\phi_{\mathbf{e}}\in\{\phi_{\mathbf{x}},\phi_{\mathbf{v}}\}$ with $\phi_{\mathbf{x}}=e^{-\varpi\langle v\rangle t}\frac{\alpha(x,v)}{\langle v\rangle^2}$ and $\phi_{\mathbf{v}}=e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2}$. We have

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\phi_{\mathbf{e}}(v)[\alpha(x,v)]^{\beta_{\mathbf{e}}}\mathbf{II_e} \\
\lesssim\; & e^{-\varpi\langle v\rangle t}\phi_{\mathbf{e}}(v)[\alpha(x,v)]^{\beta_{\mathbf{e}}}\Big\{1+(1+t)e^{-\frac{\theta}{2}|v|^2}||e^{\theta|v|^2}f||_\infty\Big\} \\
& \times\Big\{\int_0^t\sum_{j=0}^{\ell_*(0)}\mathbf{1}_{[t^{j+1},t^j)}(s)|\partial_{\mathbf{e}}t^j|\langle v\rangle^\kappa\mathrm{d}s\times||e^{\theta|v|^2}\partial_t f||_\infty && \text{(A.130)} \\
& +\int_0^t\sum_{j=0}^{\ell_*(0)}\mathbf{1}_{[t^{j+1},t^j)}(s)\{|\partial_{\mathbf{e}}x^\ell|+t|\partial_{\mathbf{e}}v^\ell|\}\nu(\sqrt{\mu}\partial_x f^{m-\ell})(s,X_{\mathbf{cl}}(s),V_{\mathbf{cl}}(s))\mathrm{d}s && \text{(A.131)} \\
& +\int_0^t\sum_{j=0}^{\ell_*(0)}\mathbf{1}_{[t^{j+1},t^j)}(s)|\partial_{\mathbf{e}}v^\ell|\int_{\mathbb{R}^3}|V_{\mathbf{cl}}(s)-u|^{\kappa-1}\sqrt{\mu(u)}f^{m-\ell}(s,X_{\mathbf{cl}}(s),u)\mathrm{d}u\mathrm{d}s && \text{(A.132)} \\
& +\int_0^t\sum_{\ell=0}^{\ell_*(0)}\mathbf{1}_{[t^{\ell+1},t^\ell)}(s)|\partial_{\mathbf{e}}t^\ell|\big[|\Gamma_{\mathrm{gain}}(\partial_t f^{m-\ell},f^{m-\ell})|+|\Gamma_{\mathrm{gain}}(f^{m-\ell},\partial_t f^{m-\ell})|\big]\mathrm{d}s && \text{(A.133)} \\
& +\int_0^t\sum_{\ell=0}^{\ell_*(0)}\mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\{|\partial_{\mathbf{e}}x^\ell|+t|\partial_{\mathbf{e}}v^\ell|\}\big[|\Gamma_{\mathrm{gain}}(\partial_x f^{m-\ell},f^{m-\ell})|+|\Gamma_{\mathrm{gain}}(f^{m-\ell},\partial_x f^{m-\ell})|\big]\mathrm{d}s && \text{(A.134)} \\
& +\int_0^t\sum_{\ell=0}^{\ell_*(0)}\mathbf{1}_{[t^{\ell+1},t^\ell)}(s)|\partial_{\mathbf{e}}v^\ell|\big[|\Gamma_{\mathrm{gain},v}(f^{m-\ell},f^{m-\ell})| \\
& \qquad +|\Gamma_{\mathrm{gain}}(f^{m-\ell},\partial_v f^{m-\ell})|+|\Gamma_{\mathrm{gain}}(\partial_v f^{m-\ell},f^{m-\ell})|\big]\mathrm{d}s\Big\}. && \text{(A.135)}
\end{aligned}
$$

Firstly, we consider $\partial_{\mathbf{e}}t^j-$contribution. Then from Lemma A.11 and *(2)* of Lemma A.5

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{\alpha(x,v)}{\langle v\rangle^2}\{(A.130)_{\mathbf{x}}+(A.133)_{\mathbf{x}}\} \\
\lesssim\; & e^{-\varpi\langle v\rangle t}\frac{\alpha(x,v)}{\langle v\rangle^2}e^{-\frac{\theta}{2}|v|^2}t\frac{t|v|^2}{\alpha(x,v)}\langle v\rangle||e^{\theta|v|^2}f||_\infty||e^{\theta|v|^2}\partial_t f||_\infty \\
& +e^{-\varpi\langle v\rangle t}\frac{\alpha(x,v)}{\langle v\rangle^2}(1+t)||e^{\theta|v|^2}f||_\infty t\frac{t|v|^2}{\alpha(x,v)}e^{-\frac{\theta}{2}|v|^2}||e^{\theta|v|^2}\partial_t f||_\infty \\
\lesssim_t\; & 1+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)+P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2}\{(A.130)_{\mathbf{v}}+(A.133)_{\mathbf{x}}\} \\
\lesssim_t\; & \frac{|v|}{\langle v\rangle^2}e^{-C_\theta|v|^2}\big[P(||e^{\theta|v|^2}\partial_t f_0||_\infty)+P(||e^{\theta|v|^2}f_0||_\infty)\big] \\
\lesssim_t\; & 1+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)+P(||e^{\theta|v|^2}f_0||_\infty).
\end{aligned}
$$

Secondly, we consider the terms $(A.131), (A.133)$, which include $|\partial_{\mathbf{e}} x^\ell| + t|\partial_{\mathbf{e}} v^\ell|$. We use *(2)* of Lemma A.5 and Lemma A.11, $|\partial_x x^\ell| + t|\partial_x v^\ell| \lesssim \frac{|v|}{\sqrt{\alpha(x,v)}}$, and (A.124)

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{\alpha(x,v)}{\langle v\rangle^2}\{(A.131)_{\mathbf{x}} + (A.133)_{\mathbf{x}}\} \\
&\lesssim_t \left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \\
&\quad \times \sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell}\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^2}\alpha(x,v)^{1/2}\frac{e^{-C_\theta|u-v^\ell|^2}}{|u-v^\ell|^{2-\kappa}}|\partial_x f^{m-\ell}(s, X_{\mathbf{cl}}(s), u)|\mathrm{d}u\mathrm{d}s, \\
&\lesssim_t \left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \max_{0\le\ell\le m}\sup_{0\le s\le t}\|e^{-\varpi\langle v\rangle s}\frac{\alpha}{\langle v\rangle^2}\partial_x f^{m-\ell}(s)\|_\infty \\
&\quad \times \int_0^t \sum_{\ell=0}^{\ell_*(0;t,x,v)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\int_{\mathbb{R}^3} e^{-\frac{\varpi}{2}\langle v\rangle(t-s)}\frac{\langle u\rangle^2}{\langle v\rangle^2}\frac{|v|\alpha(x,v)^{\frac12}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}\alpha(X_{\mathbf{cl}}(s),u)}e^{-C_\theta|v-u|^2}\mathrm{d}u\mathrm{d}s.
\end{aligned}
$$

We use $\frac{\langle u\rangle^2}{\langle v\rangle^2} \lesssim \langle v-u\rangle^2$ and (A.51) to have

$$
\begin{aligned}
&\lesssim_t \left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \max_{0\le\ell\le m}\sup_{0\le s\le t}\|e^{-\varpi\langle v\rangle s}\frac{\alpha}{\langle v\rangle^2}\partial_x f^{m-\ell}(s)\|_\infty \\
&\quad \times \frac{O(\delta)}{\langle v\rangle\alpha(x,v)^{1/2}}|v|\alpha(x,v)^{1/2} \\
&\lesssim O(\delta)\left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \max_{0\le\ell\le m}\sup_{0\le s\le t}\|e^{-\varpi\langle v\rangle s}\frac{\alpha}{\langle v\rangle^2}\partial_x f^{m-\ell}(s)\|_\infty.
\end{aligned}
$$

Similarly we further use $|\partial_v x^\ell| + t|\partial_v v^\ell| \lesssim \frac{1}{|v|}$ from Lemma A.11

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2}\{(A.131)_{\mathbf{v}} + (A.133)_{\mathbf{v}}\} \\
&\lesssim_t \left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \\
&\quad \times \sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell}\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle t}\frac{|v|}{\langle v\rangle^2}(\frac{1}{|v|}+1)\alpha(x,v)^{1/2}\frac{e^{-C_\theta|u-v^\ell|^2}}{|u-v^\ell|^{2-\kappa}}|\partial_x f^{m-\ell}(s, X_{\mathbf{cl}}(s), u)|\mathrm{d}u\mathrm{d}s, \\
&\lesssim_t \left[1 + P(\|e^{\theta|v|^2}\partial_t f_0\|_\infty) + P(\|e^{\theta|v|^2} f_0\|_\infty)\right] \max_{0\le\ell\le m}\sup_{0\le s\le t}\|e^{-\varpi\langle v\rangle t}\frac{|u|\alpha^{1/2}}{\langle u\rangle^2}\partial_x f^{m-\ell}(s, X_{\mathbf{cl}}(s), u)\|_\infty \\
&\quad \times \sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell}\int_{\mathbb{R}^3} e^{-\frac{\varpi}{2}\langle v\rangle(t-s)}\frac{|v|\langle u\rangle^2}{\langle v\rangle^2}\frac{(\frac{1}{|v|}+1)\alpha(x,v)^{1/2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}\alpha(x,u)}\mathrm{d}u\mathrm{d}s.
\end{aligned}
$$

From $\frac{\langle u\rangle^2}{\langle v\rangle^2} \lesssim \langle v-u\rangle^2$, the last integration is bounded by

$$
\sum_{\ell=0}^{\ell_*(0;t,x,v)} \int_{t^{\ell+1}}^{t^\ell}\int_{\mathbb{R}^3} e^{-\frac{\varpi}{2}\langle v\rangle(t-s)}\langle v-u\rangle^2\frac{\langle v\rangle\alpha(x,v)^{1/2}}{\alpha(x,u)}\frac{e^{-C|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}\mathrm{d}u\mathrm{d}s.
$$

By the dynamical non-local to local estimate (A.16), this is bounded by

$$
O(\delta)\left[1 + P(\|e^{\theta|v|^2}\partial_t f\|_\infty) + P(\|e^{\theta|v|^2} f\|_\infty)\right] \max_{0\le\ell\le m}\sup_{0\le s\le t}\|e^{-\varpi\langle v\rangle s}\frac{\alpha(x,v)}{\langle v\rangle^2}\partial_x f^{m-\ell}(s)\|_\infty.
$$

Thirdly, we consider $\partial_{\mathbf{e}} v^\ell-$contribution, $(A.132)$ and $(A.135)$. Note that $(A.132)_{\mathbf{x}} = 0 = (A.135)_{\mathbf{x}}$

since $\partial_x v^j \equiv 0$. From Lemma A.11 and *(3)* of Lemma A.5

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2}\{(A.132)_{\mathbf{v}}+(A.135)_{\mathbf{v}}\} \\
\lesssim & \left[1+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)+P(||e^{\theta|v|^2}f_0||_\infty)\right] \\
& \times \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s) e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2} e^{-C|v|^2}\int_{\mathbb{R}^3}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}|\partial_v f^{m-\ell}(s,X_{\mathbf{cl}}(s),u)|\mathrm{d}u\mathrm{d}s \\
\lesssim & \left[1+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)+P(||e^{\theta|v|^2}f_0||_\infty)\right] \\
& \times \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle t}e^{-\varpi\langle u\rangle s}e^{-C|v|^2}\frac{|v|\langle u\rangle^2\alpha(x,v)^{1/2}}{|u|\langle v\rangle^2\alpha(X_{\mathbf{cl}}(s),u)^{1/2}}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}\mathrm{d}u\mathrm{d}s \\
& \times \sup_{0\le s\le t}\max_{0\le\ell\le m}||e^{-\varpi\langle u\rangle s}\frac{|u|\alpha(x,u)^{1/2}}{\langle u\rangle^2}\partial_v f^{m-\ell}(s,x,u)||_\infty.
\end{aligned}
$$

Now we choose $\beta'\in(\frac12,1)$ and use $\alpha(x,u)\lesssim|u|^2$ to have

$$\frac{1}{[\alpha(X_{\mathbf{cl}}(s),u)]^{1/2}} \lesssim \frac{|u|^{2(\beta'-\frac12)}}{[\alpha(X_{\mathbf{cl}}(s),u)]^{\beta'}}.$$

Now we use (A.124) to bound the integration by

$$\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\int_{\mathbb{R}^3} e^{-\varpi\langle v\rangle(t-s)}\frac{|v|}{|u|}\frac{|u|^{2\beta'-1}\alpha(x,v)^{1/2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}\alpha(X_{\mathbf{cl}}(s),u)^{\beta'}}e^{-C|v|^2}e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}\mathrm{d}u\mathrm{d}s$$

Now we use $|u|^{2\beta'-1}\le\langle v\rangle^{2\beta'-1}\langle u-v\rangle^{2\beta'-1}$ and we apply (A.51) to bound this integration by

$$O(\delta)\langle v\rangle^{-2+2\beta'}\alpha(x,v)^{1-\beta'} \lesssim O(\delta),$$

Hence

$$
\begin{aligned}
& e^{-\varpi\langle v\rangle t}\frac{|v|\alpha(x,v)^{1/2}}{\langle v\rangle^2}\{(A.132)_{\mathbf{v}}+(A.135)_{\mathbf{v}}\} \\
\lesssim & \left[1+P(||e^{\theta|v|^2}f_0||_\infty)+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)\right]\sup_{0\le s\le t}\max_{0\le\ell\le m}||e^{-\varpi\langle v\rangle s}\frac{|u|\alpha(x,u)^{1/2}}{\langle u\rangle^2}\partial_v f^{m-\ell}(s,x,u)||_\infty \\
& \times\left\{\frac{O(\delta)}{\langle v\rangle[\alpha(x,v)]^{\beta'-1/2}}\alpha(x,v)^{1/2}e^{-C_\theta|v|^2}+O(\delta)\right\} \\
\lesssim & \left[1+P(||e^{\theta|v|^2}f_0||_\infty)+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)\right] \\
& +O(\delta)\left[P(||e^{\theta|v|^2}f_0||_\infty)+P(||e^{\theta|v|^2}\partial_t f_0||_\infty)\right]\sup_{0\le s\le t}\max_{0\le\ell\le m}||e^{-\varpi\langle v\rangle s}\frac{|u|\alpha(x,u)^{1/2}}{\langle u\rangle^2}\partial_v f^{m-\ell}(s,x,u)||_\infty.
\end{aligned}
$$

Now we gather all the estimates with small $0<\delta\ll1$ to close the estimate. Then we follow the exactly same argument as the specular case and this complete the proof of Theorem A.4.

$\square$

A.7 Appendix. Non-Existence of Second Derivatives

In the previous theorem, we consider the *first-order derivative* of the Boltzmann solution with several boundary conditions. Now we show that some second order spatial derivative does not exist up to the boundary in general so that our result is quite optimal.

Assume that all the second order spatial derivatives exist away from the grazing set $\gamma_0=\{(x,v)\in\partial\Omega\times\mathbb{R}^3 : n(x)\cdot v=0\}$ but up to some boundary $\partial\Omega\times\mathbb{R}^3$. Taking the normal derivative $\partial_n=n(x)\cdot\nabla_x=\frac{\nabla_x\xi(x)}{|\nabla_x\xi(x)|}\cdot\nabla_x$ to the Boltzmann equation directly yields

$$v\cdot\partial_n\nabla_x f=-\partial_n\partial_t f-\nu(\sqrt{\mu}f)\partial_n f+\underbrace{\partial_n\Gamma_{\mathrm{gain}}(f,f)-\partial_n\nu(\sqrt{\mu}f)f}.$$

From previous Theorem we know that $\partial_n \partial_t f,\ \nu(\sqrt{\mu} f)\partial_n f \sim \frac{1}{\alpha^a}$ with some $a > 0$. In this section we show that the underbraced term blows up at the boundary with any velocity for symmetric domains.

Assume $f_0 \sim (\sqrt{\mu})^{1-\delta}$ for some $0 < \delta \ll 1$. Then there exists $\mathbf{k}_{f_0}(v,u)$ such that

$$\Gamma_{\text{gain}}(f, f_0) + \Gamma_{\text{gain}}(f_0, f) - \nu(\sqrt{\mu} f) f_0 := \int_{\mathbb{R}^3} \mathbf{k}_{f_0}(v,u) f(u) \mathrm{d}u.$$

First consider the diffuse reflection boundary condition. Theorem 2 plays an important role in our proof.

Proposition A.3 (Diffuse BC)**.** *Assume $\Omega = \{x \in \mathbb{R}^3 : |x| < 1\}$ and $\xi(x) = |x|^2 - 1$. Assume the initial datum f_0 satisfies, for some $x_0 \in \partial\Omega$,*

$$\Big[\int_{n(x_0)\cdot u_\tau = 0} \mathbf{k}_{f_0}(v,u) u \cdot n(x_0) \partial_n f_0(x_0, u) \mathrm{d}u_\tau \Big]_{u \cdot n(x_0) = 0} > C > 0. \tag{A.134}$$

Then there exist $t > 0$ such that for all $v \in \mathbb{R}^3$,

$$\partial_n \Gamma_{\text{gain}}(f,f)(t, x_0, v) - \partial_n \nu(\sqrt{\mu} f) f(t, x_0, v) = \infty. \tag{A.135}$$

We remark that for $0 < \theta < \frac{1}{4}$ we have $\sup_t ||e^{\theta|v|^2} f(t)||_\infty \lesssim ||e^{\theta|v|^2} f_0||_\infty$ due to Lemma A.6 or [75, 67] and $||\alpha^{1/2} \partial f(t)||_\infty \lesssim 1$ due to Theorem 2. We also remark that the condition (A.134) is very natural for the diffuse BC.

Proof. We denote the different quotient

$$\triangle_\varepsilon f(t,x,v) := \frac{f(t, x + \varepsilon[-n(x)], v) - f(t,x,v)}{\varepsilon}.$$

Then

$$\triangle_\varepsilon \{\Gamma_{\text{gain}}(f,f)\} - \nu(\sqrt{\mu} \triangle_\varepsilon f) f = \Gamma_{\text{gain}}(\triangle_\varepsilon f, f) + \Gamma_{\text{gain}}(f, \triangle_\varepsilon f) - \nu(\sqrt{\mu} \triangle_\varepsilon f) f.$$

Assuming $f \sim f_0 \sim (\sqrt{\mu})^{1-\delta}$ for $0 < \delta \ll 1$, we have

$$\begin{aligned} &\Gamma_{\text{gain}}(\triangle_\varepsilon f, f) + \Gamma_{\text{gain}}(f, \triangle_\varepsilon f) - \nu(\sqrt{\mu} \triangle_\varepsilon f) f \\ &\sim \int_{\mathbb{R}^3} \mathbf{k}_{f_0}(v,u) \triangle_\varepsilon f(x,u) \mathrm{d}u \sim \int_{\mathbb{R}^3} \mathbf{k}_{f_0}(v,u) \frac{f(x - \varepsilon n(x), u) - f(x,u)}{\varepsilon} \mathrm{d}u, \end{aligned} \tag{A.136}$$

where $\mathbf{k}_{f_0}(v,u) \sim \mathbf{k}(v,u)$ in (A.24) with slightly different exponents. For simplicity let us assume $\mathbf{k}_{f_0}(v,u)$ is bounded. We split as

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathbf{k}_{f_0}(v,u) \frac{f(t, x - \varepsilon n(x), u) - f(t,x,u)}{\varepsilon} \mathrm{d}u \\ &= \underbrace{\int_{|n(x)\cdot u| \le \varepsilon}}_{\mathbf{I}} + \underbrace{\int_{\varepsilon \le |n(x)\cdot u| \le \sigma}}_{\mathbf{II}} + \underbrace{\int_{\sigma \le |n(x)\cdot u|}}_{\mathbf{III}}. \end{aligned} \tag{A.137}$$

The first term is bounded as $\mathbf{I} \lesssim O(1)||e^{\theta|v|^2} f||_\infty$. The last term is bounded due to Theorem A.1. Since $\xi(x) = |x|^2 - 1$, for all $0 < r < \varepsilon \ll 1$,

$$\begin{aligned} \nabla\xi(x - rn(x)) \cdot u &= \nabla\xi(x) \cdot u - \int_0^r \big\{ \nabla\xi(x) \cdot \nabla^2 \xi(x - r' n(x)) \cdot u \big\} \mathrm{d}r' \\ &= \nabla\xi(x) \cdot u - 2 \int_0^r \nabla\xi(x) \cdot u \mathrm{d}r' \\ &= \nabla\xi(x) \cdot u + O(\varepsilon) |\nabla\xi(x) \cdot u| \\ &\sim \nabla\xi(x) \cdot u. \end{aligned} \tag{A.138}$$

Therefore $\sigma \le |n(x) \cdot u|$ implies $\sigma \lesssim \sqrt{\alpha(x,u)}$ and

$$\begin{aligned} \mathbf{III} &\lesssim ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \int_{\sigma \lesssim \sqrt{\alpha}} \frac{e^{\varpi\langle u\rangle t}}{\sqrt{\alpha}} \mathbf{k}_{f_0}(v,u) \mathrm{d}u \\ &= \int_{\sigma \le \sqrt{\alpha}, |u| \le N} + \int_{\sigma \le \sqrt{\alpha}, |u| \ge N} \lesssim \frac{O(1) + e^{CNt}}{\sigma}. \end{aligned}$$

For the second term of (A.137) we use (A.138) to conclude, for $0 \le r \le \varepsilon$,

$$\varepsilon \lesssim |n(x - rn(x)) \cdot u| \lesssim \sigma.$$

Therefore $f(t, x - \varepsilon n(x), u)$ is differentiable so that

$$\frac{f(t, x - \varepsilon n(x), u) - f(t, x, u)}{\varepsilon} = \int_0^1 \partial_n f(t, x - \varepsilon rn(x), u) \mathrm{d}r. \tag{A.139}$$

We further split $\mathbf{II}$ as

$$\mathbf{II} = \underbrace{\int_{\substack{\varepsilon \le |n(x)\cdot u| \le \sigma \\ \frac{1}{N} \le |u| \le N}}}_{\mathbf{II}_a} + \underbrace{\int_{\substack{\varepsilon \le |n(x)\cdot u| \le \sigma \\ |u| \le \frac{1}{N}, |u| \ge N}}}_{\mathbf{II}_b}.$$

For the second term we use Theorem A.1 to have

$$\begin{aligned}
\mathbf{II}_b &\lesssim e^{-N} \int_0^1 \mathrm{d}r \int_{\varepsilon \lesssim |u_n| \lesssim \sigma} \mathrm{d}u_n \int_{|u_\tau| \gtrsim N} \mathrm{d}u_\tau \ \mathbf{k}_{f_0}(v, u) \partial_n f(t, x - \varepsilon rn(x), u) \\
&\lesssim e^{-N} \int_0^1 \mathrm{d}r \int_{\varepsilon \lesssim |u_n| \lesssim \sigma} \mathrm{d}u_n \int_{|u_\tau| \gtrsim N} \mathrm{d}u_\tau \ \frac{\mathbf{k}_{f_0}(v, u)}{\sqrt{|u_n|^2 + Cr\varepsilon N^2}},
\end{aligned} \tag{A.140}$$

where we used

$$\xi(x - \varepsilon rn(x)) = \xi(x) + C\varepsilon r = C\varepsilon r.$$

The main term is $\mathbf{II}_a$:

$$\mathbf{II}_a = \int_0^1 \mathrm{d}r \iint_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \le |u| \le N}} \mathrm{d}u_\tau \mathrm{d}u_n \ \mathbf{k}_{f_0}(v, u) \partial_n f(t, x - \varepsilon rn(x), u).$$

From (A.47), for $\varepsilon \lesssim |u_n| \lesssim \sigma$ and $\frac{1}{N} \le |u| \le N$,

$$t_{\mathbf{b}}(x - \varepsilon rn(x), u) \lesssim \frac{\sqrt{\alpha(x - \varepsilon rn(x), u)}}{|u|^2} \lesssim \frac{\sqrt{\sigma^2 + \varepsilon r N^2}}{\frac{1}{N^2}} \lesssim N^2 \sqrt{\sigma^2 + \varepsilon N^2}.$$

Let $x(r) = x - \varepsilon rn(x)$. For $\varepsilon \lesssim |u_n| \lesssim \sigma$ and $\frac{1}{N} \le |u| \le N$ and $t \gtrsim N^2 \sqrt{\sigma^2 + \varepsilon N^2}$,

$$\begin{aligned}
&\partial_n f(t, x(r), u) \\
&= n(x(r)) \cdot \nabla_x \Big\{ f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) + \int_0^{t_{\mathbf{b}}} [\Gamma_{\text{gain}}(f, f) - \nu(F) f](t - s, x(r) - su, u) \mathrm{d}s \Big\} \\
&= \sum_{i=1}^{2} n(x(r)) \cdot \tau_i(x_{\mathbf{b}}) \partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) + \frac{n(x(r)) \cdot n(x_{\mathbf{b}})}{n(x_{\mathbf{b}}) \cdot u} \underline{u \cdot n(x_{\mathbf{b}}) \partial_n f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)} \\
&\quad + \int_0^{t_{\mathbf{b}}} n(x(r)) \cdot \{\Gamma_{\text{gain}}(\nabla_x f, f) + \Gamma_{\text{gain}}(f, \nabla_x f) - \nu(\sqrt{\mu} \nabla_x f) f - \nu(\sqrt{\mu} f) \nabla_x f\}(t - s, x(r) - su, u) \mathrm{d}s.
\end{aligned}$$

Now we expand in time for the underlined term and choose $0 < t \ll 1$ ($N^2 \sqrt{\sigma^2 + \varepsilon N^2} \ll 1$) so that

$$\begin{aligned}
&u \cdot n(x_{\mathbf{b}}) \partial_n f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u) \\
&\quad = u \cdot n(x_{\mathbf{b}}) \partial_n f_0(x_{\mathbf{b}}, u) + \int_0^{t - t_{\mathbf{b}}} \{u \cdot n(x_{\mathbf{b}})\} \partial_t \partial_n f(s, x_{\mathbf{b}}, u) \mathrm{d}s \\
&\quad = u \cdot n(x_{\mathbf{b}}) \partial_n f_0(x_{\mathbf{b}}, u) + O(1) t e^{\varpi N t} ||e^{-\varpi \langle v \rangle t} \sqrt{\alpha} \partial_t \partial_n f(t)||_\infty.
\end{aligned}$$

The tangential derivative term is bounded by

$$\begin{aligned}
&|n(x(r)) \cdot \tau_i(x_{\mathbf{b}}(x(r), u))| |\partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim |n(x_{\mathbf{b}}) \cdot \tau_i(x_{\mathbf{b}}) + O(t_{\mathbf{b}}(x(r), u)) u \cdot \nabla_x n(x(r))| |\partial_{\tau_i} f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim \frac{\sqrt{\alpha(x_{\mathbf{b}}, u)}}{|u|} |\nabla_x f(t - t_{\mathbf{b}}, x_{\mathbf{b}}, u)| \\
&\lesssim N e^{\varpi N t} ||e^{-\varpi \langle v \rangle t} \sqrt{\alpha} \nabla_x f(t, x, v)||_\infty,
\end{aligned}$$

and the time integration terms are bounded by

$$
\begin{aligned}
&||e^{\theta|v|^2} f||_\infty \int_0^{t_{\mathbf{b}}} \int_{\mathbb{R}^3} \frac{e^{-C|u-u'|^2}}{|u-u'|^{2-\kappa}} |\partial_x f(t-s, x(r)-su, u')| \mathrm{d}u' \mathrm{d}s \\
&+ N e^{\varpi N t} ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi \langle v \rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \\
&\lesssim ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \times e^{\varpi N t} \Big\{ \int_0^{t_{\mathbf{b}}} \int_{\mathbb{R}^3} e^{-\varpi \langle u \rangle (t-s)} \frac{e^{-C|u-u'|^2}}{|u-u'|^{2-\kappa}} \frac{|u'|^\delta}{\alpha(x(r)-su, u')^{\frac{1+\delta}{2}}} \mathrm{d}u' \mathrm{d}s \Big\} \\
&\lesssim ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \frac{e^{\varpi N t} C_N}{[\alpha(x(r), u)]^{\delta/2}}.
\end{aligned}
$$

Now we plug these estimates into $\mathbf{II}_a$ to have

$$
\begin{aligned}
\mathbf{II}_a + \mathbf{II}_b \gtrsim & \int_0^1 \int_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{\alpha(x_0 - \varepsilon r n(x_0), u)}} \Big[\int_{\cdot n(x_0) \cdot u_\tau = 0} \mathbf{k}_{f_0}(v,u) u \cdot n(x_0) \partial_n f_0(x_0, u) \mathrm{d}u_\tau \Big]_{u \cdot n(x_0) = 0} \\
& - \Big\{ O(t) e^{-\varpi N t} ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \partial_t \partial_n f(t)||_\infty + e^{-N} \Big\} \int_0^1 \iint_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{\alpha(x_0 - \varepsilon r n(x_0), u)}} \\
& - O(1) N e^{\varpi N t} ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \\
& - O_N(1) e^{\varpi N t} ||e^{\theta|v|^2} f_0||_\infty ||e^{-\varpi\langle v\rangle t} \sqrt{\alpha} \nabla_x f(t)||_\infty \int_0^1 \iint_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{[\alpha(x_0 - \varepsilon r n(x_0), u)]^{\delta/2}}.
\end{aligned}
$$

Due to (A.134), for $N \gg 1$ and $t \ll 1$ with $N^2 \sqrt{\sigma^2 + \varepsilon N^2} \ll 1$

$$
\begin{aligned}
\mathbf{II} &\gtrsim \int_0^1 \int_{\substack{\varepsilon \lesssim |u_n| \lesssim \sigma \\ \frac{1}{N} \lesssim |u| \lesssim N}} \frac{1}{\sqrt{|u_n|^2 + C\varepsilon r |u_\tau|^2}} \mathrm{d}u_n \mathrm{d}u_\tau \mathrm{d}r \\
&\gtrsim \int_{\varepsilon \leq |u_n| \leq \sigma} \frac{N^2}{|u_n| + \sqrt{\varepsilon} N} \mathrm{d}u_\tau \mathrm{d}u_n \\
&\gtrsim N^2 \ln \frac{1}{\varepsilon + \sqrt{\varepsilon} N} - O_{N,\sigma}(1) \\
&\gtrsim \frac{N^2}{2} \ln \frac{1}{\varepsilon} - o(1) \ln \frac{1}{\varepsilon} - O_{N,\sigma}(1) \to \infty.
\end{aligned}
$$

□

For the bounce-back case, we identify the condition for non-existence of $\nabla^2 f$ up to the boundary :

Proposition A.4 (Bounce-Back BC)**.** *Assume $\Omega = \{x \in \mathbb{R}^3 : |x| < 1\}$ and $\xi(x) = |x|^2 - 1$. Assume the initial datum f_0 satisfies, for some $x_0 \in \partial\Omega$ and some $v_0 \in \mathbb{R}^3$ with $|v_0| \sim 1$ with $n(x_0) \cdot v_0 = 0$,*

$$
\int_{n(x_0) \cdot u_\tau = 0} \mathbf{k}_{f_0}(v,u) v_0 \cdot \nabla_x f_0(x_0, v_0) \mathrm{d}u_\tau > C > 0, \tag{A.141}
$$

where $u_\tau = u - [u \cdot n(x_0)] n(x_0)$. Then there exists $t > 0$ we have (A.135).

We remark that $v_0 \cdot \nabla_x f_0(x_0, v_0)$ is rather arbitrary for $v_0 \cdot n(x_0) = 0$.

Proof. We choose $(x, v) \in \bar{\Omega} \times \mathbb{R}^3$ so that $x^\ell \sim x_0$ and $v^\ell \sim \pm v_0$ for all $\ell \in \mathbb{N}$. Then

$$
\begin{aligned}
& \int_{\mathbb{R}^3} \mathbf{k}_{f_0}(v,u) \frac{f(t, x - \varepsilon n(x), u) - f(t,x,u)}{\varepsilon} \mathrm{d}u \\
= & \int_{|n(x) \cdot u| \leq \varepsilon} + \int_{\varepsilon \leq |n(x) \cdot u|}.
\end{aligned}
$$

The first terms is bounded. Due to (A.138) we have $|n(x)\cdot u|\geq\varepsilon$ implies $|n(x-rn(x))\cdot u|\gtrsim\varepsilon$ for all $0\leq r\leq\varepsilon$. Then by Theorem A.4, the function f is differentiable and the second term equals

$$\begin{aligned}
&\int_{|n(x)\cdot u|\geq\varepsilon}\mathbf{k}_{f_0}(v,u)\frac{f(t,x-\varepsilon n(x),u)-f(t,x,u)}{\varepsilon}\mathrm{d}u\\
=&\int_0^1\int_{|n(x)\cdot u|\geq\varepsilon}\mathbf{k}_{f_0}(v,u)\partial_n f(t,x-\varepsilon rn(x),u)\mathrm{d}u\mathrm{d}r\\
=&\int_0^1\int_{\varepsilon\leq|n(x)\cdot u|\leq 1,|\tau(x)\cdot u|\leq N}+\int_0^1\int_{\varepsilon\leq|n(x)\cdot u|\leq 1,|\tau(x)\cdot u|\geq N}+\int_0^1\int_{|n(x)\cdot u|\geq 1}.
\end{aligned}\tag{A.142}$$

For the third term of (A.142) we use Theorem A.4 to have

$$|\partial_n f(t,x-\varepsilon rn(x),u)|\lesssim\frac{\langle u\rangle^2 e^{\varpi\langle u\rangle t}}{\alpha(x-\varepsilon rn(x),u)}\lesssim\langle u\rangle^2e^{\varpi\langle u\rangle t},$$

and therefore the third term of (A.142) is bounded. For the second term of (A.142) we use Theorem A.4 to bound

$$\begin{aligned}
&||e^{-\varpi\langle v\rangle t}\frac{\alpha}{\langle v\rangle^2}\nabla_x f(t)||_\infty\times\int_0^1\mathrm{d}r\int_\varepsilon^1\mathrm{d}u_n\frac{e^{\varpi\delta}N^2}{|u_n|^2+Cr\varepsilon N^2}\int_{\mathbb{R}^2}\mathrm{d}u_\tau\mathbf{k}_{f_0}(v,u)\\
&\lesssim e^{-N}\times\int_0^1\mathrm{d}r\int_\varepsilon^1\mathrm{d}u_n\frac{1}{|u_n|^2+Cr\varepsilon N^2}.
\end{aligned}\tag{A.143}$$

Now we focus on the first and the second terms of (A.142). Set $y=x-\varepsilon rn(x)$ for $|\partial_n f(t,x-\varepsilon' n(x),u)|$. We use (A.129), Theorem A.4, and Lemma A.11, we have

$$\begin{aligned}
&\partial_n f(t,y,u)\\
&=e^{-\int_0^t\nu(\sqrt{\mu}f)(\tau)\mathrm{d}\tau}\Big\{[\partial_n x^{\ell_*(0)}-\partial_n t^{\ell_*(0)}v^{\ell_*(0)}]\cdot\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))+v^{\ell_*(0)}\cdot\nabla_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))\Big\}\\
&+O(||e^{\theta|v|^2}f_0||_\infty)\frac{t^2|u|^2}{\alpha(y,u)}e^{-\frac{\theta}{4}|u|^2}||e^{\theta|v|^2}\partial_t f_0||_\infty+O(||e^{\theta|v|^2}f_0||_\infty)\frac{t(1+t)|u|^2}{\alpha(y,u)}e^{-\frac{\theta}{4}|u|^2}\\
&+O(||e^{\theta|v|^2}f_0||_\infty)\sup_{0\leq s\leq t}||e^{-\varpi\langle v\rangle t}\alpha\partial_x f(t)||_\infty\\
&\quad\times\int_0^t\int_{\mathbb{R}^3}\sum_\ell\mathbf{1}_{[t^{\ell+1},t^\ell)}(s)\frac{e^{-\frac{\theta}{8}|v^\ell-u'|^2}}{|v^\ell-u'|^{2-\kappa}}\frac{|\partial_n x^\ell|}{e^{-\varpi\langle u'\rangle s}\alpha(X_{\mathbf{cl}}(s),u')}\mathrm{d}u'\mathrm{d}s.
\end{aligned}$$

Using Lemma A.16, Lemma A.11, and (A.124), for $0<\varepsilon\ll 1$ we bound the last integration by

$$\begin{aligned}
&e^{\varpi\langle u\rangle t}\frac{|u|}{\sqrt{\alpha(y,u)}}\int_0^t\int_{\mathbb{R}^3}e^{-\varpi\langle u\rangle(t-s)}\frac{e^{-\frac{\theta}{8}|V_{\mathbf{cl}}(s)-u'|^2}}{|V_{\mathbf{cl}}(s)-u'|^{2-\kappa}}\frac{1}{\alpha(X_{\mathbf{cl}}(s),u')}\mathrm{d}u'\mathrm{d}s\\
&\lesssim O(\varepsilon)e^{\varpi\langle u\rangle t}\frac{|u|}{\langle u\rangle}\frac{1}{\alpha(y,u)}.
\end{aligned}$$

Now by the explicit computations in Lemma A.11

$$\begin{aligned}
&e^{-\int_0^t\nu(\sqrt{\mu}f)(\tau)\mathrm{d}\tau}\Big\{[\partial_n x^{\ell_*(0)}-\partial_n t^{\ell_*(0)}v^{\ell_*(0)}]\cdot\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))+v^{\ell_*(0)}\cdot\nabla_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))\Big\}\\
&\geq e^{-t\langle u\rangle||e^{\theta|v|^2}f_0||_\infty}\underbrace{\Big\{\ell_*(0)\frac{n(y)\cdot\nabla\xi(x^1)}{v\cdot\nabla\xi(x^1)}+(\ell_*(0)-1)\frac{n(y)\cdot\nabla\xi(x^2)}{-v\cdot\nabla\xi(x^2)}\Big\}}V_{\mathbf{cl}}(0)\cdot\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))\\
&\quad-C_\xi\frac{|u|}{\sqrt{\alpha(y,u)}}|\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|-C_\xi|u||\nabla_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|\\
&\geq e^{-t\langle u\rangle||e^{\theta|v|^2}f_0||_\infty}O_\xi(1)\frac{t|u|^2}{\alpha(y,u)}V_{\mathbf{cl}}(0)\cdot\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))\\
&\quad-\frac{O_\xi(1+t|u|)}{\sqrt{\alpha(y,u)}}|u||\nabla_x f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|-C_\xi|u||\nabla_v f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))|,
\end{aligned}$$

where for the underbraced term we used

$$
\begin{aligned}
& n(y) \cdot \left\{ \frac{n(x_{\mathbf{b}})}{n(x_{\mathbf{b}}) \cdot v} - \frac{n(y)}{n(y) \cdot v} \right\} \\
= \; & \frac{n(y) \cdot \nabla\xi(y - t_{\mathbf{b}} v)\big(\nabla\xi(y) \cdot v\big) - n(y) \cdot \nabla\xi(y)\big(\nabla\xi(y - t_{\mathbf{b}} v) \cdot v\big)}{\big(\nabla\xi(y) \cdot v\big)\big(\nabla\xi(y - t_{\mathbf{b}} v) \cdot v\big)} \\
= \; & \frac{t_{\mathbf{b}}\big\{\big(n(y) \cdot [v \cdot \nabla]\nabla\xi(y - \tilde{\tau} v)\big)\big(\nabla\xi(y) \cdot v\big) - n(y) \cdot \nabla\xi(y)\big(v \cdot \nabla^2\xi(y - \tilde{\tau} v) \cdot v\big)\big\}}{\big(\nabla\xi(y) \cdot v\big)\big(- \nabla\xi(y - t_{\mathbf{b}} v) \cdot v\big)} \\
= \; & - \frac{t_{\mathbf{b}}}{(-\nabla\xi(x_{\mathbf{b}}) \cdot v)} \frac{\big(v \cdot \nabla^2\xi(y - \tilde{\tau} v) \cdot v\big)}{n(y) \cdot v} + \frac{t_{\mathbf{b}}}{(-\nabla\xi(x_{\mathbf{b}}) \cdot v)}\big(n(y) \cdot [v \cdot \nabla]\nabla\xi(y - \tilde{\tau} v)\big) \\
:= \; & - \frac{A(y, v)}{n(y) \cdot v} + B(y, v),
\end{aligned}
\tag{A.144}
$$

where for some $\tilde{\tau} \in [0, t_{\mathbf{b}}]$, and from (A.46), (A.47), and the Velocity lemma (Lemma A.1) we have $A \geq 0$ and

$$
A(y, v) \geq C_\xi \frac{v}{|v|} \cdot \nabla^2\xi(y - \tilde{\tau} v) \cdot \frac{v}{|v|} \gtrsim_\Omega 1, \quad B(y, v) \sim_\Omega \frac{1}{|v|},
$$

and therefore finally the underbraced term has the following explicit lower bound :

$$
\begin{aligned}
& \ell_*(0)\Big[\frac{n(y) \cdot \nabla\xi(x^1)}{v \cdot \nabla\xi(x^1)} - \frac{n(y) \cdot \nabla\xi(x^2)}{v \cdot \nabla\xi(x^2)}\Big] + \frac{n(y) \cdot \nabla\xi(x^2)}{v \cdot \nabla\xi(x^2)} \\
& = \ell_*(0)\frac{A(y, v)}{n(x^1) \cdot v} + \ell_*(0)B(y, v) + O\Big(\frac{1}{n(x^1) \cdot v}\Big) \\
& = O_\xi(1)\frac{t|v|^2}{\alpha(y, v)} + \frac{O_\xi(1 + t|v|)}{\sqrt{\alpha(y, v)}}.
\end{aligned}
$$

Therefore

$$
\begin{aligned}
\partial_n f(t, y, u) \geq \; & e^{-t\langle u\rangle||e^{\theta|v|^2} f_0||_\infty} O_\xi(1)\frac{t|u|^2}{\alpha(y, u)} V_{\mathbf{cl}}(0) \cdot \nabla_x f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \\
& - \frac{O_\xi(1 + t|u|)}{\sqrt{\alpha(y, u)}}|u||\nabla_x f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0))| - C_\xi|u||\nabla_v f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0))| \\
& - O(||e^{\theta|v|^2} f_0||_\infty)\frac{t^2|u|^2}{\alpha(y, u)} e^{-\frac{\theta}{4}|u|^2}||e^{\theta|v|^2}\partial_t f_0||_\infty \\
& - O(||e^{\theta|v|^2} f_0||_\infty)\frac{t(1 + t)|u|^2}{\alpha(y, u)} e^{-\frac{\theta}{4}|v|^2} \\
& - O(||e^{\theta|v|^2} f_0||_\infty) \sup_{0 \leq s \leq t} ||e^{-\varpi\langle v\rangle t}\alpha\partial_x f(t)||_\infty \times O(\varepsilon)e^{\varpi\langle u\rangle t}\frac{|u|}{\langle u\rangle}\frac{1}{\alpha(y, u)}.
\end{aligned}
\tag{A.145}
$$

Choose $y = x - \varepsilon r n(x)$. First consider the first contribution of (A.145). It has following lower bound as

$$
\begin{aligned}
& \int_0^1 \int_{\varepsilon \leq |n(x) \cdot u| \leq 1} \int_{|\tau(y) \cdot u| \leq N} \\
\gtrsim \; & \int_0^1 \mathrm{d}r \int_{\varepsilon \leq |u_n| \leq 1} \mathrm{d}u_n \int_{|u_\tau| \leq N} \mathrm{d}u_\tau \frac{1}{|u_n|^2 + Cr\varepsilon N^2} \mathbf{k}_{f_0}(v, u) V_{\mathbf{cl}}(0) \cdot \nabla_x f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \\
\sim \; & \int_0^1 \mathrm{d}r \int_{\varepsilon \leq |u_n| \leq 1} \frac{\mathrm{d}u_n}{|u_n|^2 + Cr\varepsilon N^2} \int_{|u_\tau| \leq N} \mathrm{d}u_\tau \mathbf{k}_{f_0}(v, u) v_0 \cdot \nabla_x f_0(x_0, v_0).
\end{aligned}
\tag{A.146}
$$

Now we use the condition (A.141) for $\varepsilon \sim 0$ and $u_n \sim 0$

$$
\begin{aligned}
& \int_{|u_\tau| \geq N} \mathbf{k}_{f_0}(v, u) V_{\mathbf{cl}}(0) \cdot \nabla_x f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \mathrm{d}u_\tau \\
& \sim \int_{n(x_0) \cdot u_\tau = 0} \mathbf{k}_{f_0}(v_0, u) v_0 \cdot \nabla_x f_0(x_0, v_0) \mathrm{d}u_\tau = C \neq 0.
\end{aligned}
$$

We combine this term with the second term of (A.142) to conclude

$$\begin{aligned}(A.146)-(A.143) &\gtrsim \{C-e^{-N}\}\int_{\varepsilon}^{1}\mathrm{d}u_n\int_0^1 \frac{\mathrm{d}r}{|u_n|^2+Cr\varepsilon N^2}\\ &\gtrsim \int_\varepsilon^1 \frac{1}{C\varepsilon N^2}\ln\Big(1+\frac{C\varepsilon N^2}{|u_n|^2}\Big)\mathrm{d}u_n \gtrsim \frac{1}{N^2}\frac{1}{\varepsilon}.\end{aligned}\tag{A.147}$$

Now the all the other terms of (A.145) except the first term are bounded by

$$\begin{aligned}&\int_\varepsilon^1 \mathrm{d}u_n\frac{1}{|u_n|}+O(||e^{\theta|v|^2}f_0||_\infty)\int_\varepsilon^1\mathrm{d}u_n\frac{1}{|u_n|^2}\\ &\lesssim |\ln\varepsilon|+O(||e^{\theta|v|^2}f_0||_\infty)\frac{1}{\varepsilon}.\end{aligned}$$

Finally we choose large $N>0$ and small $\delta>0$ and small $||e^{\theta|v|^2}f_0||_\infty$ to conclude for small $\varepsilon>0$

$$(A.142)\gtrsim\frac{1}{\varepsilon}.$$

Therefore we conclude (A.135). □

In order to show the non-existence of $\nabla^2 f$ up to the boundary for the specular reflection BC (Proposition A.5) we first obtain the explicit lower bound of (A.20) with a a lower dimensional symmetric domain, 2D disk.

Example A.1. *Let $\Omega=\{\bar{x}=(x_1,x_2)\in\mathbb{R}^2:|x_1|^2+|x_2|^2<1\}$. Define*

$$\begin{aligned}&r:=\sqrt{x_1^2+x_2^2}\in[0,1],\quad \theta\in[0,2\pi)\ \ \textit{such that}\ \ (\cos\theta,\sin\theta)=\frac{1}{\sqrt{x_1^2+x_2^2}}(x_1,x_2),\\ &\bar{v}_n:=v_1\cos\theta+v_2\sin\theta,\quad \bar{v}_\theta:=-v_1\sin\theta+v_2\cos\theta.\end{aligned}$$

We claim that as $\alpha\to 0$ (therefore $r\sim 1,\bar{v}_n\sim 0$) asymptotically

$$\begin{aligned}|\partial_n\bar{X}_{\mathbf{cl}}(s;t,x,v)\cdot\bar{n}^\perp(\bar{X}_{\mathbf{cl}}(s;t,x,v))| &\sim \frac{|t-s||\bar{v}_\theta|^2}{\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}\sim\frac{|t-s||\bar{v}|^2}{\sqrt{\alpha(x,v)}},\\ |\partial_n\bar{V}_{\mathbf{cl}}(s;t,x,v)\cdot\bar{n}(\bar{X}_{\mathbf{cl}}(s;t,x,v))| &\sim \frac{|t-s||\bar{v}|^4}{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}\sim\frac{|t-s||\bar{v}|^4}{\alpha(x,v)},\end{aligned}\tag{A.148}$$

where $\bar{n}^\perp=\begin{bmatrix}0&-1\\1&0\end{bmatrix}\bar{n}.$

Proof. Explicitly $x=(r\cos\theta,r\sin\theta,x_3)$, and $v=(\bar{v}_n\cos\theta-\bar{v}_\theta\sin\theta,\bar{v}_n\sin\theta+\bar{v}_\theta\cos\theta,v_3)$, and

$$\begin{aligned}x^\ell&=(\cos\theta^\ell,\sin\theta^\ell,x_3-(t-t^\ell)v_3),\\ v^\ell&=(\sqrt{\bar{v}_n^2+\bar{v}_\theta^2}\cos\psi^\ell,\sqrt{\bar{v}_n^2+\bar{v}_\theta^2}\sin\psi^\ell,v_3),\\ t^1&=t-\frac{r|\bar{v}_n|+\sqrt{(1-r^2)\bar{v}_\theta^2+\bar{v}_n^2}}{\bar{v}_n^2+\bar{v}_\theta^2},\\ t^\ell&=t-\frac{r|\bar{v}_n|+(2\ell-1)\sqrt{(1-r^2)\bar{v}_\theta^2+\bar{v}_n^2}}{\bar{v}_n^2+\bar{v}_\theta^2},\end{aligned}$$

and

$$\ell_*(s;t,x,v)\le\frac{(t-s)|\bar{v}|^2}{2\sqrt{(1-r^2)\bar{v}_\theta^2+\bar{v}_n^2}}-\frac{r|\bar{v}_n|}{2\sqrt{(1-r^2)\bar{v}_\theta^2+\bar{v}_n^2}}+\frac{1}{2}<\ell_*(s;t,x,v)+1,$$

where, for $\ell\ge 1$

$$\begin{aligned}&\theta^0=\theta,\quad \theta^\ell=\theta-\cos^{-1}\Big(\frac{\bar{v}_\theta}{\sqrt{\bar{v}_\theta^2+\bar{v}_n^2}}\Big)-(2\ell-1)\cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2+\bar{v}_\theta^2}}\Big),\\ &\psi^0=\cos^{-1}\Big(\frac{\bar{v}_n\cos\theta-\bar{v}_\theta\sin\theta}{\sqrt{\bar{v}_n^2+\bar{v}_\theta^2}}\Big),\quad \psi^\ell=\psi^0-2\ell\cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2+\bar{v}_\theta^2}}\Big).\end{aligned}$$

Therefore, if $t^{\ell+1} < s < t^{\ell}$,

$$X_{\mathbf{cl}}(s) = x^{\ell} - (t^{\ell} - s)v^{\ell}, \quad V_{\mathbf{cl}}(s) = v^{\ell},$$

and

$$\begin{aligned}
r(s) &= |\bar{X}_{\mathbf{cl}}(s)| = |\bar{x}^{\ell} - (t^{\ell} - s)\bar{v}^{\ell}|, \\
\bar{v}_n(s) &= \bar{V}_{\mathbf{cl}}(s) \cdot \frac{\bar{X}_{\mathbf{cl}}(s)}{|\bar{X}_{\mathbf{cl}}(s)|}, \quad \bar{v}_\theta(s) = \bar{V}_{\mathbf{cl}}(s) \cdot \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{\bar{X}_{\mathbf{cl}}(s)}{|\bar{X}_{\mathbf{cl}}(s)|}, \\
v_3(s) &= v_3.
\end{aligned}$$

Directly

$$\begin{aligned}
&\partial_\theta \bar{v}_n = v_\theta, \quad \partial_\theta \bar{v}_\theta = -\bar{v}_n, \\
&\partial_n \cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{-\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}, \\
&\partial_\theta \cos^{-1}\Big(\frac{\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = 1, \quad \partial_\theta \cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{r\bar{v}_n}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}, \\
&\partial_{\bar{v}_n} \cos^{-1}\Big(\frac{\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{\bar{v}_\theta}{\bar{v}_n^2 + \bar{v}_\theta^2}, \quad \partial_{\bar{v}_n} \cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{r\bar{v}_\theta}{\bar{v}_n^2 + \bar{v}_\theta^2}, \\
&\partial_{\bar{v}_\theta} \cos^{-1}\Big(\frac{\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{-\bar{v}_n}{\bar{v}_n^2 + \bar{v}_\theta^2}, \quad \partial_{\bar{v}_\theta} \cos^{-1}\Big(\frac{r\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{-r\bar{v}_n}{\bar{v}_n^2 + \bar{v}_\theta^2}, \\
&\partial_{\bar{v}_n} \cos^{-1}\Big(\frac{\bar{v}_n \cos\theta - \bar{v}_\theta \sin\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{\bar{v}_\theta}{\bar{v}_n^2 + \bar{v}_\theta^2}, \quad \partial_{\bar{v}_\theta} \cos^{-1}\Big(\frac{\bar{v}_n \cos\theta - \bar{v}_\theta \sin\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = \frac{\bar{v}_n}{\bar{v}_n^2 + \bar{v}_\theta^2}, \\
&\partial_\theta \cos^{-1}\Big(\frac{\bar{v}_n \cos\theta - \bar{v}_\theta \sin\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big) = 0 = \partial_n \cos^{-1}\Big(\frac{\bar{v}_n \cos\theta - \bar{v}_\theta \sin\theta}{\sqrt{\bar{v}_n^2 + \bar{v}_\theta^2}}\Big),
\end{aligned}$$

and

$$\begin{aligned}
\partial_{\bar{v}_\theta} \theta^{\ell} &= \frac{|\bar{v}_n|}{|\bar{v}|^2} + |t-s|, \quad \partial_{\bar{v}_r} \theta^{\ell} = -\frac{\bar{v}_\theta}{|\bar{v}|^2} - (2\ell - 1)\frac{r\bar{v}_\theta}{|\bar{v}|^2}, \\
\partial_\theta \theta^{\ell} &\lesssim \frac{|t-s||\bar{v}|^2|\bar{v}_n|}{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}, \ \partial_n \theta^{\ell} = \frac{(2\ell-1)\bar{v}_\theta}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}},
\end{aligned}$$

and

$$\begin{aligned}
&\partial_\theta \psi^{\ell} \lesssim \frac{|t-s||\bar{v}|^2|\bar{v}_n|}{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}, \quad \partial_n \psi^{\ell} = \frac{2\ell \bar{v}_\theta}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}, \\
&\partial_{\bar{v}_\theta} \psi^{\ell} \lesssim \frac{|t-s||\bar{v}_n|}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} \lesssim |t-s|, \quad \partial_{\bar{v}_n} \psi^{\ell} = -2\ell \frac{r\bar{v}_\theta}{\bar{v}_n^2 + \bar{v}_\theta^2} + O_\xi(1)\frac{1}{|\bar{v}|},
\end{aligned}$$

and

$$\begin{aligned}
t^{\ell} - t^{\ell+1} &\leq \frac{2\sqrt{(1-r^2)\bar{v}_\theta^2 + \bar{v}_n^2}}{\bar{v}_n^2 + \bar{v}_\theta^2}, \\
\ell_*(s) &\leq \frac{|t-s||\bar{v}|^2}{2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} - \frac{r|\bar{v}_n|}{2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} + \frac{1}{2} \leq \ell_*(s) + 1,
\end{aligned}$$

and

$$\begin{aligned}
\partial_r t^{\ell} &= \frac{-|\bar{v}_n|}{\bar{v}_n^2 + \bar{v}_\theta^2} + (2\ell - 1)\frac{r\bar{v}_\theta^2}{|\bar{v}|^2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}, \\
\partial_\theta t^{\ell} &= \frac{-(2\ell-1)\bar{v}_n\bar{v}_\theta r^2}{|\bar{v}|^2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} \lesssim \frac{|t-s||\bar{v}_\theta|r^2}{\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}, \\
\partial_{\bar{v}_n} t^{\ell} &= -(2\ell - 1)\frac{\bar{v}_n}{|\bar{v}|^2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} + O_\xi(1)\frac{1 + |\bar{v}||t-s|}{|\bar{v}|^2}, \\
\partial_{\bar{v}_\theta} t^{\ell} &\leq (2\ell - 1)\frac{(1-r^2)|\bar{v}_\theta|}{|\bar{v}|^2\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}} + 2(2\ell-1)\frac{|\bar{v}_\theta|\sqrt{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2}}{|\bar{v}|^4} \\
&\lesssim |t-s|\frac{(1-r^2)|\bar{v}_\theta|}{\bar{v}_n^2 + (1-r^2)\bar{v}_\theta^2} + |t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}.
\end{aligned}$$

If $r<\frac{1}{2}$ then $(1-r^2)\bar{v}_\theta^2+\bar{v}_n^2\geq\frac{3}{4}|\bar{v}|^2$ and $\partial_{\bar{v}_\theta}t^\ell\lesssim|t-s|\frac{4|\bar{v}_\theta|}{3|\bar{v}|^2}+|t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}\lesssim|t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}$. If $r\geq\frac{1}{2}$ and $|\bar{v}_\theta|\leq|\bar{v}_n|$ then $\partial_{\bar{v}_\theta}t^\ell\lesssim\frac{|t-s||\bar{v}_\theta|}{\frac{\bar{v}_n^2}{2}+\frac{\bar{v}_n^2}{2}}+|t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}\lesssim|t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}$. If $r\geq\frac{1}{2}$ and $|\bar{v}_\theta|\geq|\bar{v}_n|$ then $\partial_{\bar{v}_\theta}t^\ell\lesssim|t-s|\frac{(1-r^2)|\bar{v}_\theta|}{(1-r^2)|\bar{v}_\theta|(\frac{|\bar{v}_\theta|}{2}+\frac{|\bar{v}_\theta|}{2})}+|t-s|\frac{|\bar{v}_\theta|}{|\bar{v}|^2}\lesssim\frac{|t-s|}{|\bar{v}|}$.

Therefore
$$\partial_{\bar{v}_\theta}t^\ell\lesssim\frac{|t-s|}{|\bar{v}|}.$$

Directly
$$\begin{aligned}\partial_n\bar{X}_{\mathbf{cl}}(s)&=\partial_n\theta^\ell\begin{pmatrix}-\sin\theta^\ell\\ \cos\theta^\ell\end{pmatrix}-\frac{\partial t^\ell}{\partial n}|\bar{v}|\begin{pmatrix}\cos\psi^\ell\\ \sin\psi^\ell\end{pmatrix}-(t^\ell-s)|\bar{v}|\frac{\partial\psi^\ell}{\partial n}\begin{pmatrix}-\sin\psi^\ell\\ \cos\psi^\ell\end{pmatrix}\\&=\frac{(2\ell-1)\bar{v}_\theta^2}{|\bar{v}|\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}\begin{pmatrix}-\sin\theta^\ell-\cos\psi^\ell\\ \cos\theta^\ell-\sin\psi^\ell\end{pmatrix}\\&\quad+O_\xi(1)\Big\{\frac{(2\ell-1)|\bar{v}_\theta||\bar{v}_n|}{|\bar{v}|\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}+\frac{(2\ell-1)(1-r)|\bar{v}_\theta|^2}{|\bar{v}|\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}+\frac{|\bar{v}_n|}{|\bar{v}|}+\ell|t^\ell-t^{\ell+1}|\Big\},\end{aligned}$$

where $O_\xi(1)-$remainder is bounded by
$$\begin{aligned}&\lesssim\frac{|t-s||\bar{v}|^2}{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}\Big\{\frac{|\bar{v}_\theta||\bar{v}_n|}{|\bar{v}|}+\frac{|1-r||\bar{v}_\theta^2|}{|\bar{v}|}+\frac{\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}{|\bar{v}|}\Big\}+\frac{|\bar{v}_n|}{|\bar{v}|}\\&\lesssim\frac{|t-s||\bar{v}|(1+|\bar{v}|)}{\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}+|t-s||\bar{v}|+\frac{|\bar{v}_n|}{|\bar{v}|}.\end{aligned}$$

Now we use some trigonometric identities to have
$$\begin{aligned}&\sin\theta^\ell+\cos\psi^\ell\\=&\sin\theta\cos\big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})+(2\ell-1)\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\big)-\cos\theta\sin\big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})+(2\ell-1)\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\big)\\&+\frac{\bar{v}_n\cos\theta-\bar{v}_\theta\sin\theta}{|\bar{v}|}\cos(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|}))+\sin\big(\cos^{-1}(\frac{\bar{v}_n\cos\theta-\bar{v}_\theta\sin\theta}{|\bar{v}|})\big)\sin\big(-2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\big).\end{aligned}$$

Here
$$\begin{aligned}&\cos\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})+2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\\=&\cos\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\cos\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)-\sin\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\sin\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\\=&\cos\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)+O_\xi(1)\Big|1-\cos\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\Big|\\&+O_\xi(1)\Big|\sin\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\sin\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\Big|\\=&\cos\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)+O_\xi(1)\Big\{\Big|1-\frac{r\bar{v}_\theta^2}{|\bar{v}|^2}-\frac{\bar{v}_n\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}{|\bar{v}|^2}\Big|+\Big|\frac{r\bar{v}_n\bar{v}_\theta}{|\bar{v}|^2}-\frac{\bar{v}_\theta\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}{|\bar{v}|^2}\Big|\Big\}\\=&\cos\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)+O_\xi(1)\Big\{\frac{(1-r)\bar{v}_\theta^2}{|\bar{v}|^2}+\frac{\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}{|\bar{v}|}\Big\},\end{aligned}$$

and
$$\begin{aligned}&\sin\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})+2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\\=&\sin\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\cos\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\Big)\\&+\cos\Big(\cos^{-1}(\frac{\bar{v}_\theta}{|\bar{v}|})-\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\sin\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)\Big)\\=&\sin\Big(2\ell\cos^{-1}(\frac{r\bar{v}_\theta}{|\bar{v}|})\Big)+O_\xi(1)\Big\{\frac{(1-r)\bar{v}_\theta^2}{|\bar{v}|^2}+\frac{\sqrt{\bar{v}_n^2+(1-r^2)\bar{v}_\theta^2}}{|\bar{v}|}\Big\}.\end{aligned}$$

Therefore

$$\begin{aligned}\sin\theta^\ell+\cos\psi^\ell &= (1-\frac{|\bar v_\theta|}{|\bar v|})\sin\theta\cos\Big((2\ell-1)\cos^{-1}(\frac{r\bar v_\theta}{|\bar v|})\Big)-(1-\frac{|\bar v_\theta|}{|\bar v|})\cos\theta\sin\Big(2\ell\cos^{-1}(\frac{r\bar v_\theta}{|\bar v|})\Big)\\ &\quad+O_\xi(1)\{\frac{(1-r)\bar v_\theta^2}{|\bar v|^2}+\frac{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}{|\bar v|}\}\\ &\sim\frac{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}{|\bar v|}.\end{aligned}$$

Since $\cos\theta^\ell-\sin\psi^\ell=\sin(\theta^\ell+\frac{\pi}{2})+\cos(\psi^\ell+\frac{\pi}{2})$,

$$\cos\theta^\ell-\sin\psi^\ell\sim\frac{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}{|\bar v|}.$$

Therefore we conclude our claim for $\partial_n\bar X_{\mathbf{cl}}$.

Using the same estimates

$$\begin{aligned}\partial_{\bar v_n}\bar X_{\mathbf{cl}}(s) &= (2\ell-1)\Big\{\frac{-r\bar v_\theta}{|\bar v|^2}\begin{pmatrix}-\sin\theta^\ell\\ \cos\theta^\ell\end{pmatrix}+\frac{\bar v_n}{|\bar v|\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}\begin{pmatrix}\cos\psi^\ell\\ \sin\psi^\ell\end{pmatrix}\Big\}+O_\xi(1)\frac{1+|\bar v||t-s|}{|\bar v|}\\ &=\frac{2\ell-1}{|\bar v|}\begin{pmatrix}\sin\theta^\ell+\cos\psi^\ell\\ -\cos\theta^\ell+\sin\psi^\ell\end{pmatrix}+O_\xi(1)\frac{1+|\bar v||t-s|}{|\bar v|}\lesssim\frac{1}{|\bar v|}.\end{aligned}$$

Since $t^{\ell_*+1}<0<t^{\ell_*}$,

$$\partial_n v^\ell=\partial_n\psi^\ell(-|\bar v|\sin\psi^\ell,|\bar v|\cos\psi^\ell,0)=\frac{|t-s||\bar v|^2|\bar v_\theta|}{\bar v_n^2+(1-r^2)\bar v_\theta^2}(-|\bar v|\sin\psi^\ell,|\bar v|\cos\psi^\ell,0).$$

Therefore we conclude our claim for $\partial_n\bar V_{\mathbf{cl}}(0)$. Moreover

$$\begin{aligned}&|\partial_\theta\bar X_{\mathbf{cl}}(s)|\lesssim\frac{|\bar v|}{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}|\bar v||t-s|,\quad|\partial_\theta\bar V_{\mathbf{cl}}(s)|\lesssim\frac{|\bar v|^2}{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}}|\bar v||t-s|,\\ &|\partial_{\bar v_n}\bar V_{\mathbf{cl}}(s)|\lesssim 1+\frac{|\bar v|^2|t-s|}{\sqrt{\bar v_n^2+(1-r^2)\bar v_\theta^2}},\quad|\partial_{\bar v_\theta}\bar X_{\mathbf{cl}}(s)|\lesssim\frac{1}{|\bar v|},\quad|\partial_{\bar v_\theta}\bar V_{\mathbf{cl}}(s)|\lesssim 1+|\bar v||t-s|.\end{aligned}\tag{A.149}$$

□

Based on Example 1, we naturally consider the 2D specular problem. We consider the 2D specular problem for $f(t,x_1,x_2,v_1,v_2,v_3)$ solving

$$\partial_t f+v_1\partial_{x_1}f+v_2\partial_{x_2}f=\Gamma_{\text{gain}}(f,f)-\nu(\sqrt{\mu}f)f,\tag{A.150}$$

where v_3 is a paramter. Here $(x_1,x_2)\in\Omega=\{x\in\mathbb{R}^2:\xi(x)>0\}$ and the convexity (A.3) is valid for all $\zeta\in\mathbb{R}^2$. We study (A.150) with specular boundary condition (A.10). Denote $v:=(\bar v,v_3)=(v_1,v_2;v_3)\in\mathbb{R}^3$. We define

$$\alpha(x,\bar v)=|\bar v\cdot\nabla\xi(x)|^2-2\{\bar v\cdot\nabla^2\xi(x)\cdot\bar v\}\xi(x).$$

Note that $\nabla\xi(x)=(\partial_{x_1}\xi(x),\partial_{x_2}\xi(x),0)$.

The following estimate is crucial to establish the weighted C^1 estimate (Theorem A.5) and non-existence of $\nabla^2 f$ up to the boundary (Proposition A.5).

Lemma A.12. *For $\theta>0$ and for $i=1,2$,*

$$\begin{aligned}&e^{-\varpi\langle v\rangle s}|\partial_{v_i}\Gamma_{\text{gain}}(f,f)|\\ &\lesssim||e^{\theta|v|^2}f||_\infty\Big\{||e^{\theta|v|^2}f||_\infty+||\partial_{v_3}f||_\infty+\Big|\Big|e^{-\varpi\langle v\rangle s}\frac{|\bar v|}{\langle\bar v\rangle}\alpha^{1/2}\nabla_{\bar v}f\Big|\Big|_\infty\Big\},\end{aligned}\tag{A.151}$$

where $v=(\bar v,v_3)=(v_1,v_2,v_3)$.

Proof. The key is to use the splitting $u_{||,3}$ with respect to $|\bar{v}+\bar{u}_\perp|\sqrt{\alpha(\bar{v}+\bar{u}_\perp)}$.

Recall from [74] that the gain term of the nonlinear Boltzmann operator in (A.8) equals

$$\begin{aligned}
&\Gamma_{\text{gain}}(g_1,g_2)(v)\\
=&C\int_{\mathbb{R}^3}\mathrm{d}u\int_{u\cdot w=0}\mathrm{d}w\ g_1(v+w)g_2(v+u)q_0^*(\frac{|u|}{|u+w|})\frac{|u+w|^{\kappa-1}}{|u|}e^{-\frac{|u+v+w|^2}{4}},\\
=&C\int_{\mathbb{R}^3}\mathrm{d}u\int_{u\cdot w=0}\mathrm{d}w\ g_2(v+w)g_1(v+u)q_0^*(\frac{|u|}{|u+w|})\frac{|u+w|^{\kappa-1}}{|u|}e^{-\frac{|u+v+w|^2}{4}},\\
=&C\int_{\mathbb{R}^3}\mathrm{d}u\int_{(u-v)\cdot w=0}\mathrm{d}w\ g_1(v+w)g_2(u)q_0^*(\frac{|u-v|}{|u-v+w|})\frac{\left|u-v+w\right|^{\kappa-1}}{|u-v|}e^{-\frac{|u+w|^2}{4}},\\
=&C\int_{\mathbb{R}^3}\mathrm{d}u\int_{(u-v)\cdot w=0}\mathrm{d}w\ g_2(v+w)g_1(u)q_0^*(\frac{|u-v|}{|u-v+w|})\frac{\left|u-v+w\right|^{\kappa-1}}{|u-v|}e^{-\frac{|u+w|^2}{4}},
\end{aligned}\tag{A.152}$$

where $q_0^*(\cos\theta)=\frac{q_0(\cos\theta)}{|\cos\theta|}$. This is due to two change of variables (37),(38) and page 316 of [74]. Then

$$\begin{aligned}
&\partial_{v_i}\Gamma_{\text{gain}}(f,f)\\
=&\ 2\Gamma_{\text{gain}}(\partial_{v_i}f,f)\\
&+C\int_{\mathbb{R}^3}\mathrm{d}u_\parallel\int_{u_\parallel\cdot u_\perp=0}\mathrm{d}wf(v+u_\perp)f(v+u_\parallel)\\
&\qquad\times q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})\frac{|u_\parallel+u_\perp|^{\kappa-1}}{|u_\parallel|}e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}(-\frac{\mathbf{e}_i}{2})\cdot(u_\parallel+v+u_\perp)\\
=&\ 2\Gamma_{\text{gain}}(\partial_{v_i}f,f)+O_\xi(1)e^{-C|v|^2}||e^{\theta|v|^2}f||_\infty^2.
\end{aligned}$$

Denote the standard cutoff function $\chi\geq 0:\chi\equiv 1$ on $[0,1]$ and $\chi\equiv 0$ for $[2,\infty)$. We have

$$\Gamma_{\text{gain}}(\partial_{v_i}f,f)=\int_{\mathbb{R}^3}\mathrm{d}u_{||}f(v+u_{||})\int_{\mathbb{R}^2}\mathrm{d}u_\perp\partial_{v_i}f(v+u_\perp)e^{-\frac{|u_\parallel+u_\perp+v|^2}{4}}q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})\frac{|u_\parallel+u_\perp|^{\kappa-1}}{|u_{||}|}.$$

We further split it into, for $0<\varepsilon\ll 1$,

$$\begin{aligned}
&\int_{\mathbb{R}^3}\mathrm{d}u_{||}f(v+u_{||})\int_{\mathbb{R}^2}\chi\left(\frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right)\\
&\quad\times\partial_{v_i}f(v+u_\perp)e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})\frac{|u_\parallel+u_\perp|^{\kappa-1}}{|u_{||}|}\mathrm{d}u_\perp\\
&+\int_{\mathbb{R}^3}du_{||}f(v+u_{||})\int_{\mathbb{R}^2}\left\{1-\chi\left(\frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right)\right\}\\
&\quad\times\partial_{v_i}f(v+u_\perp)e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})\frac{|u_\parallel+u_\perp|^{\kappa-1}}{|u_{||}|}\mathrm{d}u_\perp.
\end{aligned}$$

For the first part, $|u_{||,3}|\geq|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}$, and we parametrize $u_\perp$ as $u_{\perp,3}=-\frac{\bar{u}_{||}\cdot\bar{u}_\perp}{u_{||,3}}$ so that

$$\mathrm{d}u_\perp=\frac{|u_{||}|}{|u_{||,3}|}\mathrm{d}\bar{u}_\perp:=\frac{|u_{||}|}{|u_{||,3}|}\mathrm{d}u_{\perp,1}\mathrm{d}u_{\perp,2},\tag{A.153}$$

and the first part equals

$$\begin{aligned}
&\textstyle\int_{\mathbb{R}^3}\mathrm{d}u_{||}f(v+u_{||})\int_{\mathbb{R}^2}\mathrm{d}\bar{u}_\perp\partial_{v_i}f(v_1+u_{\perp,1},v_2+u_{\perp,2},v_3-\frac{\bar{u}_{||}\cdot\bar{u}_\perp}{u_{||,3}})\\
&\quad\times\chi\left(\frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right)e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}\frac{q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})}{|u_{||,3}||u_\parallel+u_\perp|^{1-\kappa}}.
\end{aligned}$$

We now integrate by part in $u_{\perp,i}$ for $i=1,2$ to get

$$
\begin{aligned}
&-\int_{\mathbb{R}^3} \mathrm{d}u_{||} f(v+u_{||}) \int_{\mathbb{R}^2} \partial_{v_3} f(\bar v+\bar u_\perp, v_3 - \frac{\bar u_{||}\cdot \bar u_\perp}{u_{||,3}}) \\
&\qquad \times \chi\left(\frac{|\bar v+\bar u_\perp|^{1-}\alpha^{1/2-}}{u_{||,3}}\right) e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}} \frac{q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})u_{||,i}\mathrm{d}\bar u_\perp}{|u_{||,3}|^2|u_{||}+u_\perp|^{1-\kappa}} \\
&-\int_{\mathbb{R}^3} \mathrm{d}u_{||} f(v+u_{||}) \int_{\mathbb{R}^2} f(\bar v+\bar u_\perp, v_3 - \frac{\bar u_{||}\cdot \bar u_\perp}{u_{||,3}}) \\
&\qquad \times \partial_{u_\perp,i}\left\{\chi\left(\frac{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right) e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}} \frac{q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})\bar u_{||,i}}{|u_{||,3}||u_{||}+u_\perp|^{1-\kappa}}\right\}\mathrm{d}\bar u_\perp.
\end{aligned}
$$

Directly we have $|\partial_{u_\perp,i}\alpha(\bar v+\bar u_\perp)|\lesssim \alpha(\bar v+\bar u_\perp)^{1/2}$ and $|\frac{du_{\perp,3}}{du_{\perp,i}}|\le \frac{|\bar u_\parallel|}{|u_{\parallel,3}|}$ to conclude

$$
\begin{aligned}
|\partial_{u_\perp,i}\{\ \}| \sim\ & \chi' \frac{|\bar v+\bar u_\perp|^{-\varepsilon}\alpha^{1/2-\varepsilon}+|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}}{u_{\parallel,3}} e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}} \frac{||q_0^*||_\infty|\bar u_{||}|}{|u_{||,3}||u_{||}+u_\perp|^{1-\kappa}} \\
&+\chi e^{-C|u_\parallel+u_\perp+v|^2}\Big\{\frac{||q_0^*||_\infty|\bar u_\parallel|^2}{|u_{\parallel,3}|^2|u_\parallel+u_\perp|^{1-\kappa}}+\frac{||q_0^*||_{C^1}|\bar u_\parallel|^2}{|u_{\parallel,3}|^2|u_\parallel+u_\perp|^{3-\kappa}}+\frac{||q_0^*||_\infty|\bar u_\parallel|(1+\frac{|\bar u_\parallel|}{|u_{\parallel,3}|})}{|u_{\parallel,3}||u_\parallel+u_\perp|^{2-\kappa}}\Big\} \\
\lesssim_{q_0^*}\ & \mathbf{1}_{\{u_{\parallel,3}\sim|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}\}}\Big\{\frac{1}{|\bar v+\bar u_\perp|}+\frac{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}}{|u_{\parallel,3}|}\Big\}\frac{e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}|\bar u_{||}|}{|u_{||,3}||u_{||}+u_\perp|^{1-\kappa}} \\
&+\mathbf{1}_{\{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}\le u_{\parallel,3}\}}\frac{|\bar u_\parallel|(1+|\bar u_\parallel|)}{|u_{\parallel,3}|^2|u_\parallel+u_\perp|^{1-\kappa}}(1+\frac{1}{|u_\parallel+u_\perp|^2})e^{-C|u_\parallel+v+u_\perp|^2}.
\end{aligned}
$$

Note that $|f(v+u_\parallel)|\lesssim e^{-C|v+u_\parallel|^2}||e^{\theta|v|^2}f||_\infty$ and

$$
|f(\bar v+\bar u_\perp, v_3-\frac{\bar u_\parallel\cdot\bar u_\perp}{u_{\parallel,3}})|\lesssim e^{-C|\bar v+\bar u_\perp|^2-C|v_3+u_{\perp,3}(u_\parallel,\bar u_\perp)|^2}||e^{\theta|v|^2}f||_\infty, \tag{A.154}
$$

and

$$
e^{-|u_\parallel+u_\perp+v|^2}e^{-C|v+u_\parallel|^2}e^{-C|\bar v+\bar u_\perp|^2-C|v_3+u_{\perp,3}(u_\parallel,\bar u_\perp)|^2}\lesssim e^{-C'|v|^2}e^{-C'|u_\perp|^2}e^{-C|v+u_\parallel|^2},
$$

where $v:=v_\parallel+v_\perp$ with $v_\parallel:=v\cdot\frac{u_\parallel}{|u_\parallel|}$ and

$$
|v+u_\parallel|^2+|v+u_\perp|^2=|v_\parallel+u_\parallel|^2+|v_\perp|^2+|v_\perp+u_\perp|^2+|v_\parallel|^2\ge|v|^2.
$$

The $\partial_{u_\perp,i}\{\ \}-$contribution are bounded by following three estimates : For the first term

$$
e^{-|v|^2}||e^{\theta|v|^2}f||_\infty^2\int_{\mathbb{R}^2}\frac{e^{-|u_\perp|^2}\mathrm{d}\bar u_\perp}{|\bar v+\bar u_\perp|}\int_{\mathbb{R}^2}|\bar u_\parallel|^\kappa e^{-|\bar v+\bar u_\parallel|^2}\mathrm{d}\bar u_\parallel\int_{u_{\parallel,3}\sim|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{\frac12-\varepsilon}}\frac{\mathrm{d}u_{\parallel,3}}{|u_{\parallel,3}|}\lesssim e^{-C'|v|^2}.
$$

For the second term we use $f(\bar v+\bar u_\perp, v_3-\frac{\bar u_\parallel\cdot\bar u_\perp}{u_{\parallel,3}})\lesssim e^{-C|v+u_\perp|^2}||e^{\theta|v|^2}f||_\infty\frac{1}{1+(v_3-\frac{\bar u_\parallel\cdot\bar u_\perp}{|u_{\parallel,3}|})^\varepsilon}$ such that

$$
\begin{aligned}
& f(v+u_\parallel)\frac{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}}{|u_{\parallel,3}|^2}f(v_3-\frac{\bar u_\parallel\cdot\bar u_\perp}{u_{\parallel,3}})\frac{e^{-\frac{|u_\parallel+u_\perp+v|^2}{4}}|\bar u_\parallel|}{|u_\parallel+u_\perp|^{1-\kappa}} \\
\lesssim & e^{-|v|^2}e^{-|v+u_\parallel|^2}e^{-|u_\perp|^2}||e^{\theta|v|^2}f||_\infty^2\frac{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}|\bar u_\parallel|}{|u_\parallel+u_\perp|^{1-\kappa}}\frac{1}{|u_{\parallel,3}|^{2-\varepsilon}}\frac{1}{|u_{\parallel,3}|^\varepsilon+[v_3u_{\parallel,3}-\bar u_\parallel\cdot\bar u_\perp]^\varepsilon} \\
\lesssim & e^{-|v|^2}e^{-|v+u_\parallel|^2}e^{-|u_\perp|^2}||e^{\theta|v|^2}f||_\infty^2\frac{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}\langle v\rangle}{|u_\parallel+u_\perp|^{1-\kappa}}\frac{1}{|u_{\parallel,3}|^{2-\varepsilon}|\bar u_\perp|^\varepsilon}\frac{1}{\big[\frac{v_3u_{\parallel,3}}{|\bar u_\perp|}-\bar u_\parallel\cdot\frac{\bar u_\perp}{|\bar u_\perp|}\big]^\varepsilon},
\end{aligned}
$$

where we have used $e^{-|v+u_\parallel|^2}|u_\parallel|\lesssim\{|u_\parallel+v|+|v|\}e^{-|v+u_\parallel|^2}\lesssim(1+|v|)e^{-C|v+u_\parallel|^2}$.

Now we decompose $\bar{u}_{\|} = \bar{u}_{\|,a} + \bar{u}_{\|,b} := \bar{u}_{\|} \cdot \frac{\bar{u}_\perp}{|\bar{u}_\perp|} + (\bar{u}_{\|} - \bar{u}_{\|} \cdot \frac{\bar{u}_\perp}{|\bar{u}_\perp|})$ and bound $e^{-|v|^2}||e^{\theta|v|^2}f||_\infty^2 \times$

$$\begin{aligned}
&\int_{u_{\|,3}\sim|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{\frac{1}{2}-\varepsilon}} \mathrm{d}u_{\|,3} \int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-|\bar{u}_\perp|^2} \frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{-\varepsilon}}{|\bar{u}_\perp|^\varepsilon |u_{\|,3}|^{2-\varepsilon}} \\
&\times \int_{\mathbb{R}} \frac{e^{-|\bar{u}_{\|,b}+(v-v\cdot\frac{\bar{u}_\perp}{|\bar{u}_\perp|})|^2}\mathrm{d}\bar{u}_{\|,b}}{|\bar{u}_{\|,b}|^{1-\kappa}} \int_{\mathbb{R}} \frac{\mathrm{d}\bar{u}_{\|,a} e^{-|\bar{u}_{\|,a}|^2}}{[\bar{u}_{\|,a} - \frac{v_3 u_{\|,3}}{|\bar{u}_\perp|}]^\varepsilon} \\
\lesssim &\int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-|\bar{u}_\perp|^2} \int_{u_{\|,3}\sim|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{\frac{1}{2}-\varepsilon}} \mathrm{d}u_{\|,3} \frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha(\bar{v}+\bar{u}_\perp)^{-\varepsilon}}{|\bar{u}_\perp|^\varepsilon |u_{\|,3}|^{2-\varepsilon}},
\end{aligned}$$

where we have used $\bar{u}_{\|,a} \mapsto \bar{u}_{\|,a} - v \cdot \frac{\bar{u}_\perp}{|\bar{u}_\perp|}$. The $u_{\|,3}-$integration yields

$$\begin{aligned}
&\lesssim \int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-|\bar{u}_\perp|^2} \frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha(\bar{v}+\bar{u}_\perp)^{-\varepsilon}}{|\bar{u}_\perp|^\varepsilon} \int_{u_{\|,3}\sim|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{\frac{1}{2}-\varepsilon}} \frac{\mathrm{d}u_{\|,3}}{|u_{\|,3}|^{2-\varepsilon}} \\
&\lesssim \int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-|\bar{u}_\perp|^2} \frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha(\bar{v}+\bar{u}_\perp)^{-\varepsilon}}{|\bar{u}_\perp|^\varepsilon} \frac{1}{|\bar{v}+\bar{u}_\perp|^{(1-\varepsilon)(1-\varepsilon)}} \frac{1}{\alpha(\bar{v}+\bar{u}_\perp)^{(\frac{1}{2}-\varepsilon)(1-\varepsilon)}} \\
&\lesssim \int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-|\bar{u}_\perp|^2} \frac{|\bar{v}+\bar{u}_\perp|^{\varepsilon(1-\varepsilon)}}{|\bar{u}_\perp|^\varepsilon} \frac{1}{\alpha(\bar{v}+\bar{u}_\perp)^{\frac{1}{2}-(1-\varepsilon)\varepsilon}}.
\end{aligned}$$

Note that $\alpha(\bar{v}+\bar{u}_\perp)^{\frac{1}{2}-\varepsilon(1-\varepsilon)} \gtrsim [n(x)\cdot(\bar{v}+\bar{u}_\perp)]^{1-\varepsilon(1-\varepsilon)}$ and $|\bar{u}_\perp|^\varepsilon \gtrsim [n^\perp \cdot \bar{u}_\perp]^\varepsilon$ to bound

$$\lesssim \langle v\rangle \int_{\mathbb{R}} \frac{e^{-|n\cdot\bar{u}_\perp|^2}}{[n\cdot\bar{u}_\perp + n\cdot\bar{v}]^{1-2\varepsilon(1-\varepsilon)}} \mathrm{d}[n\cdot\bar{u}_\perp] \int_{\mathbb{R}} \frac{e^{-|n^\perp\cdot\bar{u}_\perp|^2}}{|n^\perp\cdot\bar{u}_\perp|^\varepsilon} \mathrm{d}[n^\perp\cdot\bar{u}_\perp] \lesssim \langle v\rangle.$$

For the third term is bounded by $||e^{\theta|v|^2}f||_\infty^2 \times$

$$\begin{aligned}
&\int_{\mathbb{R}^3} d\bar{u}_{||} \int_{\mathbb{R}^2} d\bar{u}_\perp \left\{ \int_{|u_{||,3}|\geq|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}} \frac{e^{-|u_{||,3}-v_3|^2}}{|u_{||,3}|^2} du_{||,3} \right\} \\
&\qquad\qquad \times \frac{\langle u_{||}\rangle^2 e^{-C\{|u_{||}+v|^2-|u_\perp|^2\}}}{|u+w|^{1-\kappa}}(1+\frac{1}{|u_{||}+u_\perp|^2}) \\
\lesssim\; &\int_{\mathbb{R}^3} d\bar{u}_{||} \left\{ \int_{\mathbb{R}^2} \frac{e^{-C|u_\perp|^2} d\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}} \right\} \frac{\langle \bar{u}_{||}\rangle^2 e^{-C\{|u_{||}+v|^2\}}}{|u_{\|}+u_\perp|^{1-\kappa}}(1+\frac{1}{|u_{||}+u_\perp|^2}),
\end{aligned}$$

where we have used

$$\begin{aligned}
&\int_{|u_{\|,3}|\geq|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{\frac{1}{2}-\varepsilon}} \frac{e^{-|u_{\|,3}-v_3|^2}}{|u_{\|,3}|^{1-\varepsilon}} \frac{1}{|u_{\|,3}|^{1+\varepsilon}} \mathrm{d}u_{\|,3} \\
&\lesssim \frac{1}{|\bar{v}+\bar{u}_\perp|^{(1-\varepsilon)(1+\varepsilon^2)}\alpha^{(\frac{1}{2}-\varepsilon)(1+\varepsilon^2)}} \int_{\mathbb{R}} \frac{e^{-|u_{\|,3}-v_3|^2}}{|u_{\|,3}|^{1-\varepsilon^2}} \mathrm{d}u_{\|,3} \\
&\lesssim \frac{1}{|\bar{v}+\bar{u}_\perp|^{1-(1-\varepsilon)(1+\varepsilon^2)}\alpha^{\frac{1}{2}-(1-\varepsilon)(1+\varepsilon^2)}}.
\end{aligned}$$

We note that, by separating $|\xi|\geq\delta$ or $|\xi|\leq\delta$, we can write $\alpha^{1/2-(1-\varepsilon)(1+\varepsilon^2)} \geq \{n\cdot[\bar{v}+\bar{u}_\perp]\}^{1-(1-\varepsilon)(1+\varepsilon^2)}$ and $|\bar{v}+\bar{u}_\perp|^{1-(1-\varepsilon)(1+\varepsilon^2)} \geq \{n^\perp\cdot[\bar{v}+\bar{u}_\perp]\}^{1-(1-\varepsilon)(1+\varepsilon^2)}$, where $n^\perp = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} n, x$ so that the inner 2D integral are two convergent 1D one

$$\begin{aligned}
&\int_{|(\bar{v}+\bar{u}_\perp)\cdot n^\perp|\geq 1} \frac{e^{-C|u_\perp|^2}d\bar{u}_\perp}{\alpha^{1/2-\varepsilon}} + \int_{|\bar{v}+\bar{u}_\perp|\leq 1, |n^\perp\{\bar{v}+\bar{u}_\perp\}|\leq 1} \frac{d\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}} \\
\leq\;& 1 + \int_{|n^\perp\{\bar{v}+\bar{u}_\perp\}|\leq 1} \frac{e^{-C|u_\perp|^2}d\bar{u}_\perp}{\alpha^{1/2-\varepsilon}} + \int_{|n^\perp\{\bar{v}+\bar{u}_\perp\}|\leq 1} \frac{d\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}} \\
&+ \int_{|n^\perp\{\bar{v}+\bar{u}_\perp\}|\leq 1} \frac{e^{-C|u_\perp|^2}d\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}} \\
<\;& +\infty.
\end{aligned}$$

Similarly, the first term is bounded by

$$||\langle v\rangle^{\zeta} e^{\theta|v|^2} f||_\infty ||\partial_{v_3} f|| \int_{\mathbb{R}^3} du_{||} \left\{ \int_{|u_{||,3}|\geq |\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}} \frac{e^{-|v_3-u_{||,3}|^2}}{|u_{||,3}|^2} \right\} \frac{q_0^*(\frac{|u|}{|v+w|})u_{||,i}\mathrm{d}\bar{u}_\perp}{|u_{||}+u_\perp|^{\kappa-1}} e^{-\frac{|u+v+w|^2}{4}},$$

and the same argument yields the same bound.

We now turn to

$$e^{-\varpi\langle v\rangle s}\int_{\mathbb{R}^3} \mathrm{d}u_{||} f(v+u_{||}) \int_{\mathbb{R}^2} \left\{1-\chi\left(\frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right)\right\} \mathrm{d}u_\perp \partial_{v_i} f(v+u_\perp) e^{-\frac{|u+v+w|^2}{4}} \frac{q_0^*(\frac{|u|}{|v+w|})}{|u_{||}||u+w|^{1-\kappa}}.$$

In this case,

$$|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon} \geq |u_{||,3}|.$$

We now parametrize $\mathrm{d}u_\perp$ in two different ways.

We decompose

$$\bar{u}_{\|} = \bar{u}_{\|,n} + \bar{u}_{\|,n^\perp} := \bar{u}_{\|}\cdot n + \bar{u}_{\|}\cdot n^\perp. \tag{A.155}$$

If $|u_{||,3}| \geq |\bar{u}_{\|,n^\perp}|$, then we use the same parametrization to get

$$\begin{aligned}
&e^{-\varpi\langle v\rangle s} e^{\varpi\langle v+u_\perp\rangle s}\int_{\mathbb{R}^3} \mathrm{d}u_{||} f(v+u_{||}) \int_{\mathbb{R}^2} \mathrm{d}\bar{u}_\perp e^{-\varpi\langle v+u_\perp\rangle s}\partial_{v_i} f(\bar{v}+\bar{u}_\perp, v_3 - \frac{\bar{u}_{\|}\cdot\bar{u}_\perp}{u_{||,3}}) \\
&\times[1-\chi\left(\frac{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}}{u_{||,3}}\right)] e^{-\frac{|u_{\|}+v+u_\perp|^2}{4}} \frac{q_0^*(\frac{|u_{\|}|}{|u_{\|}+u_\perp|})}{|u_{||,3}||u_{\|}+u_\perp|^{1-\kappa}} \\
\lesssim_s\ & ||e^{\theta|v|^2} f||_\infty ||e^{-\varpi\langle v\rangle s}\frac{\bar{v}\alpha^{1/2}}{\langle\bar{v}\rangle}\partial_{v_i} f(s)||_\infty \\
&\times \int_{\mathbb{R}^3}\mathrm{d}u_{||}\int_{|\bar{v}+\bar{u}_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}\geq u_{||,3}} \frac{\mathrm{d}\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|\alpha^{1/2}} \frac{e^{-C|u_\perp|^2}e^{-C|v+u_{\|}|^2}}{|u_{||,3}||u_{\|}+u_\perp|^{1-\kappa}}.
\end{aligned}$$

First we integrate $u_{\|,n}$ to drop $\frac{1}{|u_{\|}+u_\perp|^{1-\kappa}}$ singular term for $0<\kappa\leq 1$

$$\int \frac{e^{-|v_n+u_{\|,n}|^2}}{|u_{\|}-u_\perp|^{1-\kappa}}\mathrm{d}u_{\|,n} \leq \int \frac{e^{-|v_n+u_{\|,n}|^2}}{|u_{\|,n}-u_{\perp,n}|^{1-\kappa}}\mathrm{d}u_{\|,n} < \infty,$$

so that we only need to bound

$$\begin{aligned}
&\int \mathrm{d}\bar{u}_{||,n^\perp}\int \frac{e^{-|\bar{u}_\perp|^2-|v+u_{||}|^2}\mathrm{d}\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{2\varepsilon}\alpha^{2\varepsilon}|\bar{v}+\bar{u}_\perp|^{1-2\varepsilon}\alpha^{1/2-2\varepsilon}}\frac{1}{|u_{||,3}|} \\
\leq\ & \int \mathrm{d}\bar{u}_{||,n^\perp}\left\{\int \frac{e^{-|\bar{u}_\perp|^2}\mathrm{d}\bar{u}_\perp}{|\bar{v}+\bar{u}_\perp|^{\varepsilon}\alpha^{\varepsilon}}\right\}\frac{e^{|v+u_{\|}+u_\perp|^2}e^{-|v+u_{||}|^2}}{|u_{||,3}|^{2-2\varepsilon}}.
\end{aligned}$$

The inner integral is finite, since $\alpha \geq |n\cdot\{\bar{v}+\bar{u}_\perp\}| = |\bar{v}\cdot n + \bar{u}_{\perp,n}|$, and the integral is a 1D integral :

$$\int_{\mathbb{R}} \frac{e^{-|\bar{u}_{\perp,n}|^2}\mathrm{d}\bar{u}_{\perp,n}}{|n\cdot\bar{v}+\bar{u}_{\perp,n}|^{3\varepsilon}} < +\infty.$$

Moreover, from $|u_{||,3}| \geq |\bar{u}_{||,n^\perp}|$, the outer integral takes the form

$$\int_{\mathbb{R}} \frac{e^{-|u_{\|,3}+v_3|^2}e^{-|v_{\|,n^\perp}+u_{\|,n^\perp}|^2}\mathrm{d}u_{||,3}\mathrm{d}u_{\|,n^\perp}}{|u_{||,3}|^{2-\varepsilon}} \leq \int \frac{e^{-|u_{\|,3}+v_3|^2}e^{-|v_{\|,n^\perp}+u_{\|,n^\perp}|^2}\mathrm{d}u_{||},_{n^\perp}\,\mathrm{d}u_{||,3}}{\{|u_{||,n^\perp}|+|u_{||,3}|\}^{2-\varepsilon}} < \infty.$$

We are done in this case.

We now consider the case $|u_{||,3}| \leq |u_{\|,n^\perp}|$. We now choose a different parametrization. We define

$$u_{\perp,n} := u_\perp\cdot n,\quad u_{\perp,n^\perp} := u_\perp\cdot n^\perp.$$

Now we choose $u_{\perp,n}$ and $u_{\perp,3}$ as parameters so that $u_{\perp,n^\perp} = -\frac{u_{\perp,n}u_{||,n}+u_{\perp,3}u_{||,3}}{u_{||,n^\perp}}$ and

$$\mathrm{d}u_\perp = \frac{|u_{||}|}{|u_{||,n^\perp}|}\mathrm{d}u_{\perp,n}\mathrm{d}u_{\perp,3},$$

so that we need to bound

$$\begin{aligned}
&e^{-\varpi\langle v\rangle s}\int_{\mathbb{R}^3}\mathrm{d}u_{||}\\
&\times f(v+u_{||})\int_{\mathbb{R}^2}\mathrm{d}u_{\perp,n}\mathrm{d}u_{\perp,3}\partial_{v_i}f(v_n+u_{\perp,n},v_{n^\perp}-\frac{u_{\perp,n}u_{||,n}+u_{\perp,3}u_{||,3}}{u_{||,n^\perp}},v_3+u_{\perp,3})\frac{|u_{||}|}{|u_{||,n^\perp}|}\\
&\times\Big\{1-\chi\Big(\frac{|\bar v+\bar u_\perp|^{1-}\alpha^{1/2-}}{u_{||,3}}\Big)\Big\}e^{-\frac{|u_\parallel+v+u_\perp|^2}{4}}\frac{q_0^*(\frac{|u_\parallel|}{|u_\parallel+u_\perp|})}{|u_{||}||u_\parallel+u_\perp|^{1-\kappa}}.
\end{aligned}$$

Directly this is bounded by $||e^{\theta|v|^2}f||_\infty||e^{-\varpi\langle v\rangle s}\frac{|\bar v|\alpha^{1/2}\partial_{v_i}f}{\langle\bar v\rangle}||_\infty\times$

$$\begin{aligned}
&\int_{\mathbb{R}^3}\mathrm{d}u_{||}\int_{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}\geq|u_{||,3}|}\frac{\langle\bar v+\bar u_\perp\rangle e^{-|\bar u_\perp|^2-|v+u_{||}|^2}\mathrm{d}u_{\perp,n}\mathrm{d}u_{\perp,3}}{|\bar v+\bar u_\perp|\alpha^{1/2}}\frac{\mathrm{d}u_\parallel}{|u_{||,n^\perp}||u_\parallel+u_\perp|^{1-\kappa}}\\
\lesssim_s\ &\int_{\mathbb{R}^3}\mathrm{d}u_{||}\int_{|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{1/2-\varepsilon}\geq|u_{||,3}|}\frac{\langle\bar v+\bar u_\perp\rangle e^{-|\bar u_{\perp,n}|^2-|v+u_{||}|^2}}{|\bar v+\bar u_\perp|^{2\varepsilon}\alpha^{2\varepsilon}|\bar v+\bar u_\perp|^{1-2\varepsilon}\alpha^{1/2-2\varepsilon}}\frac{1}{|u_{||,n^\perp}|}\mathrm{d}\bar u_{\perp,n}.
\end{aligned}$$

where we integrate $u_{\perp,3}$ first to drop $\int_{\mathbb{R}}\frac{e^{-C|u_{\perp,3}|^2}\mathrm{d}u_{\perp,3}}{|u_\parallel+u_\perp|^{1-\kappa}}\lesssim\int_{\mathbb{R}}\frac{e^{-C|u_{\perp,3}|^2}\mathrm{d}u_{\perp,3}}{|u_{\parallel,3}+u_{\perp,3}|^{1-\kappa}}<+\infty$.

In the case of $|\bar v+\bar u_\perp|\leq 1$, this is bounded by

$$\begin{aligned}
\lesssim_s\ &\int_{\mathbb{R}^3}\mathrm{d}u_{||}\int\frac{e^{-|u_\perp|^2-|v+u_{||}|^2}\mathrm{d}u_{\perp,n}}{|\bar v+\bar u_\perp|^{2\varepsilon}\alpha^{2\varepsilon}}\frac{1}{|u_{||,n^\perp}||u_{||,3}|^{1-\varepsilon}}\\
\lesssim_s\ &\int_{\mathbb{R}^3}du_{||}\int\frac{e^{-|u_\perp|^2-|v+u_{||}|^2}\mathrm{d}u_{\perp,n}}{|\bar u_{\perp,n}+\bar v_n|^{4\varepsilon}}\frac{1}{|u_{||,n^\perp}||u_{||,3}|^{1-\varepsilon}}\\
\lesssim_s\ &\int_{\mathbb{R}^3}\mathrm{d}u_{||}\Big\{\int\frac{e^{-|\bar u_{\perp,n}|^2}\mathrm{d}u_{\perp,n}}{|\bar u_{\perp,n}+\bar v_n|^{4\varepsilon}}\Big\}\frac{e^{-|v+u_{||}|^2}}{|u_{||,n^\perp}||u_{||,3}|^{1-\varepsilon}},
\end{aligned}$$

where the inner integral is 1D which is finite and bounded. On the other hand, from the assumption $|u_{||,3}|\leq|\bar u_{||,n^\perp}|$, the outer integral is

$$\begin{aligned}
&\int\frac{e^{-|v+u_{||}|^2}\mathrm{d}\bar u_{||,n^\perp}\mathrm{d}\bar u_{\parallel,n}\mathrm{d}u_{||,3}}{|\bar u_{||,n^\perp}||u_{||,3}|^{1-\varepsilon}}\\
\leq\ &\int\Big\{\int_0^{|\bar u_{||,n^\perp}|}\frac{\mathrm{d}u_{||,3}}{|u_{||,3}|^{1-\varepsilon}}\Big\}\frac{e^{-|\bar v_n+\bar u_{||,n}|^2}e^{-|\bar v_{n^\perp}+\bar u_{||,n^\perp}|^2}}{|\bar u_{||,n^\perp}|}\mathrm{d}\bar u_{||,n^\perp}\mathrm{d}\bar u_{||,n}\\
\leq\ &\iint_{\mathbb{R}^2}\frac{e^{-|\bar v_n+\bar u_{||,n}|^2}e^{-|\bar v_{n^\perp}+\bar u_{||,n^\perp}|^2}}{|\bar u_{||,n^\perp}|}\mathrm{d}\bar u_{||,n^\perp}\mathrm{d}\bar u_{||,n}<\infty.
\end{aligned}$$

In the case of $|\bar v+\bar u_\perp|\geq 1$ we bound the integration as

$$\begin{aligned}
&\int_{\mathbb{R}^3}\int_{\mathbb{R}}\frac{\langle\bar v+\bar u_\perp\rangle^\varepsilon\langle\bar v+\bar u_\perp\rangle^{1-\varepsilon}}{|u_{\parallel,3}|^{\frac{2\varepsilon}{1-2\varepsilon}}|\bar v+\bar u_\perp|^{1-\varepsilon}\alpha^{\frac12-\varepsilon}}\frac{e^{-|\bar u_{\perp,n}|^2}e^{-|v+u_\parallel|^2}}{|u_{\parallel,n^\perp}||u_\parallel+u_\perp|^{1-\kappa}}\mathrm{d}\bar u_{\perp,n}\mathrm{d}u_\parallel\\
\lesssim&\int_{\mathbb{R}^3}\mathrm{d}u_\parallel\int\frac{\langle\bar v_n+\bar u_{\perp,n}\rangle^\varepsilon\langle\bar v_{n^\perp}\rangle^\varepsilon e^{-|\bar u_{\perp,n}|^2}e^{-|v+u_\parallel|^2}}{|u_{\parallel,3}|^{\frac{2\varepsilon}{1-2\varepsilon}}[\bar u_{\perp,n}+\bar v_n]^{2(\frac12-\varepsilon)}|\bar u_{\parallel,n^\perp}|}\mathrm{d}\bar u_{\perp,n}.
\end{aligned}$$

Again $\int_0^{|\bar u_{\parallel,n^\perp}|}\frac{\mathrm{d}u_{\parallel,3}}{|u_{\parallel,3}|^{\frac{2\varepsilon}{1-2\varepsilon}}}\lesssim|\bar u_{\parallel,n^\perp}|^{1-\frac{2\varepsilon}{1-2\varepsilon}}$ and hence the integration is bounded by

$$\langle\bar v_n\rangle^\varepsilon\langle\bar v_{n^\perp}\rangle^\varepsilon\iint\frac{e^{-|\bar u_{\perp,n}|^2}e^{-|\bar v+\bar u_\parallel|^2}}{|\bar u_{\parallel,n^\perp}|^{\frac{2\varepsilon}{1-2\varepsilon}}|\bar u_{\perp,n}+\bar v_n|^{1-2\varepsilon}}\leq\langle\bar v_n\rangle^\varepsilon\langle\bar v_{n^\perp}\rangle^\varepsilon\langle\bar v_{n^\perp}\rangle^{-\frac{2\varepsilon}{1-2\varepsilon}}\langle\bar v_n\rangle^{-(1-2\varepsilon)}\lesssim 1.$$

□

Our main result for 2D specular case is the following.

Theorem A.5. *Assume a stronger cut-off assumption on $q_0(\theta)$ of (A.2)*

$$\Big|\nabla_v q_0(\frac{v-u}{|v-u|}\cdot\omega)\Big|\Big/\Big|\frac{v-u}{|v-u|}\cdot\omega\Big| \lesssim 1. \tag{A.156}$$

Assume $f_0 \in W^{1,\infty}$ with (A.10). Assume that

$$\sup_{0<t\leq T}\{||e^{\theta|v|^2}f(t)||_\infty + ||\partial_{v_3}f(t)||_\infty\} \leq c_{T,\zeta,f_0} < +\infty,$$

then

$$\begin{aligned}&\sup_{0\leq t\leq T}\{||e^{-\varpi\langle\bar{v}\rangle t}\frac{\alpha}{1+|\bar{v}|^2}\nabla_x f(t)||_\infty + ||e^{-\varpi\langle\bar{v}\rangle t}\frac{|\bar{v}|}{\langle\bar{v}\rangle}\sqrt{\alpha}\nabla_v f(t)||_\infty\}\\ &\lesssim_{T,\Omega,L} ||\frac{\alpha^{1/2}}{\langle\bar{v}\rangle}\nabla_{\bar{x}}f_0||_\infty + ||\frac{|\bar{v}|^2}{\langle v\rangle}\nabla_{\bar{v}}f_0||_\infty + ||\partial_{v_3}f||_\infty + P(||e^{\theta|v|^2}f_0||_\infty),\end{aligned}$$

where P is some polynomial. If $f_0 \in C^1$ and the compatibility conditions (A.17) and (A.19) are satisfied, then $f \in C^1$ away from the grazing set γ_0. Furthermore, if $||e^{\theta|v|^2}f_0||_\infty \ll 1$, and $\partial\Omega$ (therefore ξ) is real analytic, then T can be arbitrarily large.

We remark that powers of singularity α and $\sqrt{\alpha}$ are barely missed in 3D case (borderline case).

Proof. We repeat our program in 3D for the simpler 2D case, and we only point out the differences. Lemma A.6 is valid with easy adaptations. The new $\partial_{v_3}f(t)$ estimate follows from taking the v_3 derivative

$$\begin{aligned}&\{\partial_t + v_1\partial_{x_1} + v_2\partial_{x_2}\}\partial_{v_3}f + \nu(F)\partial_{v_3}f\\ &= \Gamma_{\mathrm{gain},v_3}(f,f) + \Gamma_{\mathrm{gain}}(\partial_{v_3}f,f) + \Gamma_{\mathrm{gain}}(f,\partial_{v_3}f) - \nu_{v_3}(\sqrt{\mu}f)f - \nu(\sqrt{\mu}\partial_{v_3}f)f.\end{aligned}$$

Since

$$\begin{aligned}|\nu_{v_3}(\sqrt{\mu}f)f| + |\Gamma_{\mathrm{gain},v_3}(f,f)| &\lesssim P(||e^{\theta|v|^2}f||_\infty),\\ |\nu(\sqrt{\mu}\partial_{v_3}f)f| + |\Gamma_{\mathrm{gain}}(\partial_{v_3}f,f)| &\lesssim P(||e^{\theta|v|^2}f||_\infty)\int\frac{e^{-C|v-u|^2}}{|v-u|^{2-\kappa}}|\partial_{v_3}f(u)|\mathrm{d}u,\end{aligned}$$

and for $(x,v)\in\gamma_-$

$$\partial_{v_3}f(t,x,v) = \partial_{v_3}f(t,x,R_xv),$$

then we follow the proof of Lemma A.6 (similar to $\partial_t f$ proof) to conclude

$$||\partial_{v_3}f(t)||_\infty \lesssim ||\partial_{v_3}f_0||_\infty + P(||e^{\theta|v|^2}f||_\infty).$$

The Velocity lemma (Lemma A.1) is valid with changing v to $\bar{v}$. The non-local to local estimates (A.15) and (A.16) are valid for $0<\kappa\leq 1$ for $\bar{v}=(v_1,v_2)$: In the proof of (A.15) in Lemma A.2, Step 1, the claim (7.60) is valid. *Step 2*, (7.61) and (7.62) is valid with $\alpha(x,\bar{v})$. In Step 3 we define $\tilde{\sigma}_1$ and $\tilde{\sigma}_2$ with changing v to $\bar{v}$. Then (7.64), and (7.66) hold with changing v to $\bar{v}$. We follow the same proof of *Step 4* to bound $\int_0^{t_{\mathbf{b}}(x,\bar{v})}\frac{e^{-l\langle\bar{v}\rangle(t-s)}}{|v|^{2\beta-1}|\xi|^{\beta-\frac{1}{2}}}Z(s,v)\mathrm{d}s$. We use $\frac{1}{|v|}\leq\frac{1}{|\bar{v}|}$ to conclude (A.15). For the proof of (A.16) in Lemma A.2, we use the same time splitting of (A.49) with changing $|v|$ to $|\bar{v}|$. Then all the proofs are followed and we conclude the proof using $\frac{1}{|v|}\leq\frac{1}{|\bar{v}|}$.

The fundamental Theorem A.3 is valid with simpler proof with changing all v to $\bar{v}$. In fact, due to topological advantage, we can use a global chart $x_{||}=\theta$ in $\mathbb{R}^1$ (such as the polar co-ordinates) for the boundary as

$$\eta(x_{||}) = [R(x_{||})\cos x_{||}, R(x_{||})\sin x_{||}],$$

(vector-valued function) with a global ODE for in the polar co-ordinate system near the boundary! The proof of Theorem A.3 follows step by step of the 3D case but with simpler argument without changes of charts. The estimate of $e^{-\varpi\langle v\rangle t}\frac{\alpha}{1+|v|^2}\nabla_x f(t)$ exactly as in 3D case, valid for α. The most delicate part is to estimate $\partial_{v_3}\Gamma_{\mathrm{gain}}(f,f)$, where a weight stronger than $\sqrt{\alpha}$, due to $\beta>1/2$ in (A.16). It is important to know, that we are unable to establish (A.16) in the 2D case with $\beta=1/2$. However, we are able to close the estimate by using additional bounds on $\partial_{v_3}f$.

Basically we follow the *Proof of Theorem A.2* but we use Lemma A.12 when derivatives act on $\bar{V}_{\mathbf{cl}}(s)$ argument of $\Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})(s, X_{\mathbf{cl}}(s), \bar{V}_{\mathbf{cl}}(s), v_3)$.

More precisely we use Lemma A.5 for $\mathbf{e} \in \{x_1, x_2, v_1, v_2\}$

$$
\begin{aligned}
&\mathrm{II}_{\mathbf{e}} \text{ of } (A.123)\\
&= \int_0^t \mathrm{d}s \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1}, t^{\ell})}(s) e^{-\int_s^t \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau}\\
&\quad \times \Big\{ \partial_{\mathbf{e}} \bar{X}_{\mathbf{cl}}(s) \cdot \big[\Gamma_{\text{gain}}(\nabla_{\bar{x}} f^{m-\ell}, f^{m-\ell}) + \Gamma_{\text{gain}}(f^{m-\ell}, \nabla_{\bar{x}} f^{m-\ell})\big](s, \bar{X}_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\\
&\qquad + \partial_{\mathbf{e}} \bar{V}_{\mathbf{cl}}(s) \cdot \nabla_{\bar{v}} \big[\Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})\big](s, \bar{X}_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s)) \Big\}\\
&- \int_0^t \mathrm{d}s \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1}, t^{\ell})}(s) e^{-\int_s^t \sum_j \mathbf{1}_{[t^{j+1},t^j)}(\tau)\nu(F^{m-j})(\tau)\mathrm{d}\tau} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})(s, \bar{X}_{\mathbf{cl}}(s), V_{\mathbf{cl}}(s))\\
&\quad \times \int_s^t \mathrm{d}\tau \sum_{j=0}^{\ell_*(s)} \mathbf{1}_{[t^{j+1},t^j)}(\tau) \Big\{ \partial_{\mathbf{e}} \bar{X}_{\mathbf{cl}}(s) \cdot \nu(\sqrt{\mu} \nabla_{\bar{x}} f^{m-j})(\tau, \bar{X}_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))\\
&\qquad + \int_{\mathbb{R}^3} \partial_{\mathbf{e}} \bar{V}_{\mathbf{cl}}(s) \cdot \nabla_{\bar{v}} B(v-u, \omega) \sqrt{\mu(u)} f^{m-j}(\tau, \bar{X}_{\mathbf{cl}}(\tau), u) \mathrm{d}u \Big\}\\
&- e^{-\int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1},t^{\ell})}(s)\nu(F^{m-\ell})(s)\mathrm{d}s}\, f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \int_0^t \sum_{\ell=0}^{\ell_*(0)} \mathbf{1}_{[t^{\ell+1}, t^{\ell})}(s)\\
&\quad \times \Big\{ \partial_{\mathbf{e}} \bar{X}_{\mathbf{cl}}(s) \cdot \nu(\sqrt{\mu} \nabla_{\bar{x}} f^{m-j})(\tau, \bar{X}_{\mathbf{cl}}(\tau), V_{\mathbf{cl}}(\tau))\\
&\qquad + \int_{\mathbb{R}^3} \partial_{\mathbf{e}} \bar{V}_{\mathbf{cl}}(s) \cdot \nabla_{\bar{v}} B(v-u, \omega) \sqrt{\mu(u)} f^{m-j}(\tau, \bar{X}_{\mathbf{cl}}(\tau), u) \mathrm{d}u \Big\}.
\end{aligned}
$$

We use the crucial lemma (A.20) for the terms containing $\partial_{\bar{v}} \Gamma_{\text{gain}}$ as

$$
\begin{aligned}
&\int_0^t e^{-\varpi\langle v\rangle t} \frac{\alpha(x,\bar{v})}{\langle \bar{v}\rangle^2} |\partial_{\bar{x}} \bar{V}_{\mathbf{cl}}(s)| |\partial_{\bar{v}} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})| \mathrm{d}s\\
&\lesssim \int_0^t e^{-\varpi\langle v\rangle (t-s)} \frac{|\bar{v}|^3 e^{C|\bar{v}||t-s|}}{\langle \bar{v}\rangle^2} |e^{\varpi\langle v\rangle s} \partial_{\bar{v}} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})| \mathrm{d}s\\
&\lesssim \int_0^t e^{-\varpi\langle \bar{v}\rangle (t-s)} |\bar{v}| \mathrm{d}s \times \{ \text{ RHS of } (A.151)\}\\
&\lesssim \frac{1}{\varpi} P(||e^{\theta|v|^2} f_0||_\infty)\{1 + ||\partial_{v_3} f_0||_\infty + \Big|\Big| e^{-\varpi\langle v\rangle s} \frac{|\bar{v}|}{\langle \bar{v}\rangle} \alpha^{1/2} \partial_{\bar{v}} f \Big|\Big|_\infty \}.
\end{aligned}
$$

Similarly

$$
\begin{aligned}
&\int_0^t e^{-\varpi\langle v\rangle t} \frac{\alpha(x,\bar{v})}{\langle \bar{v}\rangle^2} |\partial_{\bar{v}} \bar{V}_{\mathbf{cl}}(s)| |\partial_{\bar{v}} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})| \mathrm{d}s\\
&\lesssim \int_0^t e^{-\varpi\langle v\rangle (t-s)} \frac{|\bar{v}|^2 e^{C|\bar{v}||t-s|}}{\langle \bar{v}\rangle} |e^{\varpi\langle v\rangle s} \partial_{\bar{v}} \Gamma_{\text{gain}}(f^{m-\ell}, f^{m-\ell})| \mathrm{d}s\\
&\lesssim \int_0^t e^{-\varpi\langle \bar{v}\rangle (t-s)} |\bar{v}| \mathrm{d}s \times \{ \text{ RHS of } (A.151)\}\\
&\lesssim \frac{1}{\varpi} P(||e^{\theta|v|^2} f_0||_\infty)\{1 + ||\partial_{v_3} f_0||_\infty + \Big|\Big| e^{-\varpi\langle v\rangle s} \frac{|\bar{v}|}{\langle \bar{v}\rangle} \alpha^{1/2} \partial_{\bar{v}} f \Big|\Big|_\infty \}.
\end{aligned}
$$

For the term containing $\partial_x \bar{V}_{\mathbf{cl}}(s) \cdot \nabla_{\bar{v}} B(v-u, \omega)$ we use (A.156). The estimate for the other terms are same as the proof of Theorem A.2. □

Proposition A.5 (Specular BC)**.** *Assume* $\Omega := \{\bar{x} \in \mathbb{R}^2 : |\bar{x}| < 1\}$ *be 2D disk and* $\xi(\bar{x}) = |\bar{x}|^2 - 1$*. For any* $1 \leq k$ *assume the compatibility conditions for* $0 \leq i \leq k-1$

$$\partial_t^i f_0(x,v) = \partial_t^i f_0(x, R_x v) \quad \text{on } \gamma_-,$$

and for some $x_0 \in \partial\Omega$ and some $u_0 \in \mathbb{R}^3$ with $|u_0| \sim 1$ and $n(x_0)\cdot u_0 = 0$,

$$\int_{\substack{n(x_0)\cdot u_\tau = 0\\ u_\tau \sim u_0}} \mathbf{k}_{f_0}(v,u)\partial_{v_n}\partial_t^k f_0(x_0,u)\mathrm{d}u_\tau > C > 0, \tag{A.157}$$

where $\mathbf{k}_{f_0}$ is defined in (A.136). Then there exists $t>0$ such that if $X_{\mathbf{cl}}(0;t,x,v)\sim x_0$ then for all $v\in\mathbb{R}^3$ we have a blow-up (A.135).

Proof. The crucial ingredients of the proof is a 2D borderline estimate of Theorem A.5 (due to Lemma A.12) and the explicit lower bound of (A.148) in Example 1.

For simplicity we only consider the case of $k=1$. In order to show (A.135) it suffices to show

$$\partial_n\partial_t\Gamma_{\text{gain}}(f,f)(t,x_0,v) - \partial_n\partial_t\nu(\sqrt{\mu}f)f(t,x_0,v) = +\infty. \tag{A.158}$$

This is due to the fundamental theory of calculus

$$\begin{aligned}
&\partial_n\Gamma_{\text{gain}}(f,f)(t,x_0,v) - \partial_n\nu(\sqrt{\mu}f)f(t,x_0,v)\\
=&\partial_n\Gamma_{\text{gain}}(f_0,f_0)(x_0,v) - \partial_n\nu(\sqrt{\mu}f_0)f_0(x_0,v) + \int_0^t \partial_n\partial_s\Gamma_{\text{gain}}(f,f)(s,x_0,v) - \partial_n\partial_s\nu(\sqrt{\mu}f)f(s,x_0,v)\mathrm{d}s,
\end{aligned}$$

where we can choose the initial datum as good as possible.

We decompose

$$\int_{\mathbb{R}^3}\mathbf{k}_{f_0}(v,u)\frac{\partial_t f(t,x-\varepsilon n(x),u) - \partial_t f(t,x,u)}{\varepsilon} = \int_{|n(x)\cdot u|\le\varepsilon} + \underbrace{\int_{\varepsilon\le|n(x)\cdot u|\le 1}}_{\mathbf{II}} + \int_{1\le|n(x)\cdot u|}.$$

By Lemma A.6, the first term is bounded by

$$\int_{|n(x)\cdot u|\le\varepsilon} \lesssim O(1)||\partial_t f||_\infty.$$

Due to (A.138), $1\le|n(x)\cdot u|$ implies $1\lesssim|n(x-\varepsilon n(x))\cdot u|$ for $0\le\varepsilon\ll 1$. Therefore we use Theorem A.5 to bound the third term as

$$\begin{aligned}
\int_{1\le|n(x)\cdot u|} &\lesssim \int e^{\varpi\langle\bar{u}\rangle t}\frac{1+|\bar{u}|^2}{1+\varepsilon|\bar{u}|^2}\mathbf{k}_{f_0}(v,u)\mathrm{d}u \times ||e^{-\varpi\langle\bar{v}\rangle t}\frac{\alpha}{1+|\bar{v}|^2}\partial_t\nabla_{\bar{x}}f(t)||_\infty\\
&\lesssim O_{N,t}(1)||e^{-\varpi\langle\bar{v}\rangle t}\frac{\alpha}{1+|\bar{v}|^2}\partial_t\nabla_{\bar{x}}f(t)||_\infty.
\end{aligned}$$

Now we focus on the second term $\mathbf{II}$. Due to (A.138), $\partial_t f(t,x-\varepsilon rn(x),u)$ is differentiable for all $0\le r\le 1$ and we have (A.139). We further decompose

$$\mathbf{II} = \int_{\varepsilon\le|n(x)\cdot u|\le 1}\int_0^1 \mathbf{k}_{f_0}(v,u)\partial_n\partial_t f(t,x-\varepsilon rn(x),u)\mathrm{d}r\mathrm{d}u = \int_{\substack{\varepsilon\le|u_n|\le 1\\ |u_\tau|\le N}} + \int_{\substack{\varepsilon\le|u_n|\le 1\\ |u_\tau|\ge N}}.$$

Set $x(r) := x-\varepsilon rn(x)$. Now we use (A.123) for the first term and apply Theorem A.5 to the second term ($|u_\tau|\ge N$) to have

$$\begin{aligned}
\mathbf{II} \gtrsim& \int_{\substack{\varepsilon\le|u_n|\le 1\\ |u_\tau|\le N}}\mathrm{d}u\int_0^1\mathrm{d}r\ \mathbf{k}_{f_0}(v,u)\big\{\partial_n\bar{X}_{\mathbf{cl}}(0)\cdot\nabla_{\bar{x}}\partial_t f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0)) + \underbrace{\partial_n\bar{V}_{\mathbf{cl}}(0)\cdot\nabla_{\bar{v}}\partial_t f_0(X_{\mathbf{cl}}(0),V_{\mathbf{cl}}(0))}\big\}\\
&- P(||e^{\theta|v|^2}f_0||_\infty)\int_{\substack{\varepsilon\le|u_n|\le 1\\ |u_\tau|\le N}}\mathrm{d}u\int_0^1\mathrm{d}r\ \mathbf{k}_{f_0}(v,u)\\
&\times\Big\{\int_0^t|\partial_n\bar{X}_{\mathbf{cl}}(s)|\int_{\mathbb{R}^3}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}|\nabla_{\bar{x}}f(s)|\mathrm{d}u\mathrm{d}s + \int_0^t|\partial_n\bar{V}_{\mathbf{cl}}(s)|\int_{\mathbb{R}^3}\frac{e^{-C_\theta|V_{\mathbf{cl}}(s)-u|^2}}{|V_{\mathbf{cl}}(s)-u|^{2-\kappa}}|\nabla_{\bar{v}}f(s)|\mathrm{d}u\mathrm{d}s\\
&\quad+\langle u\rangle^\kappa e^{-\theta|u|^2}\sup_{0\le s\le t}|\partial_n\bar{V}_{\mathbf{cl}}(s;t,x,v)|\Big\}\\
&- O(1)\int_0^1\int_{\varepsilon\le|u_n|\le 1}\frac{e^{-N}}{|u_n|^2+C\varepsilon rN^2}\mathrm{d}u_n\mathrm{d}r.
\end{aligned}$$

We use (A.148) and (A.157) and (A.147) to bound (lower) the underbraced term

$$\begin{aligned}
&\gtrsim \int_0^1 \mathrm{d}r \int_{\varepsilon \leq |u_n| \leq 1} \mathrm{d}u_n \int_{|u_\tau| \leq N} \mathrm{d}u_\tau \frac{t|\bar{u}_\tau|^4}{|u_n|^2 + C\varepsilon r N^2} \mathbf{k}_{f_0}(v,u) \partial_{v_n} \partial_t f_0(X_{\mathbf{cl}}(0), V_{\mathbf{cl}}(0)) \\
&\sim \int_0^1 \mathrm{d}r \int_{\varepsilon \leq |u_n| \leq 1} \mathrm{d}u_n \frac{1}{|u_n|^2 + C\varepsilon r N^2},
\end{aligned}$$

where $X_{\mathbf{cl}}(0) \sim x_0$ and $V_{\mathbf{cl}}(0) \sim u_0$.

Except the underbraced term, all the other terms are bounded, by Theorem A.5 and (A.148) and (A.16),

$$\begin{aligned}
&\gtrsim - \int_{\varepsilon \leq |u_n| \leq 1} \mathrm{d}u_n \int_{|u_\tau| \leq N} \mathrm{d}u_\tau \mathbf{k}_{f_0}(v,u) \frac{t|\bar{u}|^2}{\sqrt{|u_n|^2 + C\varepsilon r N^2}} ||\nabla_{\bar{x}} \partial_t f_0||_\infty \\
&\quad - P(||e^{\theta|v|^2} f_0||_\infty) \int_{\substack{\varepsilon \leq |u_n| \leq 1 \\ |u_\tau| \leq N}} \mathrm{d}u \int_0^1 \mathrm{d}r \; \mathbf{k}_{f_0}(v,u) \int_0^t \int_{\mathbb{R}^3} \frac{|t-s||\bar{u}'|^2(1+|\bar{u}'|^2) e^{\varpi \langle \bar{u}' \rangle s}}{\alpha(X_{\mathbf{cl}}(s), u')^{3/2}} \mathrm{d}u' \mathrm{d}s \\
&\quad - P(||e^{\theta|v|^2} f_0||_\infty) \int_{\substack{\varepsilon \leq |u_n| \leq 1 \\ |u_\tau| \leq N}} \mathrm{d}u \int_0^1 \mathrm{d}r \; \mathbf{k}_{f_0}(v,u) \langle u \rangle^\kappa e^{-\theta|u|^2} \frac{|t||\bar{u}|^4}{|u_n|^2 + C\varepsilon r N^2} \\
&\quad - O(1) \int_0^1 \int_{\varepsilon \leq |u_n| \leq 1} \frac{e^{-N}}{|u_n|^2 + C\varepsilon r N^2} \mathrm{d}u_n \mathrm{d}r \\
&\gtrsim - O_N(1) ||\nabla_x \partial_t f_0||_\infty \ln(\frac{1}{\varepsilon}) - o(1) \int_0^1 \int_{\varepsilon \leq |u_n| \leq 1} \frac{e^{-N}}{|u_n|^2 + C\varepsilon r N^2} \mathrm{d}u_n \mathrm{d}r.
\end{aligned}$$

Collecting the terms and using (A.147)

$$\mathbf{II} \gtrsim \int_0^1 \mathrm{d}r \int_{\varepsilon \leq |u_n| \leq 1} \mathrm{d}u_n \frac{1}{|u_n|^2 + C\varepsilon r N^2} - \ln(\frac{1}{\varepsilon}) \gtrsim_N \frac{1}{\varepsilon} \to +\infty,$$

and $\varepsilon \to 0$ and this proves (A.158). $\square$

Annexe B

Bibliographie

B.1 Autour des systèmes de diffusion croisée (Parties I et II)

[1] H. Amann. Dynamic theory of quasilinear parabolic equations. I. Abstract evolution equations. *Nonlinear Anal.*, 12(9) :895–919, 1988.

[2] H. Amann. Dynamic theory of quasilinear parabolic equations. II. Reaction-diffusion systems. *Differential Integral Equations*, 3(1) :13–75, 1990.

[3] H. Amann. Erratum : "Dynamic theory of quasilinear parabolic systems. III. Global existence" [Math. Z. **202** (1989), no. 2, 219–250 ; MR1013086 (90i :35125)]. *Math. Z.*, 205(2) :331, 1990.

[4] M. Bendahmane, T. Lepoutre, A. Marrocco, and B. Perthame. Conservative cross diffusions and pattern formation through relaxation. *Journal de Mathématiques Pures et Appliquées*, 92(6) :651 – 667, 2009.

[5] N. Boudiba and M. Pierre. Global existence for coupled reaction-diffusion systems. *J. Math. Anal. Appl.*, 250 :1–12, 2000.

[6] L. Boudin, B. Grec, and F. Salvarani. A mathematical and numerical analysis of the Maxwell-Stefan diffusion equations. *Discrete Contin. Dyn. Syst. Ser. B*, 17(5) :1427–1440, 2012.

[7] J. Canizo, L. Desvillettes, and K. Fellner. Improved duality estimates and applications to reaction-diffusion equations. *Communications in Partial Differential Equations*, 39(6) :1185–1204, 2014.

[8] L. Chen and A. Jüngel. Analysis of a parabolic cross-diffusion population model without self-diffusion. *J. Differential Equations*, 224(1) :39–59, 2006.

[9] Y. Chen, C. Tian, and Z. Ling. Cross-diffusion induced turing instability in two-prey one-predator system. arXiv :1501.05708v1.

[10] Y. S. Choi, R. Lui, and Y. Yamada. Existence of global solutions for the Shigesada-Kawasaki-Teramoto model with weak cross-diffusion. *Discrete Contin. Dyn. Syst.*, 9(5) :1193–1200, 2003.

[11] Y. S. Choi, R. Lui, and Y. Yamada. Existence of global solutions for the Shigesada-Kawasaki-Teramoto model with strongly coupled cross-diffusion. *Discrete Contin. Dyn. Syst.*, 10(3) :719–730, 2004.

[12] F. Conforto and L. Desvillettes. Rigorous passage to the limit in a system of reaction-diffusion equations towards a system including cross diffusions. *Commun. Math. Sci*, 12(3) :457–472, 2014.

[13] L. Desvillettes. About entropy methods for reaction-diffusion equations. *Riv. Mat. Univ. Parma*, 7(7) :81–123, 2007.

[14] L. Desvillettes, K. Fellner, M. Pierre, and J. Vovelle. Global existence for quadratic systems of reaction-diffusion. *Adv. Nonlinear Stud.*, 7(3) :491–511, 2007.

[15] L. Desvillettes, T. Lepoutre, and A. Moussa. Entropy, duality, and cross diffusion. *SIAM Journal on Mathematical Analysis*, 46(1) :820–853, 2014.

[16] L. Desvillettes, T. Lepoutre, A. Moussa, and A. Trescases. On the entropic structure of reaction-cross diffusion systems. *Communications in Partial Differential Equations*, 40(9) :1705–1747, 2015.

[17] L. Desvillettes and A. Trescases. New results for triangular reaction cross diffusion system. *Journal of Mathematical Analysis and Applications*, 430 :32–59, 2015.

[18] M. Dreher and A. Jüngel. Compact families of piecewise constant functions in $L^p(0,T;B)$. *Nonlinear Analysis : Theory, Methods & Applications*, 75(6) :3072–3077, 2012.

[19] A. Einstein. *Investigations on the theory of the Brownian movement.* Dover Publications, Inc., New York, 1956. Edited with notes by R. Fürth, Translated by A. D. Cowper.

[20] J. Fontbona and S. Méléard. Non local Lotka-Volterra system with cross-diffusion in an heterogeneous medium. *J. Math. Biol.*, 70(4) :829–854, 2015.

[21] D. Gilbarg and N. S. Trudinger. *Elliptic partial differential equations of second order*, volume 224 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences].* Springer-Verlag, Berlin, second edition, 1983.

[22] M. E. Gilpin and F. J. Ayala. Global models of growth and competition. *Proceedings of the National Academy of Sciences of the United States of America*, 70(12 Pt 1-2), 1973.

[23] M. E. Gilpin and K. E. Justice. Animal dispersion in relation to social behavior. *Nature*, 236(8) :273–303, 1972.

[24] W. Gordon. On the diffeomorphisms of euclidean space. *American Mathematical Monthly*, pages 755–759, 1972.

[25] P. Grisvard. *Elliptic problems in nonsmooth domains*, volume 24 of *Monographs and Studies in Mathematics.* Pitman (Advanced Publishing Program), Boston, MA, 1985.

[26] L. T. Hoang, T. V. Nguyen, and T. V. Phan. Self-diffusion and cross-diffusion equations : $W^{1,p}$-estimates and global existence of smooth solutions. arXiv : 1311.6828.

[27] M. Iida, M. Mimura, and H. Ninomiya. Diffusion, cross-diffusion and competitive interaction. *J. Math. Biol.*, 53(4) :617–641, 2006.

[28] H. Izuhara and M. Mimura. Reaction-diffusion system approximation to the cross-diffusion competition system. *Hiroshima Math. J.*, 38(2) :315–347, 2008.

[29] A. Jüngel. The boundedness-by-entropy principle for cross-diffusion systems. *Nonlinearity*, 28(6) :1963–2001, 2015.

[30] A. Jüngel and N. Zamponi. Boundedness of weak solutions to cross-diffusion systems from population dynamics. *arXiv :1404.6054*, 2014.

[31] A. Jüngel and N. Zamponi. Analysis of degenerate cross-diffusion population models with volume filling. *arXiv preprint arXiv :1502.05617*, 2015.

[32] K. Kuto and Y. Yamada. Multiple coexistence states for a prey-predator system with cross- diffusion. *J. Differ. Equ.*, 197 :315–348, 2004.

[33] O. A. Ladyzhenskaya, V. A. Solonnikov, and N. N. Ural'ceva. *Linear and quasilinear equations of parabolic type*, volume 23 of *Translations of Mathematical Monographs.* Amercian Mathematical Society, Providence, 1968.

[34] Y. Lou and W.-M. Ni. Diffusion, self-diffusion and cross-diffusion. *J. Differential Equations*, 131(1) :79–131, 1996.

[35] Y. Lou, W.-M. Ni, and Y. Wu. On the global existence of a cross-diffusion system. *Discrete Contin. Dynam. Systems*, 4(2) :193–203, 1998.

[36] R. H. Martin, Jr. and M. Pierre. Nonlinear reaction-diffusion systems. In *Nonlinear equations in the applied sciences*, volume 185 of *Math. Sci. Engrg.*, pages 363–398. Academic Press, Boston, MA, 1992.

[37] H. Matano and M. Mimura. Pattern formation in competition-diffusion systems in nonconvex domains. *Publ. Res. Inst. Math. Sci.*, 19(3) :1049–1079, 1983.

[38] M. Mimura. Stationary pattern of some density-dependent diffusion system with competitive dynamics. *Hiroshima Math. J.*, 11(3) :621–635, 1981.

[39] A. Moussa. Some variants of the classical Aubin-Lions lemma. *arXiv :1401.7231*, 2014.

[40] H. Murakawa. A relation between cross-diffusion and reaction-diffusion. *Discrete Contin. Dyn. Syst.*, Ser. S 5(1) :147–158, 2012.

[41] A. Okubo. *Diffusion and ecological problems : mathematical models*, volume 10 of *Biomathematics.* Springer-Verlag, Berlin-New York, 1980. An extended version of the Japanese edition, ıt Ecology and diffusion, Translated by G. N. Parker.

[42] M. Pierre. Weak solutions and supersolutions in L^1 for reaction-diffusion systems. *J. Evol. Equ.*, 3(1) :153–168, 2003. Dedicated to Philippe Bénilan.

[43] M. Pierre and D. Schmitt. Blowup in reaction-diffusion systems with dissipation of mass. *SIAM J. Math. Anal.*, 28(2) :259–269, 1997.

[44] M. A. Pozio and A. Tesei. Global existence of solutions for a strongly coupled quasilinear parabolic system. *Nonlinear Anal.*, 14(8) :657–689, 1990.

[45] N. Shigesada, K. Kawasaki, and E. Teramoto. Spatial segregation of interacting species. *J. Theoret. Biol.*, 79(1) :83–99, 1979.

[46] S.-A. Shim. Uniform boundedness and convergence of solutions to the systems with a single nonzero cross-diffusion. *J. Math. Anal. Appl.*, 279(1) :1–21, 2003.

[47] J. Simon. Compact sets in the space $L^p(0,T;B)$. *Ann. Mat. Pura Appl. (4)*, 146 :65–96, 1987.

[48] A. Trescases. On triangular reaction cross-diffusion systems with possible self-diffusion. *arXiv :1503.07468, soumis*, 2015.

[49] P. V. Tuoc. Global existence of solutions to Shigesada-Kawasaki-Teramoto cross-diffusion systems on domains of arbitrary dimensions. *Proc. Amer. Math. Soc.*, 135(12) :3933–3941 (electronic), 2007.

[50] P. V. Tuoc. On global existence of solutions to a cross-diffusion system. *J. Math. Anal. Appl.*, 343(2) :826–834, 2008.

[51] A. Turing. The chemical basis of morphogenesis. *Philos. Trans. R. Soc*, B 237 :37–72, 1952.

[52] Y. Wang. The global existence of solutions for a cross-diffusion system. *Acta Math. Appl. Sin. Engl. Ser.*, 21(3) :519–528, 2005.

[53] A. Yagi. Global solution to some quasilinear parabolic system in population dynamics. *Nonlinear Anal.*, 21(8) :603–630, 1993.

[54] Y. Yamada. Global solutions for quasilinear parabolic systems with cross-diffusion effects. *Nonlinear Anal.*, 24(9) :1395–1412, 1995.

B.2 Autour de l'équation de Boltzmann (Parties I et III)

[55] K. Aoki, C. Bardos, C. Dogbe, and F. Golse. A note on the propagation of boundary induced discontinuities in kinetic theory. *Math. Models Methods Appl. Sci.*, 11(9) :1581–1595, 2001.

[56] K. Aoki, S. Takata, H. Aikawa, and F. Golse. A rarefied gas flow caused by a discontinuous wall temperature. *Phys. Fluids*, 13(9) :2645–2661, 2001.

[57] L. Arkeryd and A. Heintz. On the solvability and asymptotics of the Boltzmann equation in irregular domains. *Comm. Partial Differential Equations*, 22(11-12) :2129–2152, 1997.

[58] L. Arkeryd and N. Maslova. On diffuse reflection at the boundary for the Boltzmann equation and related equations. *J. Statist. Phys.*, 77(5-6) :1051–1077, 1994.

[59] L. Bernis and L. Desvillettes. Propagation of singularities for classical solutions of the Vlasov-Poisson-Boltzmann equation. *Discrete Contin. Dyn. Syst.*, 24(1) :13–33, 2009.

[60] L. Boudin and L. Desvillettes. On the singularities of the global small solutions of the full Boltzmann equation. *Monatshefte Math.*, 131 :91–108, 2000.

[61] C. Cercignani. On the initial-boundary value problem for the Boltzmann equation. *Arch. Rational Mech. Anal.*, 116(4) :307–315, 1992.

[62] C. Cercignani. *Rarefied gas dynamics*. Cambridge Texts in Applied Mathematics. Cambridge University Press, 2000.

[63] C. Cercignani, R. Illner, and M. Pulvirenti. *The mathematical theory of dilute gases*, volume 106 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1994.

[64] C.-C. Chen, I.-K. Chen, T.-P. Liu, and Y. Sone. Thermal transpiration for the linearized boltzmann equation. *Commun. Pure Appl. Math.*, 60 :147–163, 2007.

[65] L. Desvillettes and C. Villani. On the trend to global equilibrium for spatially inhomogeneous kinetic systems : the Boltzmann equation. *Invent. Math.*, 159(2) :245–316, 2005.

[66] R. Duan, M.-R. Li, and T. Yang. Propagation of singularities in the solutions to the Boltzmann equation near equilibrium. *Math. Models Methods Appl. Sci.*, 18(7) :1093–1114, 2008.

[67] R. Esposito, Y. Guo, C. Kim, and R. Marra. Non-isothermal boundary in the Boltzmann theory and Fourier law. *Comm. Math. Phys.*, 323(1) :177–239, 2013.

[68] L. C. Evans. A survey of entropy methods for partial differential equations. *Bulletin AMS*, 41, 2004.

[69] L. C. Evans and R. F. Gariepy. *Measure theory and fine properties of functions*. Studies in Advanced Mathematics. CRC Press, Boca Raton, FL, 1992.

[70] R. T. Glassey. *The Cauchy problem in kinetic theory*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1996.

[71] F. Golse. De Newton à Boltzmann et Einstein : Validation des modèles cinétiques et de diffusion. In *Séminaire Bourbaki 2013–2014*, pages 1–39. 66ème année. exp. numéro 1083.

[72] J.-P. Guiraud. An H theorem for a gas of rigid spheres in a bounded domain. In *Théories cinétiques classiques et relativistes (Colloq. Internat. Centre Nat. Recherche Sci., No. 236, Paris, 1974)*, pages 29–58. Centre Nat. Recherche Sci., Paris, 1975.

[73] Y. Guo. Singular solutions of the Vlasov-Maxwell system on a half line. *Arch. Rational Mech. Anal.*, 131(3) :241–304, 1995.

[74] Y. Guo. Classical solutions to the Boltzmann equation for molecules with an angular cutoff. *Arch. Ration. Mech. Anal.*, 169(4) :305–353, 2003.

[75] Y. Guo. Decay and continuity of the Boltzmann equation in bounded domains. *Arch. Ration. Mech. Anal.*, 197(3) :713–809, 2010.

[76] Y. Guo, C. Kim, D. Tonon, and A. Trescases. Bv-regularity of the boltzmann equation in non-convex domains. arXiv :1409.0160, soumis.

[77] Y. Guo, C. Kim, D. Tonon, and A. Trescases. Regularity of the boltzmann equation in convex domains. arXiv :1212.1694v4, soumis.

[78] K. Hamdache. Initial-boundary value problems for the Boltzmann equation : global existence of weak solutions. *Arch. Rational Mech. Anal.*, 119(4) :309–353, 1992.

[79] H. J. Hwang and J. J. L. Velázquez. Global existence for the Vlasov-Poisson system in bounded domains. *Arch. Ration. Mech. Anal.*, 195(3) :763–796, 2010.

[80] A. Jüngel. Entropy dissipation methods for nonlinear partial differential equations. *Lecture Notes, Spring School, Bielefeld*, March 2012.

[81] C. Kim. Formation and propagation of discontinuity for Boltzmann equation in non-convex domains. *Comm. Math. Phys.*, 308(3) :641–701, 2011.

[82] S. Mischler. Kinetic equations with Maxwell boundary condition. *Annales scientifiques de l'ENS*, 43(5) :719–760, 2010.

[83] L. Schwartz. *Théorie des Distributions*. Hermann, 1966.

[84] Y. Shizuta and K. Asano. Global solutions of the Boltzmann equation in a bounded convex domain. *Proc. Japan Acad. Ser. A Math. Sci.*, 53(1) :3–5, 1977.

[85] Y. Sone. Thermal creep in rarefied gas. *J. Phys. Soc. Jpn.*, 21 :1836–1837, 1966.

[86] Y. Sone. *Molecular gas dynamics. Theory, techniques, and applications.* Modeling and Simulation in Science, Engineering and Technology., 2007.

[87] S. Ukai. Solutions of the Boltzmann equation. In *Patterns and waves*, volume 18 of *Stud. Math. Appl.*, pages 37–96. North-Holland, Amsterdam, 1986.

[88] S. Ukai and K. Asano. On the initial-boundary value problem of the linearized Boltzmann equation in an exterior domain. *Proc. Japan Acad. Ser. A Math. Sci.*, 56(1) :12–17, 1980.