

CONVERGENCE OF A FINITE VOLUME SCHEME FOR COAGULATION-FRAGMENTATION EQUATIONS

JEAN-PIERRE BOURGADE AND FRANCIS FILBET

ABSTRACT. This paper is devoted to the analysis of a numerical scheme for the coagulation and fragmentation equation. A time explicit finite volume scheme is developed, based on a conservative formulation of the equation. It is shown to converge under a stability condition on the time step, while a first order rate of convergence is established and an explicit error estimate is given. Finally, several numerical simulations are performed to investigate the gelation phenomenon and the long time behavior of the solution.

KEYWORDS. coagulation-fragmentation equation, finite volume method

AMS SUBJECT CLASSIFICATIONS. 65R20, 82C05

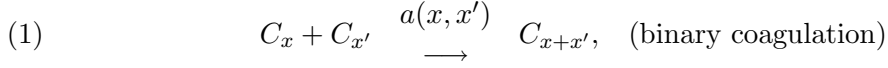
CONTENTS

1. Introduction	1
2. Numerical scheme and main results	4
3. A priori estimates	11
4. Convergence of the numerical solution	18
5. Error estimates on the numerical solution	22
6. Numerical simulations	27
6.1. Detailed balance kernels and convergence to equilibrium	27
6.2. Occurrence of gelation	28
7. Conclusion	31
Acknowledgement	31
References	31

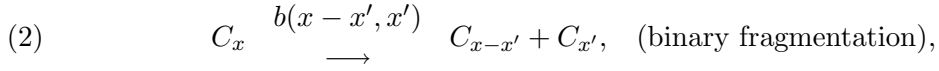
1. INTRODUCTION

Coagulation and fragmentation processes arise in the dynamics of cluster growth and describe the mechanisms by which clusters can coalesce to form larger clusters or break apart into smaller pieces. In the simplest coagulation-fragmentation models the clusters are usually assumed to be fully identified by their size (or volume, or number of particles). The coagulation-fragmentation models we consider in this paper describe the time evolution of the cluster size distribution as the system of clusters undergoes binary coagulation and binary fragmentation events. More precisely, denoting by C_x the clusters of size x

with $x \in \mathbb{R}^+ = (0, \infty)$, the basic reactions taken into account herein are



and



where a and b denote the coagulation and fragmentation rates respectively, and are assumed to depend only on the size of the clusters involved in these reactions.

The dynamics of the density function $f = f(t, x) \geq 0$ of particles with mass $x \in \mathbb{R}^+$, at time $t \geq 0$, subject to coagulation and fragmentation phenomena is governed by the following equation

$$(3) \quad \frac{\partial f}{\partial t} = \mathcal{Q}_c(f) - \mathcal{Q}_f(f),$$

where the coagulation and fragmentation terms are respectively defined by

$$\begin{aligned} \mathcal{Q}_c(f)(x) &= \frac{1}{2} \int_0^x a(x', x-x') f(x') f(x-x') dx' - \int_0^\infty a(x, x') f(x) f(x') dx' \\ \mathcal{Q}_f(f)(x) &= \frac{1}{2} \int_0^x b(x', x-x') dx' f(x) - \int_0^\infty b(x, x') f(x+x') dx'. \end{aligned}$$

The coagulation coefficient, $a = a(x, x')$, characterizes the rate at which the coalescence of two particles with respective volumes x and x' produces a particle of volume $x+x'$, whereas the fragmentation coefficient, $b = b(x, x')$, represents the rate at which the fragmentation of one particle with volume $x+x'$ produces two particles of volume x and x' . Both coefficients a and b are nonnegative symmetric functions and

$$(4) \quad a, b \in L_{loc}^\infty(\mathbb{R}^+ \times \mathbb{R}^+).$$

For symmetric kernels, we observe that during the microscopic coagulation and fragmentation processes, as depicted in equations (1)-(2), the number of particles varies with time while the total mass of particles is conserved.

In terms of f , the total number of particles and the total mass of particles at time $t \geq 0$ are respectively given by

$$M_0(t) := \int_{\mathbb{R}^+} f(t, x) dx, \quad M_1(t) := \int_{\mathbb{R}^+} x f(t, x) dx.$$

For some coefficients a and b , the total mass might not remain constant throughout time evolution. More precisely, if a increases sufficiently rapidly compared to the fragmentation kernel b for large x, x' , then the larger the particles are, the faster they merge. Then a runaway growth takes place, producing particles with “infinite” mass in finite time which are removed from the system. Unlike the local mass in the microscopic picture (1)-(2), the total mass is thereby not conserved, that is, M_1 starts to decrease, a phenomenon usually called the occurrence of gelation.

Writing equation (3) in a “conservative” form, as proposed in [21, 22], enables to describe precisely the time evolution of the total mass. Also, this formulation is particularly well

adapted to a finite volume discretization which, in turn, is expected to give a precise account of mass dissipation or conservation. Precisely, the coagulation and fragmentation terms can be written in divergence form:

$$\begin{cases} x \mathcal{Q}_c(f)(x) = -\frac{\partial \mathcal{C}(f)}{\partial x}(x), \\ x \mathcal{Q}_f(f)(x) = -\frac{\partial \mathcal{F}(f)}{\partial x}(x), \end{cases}$$

where

$$(5) \quad \mathcal{C}(f)(x) := \int_0^x \int_{x-u}^{\infty} u a(u, v) f(u) f(v) dv du, \quad x \in \mathbb{R}^+,$$

$$(6) \quad \mathcal{F}(f)(x) := \int_0^x \int_{x-u}^{\infty} u b(u, v) f(u+v) dv du, \quad x \in \mathbb{R}^+.$$

Then, the coagulation-fragmentation equation reads

$$(7) \quad \begin{cases} x \frac{\partial f}{\partial t} = -\frac{\partial \mathcal{C}(f)}{\partial x} + \frac{\partial \mathcal{F}(f)}{\partial x}, & (t, x) \in (\mathbb{R}^+)^2, \\ f(0, x) = f^{\text{in}}(x), & x \in \mathbb{R}^+ \end{cases}$$

and we assume that the initial datum f^{in} satisfies:

$$(8) \quad f^{\text{in}} \in L^1(\mathbb{R}^+) \cap L^1(\mathbb{R}^+, x dx) \text{ is a nonnegative function.}$$

Here and below, the notation $L^1(\mathbb{R}^+, x dx)$ stands for the space of the Lebesgue measurable real-valued functions on \mathbb{R}^+ which are integrable with respect to the measure $x dx$.

The main purpose of this work is to present a numerical scheme to solve (5)-(7) built upon an explicit Euler discretization with respect to the time variable t and a finite volume discretization with respect to the volume variable x . The analysis of the so-obtained scheme allows to prove the convergence of the discretized particle density towards a solution to the continuous problem. An error estimate on the approximation is given and the scheme is shown to give a first order accurate discretization of the coagulation-fragmentation equation.

Before describing more precisely our results, let us recall that the coagulation and fragmentation equations (5)-(7) have been the object of several studies recently. On the one hand, the relationship between discrete and continuous models has been considered by some authors, see the survey paper [5] and [1]. Their analysis is either performed at a formal level [1] or restricted to a particular fragmentation model (scaling technique [23]). A rigorous setting for the formal analysis performed in [1] under general assumptions on the coagulation and fragmentation coefficients has been given in [16]. Among the various approaches for the approximation of coagulation and fragmentation models, we may distinguish between deterministic and Monte Carlo methods. We refer for instance to [7, 18] for deterministic methods, [2, 6, 13] for stochastic methods, and the references therein. However, there are few results concerning the convergence analysis of numerical methods for coagulation and fragmentation models (see [17] for quasi Monte-Carlo methods).

In Reference [16], the authors obtain as a by-product of their analysis a convergence result for an explicit time discretization. However, note that the main outcome of this study is a deeper understanding of the link between the discrete and continuous Smoluchowski equations, thanks to scaling methods, whereas the present paper is rather focused on the discretization of the continuous Smoluchowski equation itself. To this aim, we use the formulation in divergence form, which is more suitable to design a finite volume scheme, and, unlike the discretization proposed in [16], this scheme is built on non-uniform meshes. Also, while reference [16] gives an analysis for unbounded domains of admissible size values, one of our goals is to assess the reliability of non-conservative truncation methods. Among other features established in this paper, these approximation methods prove to give a faithful picture of long time behaviour as well as of occurrence of gelation.

Indeed, the occurrence of gelation at finite time is a well-known feature of coagulation and fragmentation processes. It has been theoretically established in [14] with a probabilistic approach and in [8, 9] with deterministic arguments. Once gelation is known to occur, a natural question is to determine the gelation time and to investigate the behavior of $f(t)$ at the gelation time, which still constitutes an open problem. In this context, numerical simulations could give some clues on how to solve this problem and, in particular, non-conservative truncation methods of approximations may prove an efficient tool to observe gelation with accuracy.

We now briefly outline the contents of the paper. In the next section, we introduce the numerical approximation of (5)-(7) and state the convergence result which we prove in Sections 3 & 4. In Section 5, we give some error estimates when the mesh is uniform. In the final section (Section 6), some numerical simulations are performed with the numerical scheme presented in Section 2. Long time behaviour and occurrence of gelation are investigated.

2. NUMERICAL SCHEME AND MAIN RESULTS

When designing the volume discretization of the coagulation and fragmentation terms, one is confronted with two somewhat contradictory requirements. First, the coagulation and fragmentation terms should be discretized so as to allow for the simulation of gelation phenomena for instance. But occurrence of gelation depends on the behaviour of kernels a and b for large values of the volume variable x . On the other hand, discretizing these terms makes necessary to truncate the infinite integrals in formulae (5)-(6). But this means restricting the domain of action of kernels a and b to a bounded set of volumes x , that is, preventing coagulation to occur among particles with volume exceeding a fixed value.

The discretization we propose tries to overcome this conflict by using a non-conservative truncation method for the coagulation term. The following truncation has been introduced for the Smoluchowski coagulation equation in [3]. Given a positive real R , let

$$(9) \quad \mathcal{C}_{\text{nc}}^R(f)(x) := \int_0^x \int_{x-u}^R u a(u, v) f(u) f(v) dv du, \quad x \in (0, R).$$

In that case, $\mathcal{C}_{\text{nc}}^R(f)(R) \geq 0$ so that the total mass of the solution is now nonincreasing with respect to time. This approximation is particularly well suited for reproducing the gelation phenomenon [3, 4].

As regards the fragmentation term, the first idea would be to give a “non conservative” truncation as for the coagulation term, according to

$$\mathcal{F}_{\text{nc}}^R(f)(x) := \int_0^x \int_{x-u}^R u b(u, v) f(u + v) dv du, \quad x \in (0, R),$$

where R is, as above, a constant positive parameter. Obviously, if one only considers the solution to the non conservative fragmentation equation, it leads to a time increasing mass for the system. However, it is hard to conclude on the conservativity of the full model when including the coagulation term $-\partial_x \mathcal{C}_{\text{nc}}^R$ since one should have to determine the sign of

$$-\mathcal{C}_{\text{nc}}^R(t, R) + \mathcal{F}_{\text{nc}}^R(t, R), \quad t \geq 0,$$

which is not obvious (in particular, the first term is quadratical in f and depends on a , whereas the second one is linear in f and depends on b).

Possibly the most meaningful truncation is therefore a conservative truncation on the fragmentation term (while a non conservative truncation is performed on the coagulation part). We introduce

$$(10) \quad \mathcal{F}_c^R(f)(x) := \int_0^x \int_{x-u}^{R-u} u b(u, v) f(u + v) dv du.$$

Then, the conservative fragmentation operator satisfies exactly the conservation of total mass, so that the following equation is indeed a non conservative coagulation and fragmentation equation:

$$(11) \quad \begin{cases} x \frac{\partial f_R}{\partial t} = -\frac{\partial \mathcal{C}_{\text{nc}}^R(f_R)}{\partial x}(x) + \frac{\partial \mathcal{F}_c^R(f_R)}{\partial x}(x), & (t, x) \in \mathbb{R}^+ \times (0, R), \\ f(0, x) = f^{\text{in}}(x), & x \in (0, R), \end{cases}$$

since

$$\frac{d}{dt} \int_0^R x f_R(t, x) dx = -\mathcal{C}_{\text{nc}}^R(f_R)(t, R) \leq 0.$$

Convergence for large values of R has been thoroughly studied in the recent past. We briefly mention some results for the coagulation equation (that is, with $b = 0$). These results adapt easily to the coagulation-fragmentation equation but under different assumptions on the kernels.

On the one hand, when $a(x, x')/(x x') \rightarrow 0$ as $x + x' \rightarrow +\infty$, convergence as $R \rightarrow +\infty$ of the solutions to (11) toward a solution of (5)-(7) can be proven by using the approach developed in [16]. First, we observe that the previous growth assumption on $a(x, x')$ does not exclude coagulation coefficients for which the occurrence of gelation takes place. Second, when gelation does not take place, it can be shown that the solutions to (11) converge toward a solution to (5)-(7) satisfying $M_1(t) = M_1(0)$ for $t \geq 0$ (we refer to [11] for a rigorous proof). On the other hand, the convergence of the nonconservative

approximation (11) to the solution of (5)-(7) is valid when $a(x, x') \sim x x'$ for large x, x' [15]. Therefore, this approximation is well-suited for the description of both gelation and mass conservation, despite the qualitatively important gap between these regimes.

Since the convergence of solutions to (11) towards solutions of (5)-(7) is well established in rather general situations, this paper will only focus on the convergence of a sequence built on a numerical scheme towards a solution to the equation (11) *when the truncature R is fixed*. The works we have just mentioned fill in the gap to get a convergence result to solutions to the original problem. In the remainder of the paper, for the sake of clarity, we drop the subscript R and write f instead of f_R for a solution of equation (11). Parameter R being fixed, this should raise no confusion.

Now, we turn to the discretization of equation (11). Having reduced the computation to a bounded interval, the second step is to introduce the time and volume discretizations. To this end, let $h \in (0, 1)$, I^h be a large integer, and denote by $(x_{i-1/2})_{i \in \{0, \dots, I^h\}}$ a mesh of $(0, R)$, where

$$x_{-1/2} = 0, \quad x_i = (x_{i-1/2} + x_{i+1/2})/2, \quad \Delta x_i = x_{i+1/2} - x_{i-1/2} \leq h,$$

and $\Lambda_i^h = [x_{i-1/2}, x_{i+1/2})$ for $i \geq 0$. Moreover, given two integers i and j such that $x_{i+1/2} - x_j \geq 0$, we introduce integer $\gamma_{i,j} \in \{0, \dots, I^h\}$ such that

$$x_{i+1/2} - x_j \in \Lambda_{\gamma_{i,j}}^h.$$

In the general case of a non uniform mesh, we denote by $\delta_h = \min_i \Delta x_i$ and assume that there exists a positive constant (independent of the mesh) K such that

$$(12) \quad \frac{h}{\delta_h} \leq K$$

or, if the mesh has to be excessively refined in some regions (usually close to the origin), we assume that the mesh is increasing, that is

$$(13) \quad \Delta x_i \leq \Delta x_{i+1}, \quad \forall i \in \{0, \dots, I^h - 1\}.$$

Remark 2.1. *In the case of a uniform mesh (that is when $\Delta x_i = h$ for all i), there holds:*

$$x_{i-\frac{1}{2}} = ih, \quad \gamma_{i,j} = i - j.$$

In particular, whenever $x_{j-\frac{1}{2}} < x < x_{j+\frac{1}{2}}$ and $j < i$, we have

$$x_{i+\frac{1}{2}} - x \in \Lambda_{i-j}^h.$$

Let Δt denote the time step and N be a large integer such that $N\Delta t = T$, where $[0, T]$ is the time domain on which the equation is studied. We also define the time interval $\tau_n = [t_n, t_{n+1})$.

The discretization of the coagulation and fragmentation kernels will be detailed at the end of this section. For the time being, we formally set

$$(14) \quad a(u, v) \approx a^h(u, v) = a_{i,j}$$

$$(15) \quad b(u, w - u) \approx b^h(u, w - u) = b_{i,k}$$

for u in Λ_i^h , v in Λ_j^h and w in Λ_k^h , such that $i, j \in \{0, \dots, I^h\}$ and $k \in \{i+1, \dots, I^h\}$ and assume that this defines a suitable approximation of the kernels.

Let us now introduce the numerical scheme itself. For each integer $i \in \{0, \dots, I^h\}$ and each $n \in \{0, \dots, N-1\}$, we define the approximation of $f(t, x)$ for $t \in \tau_n$ and $x \in \Lambda_i^h$ as f_i^n .

The sequence $(f_i^n)_{i,n}$ is defined recursively by the following discretization of the coagulation-fragmentation equation: for $n \in \{1, \dots, N-1\}$, $i \in \{0, \dots, I^h\}$, we set

$$(16) \quad \Delta x_i x_i (f_i^{n+1} - f_i^n) = -\Delta t \left(\mathcal{C}_{i+1/2}^n - \mathcal{C}_{i-1/2}^n \right) + \Delta t \left(\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n \right),$$

where the fluxes $\mathcal{C}_{i+1/2}^n$ and $\mathcal{F}_{i+1/2}^n$ are given by

$$(17) \quad \mathcal{C}_{i+1/2}^n = \sum_{j=0}^i \sum_{k=\gamma_{i,j}}^{I^h} \Delta x_j \Delta x_k x_j a_{j,k} f_j^n f_k^n,$$

$$(18) \quad \mathcal{F}_{i+1/2}^n = \sum_{j=0}^i \sum_{k=i+1}^{I^h} \Delta x_j \Delta x_k x_j b_{j,k} f_k^n,$$

and the initial datum is approached by

$$(19) \quad f_i^{\text{in}} = \frac{1}{\Delta x_i} \int_{\Lambda_i^h} f^{\text{in}}(x) dx, \quad i \in \{0, \dots, I^h\},$$

whereas the fluxes at the boundary are

$$(20) \quad \mathcal{C}_{-1/2}^n = \mathcal{F}_{-1/2}^n = \mathcal{F}_{I^h+1/2}^n = 0, \quad n \in \{0, \dots, N-1\}.$$

This discretization obviously relies on an explicit Euler time discretization and a finite volume approach for the volume variable (see, *e.g.* [10, 19]). This will be even clearer when the discretization of a and b will be given.

We denote by $\chi_{\mathcal{A}}$ the characteristic function of a set \mathcal{A} . The following function f^h defined on $[0, T] \times [0, R]$ will be useful in the sequel.

$$(21) \quad f^h(t, x) = \sum_{n=0}^{N-1} \sum_{i=0}^{I^h} f_i^n \chi_{\tau_n}(t) \chi_{\Lambda_i^h}(x).$$

Note that this function depends on the time and volume steps and that

$$f^h(0, \cdot) = \sum_{i=0}^{I^h} \chi_{\Lambda_i^h}(\cdot) f_i^{\text{in}}$$

converges strongly to f^{in} in $L^1(0, R)$ as h goes to 0.

We may now state our main result.

Theorem 2.2. *Assume that the coagulation and fragmentation kernels satisfy (4) and f^{in} satisfies (8). Moreover, suppose that the volume mesh used in the numerical scheme*

is regular in the sense of assumptions (12) or (13) and that the time step satisfies there exists a positive constant θ such that

$$(22) \quad \max(2, K + 1) C_{T,R} \Delta t \leq \theta < 1,$$

where K is given by (12) and

$$(23) \quad C_{T,R} := \|a\|_{L^\infty} \|f^{in}\|_{L^1} e^{R\|b\|_{L^\infty} T} + R\|b\|_{L^\infty}.$$

Then, up to the extraction of a subsequence,

$$f^h \longrightarrow f \text{ in } L^\infty(0, T; L^1(0, R)),$$

where f is the weak solution to (11) on $[0, T]$ with initial datum f^{in} . More precisely, f is a nonnegative function satisfying

$$(24) \quad \begin{aligned} & \int_0^T \int_0^R x f(t, x) \frac{\partial \varphi}{\partial t}(t, x) + [C_{nc}^R(t, x) - \mathcal{F}_c^R(t, x)] \frac{\partial \varphi}{\partial x}(t, x) dx dt \\ & + \int_0^R x f^{in}(x) \varphi(0, x) dx - \int_0^T C_{nc}^R(t, R) \varphi(t, R) dt = 0, \end{aligned}$$

for all continuously differentiable function φ compactly supported in $[0, T] \times [0, R]$.

Moreover, when the mesh is uniform $\Delta x_i = h$, for all $i \in \{0, \dots, I^h\}$, we get the following error estimate

Theorem 2.3. *Assume that the coagulation and fragmentation kernels satisfy*

$$(25) \quad a, b \in W_{loc}^{1,\infty}(\mathbb{R}^+ \times \mathbb{R}^+).$$

We also assume that f^{in} satisfies

$$(26) \quad f^{in} \in W_{loc}^{1,\infty}(\mathbb{R}^+).$$

We consider a uniform volume mesh and require time step Δt to satisfy condition (22). Then, the following error estimate holds

$$(27) \quad \|f^h - f\|_{L^1} \leq C(T, R) (h + \Delta t),$$

where f is the weak solution to (11) on $[0, T]$ with initial datum f^{in} .

This implies the uniqueness of the limit, and, consequently, that the whole sequence f^h converges under these assumptions.

Of course, these results depend on the definition of a correct approximation of the coagulation and fragmentation kernels. Equations (14) and (15) are now given a precise meaning.

Unless otherwise specified, in the sequel kernels a and b are taken as in (4). On the one hand, the kernel a is approached by a finite volume approximation $a^h(u, v)$ on each space cell: for all $(u, v) \in [0, R] \times [0, R]$,

$$a^h(u, v) = \sum_{i=0}^{I^h} \sum_{j=0}^{I^h} a_{i,j} \chi_{\Lambda_i^h}(u) \chi_{\Lambda_j^h}(v),$$

where $\chi_{\mathcal{A}}$ denotes the characteristic function of set \mathcal{A} and

$$a_{i,j} = \frac{1}{\Delta x_i \Delta x_j} \int_{\Lambda_i^h \times \Lambda_j^h} a(x, y) dx dy.$$

This approximation method is well-known and yields strong convergence in the space of integrable functions provided the kernel a is in $L^1((0, R) \times (0, R))$, which is the case here according to (4)

$$\|a^h - a\|_{L^1} \rightarrow 0, \quad \text{as } h \rightarrow 0.$$

The fragmentation kernel b is discretized in a different way. Indeed, we first notice that b need not be defined on the whole square $[0, R] \times [0, R]$ and that the kernel defined on the compact set

$$\mathcal{D}_b := \{(u, v) \in [0, R] \times [0, R]; \quad 0 \leq u + v \leq R\}$$

can be used to compute the fragmentation term \mathcal{F}_c^R as given in (10). Therefore, all we need is to give an approximation b^h of the kernel b on the compact set \mathcal{D}_b . First, we define the following finite volume approximation of b , for all $(u, v) \in \mathcal{D}_b$,

$$(28) \quad \tilde{b}^h(u, v) = \sum_{i=0}^{I^h} \sum_{j=i+1}^{I^h} \tilde{b}_{i,j} \chi_{\Lambda_i^h}(u) \chi_{\Lambda_j^h}(v+u),$$

with

$$(29) \quad \tilde{b}_{i,j} = \frac{1}{\Delta x_i \Delta x_j} \int_{\Lambda_i^h \times \Lambda_j^h} b(x, y-x) dy dx, \quad 0 \leq i < j \leq I^h.$$

This sequence is particularly well suited to approach $b(u, v-u)$ since, for all $(u, v) \in [0, R] \times [0, R]$ such that $0 \leq u \leq v \leq R$,

$$\tilde{b}^h(u, v-u) = \sum_{i=0}^{I^h} \sum_{j=i+1}^{I^h} \tilde{b}_{i,j} \chi_{\Lambda_i^h}(u) \chi_{\Lambda_j^h}(v)$$

is obviously a finite volume approximation of $b(u, v-u)$. Then, since b is symmetric, one would expect that a good approximation b^h of b should satisfy

$$b^h(u, v) = b^h(v, u),$$

which would translate on the sequence $b_{i,j}$ as:

$$(30) \quad b_{i,j} = b_{j-i,j}.$$

However, this is not true in general and one can prove that, in the case of a more regular kernel b satisfying condition (25) and for a uniform mesh, equality (30) holds true only up to first order terms in h when $b_{i,j} = \tilde{b}_{i,j}$.

This motivates the following definition:

Definition 2.4. *We define the approximate kernel b^h such that*

(i) if the fragmentation b satisfies (4), then an approximation of b is defined by

$$(31) \quad b^h(u, v) = \tilde{b}^h(u, v), \quad \forall (u, v) \in \mathcal{D}_b,$$

where \tilde{b}^h is given by (28) and (29);

(ii) if the fragmentation kernel b satisfies (25) and if the mesh is taken uniform, then one introduces the following approximation of b ,

$$(32) \quad b^h(u, v) = \sum_{i=0}^{I^h} \sum_{j=i+1}^{I^h} b_{i,j} \chi_{\Lambda_i^h}(u) \chi_{\Lambda_j^h}(v+u), \quad \forall (u, v) \in \mathcal{D}_b,$$

where

$$(33) \quad b_{i,j} = \begin{cases} \frac{1}{2} (\tilde{b}_{i,j} + \tilde{b}_{j-i,j}), & i \in \{1, \dots, I^h\}, j \in \{i+1, \dots, I^h\}, \\ \tilde{b}_{0,j}, & i = 0, j \in \{1, \dots, I^h\}. \end{cases}$$

It will be useful to write, conventionally,

$$(34) \quad b_{0,0} = 0.$$

Properties of these approximations are summarized in the following Lemma.

Lemma 2.5. *The approximate kernel b^h given either by (31) or by (32) satisfies the following convergence properties.*

(i) *Let b satisfy (4), then equation (31) defines an approximation of b which converges strongly in the L^1 topology*

$$\|b^h - b\|_{L^1(\mathcal{D}_b)} \rightarrow 0, \quad \text{as } h \rightarrow 0.$$

(ii) *Let b satisfy (25), and take a uniform mesh. Then the approximation of b given by equation (32) converges in the strong topology of L^1 :*

$$\|b^h - b\|_{L^1(\mathcal{D}_b)} \rightarrow 0, \quad \text{as } h \rightarrow 0,$$

and the sequence $b_{i,j}$ defined in (33) satisfies

$$(35) \quad b_{i,j} = b_{j-i,j}, \quad i \in \{1, \dots, I^h\}, j \in \{i+1, \dots, I^h\}.$$

Proof: Strong convergence for the approximation (31) is classical: the proof is close to the convergence proof of the finite volume approximation a^h .

On the other hand, when the kernel b satisfies (25), we can perform a Taylor expansion of b and easily prove that

$$|\tilde{b}_{i,j} - \tilde{b}_{j-i,j}| \leq \|b\|_{W^{1,\infty}} h,$$

which means that up to a first order term with respect to h , the approximation (32) is equal to the approximation (31). Therefore, strong convergence for (31) implies strong convergence for (32) since the first order term in h vanishes asymptotically. \square

Remark 2.6. *It is worth mentioning that property (35) is used only in the proof of Theorem 2.3 to estimate the error between the numerical scheme and the actual solution of (11). In this case, we use approximation (32), take a uniform mesh and assume regularity (25) for b . In contrast, Theorem 2.2 can be proven without appealing to symmetry property (35) and, therefore, can be established under the weaker assumption (4), using approximation (31). Of course, it also holds true under assumption (25) and with approximation (32).*

In the convergence analysis of the numerical scheme, it will be useful to consider point-wise convergence for the coagulation and fragmentation kernels. These convergences hold true up to the extraction of subsequences. Namely, there exists a subfamily of the family \mathbb{R}_*^+ of indices h such that, for almost every $(u, v) \in [0, R] \times [0, R]$ and almost every $(x, y) \in \mathcal{D}_b$,

$$a^h(u, v) \rightarrow a(u, v), \quad b^h(x, y) \rightarrow b(x, y)$$

as h goes to 0. In the remainder of this paper, all sequences will be indexed on this subfamily of indices, so that these almost everywhere convergences can be used.

3. A PRIORI ESTIMATES

In this section, our goal is to prove that the sequence of functions $(f^h)_h$ converges in some sense to a function f as h and Δt go to 0. First, we prove that the solution f^h to the scheme (16)-(19) enjoys properties similar to those of function f given by (11) which we gather in Proposition 3.1 below. Next, we prove the weak convergence of f^h to a function f in $L^1(0, R)$.

The midpoint approximation of a point x is denoted by $X^h(x)$, *i.e.* $X^h(x) = x_i$ for $x \in \Lambda_i^h$, see section 4 for further details.

Proposition 3.1. *Assume the time step satisfies (22). Then, the distribution function f^h is a nonnegative function such that*

$$\int_0^R X^h(x) f^h(t, x) dx \leq \int_0^R X^h(x) f^h(s, x) dx, \quad 0 \leq s \leq t \leq T$$

and, for all $t \in [0, T]$,

$$(36) \quad \int_0^R f^h(t, x) dx \leq \|f^{\text{in}}\|_{L^1} e^{R\|b\|_{L^\infty} t}.$$

Proof: We proceed by induction and first notice that $f^h(0)$ is nonnegative and belongs to $L^1(0, R)$. Assume next that the function $f^h(t^n)$ is nonnegative and

$$(37) \quad \int_0^R f^h(t^n, x) dx \leq \|f^{\text{in}}\|_{L^1} e^{R\|b\|_{L^\infty} t^n}.$$

We start by proving that $f^h(t^{n+1})$ is nonnegative, and first take $i = 0$ since it involves boundary conditions,

$$\begin{aligned} x_0 f_0^{n+1} &= x_0 f_0^n - \frac{\Delta t}{\Delta x_0} \mathcal{C}_{1/2}^n + \frac{\Delta t}{\Delta x_0} \mathcal{F}_{1/2}^n, \\ &\geq \left(1 - \Delta t \sum_{k=0}^{I^h} \Delta x_k a_{0,k} f_k^n \right) x_0 f_0^n. \end{aligned}$$

Then, using condition (22) on the time step with (37), we conclude to the nonnegativity of f_0^{n+1} . For $i \geq 1$, we have

$$x_i f_i^{n+1} = x_i f_i^n - \frac{\Delta t}{\Delta x_i} \left(\mathcal{C}_{i+1/2}^n - \mathcal{C}_{i-1/2}^n \right) + \frac{\Delta t}{\Delta x_i} \left(\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n \right).$$

On the one hand, from the nonnegativity of $f^h(t^n)$, we show that

$$\begin{aligned} -\frac{\mathcal{C}_{i+1/2}^n - \mathcal{C}_{i-1/2}^n}{\Delta x_i} &= -x_i f_i^n \sum_{k=\gamma_{i,i}}^{I^h} \Delta x_k a_{i,k} f_k^n + \sum_{j=0}^{i-1} \sum_{k=\gamma_{i-1,j}}^{\gamma_{i,j}-1} \frac{\Delta x_k}{\Delta x_i} f_k^n \Delta x_j a_{j,k} x_j f_j^n \\ (38) \quad &\geq - \left(\sum_{k=0}^{I^h} \Delta x_k a_{i,k} f_k^n \right) x_i f_i^n. \end{aligned}$$

On the other hand, still using the nonnegativity of $f^h(t^n)$, we get for the discrete fragmentation operator

$$\begin{aligned} \frac{\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n}{\Delta x_i} &= \sum_{k=i+1}^{I^h} \Delta x_k x_i b_{i,k} f_k^n - \sum_{j=0}^{i-1} \Delta x_j b_{j,i} x_j f_j^n \\ (39) \quad &\geq - \left(\sum_{k=0}^{I^h} \Delta x_k b_{k,i} \right) x_i f_i^n. \end{aligned}$$

Then gathering the two inequalities (38) and (39), we get

$$x_i f_i^{n+1} \geq \left(1 - \Delta t \left(\sum_{k=0}^{I^h} \Delta x_k a_{i,k} f_k^n + \sum_{k=0}^{I^h} \Delta x_k b_{k,i} \right) \right) x_i f_i^n.$$

Using condition (22) on the time step and the L^1 -estimate (37) on $f^h(t^n)$, we finally prove that $f^h(t^{n+1})$ is nonnegative.

Next, the time monotonicity of the total mass with respect to time follows at once from the nonnegativity of f^h by summing (16) with respect to i

$$\sum_{i=0}^{I^h} \Delta x_i x_i f_i^{n+1} \leq \sum_{i=0}^{I^h} \Delta x_i x_i f_i^n - \Delta t \mathcal{C}_{I^h+1/2}^n \leq \sum_{i=0}^{I^h} \Delta x_i x_i f_i^n.$$

Now, let us prove that $f^h(t^{n+1})$ enjoys a similar estimate as (37). It follows from (16) that

$$\sum_{i=0}^{I^h} \Delta x_i f_i^{n+1} = \sum_{i=0}^{I^h} \Delta x_i f_i^n - \Delta t \sum_{i=0}^{I^h} \frac{\mathcal{C}_{i+1/2}^n - \mathcal{C}_{i-1/2}^n}{x_i} + \Delta t \sum_{i=0}^{I^h} \frac{\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n}{x_i}.$$

Of course the coagulation term decreases the number of particles ($\mathcal{C}_{i+1/2} \geq 0$, for all i)

$$-\sum_{i=0}^{I^h} \frac{\mathcal{C}_{i+1/2}^n - \mathcal{C}_{i-1/2}^n}{x_i} \leq -\sum_{i=0}^{I^h} \mathcal{C}_{i+1/2}^n \left(\frac{1}{x_i} - \frac{1}{x_{i+1}} \right) \leq 0.$$

For the fragmentation term, we observe that

$$\sum_{i=0}^{I^h} \frac{\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n}{x_i} \leq \sum_{i=0}^{I^h} \Delta x_i \sum_{k=i+1}^{I^h} \Delta x_k b_{i,k} f_k^n,$$

and using the assumption (4) on the kernel b , we finally get

$$\sum_{i=0}^{I^h} \Delta x_i f_i^{n+1} \leq (1 + R \|b\|_{L^\infty} \Delta t) \sum_{i=0}^{I^h} \Delta x_i f_i^n.$$

Thus, using estimate (37) at step n ,

$$\sum_{i=0}^{I^h} \Delta x_i f_i^{n+1} \leq \|f^{\text{in}}\|_{L^1} e^{R \|b\|_{L^\infty} t^{n+1}}.$$

□

We also remark that $f^h(0, \cdot)$ is an approximation of f^{in} , with strong convergence in $L^1(0, R)$. Moreover, the initial datum f^{in} is in $L^1(0, R)$, hence, by the La Vallée Poussin theorem, there exists a nonnegative and convex function Φ continuously differentiable on \mathbb{R}^+ with $\Phi(0) = 0$, $\Phi'(0) = 1$, such that Φ' is concave,

$$\frac{\Phi(r)}{r} \longrightarrow +\infty, \text{ as } r \rightarrow \infty$$

and

$$(40) \quad \int_0^R \Phi(f^{\text{in}})(x) dx < +\infty.$$

Let us now recall an inequality on convex functions.

Lemma 3.2. *Let $\Phi \in C^1(\mathbb{R}^+)$ be convex and such that Φ' is concave, $\Phi(0) = 0$, $\Phi'(0) = 1$, and $\Phi(r)/r \rightarrow +\infty$ as $r \rightarrow +\infty$. Then, for all (x, y) in $\mathbb{R}^+ \times \mathbb{R}^+$,*

$$(41) \quad x \Phi'(y) \leq \Phi(x) + \Phi(y).$$

Next, the following result holds.

Proposition 3.3. *Let $f^{i^n} \in L^1(0, R)$ be nonnegative, and f^h be defined for all h and Δt by (16)-(21) where Δt satisfies (22). Then the family $(f^h)_{(h, \Delta t)}$ is weakly relatively sequentially compact in $L^1((0, T) \times (0, R))$.*

Proof: Based on estimate (40), one can prove a similar estimate on the function f^h , uniformly in h . First, the integral of $\Phi(f^h)$ is clearly related to the sequence f_i^n through

$$\int_0^T \int_0^R \Phi(f^h(t, x)) dx dt = \sum_{n=0}^{N-1} \sum_{i=0}^{I^h} \Delta t \Delta x_i \Phi(f_i^n).$$

From the discrete equation (16), together with the convexity of the function Φ and the nonnegativity of Φ' , it follows

$$\begin{aligned} \sum_{i=0}^{I^h} \Delta x_i [\Phi(f_i^{n+1}) - \Phi(f_i^n)] &\leq \sum_{i=0}^{I^h} \Delta x_i (f_i^{n+1} - f_i^n) \Phi'(f_i^{n+1}) \\ &\leq \|a\|_{L^\infty} \Delta t \sum_{i=0}^{I^h} \sum_{j=0}^{i-1} \Delta x_j f_j^n \sum_{k=\gamma_{i-1, j}}^{\gamma_{i, j}-1} \Delta x_k f_k^n \Phi'(f_i^{n+1}) \\ &\quad + \|b\|_{L^\infty} \Delta t \sum_{i=0}^{I^h} \sum_{k=i+1}^{I^h} \Delta x_i \Delta x_k f_k^n \Phi'(f_i^{n+1}), \end{aligned}$$

where we have used assumption (4) and the fact that $x_j/x_i \leq 1$ whenever $j \leq i$. Then the convexity of Φ together with (41), entails

$$\begin{aligned} &\|a\|_{L^\infty} \Delta t \sum_{i=0}^{I^h} \sum_{j=0}^{i-1} \Delta x_j f_j^n \sum_{k=\gamma_{i-1, j}}^{\gamma_{i, j}-1} \Delta x_k f_k^n \Phi'(f_i^{n+1}) \\ &\leq \|a\|_{L^\infty} \Delta t \sum_{i=0}^{I^h} \sum_{j=0}^{i-1} \Delta x_j f_j^n \sum_{k=\gamma_{i-1, j}}^{\gamma_{i, j}-1} \Delta x_k [\Phi(f_k^n) + \Phi(f_i^{n+1})] \\ &= \|a\|_{L^\infty} \Delta t \sum_{j=0}^{I^h} \Delta x_j f_j^n \sum_{i=j+1}^{I^h} \sum_{k=\gamma_{i-1, j}}^{\gamma_{i, j}-1} \Delta x_k [\Phi(f_k^n) + \Phi(f_i^{n+1})], \end{aligned}$$

and still applying (41) to the fragmentation term, it yields

$$\begin{aligned} &\sum_{i=0}^{I^h} \Delta x_i [\Phi(f_i^{n+1}) - \Phi(f_i^n)] \\ &\leq \|a\|_{L^\infty} \Delta t \sum_{j=0}^{I^h} \Delta x_j f_j^n \sum_{i=j+1}^{I^h} \sum_{k=\gamma_{i-1, j}}^{\gamma_{i, j}-1} \Delta x_k [\Phi(f_k^n) + \Phi(f_i^{n+1})] \\ &\quad + \|b\|_{L^\infty} \Delta t \sum_{i=0}^{I^h} \Delta x_i \sum_{k=i+1}^{I^h} \Delta x_k [\Phi(f_k^n) + \Phi(f_i^{n+1})]. \end{aligned}$$

On the one hand, we have

$$(42) \quad \sum_{i=j+1}^{I^h} \sum_{k=\gamma_{i-1,j}}^{\gamma_{i,j}-1} \Delta x_k \Phi(f_k^n) = \sum_{k=\gamma_{j,j}}^{\gamma_{I^h,j}-1} \Delta x_k \Phi(f_k^n) \leq \sum_{k=0}^{I^h} \Delta x_k \Phi(f_k^n).$$

On the other hand, observing that

$$\sum_{k=\gamma_{i-1,j}}^{\gamma_{i,j}-1} \Delta x_k = x_{\gamma_{i,j}-1/2} - x_{\gamma_{i-1,j}-1/2}$$

and since $x_{\gamma_{i,j}-1/2}$ and $x_{\gamma_{i-1,j}-1/2}$ are defined as left point approximations of $x_{i+1/2} - x_j$ and $x_{i-1/2} - x_j$ respectively, it gives

$$\begin{aligned} x_{\gamma_{i,j}-1/2} - x_{\gamma_{i-1,j}-1/2} &= \left(x_{\gamma_{i,j}-1/2} - x_{i+1/2} \right) - \left(x_{\gamma_{i-1,j}-1/2} - x_{i-1/2} \right) + \Delta x_i \\ &= (x_{i-1/2} - x_j) - x_{\gamma_{i-1,j}-1/2} - \left((x_{i+1/2} - x_j) - x_{\gamma_{i,j}-1/2} \right) + \Delta x_i \\ &\leq (x_{i-1/2} - x_j) - x_{\gamma_{i-1,j}-1/2} + \Delta x_i. \end{aligned}$$

Either assumption (12) or assumption (13) holds, and we get, accordingly,

$$(x_{i-1/2} - x_j) - x_{\gamma_{i-1,j}-1/2} \leq h$$

or

$$(x_{i-1/2} - x_j) - x_{\gamma_{i-1,j}-1/2} \leq \Delta x_i.$$

The latter inequality is a consequence of the fact that the mesh is increasing. In the former case, however, the regularity of the mesh is such that, by (12), one has

$$h \leq K \Delta x_i.$$

Finally, both cases yield

$$x_{\gamma_{i,j}-1/2} - x_{\gamma_{i-1,j}-1/2} \leq M \Delta x_i$$

with $M = 1 + K$ or $M = 2$. Therefore,

$$\sum_{i=j+1}^{I^h} \sum_{k=\gamma_{i-1,j}}^{\gamma_{i,j}-1} \Delta x_k \Phi(f_i^{n+1}) \leq M \sum_{i=0}^{I^h} \Delta x_i \Phi(f_i^{n+1}).$$

Consequently, this result and inequality (42) lead to

$$\begin{aligned} &\sum_{i=0}^{I^h} \Delta x_i [\Phi(f_i^{n+1}) - \Phi(f_i^n)] \\ &\leq \Delta t \|a\|_{L^\infty} \left(\sum_{j=0}^{I^h} \Delta x_j f_j^n \right) \sum_{i=0}^{I^h} \Delta x_i [M \Phi(f_i^{n+1}) + \Phi(f_i^n)], \end{aligned}$$

which entails, as $\|a\|_{L^\infty} \sum \Delta x_j f_j^n$ is bounded by $C_{T,R}$ according to (23) and (36)

$$\begin{aligned} \sum_{i=0}^{I^h} \Delta x_i [\Phi(f_i^{n+1}) - \Phi(f_i^n)] &\leq \Delta t M C_{T,R} \sum_{i=0}^{I^h} \Delta x_i \Phi(f_i^{n+1}) \\ &+ \Delta t C_{T,R} \sum_{i=0}^{I^h} \Delta x_i \Phi(f_i^n). \end{aligned}$$

Finally, it appears that if the time step satisfies (22), a discrete version of Gronwall's lemma gives

$$\int_0^R \Phi(f^h(t, x)) dx \leq e^{\frac{C_{T,R}(1+M)}{1-\theta} t} \int_0^R \Phi(f^{\text{in}}(x)) dx, \quad \forall t \in [0, T]$$

and this estimate allows to conclude to the compactness of the sequence $(f^h)_h$ thanks to the La Vallée Poussin theorem. Indeed, the exponent is uniformly bounded with respect to h and Δt as long as (22) holds true. \square

Remark 3.4. *Proposition 3.3 implies that there exist a function f in $L^1((0, T) \times (0, R))$ and a subsequence of $(f^h)_h$ such that $f^h \rightharpoonup f$ as $h \rightarrow 0$. By a diagonal procedure, one can extract subsequences of $(f^h)_h$, $(a^h)_h$ and $(b^h)_h$ such that*

$$f^h \rightharpoonup f, \quad \text{in the weak topology of } L^1((0, T) \times (0, R)), \quad \text{as } \max\{h, \Delta t\} \rightarrow 0$$

and

$$\begin{aligned} a^h(u, v) &\rightarrow a(u, v), \quad \text{for almost every } (u, v) \in (0, R) \times (0, R), \quad \text{as } h \rightarrow 0, \\ b^h(u, v) &\rightarrow b(u, v), \quad \text{for almost every } (u, v) \in \mathcal{D}_b, \quad \text{as } h \rightarrow 0. \end{aligned}$$

In the sequel, these diagonally extracted subsequences are considered implicitly, unless otherwise specified.

Thus, Proposition 3.3 gives enough information to study the asymptotic behaviour of all terms in equation (16). However, the following lemma recalls a classical tool that will be needed afterwards.

Lemma 3.5. *Let Ω be an open subset of \mathbb{R}^m and let there exist a constant $\kappa > 0$ and two sequences $(v_n)_{n \in \mathbb{N}}$ and $(w_n)_{n \in \mathbb{N}}$ such that $(v_n)_{n \in \mathbb{N}} \in L^1(\Omega)$, $v \in L^1(\Omega)$ and*

$$v_n \rightharpoonup v, \quad \text{weakly in } L^1(\Omega), \quad \text{as } n \rightarrow \infty,$$

$(w_n) \in L^\infty(\Omega)$, $w \in L^\infty(\Omega)$, and for all $n \in \mathbb{N}$, $|w_n| \leq \kappa$ with

$$w_n \rightarrow w, \quad \text{almost everywhere in } \Omega, \quad \text{as } n \rightarrow \infty.$$

Then, $\lim_{n \rightarrow \infty} \|v_n(w_n - w)\|_{L^1(\Omega)} = 0$, and

$$v_n w_n \rightharpoonup v w, \quad \text{weakly in } L^1(\Omega), \quad \text{as } n \rightarrow \infty.$$

Proof: The proof of this classical result in measure theory is based on the Dunford-Pettis and Egorov theorems. \square

All the material required for the convergence proof is now gathered. The following Proposition gives, under additional assumptions on the kernels and on the mesh, some estimates which will prove useful to estimate the error in view of Theorem 2.3.

Proposition 3.6. *Let the coagulation kernel a and fragmentation kernel b satisfy property (4) and let the mesh be regular in the sense of (12) or (13), the time step Δt also satisfies (22).*

Assume that the initial datum f^{in} is bounded in $L_{\text{loc}}^\infty(\mathbb{R}^+)$. Then, the approximate solution f^h and the exact solution f to (11) are essentially bounded in $(0, T) \times (0, R)$

$$\|f^h\|_{L^\infty((0,T)\times(0,R))} \leq C(T, R), \quad \|f\|_{L^\infty((0,T)\times(0,R))} \leq C(T, R).$$

Moreover, if the kernels a and b satisfy (25) and the initial datum f^{in} satisfies the smoothness condition (26). Then, there exists a positive constant $C(T, R)$ such that

$$(43) \quad \|f(t)\|_{W^{1,\infty}(0,R)} \leq C(T, R),$$

where f is the exact solution to (11).

Proof: We prove *a priori* boundedness for the solution f to the continuous equation (11) only. The proof in the discrete case is similar to the one for the nonnegativity of f^h . Integrating equation (11) with respect to time gives

$$\begin{aligned} f(t, x) &= f^{\text{in}}(x) + \int_0^t -\frac{1}{x} \frac{\partial \mathcal{C}^R}{\partial x}(s, x) + \frac{1}{x} \frac{\partial \mathcal{F}^R}{\partial x}(s, x) ds \\ &\leq f^{\text{in}}(x) + \frac{1}{2} \int_0^t \int_0^x a(x', x - x') f(s, x') f(s, x - x') dx' ds \\ &\quad + \int_0^t \int_x^R b(x' - x, x) f(s, x') dx' ds \\ &\leq f^{\text{in}}(x) + \|b\|_{L^\infty} \|f\|_{\infty,1} t + \frac{\|a\|_{L^\infty}}{2} \|f\|_{\infty,1} \int_0^t \sup_{y \in (0,R)} f(s, y) dx, \end{aligned}$$

where $\|f\|_{\infty,1}$ denotes the norm of f in $L^\infty(0, T; L^1(0, R))$. Then, Gronwall's lemma enables to conclude the proof.

We turn to the proof of estimate (43). First, we integrate equation (11) with respect to time, divide it by x and next differentiate it with respect to volume variable x (using formulae (9) and (10) for the coagulation and fragmentation terms). Then, taking the

maximum value over all possible values of x , it yields

$$\begin{aligned} \left\| \frac{\partial f}{\partial x}(t) \right\|_{L^\infty} &= \left\| \frac{\partial f^{\text{in}}}{\partial x} \right\|_{L^\infty} + \left\{ \frac{3}{2} \|a\|_{W^{1,\infty}} \|f\|_{\infty,1} \|f\|_{L^\infty} + \frac{1}{2} \|a\|_{L^\infty} \|f\|_{L^\infty}^2 \right. \\ &\quad \left. + \frac{3}{2} \|b\|_{L^\infty} \|f\|_{L^\infty} + \|b\|_{W^{1,\infty}} \left(\|f\|_{\infty,1} + \frac{1}{2} R \|f\|_{L^\infty} \right) \right\} t \\ &\quad + \frac{3}{2} (\|a\|_{L^\infty} \|f\|_{\infty,1} + \|b\|_{L^\infty}) \int_0^t \left\| \frac{\partial f}{\partial x}(s) \right\|_{L^\infty} ds \end{aligned}$$

and, again Gronwall's lemma allows to conclude. \square

Note that, in this proof, $f \in L^\infty(0, T; L^1(0, R))$ has been extensively used. Indeed, Theorem 2.2 gives this information under the same (or weaker) assumptions as those made in Proposition 3.6. We underline that, of course, Theorem 2.2 is proven independently of this Proposition.

4. CONVERGENCE OF THE NUMERICAL SOLUTION

Proving Theorem 2.2 is achieved by interpreting the sequence f_i^n built from the numerical scheme as a sequence of step functions f^h depending on the mesh size h and on Δt . Properties (in particular weak compactness) of this sequence have been stated in details in the previous section. The proof is now reduced to writing the discrete coagulation and fragmentation operators in terms of f^h and proving (weak) convergence for these expressions towards the continuous coagulation and fragmentation operators (5)-(6). This is provided by Lemma 4.1 below. Then usual finite volumes techniques allow to conclude.

The following notations will be used throughout the analysis of the numerical scheme. First, several point approximations are defined:

$$\begin{aligned} X^h : x \in (0, R) &\rightarrow X^h(x) = \sum_{i=0}^{I^h} x_i \chi_{\Lambda_i^h}(x), \quad (\text{midpoint approximation}) \\ \Xi^h : x \in (0, R) &\rightarrow \Xi^h(x) = \sum_{i=0}^{I^h} x_{i+1/2} \chi_{\Lambda_i^h}(x), \quad (\text{right endpoint approximation}) \\ \xi^h : x \in (0, R) &\rightarrow \xi^h(x) = \sum_{i=0}^{I^h} x_{i-1/2} \chi_{\Lambda_i^h}(x), \quad (\text{left endpoint approximation}) \end{aligned}$$

and

$$\Theta^h : (x, u) \in (0, R)^2 \rightarrow \Theta^h(x, u) = \sum_{i=0}^{I^h} \sum_{j=0}^i x_{\gamma_{i,j}} \chi_{\Lambda_i^h}(x) \chi_{\Lambda_j^h}(u).$$

At this stage, note that $(X^h)_h$, $(\Xi^h)_h$ and $(\Theta^h)_h$ converge pointwisely: for all $x \in (0, R)$,

$$X^h(x) \rightarrow x, \quad \Xi^h(x) \rightarrow x,$$

as $h \rightarrow 0$ and for all $(x, u) \in (0, R)^2$, we have

$$\begin{cases} \Theta^h(x, u) \rightarrow x - u & \text{if } x \geq u, \\ \Theta^h(x, u) \rightarrow 0 & \text{if } x \leq u. \end{cases}$$

Then, the proof of Theorem 2.2 is based on the following Lemma.

Lemma 4.1. *Let us define the approximations of the coagulation and fragmentation terms according to:*

$$\begin{aligned} \mathcal{C}^h(t, x) &= \int_0^R \int_0^R \chi_{[0, \Xi^h(x)]}(u) \chi_{[\Theta^h(x, u), R]}(v) X^h(u) a^h(u, v) f^h(t, u) f^h(t, v) dv du \\ \mathcal{F}^h(t, x) &= \int_0^R \int_0^R \chi_{[0, \Xi^h(x)]}(u) \chi_{[\Xi^h(x) - u, R - u]}(v) X^h(u) b^h(u, v) f^h(t, u + v) dv du. \end{aligned}$$

There exists a subsequence of $(f^h)_h$, such that

$$\begin{aligned} \mathcal{C}^h &\rightharpoonup \mathcal{C}_{nc}^R \text{ in } L^1((0, T) \times (0, R)), \quad \text{as } h \rightarrow 0, \\ \mathcal{F}^h &\rightharpoonup \mathcal{F}_{nc}^R \text{ in } L^1((0, T) \times (0, R)), \quad \text{as } h \rightarrow 0. \end{aligned}$$

In addition, $\mathcal{C}^h(\cdot, R)$ converges weakly to $\mathcal{C}_{nc}^R(\cdot, R)$ in $L^1(0, T)$.

Proof: We consider the sequences $(f^h)_h$, $(a^h)_h$ and $(b^h)_h$ extracted according to the procedure sketched in Remark 3.4. Then, obviously for all $(t, x) \in (0, T) \times (0, R)$ and almost all $(u, v) \in (0, R) \times (0, R)$, the sequence $X^h(\cdot) a^h(\cdot, v)$ is bounded in $L^\infty(0, R)$ and

$$\chi_{[0, \Xi^h(x)]}(u) \chi_{[\Theta^h(x, u), R]}(v) X^h(u) a^h(u, v) \rightarrow \chi_{[0, x]}(u) \chi_{[x - u, R]}(v) u a(u, v),$$

as h goes to 0. Thus, applying Lemma 3.5, it yields

$$\begin{aligned} &\int_0^R \chi_{[0, \Xi^h(x)]}(u) \chi_{[\Theta^h(x, u), R]}(v) X^h(u) a^h(u, v) f^h(t, u) du \\ (44) \quad &\rightarrow \int_0^x \chi_{[x - u, R]}(v) u a(u, v) f(t, u) du \end{aligned}$$

for each t, x , and almost every v . The same argument is used to prove the pointwise convergence of \mathcal{C}^h . Indeed, for each x and t and for almost every v (44) holds true, and since f^h converges weakly, Lemma 3.5 applies again and gives:

$$\mathcal{C}^h(t, x) \rightarrow \mathcal{C}_{nc}^R(t, x)$$

for every $(t, x) \in [0, T] \times [0, R]$. This pointwise convergence obviously implies weak convergence for \mathcal{C}^h and for the boundary value $\mathcal{C}^h(\cdot, R)$.

The convergence study of \mathcal{F}^h is similar to that of \mathcal{C}^h , observing that

$$\mathcal{F}^h(t, x) = \int_0^R \int_0^R \chi_{[0, \Xi^h(x)]}(u) \chi_{[\Xi^h(x), R]}(v) X^h(u) b^h(u, v - u) f^h(t, v) dv du$$

and recalling that $b^h(u, v - u)$ converges to $b(u, v - u)$ for almost every $0 \leq u \leq v \leq R$. \square

To make the importance of this Lemma clear, it may be useful to mention that $\mathcal{C}^h(t, x)$ (*resp.* $\mathcal{F}^h(t, x)$) actually coincide with \mathcal{C}_i^n (*resp.* \mathcal{F}_i^n) whenever $t \in \tau_n$ and $x \in \Lambda_i^h$. This will be proven in the sequel.

Now, we turn to the proof of Theorem 2.2. We consider a test function $\varphi \in C^1([0, T] \times [0, R])$, which is compactly supported. On the one hand, we observe that, for Δt small enough, the support of φ with respect to the time variable satisfies $\text{Supp}_t \varphi \subset [0, t_{N-1}]$. On the other hand, we define the finite volume (in time) and left endpoint (in space) approximation of φ on $\tau_n \times \Lambda_i^h$ by

$$\varphi_i^n := \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \varphi(t, x_{i-1/2}) dt.$$

Then, multiplying equation (16) by φ_i^n and summing over $n \in \{0, \dots, N-1\}$ and $i \in \{0, \dots, I^h\}$, yields by a discrete integration by parts

$$(45) \quad \begin{aligned} & \sum_{n=0}^{N-1} \sum_{i=0}^{I^h} \Delta x_i x_i f_i^{n+1} (\varphi_i^{n+1} - \varphi_i^n) + \sum_{n=0}^{N-1} \sum_{i=0}^{I^h-1} \Delta t \left[\mathcal{C}_{i+1/2}^n - \mathcal{F}_{i+1/2}^n \right] (\varphi_{i+1}^n - \varphi_i^n) \\ & + \sum_{i=0}^{I^h} \Delta x_i x_i f_i^{\text{in}} \varphi_i^0 - \sum_{n=0}^{N-1} \Delta t \mathcal{C}_{I^h+1/2}^n \varphi_{I^h}^n = 0, \end{aligned}$$

where the boundary and initial value properties (19)-(20) have been used. The first and third terms in the left hand side of equation (45) can be written in terms of function f^h :

$$(46) \quad \begin{aligned} & \sum_{n=0}^{N-1} \sum_{i=0}^{I^h} \Delta x_i x_i f_i^{n+1} (\varphi_i^{n+1} - \varphi_i^n) + \sum_{i=0}^{I^h} \Delta x_i x_i f_i^{\text{in}} \varphi_i^0 \\ & = \sum_{n=0}^{N-1} \sum_{i=0}^{I^h} \int_{\tau_{n+1}} \int_{\Lambda_i^h} X^h(x) f^h(t, x) \frac{\varphi(t, \xi^h(x)) - \varphi(t - \Delta t, \xi^h(x))}{\Delta t} dx dt \\ & + \sum_{i=0}^{I^h} \int_{\Lambda_i^h} X^h(x) f^h(0, x) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(t, \xi^h(x)) dt dx \\ & = \int_{\Delta t}^T \int_0^R X^h(x) f^h(t, x) \frac{\varphi(t, \xi^h(x)) - \varphi(t - \Delta t, \xi^h(x))}{\Delta t} dx dt \\ & + \int_0^R X^h(x) f^h(0, x) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(t, \xi^h(x)) dt dx \end{aligned}$$

We first treat the last term of the former equality. On the one hand, $X^h(x)$ converges pointwise in $[0, R]$ whereas $f^h(0, \cdot)$ is a finite volume approximation of f^{in} and, henceforth, converges strongly in $L^1(0, R)$. On the other hand, since φ is continuously differentiable with compact support, its derivatives are bounded and, therefore, the following convergence is *uniform* with respect to t, x as $\max\{h, \Delta t\}$ goes to 0:

$$\frac{1}{\Delta t} \int_0^{\Delta t} \varphi(t, \xi^h(x)) dt \rightarrow \varphi(0, x).$$

Consequently, it first yields

$$\int_0^R X^h(x) f^h(0, x) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(t, \xi^h(x)) dt dx \rightarrow \int_0^R x f^{\text{in}}(x) \varphi(0, x) dx,$$

as $\max\{h, \Delta t\}$ goes to 0.

To deal with the first term in (46), a Taylor expansion of the smooth function φ is performed, which finally yields

$$\frac{\varphi(t, \xi^h(x)) - \varphi(t - \Delta t, \xi^h(x))}{\Delta t} \rightarrow \frac{\partial \varphi}{\partial t}(t, x)$$

uniformly as $\max\{h, \Delta t\}$ goes to 0, while $\chi_{[\Delta t, T]}(t) X^h(x)$ converges pointwise to $\chi_{[0, T]}(t) x$. Applying Lemma 3.5, together with Proposition 3.3, entails that the first term on the right hand side of (46) converges to

$$\int_0^T \int_0^R x f(t, x) \frac{\partial \varphi}{\partial t}(t, x) dx dt$$

as $\max\{h, \Delta t\}$ goes to 0.

Consider now the coagulation and fragmentation terms. As mentioned above, the approximations \mathcal{C}^h and \mathcal{F}^h coincide with the discrete coagulation and fragmentation terms. Indeed, on the one hand, for $t \in \tau_n$ and $x \in \Lambda_i^h$,

$$\begin{aligned} \mathcal{C}^h(t, x) &= \int_0^{x_{i+1/2}} \int_{\Theta^h(x, u)}^R X^h(u) a^h(u, v) f^h(t, u) f^h(t, v) dv du \\ &= \sum_{j=0}^i \int_{\Lambda_j^h} du \sum_{k=\gamma_{i,j}}^{I^h} \int_{\Lambda_k^h} dv x_j a_{j,k} f_j^n f_k^n \\ &= \mathcal{C}_{i+1/2}^n, \end{aligned}$$

where we have used that, for $x \in \Lambda_i^h$ and $u \in \Lambda_j^h$, $\Theta^h(x, u) = x_{\gamma_{i,j}}$. On the other hand, for the fragmentation operator

$$\begin{aligned} \mathcal{F}^h(t, x) &= \int_0^{x_{i+1/2}} \int_{x_{i+1/2}}^R X^h(u) b^h(u, v - u) f^h(t, v) dv du \\ &= \sum_{j=0}^i \int_{\Lambda_j^h} du \sum_{k=i+1}^{I^h} \int_{\Lambda_k^h} dv x_j b_{j,k} f_k^n \\ &= \mathcal{F}_{i+1/2}^n. \end{aligned}$$

Consequently, it is straightforward to write the second and fourth terms of the left hand side of equation (45) in terms of \mathcal{C}^h and \mathcal{F}^h :

$$\begin{aligned}
& \sum_{n=0}^{N-1} \sum_{i=0}^{I^h-1} \Delta t \left[\mathcal{C}_{i+1/2}^n - \mathcal{F}_{i+1/2}^n \right] (\varphi_{i+1}^n - \varphi_i^n) - \sum_{n=0}^{N-1} \Delta t \mathcal{C}_{I^h+1/2}^n \varphi_{I^h}^n \\
= & \sum_{n=0}^{N-1} \sum_{i=0}^{I^h-1} \int_{\tau_n} \int_{\Lambda_i^h} \left[\mathcal{C}_{i+1/2}^n - \mathcal{F}_{i+1/2}^n \right] \frac{1}{\Delta x_i} (\varphi(t, x_{i+1/2}) - \varphi(t, x_{i-1/2})) dx dt \\
& - \sum_{n=0}^{N-1} \int_{\tau_n} \mathcal{C}_{I^h+1/2}^n \varphi(t, R - \Delta x_{I^h}) dt \\
= & \int_0^T \int_0^{R-\Delta x_{I^h}} \left[\mathcal{C}^h(t, x) - \mathcal{F}^h(t, x) \right] \frac{\partial \varphi}{\partial x}(t, x) dx dt \\
& - \int_0^T \mathcal{C}^h(t, R) \varphi(t, R - \Delta x_{I^h}) dt.
\end{aligned}$$

Therefore, the weak compactness result given by Lemma 4.1 implies the convergence of the right hand side of the latter equality to the corresponding terms in (24), as expected.

5. ERROR ESTIMATES ON THE NUMERICAL SOLUTION

The error estimate is performed by giving a priori estimates on the difference $f^h - f$, where f^h is built thanks to the numerical scheme and f is the exact solution to (11). The difference $f^h - f$ is obviously a solution to the difference of equations (16) and (11) respectively divided by x_i and x . A mere integration by parts enables to give to equation (11) divided by x a convenient form. Lemma 5.1 shows that summations by parts can yield a similar result in the discrete case. Then, estimating the difference $f^h - f$ is easy thanks to Proposition 3.6.

When the mesh is uniform, that is $\Delta x_i = h$ for all $i \in \{0, \dots, I^h\}$, the discrete coagulation and fragmentation terms read

$$(47) \quad - \frac{\mathcal{C}_{i+\frac{1}{2}}^n - \mathcal{C}_{i-\frac{1}{2}}^n}{h} = h \sum_{j=0}^{i-1} x_j a_{j,i-j-1} f_j^n f_{i-j-1}^n - h \sum_{j=0}^{I^h} x_i a_{i,j} f_i^n f_j^n,$$

$$(48) \quad \frac{\mathcal{F}_{i+\frac{1}{2}}^n - \mathcal{F}_{i-\frac{1}{2}}^n}{h} = -h \sum_{j=0}^{i-1} x_j b_{j,i} f_i^n + h \sum_{j=i+1}^{I^h} x_i b_{i,j} f_j^n.$$

The following Lemma gives a simplified expression of these variation rates.

Lemma 5.1. *Assume that a and b satisfy (4) and (25) respectively and consider a uniform mesh, that is, $\Delta x_i = h$ for all i . We also assume that the initial datum f^{in} is bounded in*

$L^\infty(\mathbb{R}^+)$. Let $(s, x) \in \tau_n^h \times \Lambda_i^h$, with $n \in \{0, \dots, N-1\}$, $i \in \{0, \dots, I^h\}$. Then

$$(49) \quad -\frac{\mathcal{C}_{i+\frac{1}{2}}^n - \mathcal{C}_{i-\frac{1}{2}}^n}{x_i h} = \frac{1}{2} \int_0^{\xi^h(x)} a^h(x', x - \Xi^h(x')) f^h(s, x') f^h(s, x - \Xi^h(x')) dx' \\ - \int_0^R a^h(x, x') f^h(s, x') dx' f^h(s, x) + \varepsilon_c^h(x)$$

$$(50) \quad \frac{\mathcal{F}_{i+\frac{1}{2}}^n - \mathcal{F}_{i-\frac{1}{2}}^n}{x_i h} = -\frac{1}{2} \int_h^{\xi^h(x)} b^h(x', x - x') dx' f^h(s, x) \\ + \int_{\Xi^h(x)}^R b^h(x, x' - x) f^h(s, x') dx' + \varepsilon_f^h(x),$$

where ε_c^h and ε_f^h denote first order terms with respect to h in the strong L^1 topology:

$$(51) \quad \|\varepsilon_c^h\|_{L^1} \leq \frac{R}{4} \|f^h\|_{L^\infty}^2 \|a\|_{L^\infty} h$$

$$(52) \quad \|\varepsilon_f^h\|_{L^1} \leq \left(\frac{R}{2} \|f^h\|_{L^\infty} + \|f^h\|_{\infty,1} \right) \|b\|_{L^\infty} h.$$

Proof: First, the variation rates have to be written in such a way that the volume x_i is factored out. To this aim, we consider for instance the fragmentation term: since the mesh is uniform, there holds $x_{i+\frac{1}{2}} - x_j = x_{i-j}$ and we have, for $i \geq 1$,

$$-h \sum_{j=1}^{i-1} x_j b_{j,i} f_i^n = h \sum_{j=1}^{i-1} x_{i-j} b_{j,i} f_i^n - x_{i+\frac{1}{2}} h \sum_{j=1}^{i-1} b_{j,i} f_i^n \\ = h \sum_{j=1}^{i-1} x_j b_{i-j,i} f_i^n - x_{i+\frac{1}{2}} h \sum_{j=1}^{i-1} b_{j,i} f_i^n.$$

Thus, using the symmetry property (35) of $b_{i,j}$

$$-h \sum_{j=1}^{i-1} x_j b_{j,i} f_i^n = h \sum_{j=1}^{i-1} x_j b_{j,i} f_i^n - x_{i+\frac{1}{2}} h \sum_{j=1}^{i-1} b_{j,i} f_i^n,$$

which finally gives

$$h \sum_{j=1}^{i-1} x_j b_{j,i} f_i^n = \frac{h}{2} x_{i+\frac{1}{2}} \sum_{j=1}^{i-1} b_{j,i} f_i^n,$$

and for (48)

$$\frac{\mathcal{F}_{i+\frac{1}{2}}^n - \mathcal{F}_{i-\frac{1}{2}}^n}{h x_i} = h \left[-\frac{x_0}{x_i} b_{0,i} f_i^n - \frac{x_{i+\frac{1}{2}}}{x_i} \frac{1}{2} \sum_{j=1}^{i-1} b_{j,i} f_i^n + \sum_{j=i+1}^{I^h} b_{i,j} f_j^n \right] \\ = h \left[-\frac{x_0}{x_i} b_{0,i} f_i^n - \frac{h}{4x_i} \sum_{j=1}^{i-1} b_{j,i} f_i^n - \frac{1}{2} \sum_{j=1}^{i-1} b_{j,i} f_i^n + \sum_{j=i+1}^{I^h} b_{i,j} f_j^n \right]$$

since $x_{i+\frac{1}{2}} = x_i + \frac{h}{2}$. We have used convention (34), so that $b_{0,i}$ is equal to zero whenever $i = 0$. We define

$$\varepsilon_f^h(x) = -h \frac{x_0}{x_i} b_{0,i} f_i^n - \frac{h^2}{4x_i} \sum_{j=1}^{i-1} b_{j,i} f_j^n$$

and then get (50). Moreover, estimating the x integral of this term is equivalent to estimating the following sum

$$h \sum_{i=0}^{I^h} \left| h \frac{x_0}{x_i} b_{0,i} f_i^n + \frac{h^2}{4x_i} \sum_{j=1}^{i-1} b_{j,i} f_j^n \right|.$$

The first term in this sum is bounded if one remarks that $x_0/x_i \leq 1$ while the second one is bounded by noting that

$$\frac{h^2}{4x_i} \sum_{j=1}^{i-1} b_{j,i} \leq h \|b\|_{L^\infty} \frac{(i-1)h}{4x_i} \leq \frac{h}{4} \|b\|_{L^\infty}.$$

Hence, applying Proposition 3.6, the approximate solution is bounded in L^∞ and estimate (52) easily follows.

Now, turning to equation (47) and remarking that $x_{i-\frac{1}{2}} - x_j = x_{i-j-1}$, we similarly prove that

$$-\frac{\mathcal{C}_{i+\frac{1}{2}}^n - \mathcal{C}_{i-\frac{1}{2}}^n}{x_i h} = \frac{x_{i-\frac{1}{2}}}{2x_i} h \sum_{j=0}^{i-1} a_{j,i-j-1} f_j^n f_{i-j-1}^n - h \sum_{j=0}^{I^h} a_{i,j} f_i^n f_j^n,$$

which gives expression (49) by setting

$$\varepsilon_c^h(x) = -\frac{h^2}{4x_i} \sum_{j=0}^{i-1} a_{j,i-j-1} f_j^n f_{i-j-1}^n$$

and the estimate (51) is obtained in the same way as (52). \square

Therefore, both terms (51) and (52) have to be compared to the explicit formulation of the continuous coagulation and fragmentation terms

$$(53) \quad -\frac{1}{x} \frac{\partial \mathcal{C}^R}{\partial x}(t, x) = \frac{1}{2} \int_0^x a(x', x-x') f(t, x') f(t, x-x') dx' \\ - \int_0^R a(x, x') f(t, x') dx' f(t, x),$$

$$(54) \quad \frac{1}{x} \frac{\partial \mathcal{F}^R}{\partial x}(t, x) = -\frac{1}{2} \int_0^x b(x', x-x') dx' f(t, x) + \int_x^R b(x, x'-x) f(t, x') dx'.$$

Using formulae (49), (50), (53) and (54), equation (11) and the scheme (16), we easily get for $t \in \tau_n$,

$$(55) \quad \int_0^R \left| f^h(t, x) - f(t, x) \right| dx \leq \int_0^R \left| f^h(0, x) - f^{\text{in}}(x) \right| dx + \sum_{\alpha=1}^4 \left[\mathcal{E}_{c,\alpha}^h + \mathcal{E}_{f,\alpha}^h \right] + \mathcal{E}_{t,n}^h + \|\varepsilon_c^h\|_{L^1} + \|\varepsilon_f^h\|_{L^1},$$

where $(\mathcal{E}_{c,\alpha}^h)_{\alpha=1,\dots,4}$ are error terms related to the coagulation operator

$$\begin{aligned} \mathcal{E}_{c,1}^h &= \frac{1}{2} \int_0^t \int_0^R \int_0^{\xi^h(x)} \left| a^h(x', x - \Xi^h(x')) f^h(s, x') f^h(s, x - \Xi^h(x')) \right. \\ &\quad \left. - a(x', x - \Xi^h(x')) f(s, x') f(s, x - \Xi^h(x')) \right| dx' dx ds \\ \mathcal{E}_{c,2}^h &= \frac{1}{2} \int_0^t \int_0^R \int_0^{\xi^h(x)} \left| a(x', x - \Xi^h(x')) f(s, x') f(s, x - \Xi^h(x')) \right. \\ &\quad \left. - a(x', x - x') f(s, x') f(s, x - x') \right| dx' dx ds \\ \mathcal{E}_{c,3}^h &= \frac{1}{2} \int_0^t \int_0^R \int_{\xi^h(x)}^x a(x', x - x') f(s, x') f(s, x - x') dx' dx ds \end{aligned}$$

and

$$\mathcal{E}_{c,4}^h = \int_0^t \int_0^R \int_0^R \left| a^h(x, x') f^h(s, x) f^h(s, x') - a(x, x') f(s, x) f(s, x') \right| dx' dx ds,$$

whereas $(\mathcal{E}_{f,\alpha}^h)_{\alpha=1,\dots,4}$ are error terms related to the fragmentation operator

$$\begin{aligned} \mathcal{E}_{f,1}^h &= \frac{1}{2} \int_0^t \int_0^R \int_h^{\xi^h(x)} \left| b^h(x', x - x') f^h(s, x) - b(x', x - x') f(s, x) \right| dx' dx ds \\ \mathcal{E}_{f,2}^h &= \frac{1}{2} \int_0^t \int_0^R \int_{[0,h] \cup [\xi^h(x), x]} b^h(x', x - x') f^h(s, x) dx' dx ds \\ \mathcal{E}_{f,3}^h &= \int_0^t \int_0^R \int_{\Xi^h(x)}^R \left| b^h(x, x' - x) f^h(s, x') - b(x, x' - x) f(s, x') \right| dx' dx ds \end{aligned}$$

and

$$\mathcal{E}_{f,4}^h = \int_0^t \int_0^R \int_x^{\Xi^h(x)} b^h(x, x' - x) f^h(s, x') dx' dx ds.$$

Finally, $\mathcal{E}_{t,n}^h$ is the error due to the time discretization:

$$\begin{aligned} \mathcal{E}_{t,n}^h &= \int_{t_n}^t \left\{ \int_0^R \left[\frac{1}{2} \int_0^{\xi^h(x)} a^h(x', x - \Xi^h(x')) f^h(s, x') f^h(s, x - \Xi^h(x')) dx' \right. \right. \\ &+ \int_0^R a^h(x, x') f^h(s, x) f^h(s, x') dx' + \varepsilon_c^h(x) + \frac{1}{2} \int_h^{\xi^h(x)} b^h(x', x - x') f^h(s, x) dx' \\ &\left. \left. + \int_{\Xi^h(x)}^R b^h(x, x' - x) f^h(s, x') dx' + \varepsilon_f^h(x) \right] dx \right\} ds. \end{aligned}$$

On the one hand, the error given by $\mathcal{E}_{c,2}^h$ is estimated from the smoothness of the kernel a and of the solution f to (11). Indeed, since in this section a is taken in $W_{loc}^{1,\infty}$, we have for all $x \in (0, R)$ and $x' \in \Lambda_i^h$

$$|a(x', x - x_i) - a(x', x - x')| \leq \|a\|_{W^{1,\infty}} h$$

and applying Proposition 3.6, the $W^{1,\infty}$ estimate (43) on f gives

$$|f(t, x - x_i) - f(t, x - x')| \leq \|f(t, \cdot)\|_{W^{1,\infty}} h$$

Thus, it yields

$$(56) \quad \mathcal{E}_{c,2}^h \leq \frac{R^2}{4} \|f\|_\infty \left(\|a\|_{W^{1,\infty}} \|f\|_\infty + \|a\|_{L^\infty} \|f\|_{L^\infty(W^{1,\infty})} \right) t h.$$

On the other hand, we consider the terms $\mathcal{E}_{c,3}^h$, $\mathcal{E}_{f,2}^h$ and $\mathcal{E}_{f,4}^h$ which are all integrals on a domain of size $t R h$. Then L^∞ bounds on f and f^h give

$$(57) \quad \mathcal{E}_{c,3}^h \leq \|a\|_{L^\infty} \|f\|_{L^\infty}^2 t R h$$

and

$$(58) \quad \mathcal{E}_{f,2}^h + \mathcal{E}_{f,4}^h \leq 2 \|b\|_{L^\infty} \|f^h\|_{L^\infty} t R h.$$

The error due to the time discretization is treated similarly and it is easily seen that

$$(59) \quad \mathcal{E}_{t,n}^h \leq 2 \left\{ R^2 \|f^h\|_{L^\infty}^2 \|a\|_{L^\infty} + R^2 \|f^h\|_{L^\infty} \|b\|_{L^\infty} + \|\varepsilon_c^h\|_{L^1} + \|\varepsilon_f^h\|_{L^1} \right\} \Delta t$$

since $|t - t_n| \leq \Delta t$.

Finally, we turn to the estimation of terms $\mathcal{E}_{c,1}^h$, $\mathcal{E}_{c,4}^h$, $\mathcal{E}_{f,1}^h$ and $\mathcal{E}_{f,3}^h$. A detailed calculation is given for $\mathcal{E}_{c,1}^h$. Estimations for the other terms are obtained by using similar arguments and details are left to the reader to check. First we perform a change of variable $x \rightarrow y = x - \Xi^h(x')$ and split $\mathcal{E}_{c,1}^h$ into three parts:

$$\begin{aligned} \mathcal{E}_{c,1}^h &\leq \frac{1}{2} \int_0^t \int_0^R \int_0^R \left| a^h(x', y) - a(x', y) \right| f(s, x') f(s, y) dx' dy ds \\ &+ \frac{1}{2} \int_0^t \int_0^R \int_0^R a^h(x', y) \left| f^h(s, x') - f(s, x') \right| f(s, y) dx' dy ds \\ &+ \frac{1}{2} \int_0^t \int_0^R \int_0^R a^h(x', y) f^h(s, x') \left| f^h(s, y) - f(s, y) \right| dx' dy ds. \end{aligned}$$

Thus, it yields,

$$(60) \quad \begin{aligned} \mathcal{E}_{c,1}^h &\leq (t R^2 \|f\|_{L^\infty}^2 \|a\|_{W^{1,\infty}}) \frac{h}{2} \\ &+ \frac{R}{2} \|a\|_{L^\infty} \left(\|f^h\|_{L^\infty} + \|f\|_{L^\infty} \right) \int_0^t \|f^h(s) - f(s)\|_{L^1} ds. \end{aligned}$$

Similarly,

$$(61) \quad \begin{aligned} \mathcal{E}_{c,4}^h &\leq (t R^2 \|f\|_{L^\infty}^2 \|a\|_{W^{1,\infty}}) \frac{h}{2} \\ &+ \frac{R}{2} \|a\|_{L^\infty} \left(\|f^h\|_{L^\infty} + \|f\|_{L^\infty} \right) \int_0^t \|f^h(s) - f(s)\|_{L^1} ds. \end{aligned}$$

and

$$(62) \quad \begin{aligned} \mathcal{E}_{f,1}^h + \mathcal{E}_{f,3}^h &\leq 2 (t R^2 \|f\|_{L^\infty} \|b\|_{W^{1,\infty}}) h \\ &+ 2 R \|b\|_{L^\infty} \int_0^t \|f^h(s) - f(s)\|_{L^1} ds. \end{aligned}$$

Finally, using (55) and gathering estimates (56)-(62), we conclude thanks to Gronwall's lemma that

$$\|f^h - f\|_{L^\infty(0,T;L^1(0,R))} \leq C(T, R) \left\{ \|f^h(0, \cdot) - f^{\text{in}}\|_{L^1(0,R)} + (h + \Delta t) \right\}.$$

To get estimate (27), one only has to remember that f^{in} is taken in $W_{loc}^{1,\infty}$, so that the finite volume approximation of the initial datum by $f^h(0, \cdot)$ is actually of order 1 in L^1 with respect to h .

6. NUMERICAL SIMULATIONS

This section is devoted to the numerical study of two different phenomena: the convergence to equilibrium under the detailed balance condition and the gelation phenomenon, that is, the possible loss of matter during time evolution.

6.1. Detailed balance kernels and convergence to equilibrium. We assume that the coagulation and fragmentation coefficients fulfil the detailed balance condition: there exists a nonnegative function $M \in L^1_+(\mathbb{R}^+ \times \mathbb{R}^+)$, such that

$$(63) \quad a(x, x') M(x) M(x') = b(x, x') M(x + x'), \quad (x, x') \in \mathbb{R}^+ \times \mathbb{R}^+.$$

Observe that this condition implies that M is a stationary solution to (7), usually referred to as an equilibrium. An additional and interesting consequence of the detailed balance condition (63) is the existence of a Lyapunov functional H given by

$$H(f) := \int_{\mathbb{R}^+} f(t, x) \left(\log \left(\frac{f(t, x)}{M(x)} \right) - 1 \right).$$

Indeed, any positive solution f of the coagulation-fragmentation equation satisfies

$$\begin{aligned} \frac{d}{dt}H(f) &= -\frac{1}{2} \int_{\mathbb{R}^+ \times \mathbb{R}^+} (a(x, x') f(t, x) f(t, x') - b(x, x') f(t, x + x')) \\ &\quad (\log(a(x, x') f(t, x) f(t, x')) - \log(b(x, x') f(t, x + x'))) dx dx' \\ &\leq 0. \end{aligned}$$

Since any such solution f decays the Lyapunov functional, convergence of f towards the equilibrium state M is expected. The first series of results proposed in this section is concerned with the observation of this trend to equilibrium. We choose kernels a and b as follows:

$$a(x, x') = b(x, x') = (x x')^{1/2},$$

so that

$$M(x) = \exp(-x), \quad x \in \mathbb{R}^+.$$

As an initial datum, we take

$$f^{\text{in}}(x) = \begin{cases} 2, & \text{if } 0 \leq x \leq 1, \\ 0, & \text{else.} \end{cases}$$

with $R = 30$, $\Delta t = 0.004$.

From a numerical point of view, some care is needed to compute the small x -behavior of the stationary state, taking into account that it also depends on its values for large x . Therefore, it is important to consider a suitable mesh in order to obtain an accurate numerical solution when x is small but also for large x . We construct the following mesh:

$$x_{i-1/2} = \begin{cases} e^{-6 + \frac{7i}{N}} & \text{for } 0 \leq i \leq N, \\ e + (R - e) \left(\frac{i - N}{N} \right)^{3/2} & \text{for } N + 1 \leq i \leq 2N, \end{cases}$$

with $N = 25, 50, 100$ and 200 . This mesh satisfies the condition (13) and is extremely refined in the region close to the origin in order to describe with a lot of accuracy the solution in this region. On the other hand, the mesh Δx_i is increasing for large x in order to use a large enough truncature $R = 30$ with few points.

In Figure 1, we report the evolution of the total number of particles M_0 , the second moment of f , the Lyapunov functional $H(f)$ and the behavior of the asymptotic profile $f(+\infty, x)$. As expected, the total mass $M_1(t)$ remains constant throughout time evolution and the moments stabilize to a fixed value. As regards the asymptotic profile, our numerical results are in fair agreement with the equilibrium $M(x) = \exp(-x)$, even when using few points ($N = 25$). Moreover, in view of the comparison between the exact steady state and the numerical solution for large time, we observe that using a non uniform mesh allows to get a very good approximation in the region close to zero.

6.2. Occurrence of gelation. As already mentioned in the introduction, when the coagulation coefficient a increases sufficiently rapidly for large x, x' , a runaway growth takes place and leads to the formation of a particle of “infinite mass” in finite time. Since no such particle is taken into account in (7), some matter escapes from the system of particles

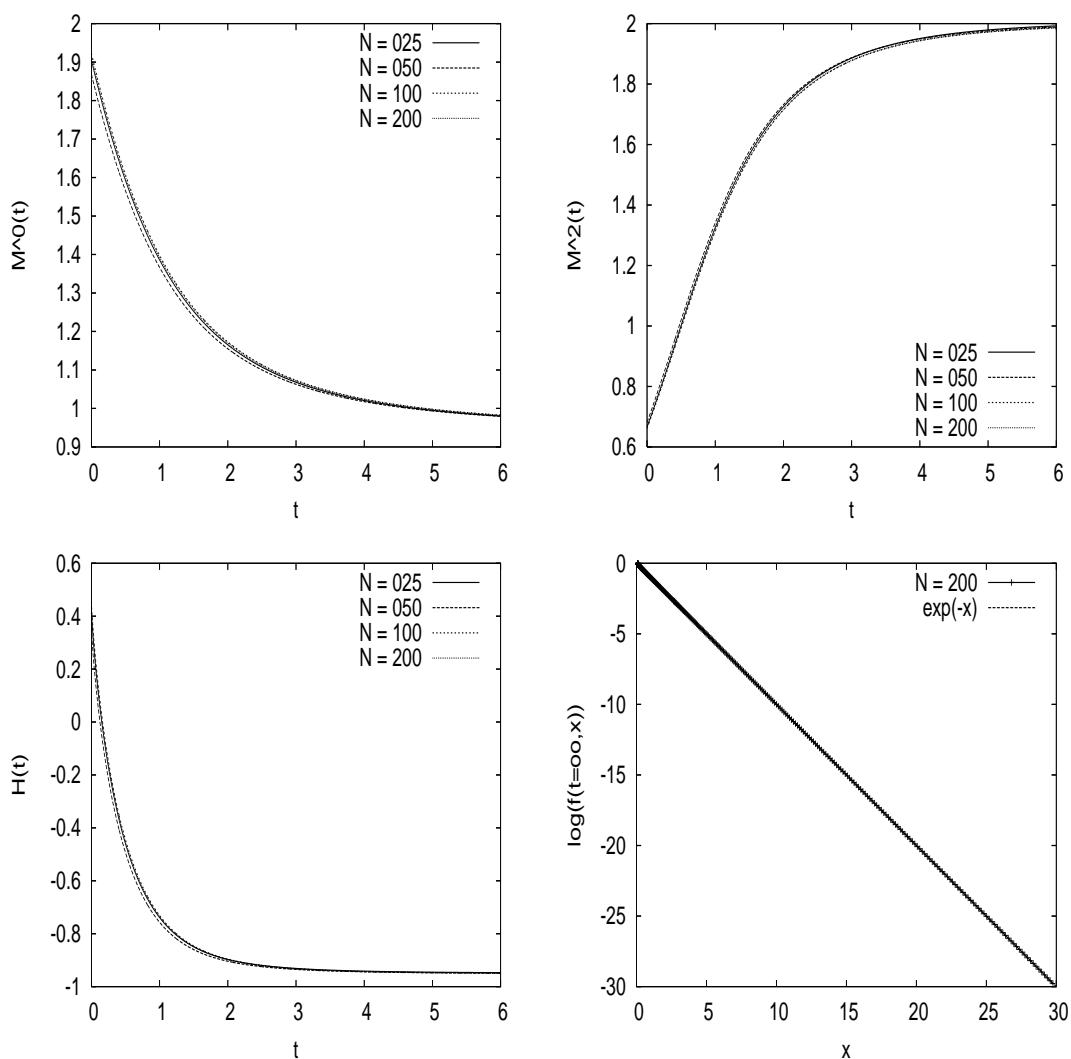


FIGURE 1. Evolution of the total number of particles M_0 , the second moment of f , the functional $H(f)$ and the stationary distribution $f(x)$ in log scale.

described by the density distribution function f . As a consequence, the total mass M_1 decreases with time, and the gelation time T_{gel} is defined by

$$(64) \quad T_{gel} := \inf \left\{ t \geq 0, \int_0^\infty x f(t, x) dx < \int_0^\infty x f(0, x) dx \right\} \in [0, +\infty].$$

Then we say that gelation occurs if $T_{gel} < +\infty$.

An elementary proof that $T_{gel} < +\infty$ was given in [20] when $a(x, x') = x x'$, and a central issue in the physical literature in the eighties was to figure out for which coagulation

coefficients a the gelation time T_{gel} is finite. We restrict our discussion here to the model case

$$(65) \quad a(x, x') = x^\mu (x')^\nu + x^\nu (x')^\mu, \quad b(x, x') = (x + x')^\gamma, \quad (x, x') \in (\mathbb{R}^+)^2,$$

with $0 \leq \mu \leq \nu \leq 1$ and $\gamma \in \mathbb{R}$. Putting $\lambda = \mu + \nu$, it follows from [9, Theorem 3.1] that there is a mass-conserving solution to (7) for any initial datum with a finite first order moment when $\gamma > \lambda - 2$. On the other hand, when $\gamma \in ((\lambda - 3)/2, \lambda - 2)$, it is proven in [9, Theorem 1.2] that gelation occurs when the initial first moment M_1 is large while there should be mass-conserving solutions when M_1 is small enough. Finally, gelation should occur for every non-zero solution when $\gamma < (\lambda - 3)/2$ [9, Section A.1].

We have first performed several computations to confirm the fact that the non conservative truncation allows to approximate as well mass-conserving solutions ($\gamma > \lambda - 2$) as gelation phenomenon ($\gamma < (\lambda - 3)/2$). In these situations, the long time behaviour does not depend on the initial mass, but only on the relative proportion of coagulation and fragmentation phenomena. Not surprisingly, the solution is well approached by the scheme in this case and we prefer to give a detailed account of the more delicate situation where the long time behaviour strongly depends on the initial mass. Thus, the main purpose of the numerical simulations presented in this section is to observe numerically the intermediate regime $\gamma \in ((\lambda - 3)/2, \lambda - 2)$, which is, due to the dependence with respect to the initial datum, the most difficult to study.

We restrict ourselves here to the model case (65) with $\mu = \nu = \lambda/2$; that is,

$$a(x, x') = (x x')^{\lambda/2}, \quad b(x, x') = (x + x')^\gamma, \quad (x, x') \in (\mathbb{R}^+)^2,$$

with $\lambda = 5/2$ and $\gamma = 0$. We take the following initial datum f_0 :

$$(66) \quad f_0(x) = M_1 \exp(-x), \quad x \in \mathbb{R}^+.$$

Thus, the gelation phenomenon does take place when the initial mass M_1 is large enough and $T_{gel} < +\infty$ (see [9, Theorem 1.2]) and the authors conjecture that for a small initial mass M_1 , there is a mass-conserving solution.

In Figure 2, we present our results for an initial mass $M_1 = 0.4$ and observe that gelation occurs at finite time ($T_{gel} \simeq 1$). We see that the choice of the truncation (9), (10) and the scheme (16)-(21) provide a good estimate of the gelation phenomenon.

Next, the moments $M_\ell(t)$ are expected to blow up as $t \rightarrow T_{gel}$ for $\ell \geq 2$. We compute numerical approximations of the solution to (7) with initial datum (66) for increasing values of the truncation parameter R . We define the moment of order $\ell \geq 0$ of the numerical approximation by

$$\mathcal{M}_\ell^h(t^n) = \sum_{i=0}^{I^h} \Delta x_i x_i^\ell f_i^n,$$

and we plot the time evolution of the moments of order 1, 2, and 3 (see Figure 2). It is clear that the gelation transition takes place in finite time and that there is a sudden growth of the moments of order 2 and 3 near the numerical gelation time. In particular, the growth rate increases for increasing values of R , which is seemingly a good evidence for occurrence of blow-up. The fact that these moments decrease after the numerical

gelation time is due to the finite length of the interval of computation $(0, R)$. Indeed, due to the non conservative approximation, the amount of mass $\mathcal{F}_{I^{h+1/2}}^n$ is lost and high order moments then start to decrease with time.

On the other hand, we perform other computations (see Figure 3) for a small initial mass $M_1 = 0.25$ and observe that in this case the solution is mass-conserving. Moreover, the numerical solution converges as time goes to infinity to an equilibrium (note that the detailed balance condition is not valid for these kernels a and b (65)): there are two different regimes in this case, the solution first spreads out and next concentrates itself to reach a steady state (see last pictures of Figure 3).

7. CONCLUSION

This paper provides an extensive study of a discrete approximation of coagulation and fragmentation equations. The scheme first introduced for the discretization to the coagulation-fragmentation equation in [12] proves unexpectedly efficient in the description of gelation as well as long time behaviour of solutions to this model. In particular, it should be emphasized that mass conservation or dissipation is obtained in strong agreement with theoretical works.

The discretization is based on a divergence formulation, which (in association with the finite volume method) makes it well adapted to the observation of the time evolution of the total mass. Finally, numerical results seem to indicate the validity and the flexibility of the present approach that, to our opinion, will make deterministic schemes much more competitive with Monte Carlo methods in several situations for coagulation and fragmentation models.

ACKNOWLEDGEMENT

The first author wishes to thank N. Mauser for providing him the best possible scientific and human conditions to complete this work. He also wants to thank, for financial support, the Austrian Ministry of Science (BM:BWK) via its grant for the Wolfgang Pauli Institute, the Austrian Science Foundation (FWF) via the START Project (Y-137-TEC) of N. Mauser, and the European network HYKE funded by the EC as contract HPRN-CT-2002-00282.

REFERENCES

- [1] M. AIZENMAN AND T.A. BAK, *Convergence to equilibrium in a system of reacting polymers*, Comm. Math. Phys. **65** (1979), pp. 203–230.
- [2] H. BABOVSKY, *On a Monte Carlo scheme for Smoluchowski's coagulation equation*, Monte Carlo Methods Appl., **5** (1999), pp. 1–18.
- [3] T. A. BAK AND O. HEILMANN, *A finite version of Smoluchowski's coagulation equation*, J. Phys. A, **24** (1991), pp. 4889–4893.
- [4] F. P. DA COSTA, *A finite-dimensional dynamical model for gelation in coagulation processes*, J. Non-linear Sci., **8** (1998), pp. 619–653.
- [5] R. L. DRAKE, *A general mathematical survey of the coagulation equation*, in Topics in Current Aerosol Research (Part 2), International Reviews in Aerosol Physics and Chemistry, Pergamon Press, Oxford, UK, (1972), pp. 203–376.

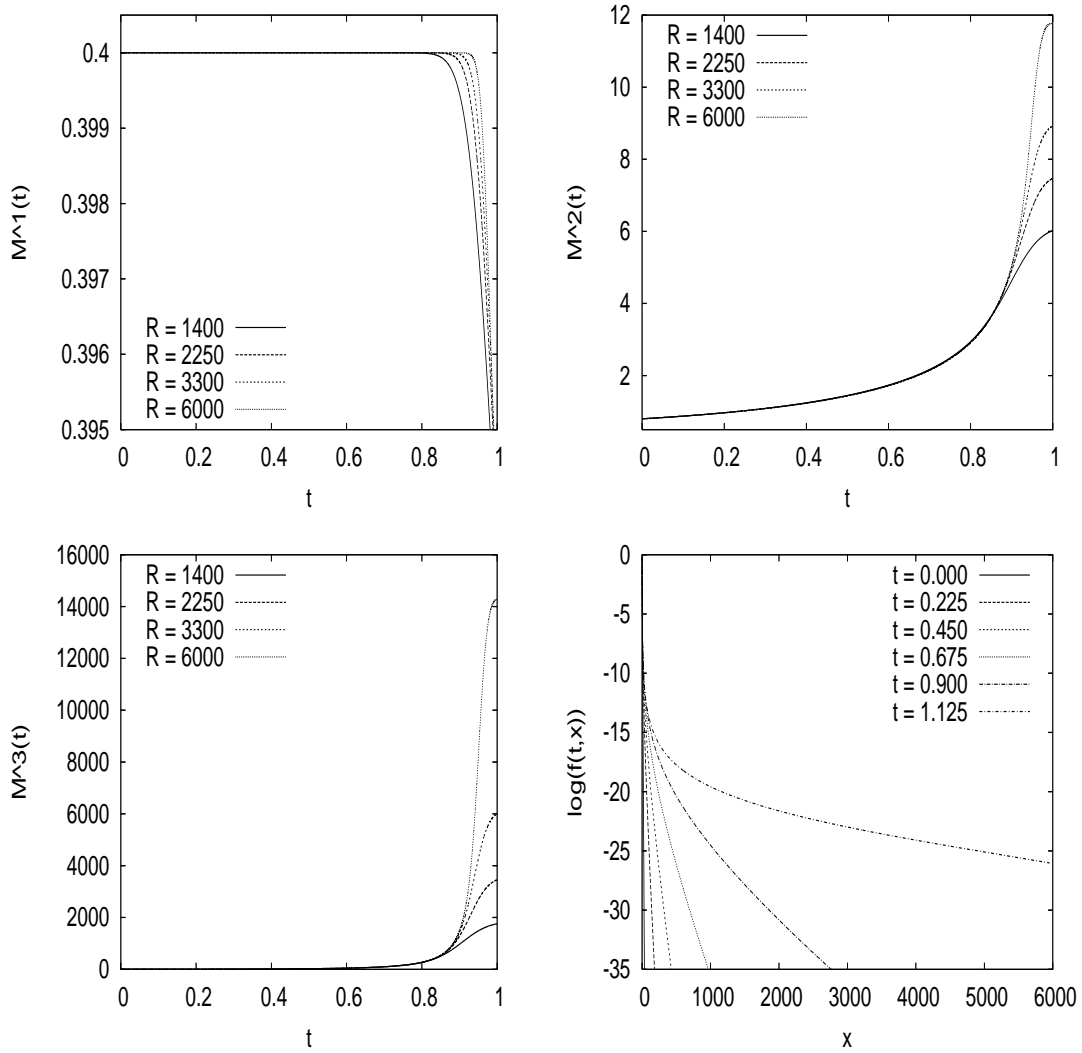


FIGURE 2. Initial mass $M_1 = 0.4$: Evolution of the total mass of particles M_1 , the second and third moments of f and the distribution $f(t, x)$ in log scale at time $t = 0, 0.225, 0.45, 0.675, 0.9$ and 1.125 (after blow-up).

- [6] A. EIBECK AND W. WAGNER, *An efficient stochastic algorithm for studying coagulation dynamics and gelation phenomena*, SIAM J. Sci. Comput., **22** (2000), pp. 802–821.
- [7] L. D. ERASMUS, D. EYRE, AND R. C. EVERSON, *Numerical treatment of the population balance equation using a Spline-Galerkin method*, Computers Chem. Engrg., **8** (1994), pp. 775–783.
- [8] M. ESCOBEDO, S. MISCHLER, AND B. PERTHAME, *Gelation in coagulation and fragmentation models*, Comm. Math. Phys., **231** (2002), pp. 157–188.
- [9] M. ESCOBEDO, PH. LAURENÇOT, S. MISCHLER, AND B. PERTHAME, *Gelation and mass conservation in coagulation-fragmentation models*, J. Differential Equations, **195** (2003), pp. 143–174.

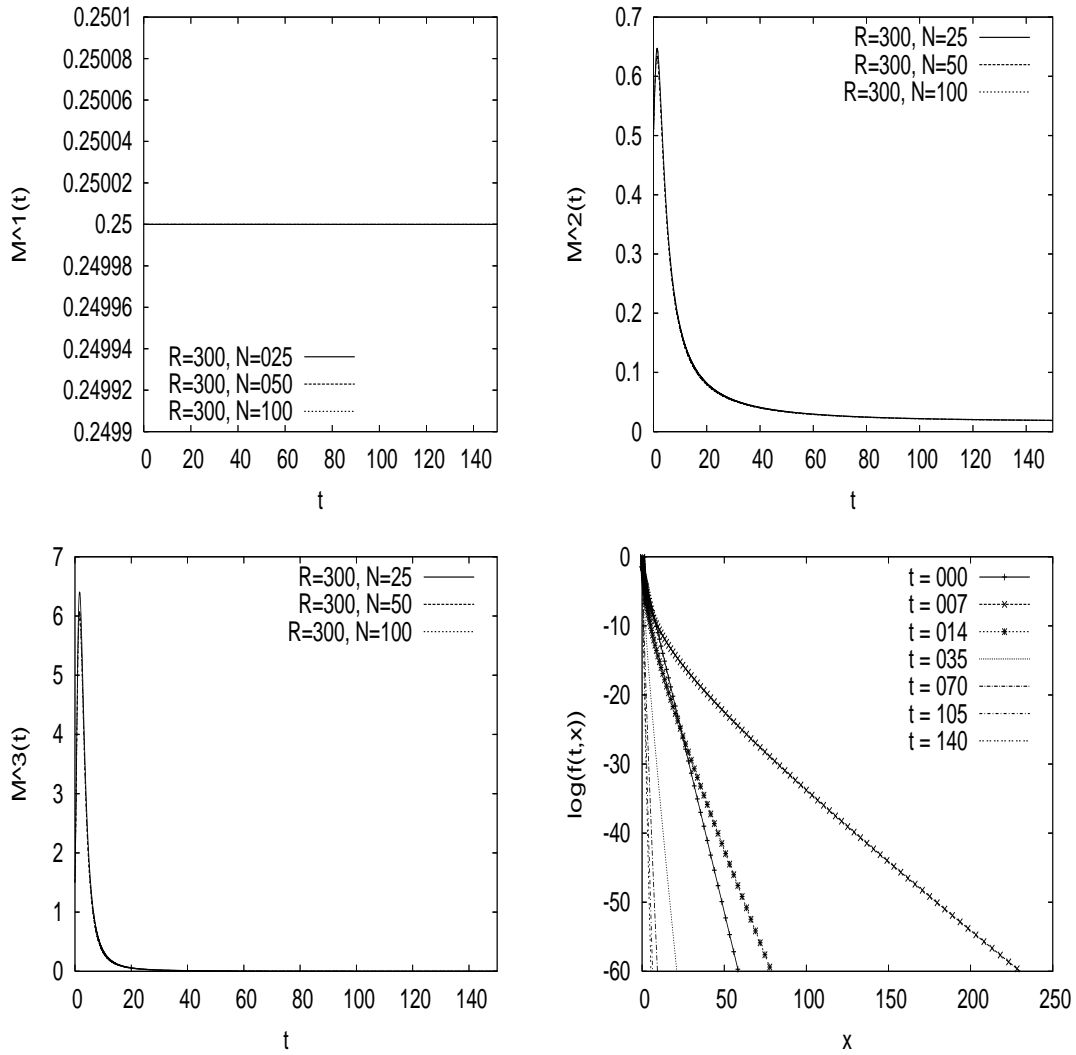


FIGURE 3. Initial mass $M_1 = 0.25$: Evolution of the total mass of particles M_1 , the second and third moments of f and the distribution $f(t, x)$ in log scale at time $t = 0, 7, 14, 35, 70, 105$ and 140 .

[10] R. EYMARD, T. GALLOUËT AND R. HERBIN, *Finite volume methods*, in Handbook of numerical analysis, Vol. VII, 713–1020, Handb. Numer. Anal., VII, North-Holland, Amsterdam, 2000.
 [11] F. FILBET AND PH. LAURENÇOT, *Mass-conserving solutions and non-conservative approximation to the Smoluchowski coagulation equation*, Arch. Math. (Basel) **83** (2004), pp. 558–567.
 [12] F. FILBET, P. LAURENÇOT, *Numerical Simulation of the Smoluchowski Coagulation Equation*, SIAM J. Sci. Comput. Vol. **25** (2004), pp. 2004–2028.
 [13] F. GUIAŞ, *A Monte Carlo approach to the Smoluchowski equations*, Monte Carlo Methods Appl., **3** (1997), pp. 313–326.

- [14] I. JEON, *Existence of gelling solutions for coagulation-fragmentation equations*, Comm. Math. Phys., **194** (1998), pp. 541–567.
- [15] PH. LAURENÇOT, *On a class of continuous coagulation-fragmentation equations*, J. Differential Equations, **167** (2000), pp. 145–174.
- [16] PH. LAURENÇOT AND S. MISCHLER, *From the discrete to the continuous coagulation-fragmentation equations*, Proc. Roy. Soc. Edinburgh Sect. A, **132** (2002), pp. 1219–1248.
- [17] C. LÉCOT AND W. WAGNER, *A quasi-Monte Carlo scheme for Smoluchowski's coagulation equation*, Math. Comp. **73** (2004), pp. 1953–1966.
- [18] M. H. LEE, *On the validity of the coagulation equation and the nature of runaway growth*, Icarus, **143** (2000), pp. 74–86.
- [19] R.J. LEVEQUE, *Numerical methods for conservation laws*, Second edition, Lectures in Mathematics ETH Zürich, Birkhäuser Verlag, Basel, 1992.
- [20] F. LEYVRAZ AND H. R. TSCHUDI, *Singularities in the kinetics of coagulation processes*, J. Phys. A, **14** (1981), pp. 3389–3405.
- [21] J. MAKINO, T. FUKUSHIGE, Y. FUNATO, AND E. KOKUBO, *On the mass distribution of planetesimals in the early runaway stage*, New Astronomy, **3** (1998), pp. 411–417.
- [22] H. TANAKA, S. INABA, AND K. NAKAZA, *Steady-state size distribution for the self-similar collision cascade*, Icarus, **123** (1996), pp. 450–455.
- [23] R.M. ZIFF AND E.D. MCGRADY, *The kinetics of cluster fragmentation and depolymerisation*, J. Phys. A **18** (1985), pp. 3027–3037.

JEAN-PIERRE BOURGADE

UNIVERSITY OF VIENNA,
NORDBERGSTRASSE 15
A-1090 VIENNA
AUSTRIA

E-MAIL: bourgade@mip.ups-tlse.fr

FRANCIS FILBET

MIP, UNIVERSITÉ PAUL SABATIER
118, ROUTE DE NARBONNE,
F-31062 TOULOUSE CEDEX 04
FRANCE

E-MAIL: filbet@mip.ups-tlse.fr