Numerical methods for computing an averaged matrix field. Application to the asymptotic analysis of a parabolic problem with stiff transport terms.

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Abstract

Parabolic problems with stiff terms are challenging to solve numerically. When the stiff terms become dominant, multiple scale effects occur and the classical numerical methods do not catch the microscopic effects. The aim of this paper is to provide a numerical method to study the behavior of parabolic problems with stiff transport terms based on recent results on the asymptotic analysis for such problems. Precisely, the behavior of the solutions can be described in terms of a composition product between a certain profile and the fast flow associated to the dominant transport operator, where the asymptotic profile solves an effective diffusion equation. A numerical method for determining the effective diffusion matrix is given, the computation of the limit profile is carried out and the error with respect to the solution of the stiff problem is studied.

Keywords: Averaging methods, Semi-Lagrangian schemes, Multiple scales.

AMS classification: 65M25, 65M06.

1 Introduction

In many applications, partial differential equations with multiple scales can occur: transport in strongly magnetized plasmas with or without collisions, heat transfer inside the plasma fusion, heat and mass transport in the chemical framework. Each of these problems makes appear multiple scales in time or space. From the numerical point of view, the study of these problems is highly constraint by the size of the small scale. Indeed, the numerical resolution must be thin enough for catching the effects caused by the small scales. But, in this case, the classical methods have a prohibitive numerical cost and are not adapted for solving this type of problems. In this work we provide a way to study numerically the behavior of a diffusion equation with a stiff convection term. We focus on the following parabolic model

\[
\begin{align*}
\partial_t \varepsilon u - \text{div}(D(y)\nabla \varepsilon u) + \frac{1}{\varepsilon} b(y) \cdot \nabla \varepsilon u &= 0, & (t, y) \in \mathbb{R}_+ \times \mathbb{R}^m, \\
\varepsilon(0, y) &= u^{in}(y), & y \in \mathbb{R}^m,
\end{align*}
\]

(1.1)

where \( b : \mathbb{R}^m \to \mathbb{R}^m \) and \( D : \mathbb{R}^m \to \mathcal{M}_m(\mathbb{R}) \) are given fields of vectors and symmetric positive definite matrices, and \( \varepsilon > 0 \) is a small parameter close to zero. The fast transport, which is related to the operator \( b \cdot \nabla_y \), introduce a fast time scale. Actually, this problem

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can be interpreted as a two-scale problem in time, after a convenient Lagrangian change of variable along the fast motion. Multiple-scale problems have been extensively studied by many authors and there exists a lot of approaches for their numerical study. The strongly anisotropic diffusion problems have been analyzed by using asymptotic preserving schemes [16], the kinetic equations [12], the multiple-scale parabolic problems [13], the Schrödinger and Klein-Gourdon equations [10] have been addressed by appealing to uniform accurate schemes. Multiple-scale methods for advection-diffusion equations are proposed in [1]. The strategy we choose in this paper will be not to solve numerically the problem (1.1), but rather an homogenized limit problem not constraint by the small parameter $\varepsilon$, and for which standard numerical solvers can be used. Indeed, the theoretical study of multiple scales problems by homogenization techniques has been done in many frameworks such as transport with disparate advection fields [4, 9, 15], transport of charged particles under high magnetic fields [7, 6, 7, 8, 18, 19], elliptic and parabolic models [2, 22] or asymptotic analysis of strongly anisotropic diffusion problems [8]. In the recent paper [3], the asymptotic analysis of the problem (1.1) has been performed through an ergodic theory result. It has been shown that the behavior of the family $(u^\varepsilon)_{\varepsilon>0}$, when $\varepsilon$ goes to zero, can be described, in the $L^2$ sense, with a convergence rate, in terms of the composition product between a profile solution of the homogenized problem and the fast oscillating flow associated to $b/\varepsilon$. Moreover, it is shown that the homogenized problem is still a parabolic problem, whose effective diffusion matrix field is given by an ergodic average of the initial diffusion matrix field $D$, along a group of linear operators. Actually the infinitesimal generator associated to this group is a transport operator which acts on matrix fields. The main goal of this article is to provide a semi-Lagrangian scheme for solving the group, and thus compute the effective diffusion matrix field. The interest of this numerical computation is not restricted to the problem (1.1). Indeed, the average of a matrix field is found in various situations and makes it possible to describe, for example, the effective system associated with a strongly anisotropic diffusion equation, cf. [8]. We illustrate this approach by observing the error between a reference solution of (1.1) and the solution of the effective diffusion problem for some particular examples.

This paper is organized as follow. In Section 2 we introduce the notations which will be used throughout this study and we recall the main asymptotic results established in [3]. A scheme based on a semi-Lagrangian method is provided in Section 3 for the computation of the effective diffusion field. Some numerical tests are done as well. In Section 4, we study the error between the solution of the effective problem, with respect to the solution of the stiff problem (1.1). We use a numerical scheme based on splitting methods for providing a reference solution for (1.1). The numerical results confirm the expected theoretical convergence rates.

## 2 Asymptotic analysis, theoretical results

In this section we introduce some notations and results which will be useful along the paper. The main points are the definition of the effective diffusion matrix field (2.4), (2.1) and the asymptotic result (2.6). We only indicate the main lines of the arguments leading to these results. For the proof details we refer to [3]. Consider $Y : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ the characteristic flow of the vector field $b$

$$\frac{dY}{ds} = b(Y(s; y)), \quad (s, y) \in \mathbb{R} \times \mathbb{R}^m, \quad Y(0; y) = y, \quad y \in \mathbb{R}^m.$$  

This flow is well defined under the standard smoothness and boundedness assumptions

\[
\begin{cases}
    b \in W^{1, \infty}_{\text{loc}}(\mathbb{R}^m), \\
    \exists C > 0 \text{ such that } |b(y)| \leq C(1 + |y|), \quad y \in \mathbb{R}^m.
\end{cases}
\]
Under the above hypotheses the flow $Y$ is global and smooth, $Y \in W_{\text{loc}}^{1,\infty}(\mathbb{R} \times \mathbb{R}^m)$. We assume that the vector field $b$ is divergence free
\[
\text{div}_yb = 0, \ y \in \mathbb{R}^m
\]
which guarantees that the transformation $y \in \mathbb{R}^m \rightarrow Y(s;y) \in \mathbb{R}^m$ is measure preserving for any $s \in \mathbb{R}$. The asymptotic analysis of (1.1) comes immediately when the operators $b \cdot \nabla_y$ and $\text{div}_y(D\nabla_y)$ are commuting, i.e. $[b \cdot \nabla_y, \text{div}_y(D\nabla_y)] = 0$. The idea is to perform the change of coordinates $z = Y(-t/\varepsilon; y)$, and therefore to replace the family $(u^\varepsilon)_{\varepsilon > 0}$ by the new family $(v^\varepsilon)_{\varepsilon > 0}$ given by
\[
u^\varepsilon(t, y) = v^\varepsilon(t, z) = v^\varepsilon(t, Y(-t/\varepsilon; y)), \ (t, y) \in \mathbb{R}^+ \times \mathbb{R}^m.
\]
The point is that, under the above commutation property, the new unknowns $(v^\varepsilon)_{\varepsilon > 0}$ satisfy
\[
\begin{cases}
\partial_t v^\varepsilon - \text{div}_z(D\nabla_z v^\varepsilon) = 0, & (t, z) \in \mathbb{R}^+ \times \mathbb{R}^m \\
v^\varepsilon(0, z) = u^m(z), & z \in \mathbb{R}^m.
\end{cases}
\]
Thus, $v^\varepsilon$ does not depend on $\varepsilon$ and therefore $u^\varepsilon$ is the composition between the profile $v = v^\varepsilon$ and the flow associated to the vector field $b/\varepsilon$. The matrix fields $D$ which ensure the commutation property are characterized in the following proposition, see [8, 3] for more details.

**Proposition 2.1.** Consider a divergence free vector field $c \in W_{\text{loc}}^{1,\infty}(\mathbb{R}^m)$ with at most linear growth at infinity and $A \in L_{\text{loc}}^1(\mathbb{R}^m, \mathcal{M}_m(\mathbb{R}))$ a matrix field.

1. The commutator between the advection operator $c \cdot \nabla_y$ and the diffusion operator $\text{div}_y(A\nabla_y)$ is still a diffusion operator, and we have
\[
[c \cdot \nabla_y, \text{div}_y(A\nabla_y)] = \text{div}_y([c, A]\nabla_y) \quad \text{in} \quad \mathcal{D}'(\mathbb{R}^m)
\]
where the associated diffusion field is defined by the bracket between the vector field $c$ and the matrix field $A$
\[
[c, A] := (c \cdot \nabla_y)A - \partial_y cA - A^t \partial_y c \quad \text{in} \quad \mathcal{D}'(\mathbb{R}^m).
\]

2. The following assertions are equivalent
(a) We have $[c, A] = 0$ in $\mathcal{D}'(\mathbb{R}^m)$
(b) For any $s \in \mathbb{R}$, we have $G(s)A = A$, where the family of linear operators $(G(s))_s$, acting on matrix fields, is defined by
\[
(G(s)A)(y) := \partial Y^{-1}(s; y)A(Y(s; y))^t \partial Y^{-1}(s; y), \ (s, y) \in \mathbb{R} \times \mathbb{R}^m.
\]

Motivated by the case in which the operators commute, we perform the asymptotic analysis not for the family $(u^\varepsilon)_{\varepsilon > 0}$ but rather for the new family of functions $(v^\varepsilon)_{\varepsilon > 0}$ given by
\[

v^\varepsilon(t, z) = u^\varepsilon(t, Y(t/\varepsilon; z)), \ (t, z) \in \mathbb{R}^+ \times \mathbb{R}^m, \ \varepsilon > 0.
\]
We expect that the family $(v^\varepsilon)_{\varepsilon > 0}$ converges when $\varepsilon$ goes to zero. Actually, when the operators $b \cdot \nabla_y$ and $\text{div}_y(D\nabla_y)$ are not commuting, the asymptotic behavior of the family $(u^\varepsilon)_{\varepsilon > 0}$, when $\varepsilon$ goes to zero, can be described asymptotically in the same way as before, that is as a composition product between a profile $v$ and the flow associated to $b/\varepsilon$. This profile $v$ is the solution of a diffusion equation with a new diffusion matrix field $\langle D \rangle$, which appears as
the orthogonal projection of $D$ over the linear space of matrix fields which are left invariant by the family $(G(s))_s$ in (2.1), with respect to some scalar product, to be precised. The definition of $\langle D \rangle$ is given by (2.4). Performing the change of variable $z = Y(-t/\varepsilon; y)$ in (1.1), for any $\varepsilon > 0$, $t \in \mathbb{R}_+$, $y \in \mathbb{R}^m$, and appealing to the chain rule (see [3] for more details) lead to a two time scales diffusion problem
\[
\begin{cases}
\partial_t v^\varepsilon - \text{div}_z ((G(t/\varepsilon)D)\nabla_z v^\varepsilon) = 0, & (t, z) \in \mathbb{R}_+ \times \mathbb{R}^m \\
v^\varepsilon(0, z) = u^\varepsilon(0, z) = u^\text{in}(z), & z \in \mathbb{R}^m, \varepsilon > 0
\end{cases}
\] (2.2)
where $(G(s))_{s \in \mathbb{R}}$ is defined by (2.1). A two-scale approach, based on Hilbert’s method, formally leads to the following effective problem
\[
\begin{cases}
\partial_t v - \text{div}_z (\langle D \rangle \nabla_z v) = 0, & (t, z) \in \mathbb{R}_+ \times \mathbb{R}^m \\
v(0, z) = u^\text{in}(z), & z \in \mathbb{R}^m,
\end{cases}
\] (2.3)
where the effective diffusion field $\langle D \rangle$ is given by the long time average
\[
\langle D \rangle = \lim_{S \to +\infty} \frac{1}{S} \int_0^S G(s)D \, ds.
\] (2.4)

**Remark 2.1** The computation of such average matrix field does not depend on the initial condition $u^\text{in}$. Thus, a pre-computation of the average matrix field is possible by knowing only $D$ and $b$.

The existence of the matrix field $\langle D \rangle$ is provided by the von Neumann ergodic theorem, see [23, 3]. Indeed, the family of linear operators $(G(s))_{s \in \mathbb{R}}$ defined by (2.1) is a $C^0$-group of unitary operators in a suitable Hilbert space $H_Q$, see (3.12). The existence of such Hilbert space is not always ensured, thus the average matrix field (2.4) is not always defined in this sense, see Section 3.4 or [3] for more details. The average matrix field (2.4) can be interpreted as a projection on the kernel of the infinitesimal generator $L$ associated to $(G(s))_{s \in \mathbb{R}}$. We have a description for the restriction of $L$ to the compactly supported smooth matrix fields as a transport operator
\[
L(A) = [b, A] = (b \cdot \nabla_y)A - \partial_y bA - A^t\partial_y b, \quad A \in C^1_c(\mathbb{R}^m).
\] (2.5)

This expression of $L$ will be useful for the computation of the group $(G(s))_s$, see Section 3. Now, we can describe the behavior of the family $(u^\varepsilon)_{\varepsilon > 0}$ when $\varepsilon$ goes to zero. It is shown in [3] that, for any initial condition $u^\text{in} \in L^2(\mathbb{R}^m)$, the family $(v^\varepsilon)_{\varepsilon > 0}$ solutions of the equation (2.2) converges strongly in $L^2_{\text{loc}}(\mathbb{R}_+; L^2(\mathbb{R}^m))$, to the unique solution $v \in L^2(\mathbb{R}_+; L^2(\mathbb{R}^m))$ of (2.3). Actually, if we consider $T > 0$, there is a constant $C_T > 0$ such that, for any $\varepsilon > 0$, we have
\[
\sup_{t \in [0, T]} \|v^\varepsilon(t, \cdot) - v(t, \cdot)\|_{L^2(\mathbb{R}^m)} \leq C_T \varepsilon
\]
and
\[
\sup_{t \in [0, T]} \|u^\varepsilon(t, \cdot) - v(t, Y(-t/\varepsilon; \cdot))\|_{L^2(\mathbb{R}^m)} \leq C_T \varepsilon.
\] (2.6)

### 3  Computation of the average matrix field

In this section, we provide a numerical method for the computation of the average matrix field (2.4). If $D : \mathbb{R}^m \to \mathcal{M}_m(\mathbb{R})$ is a matrix field, the computation of the average matrix field $\langle D \rangle$ defined by (2.4) will be provided in two steps. First, we compute numerically the matrix field $G(s)D = (G(s)D)(y)$ by using the infinitesimal generator $L$ given by (2.5). Secondly,
the computation of the long time average will be done by a quadrature method. The method is presented in Section 3.1 and the numerical scheme associated is performed in Section 3.2. In Section 3.3, the accuracy of the method is tested for several vector fields \( b \). The cases where the flow associated to the vector field \( b \) is known provide, thanks to the formula (2.1), reference curves for the one parameter group \((G(s))_{s \in \mathbb{R}}\). Finally, it seemed interesting to give an example of vector field \( b \) for which the associated average matrix field is not well defined, we propose such example in Section 3.4.

### 3.1 Computation of the matrix field \( G(s)D \)

Consider \( S > 0 \) and \( D \in C^1_b(\mathbb{R}^m, \mathcal{M}_m(\mathbb{R})) \) a compactly supported smooth matrix field. The matrix field \((G(s)D)(y)\) where \( s \in [0, S], y \in \mathbb{R}^m \) is related to the infinitesimal generator \( L \) of the group \((G(s))_{s \in \mathbb{R}}\) through the following evolution problem

\[
\begin{cases}
\frac{d}{ds} (G(s)D)(y) = L(G(s)D)(y), & (s, y) \in [0, S] \times \mathbb{R}^m \\
G(0)D(y) = D(y), & y \in \mathbb{R}^m.
\end{cases}
\]

Moreover, the operator \( L \) is a transport operator and its explicit expression is given in terms of \( b \) and its partial derivatives with respect to \( y \), see (2.5). Thus, we need to solve the following partial differential equation on the matrix field \( A(s, y) := (G(s)D)(y), (s, y) \in [0, S] \times \mathbb{R}^m \)

\[
\begin{cases}
\frac{d}{ds} A(s, y) = (b \cdot \nabla_y)A(s, y) - \partial_y b(y) A(s, y) - A(s, y)^t \partial_y b(y), & (s, y) \in [0, S] \times \mathbb{R}^m \\
A(0, y) = D(y), & y \in \mathbb{R}^m.
\end{cases}
\] (3.1)

For the resolution of this equation, we appeal to a semi-Lagrangian scheme, see [17]. Such schemes have several advantages: they are unconditionally stable, with arbitrary order of accuracy and are known to provide less numerical diffusion that the Eulerian schemes, as upwind schemes. To avoid a too prohibitive numerical cost, we are not allowed to choose a small resolution. It is the reason why, we choose a high order of accuracy (four in practice) for the computation of the diffusion matrix field \( G(s)D \) for \( s \in [0, S] \). As the time long computation of \( G(s)D \) is required, we need that the scheme be not too diffusive. All these remarks have guided us to provide a numerical scheme based on the semi-Lagrangian framework for the resolution of (3.1). We rewrite the equation (3.1) by using the Lagrangian change of coordinates \( y = Y(\cdot - s; z) \) for \((s, z) \in [0, S] \times \mathbb{R}^m \). By setting \( B(s, z) := A(s, Y(\cdot - s; z)) \), we have

\[
\begin{cases}
\frac{d}{ds} B(s, z) = -\partial_y b(Y(\cdot - s; z)) B(s, z) - B(s, z)^t \partial_y b(Y(\cdot - s; z)), & (s, z) \in [0, S] \times \mathbb{R}^m \\
B(0, z) = D(z), & y \in \mathbb{R}^m.
\end{cases}
\] (3.2)

We solve the ordinary differential equation (3.2) by a Runge-Kutta scheme of order four. The unknown change \( A(s_0, y) = B(s_0, Y(s_0; y)) \), for \( s_0 \in [0, S], y \in \mathbb{R}^m \), is performed by a semi-Lagrangian scheme. The flow \( Y(\cdot s_0; y) \) is computed by a Runge-Kutta solver, and the reconstruction of \( B(s_0, Y(s_0; y)) \), from the values of \( B(s_0, \cdot) \) on the grid points, is achieved by Lagrangian interpolation. This last step can be interpreted as the resolution of the following
transport equation

\[
\frac{d}{ds} C(s, y) = (b \cdot \nabla y) C(s, y), \quad (s, y) \in [0, S] \times \mathbb{R}^m
\]  

(3.3)

Indeed, if we use the method of characteristics method on (3.3), we obtain \( C(s_0, y) = B(s_0, Y(s_0; y)) = A(s_0, y) \). The construction of the scheme is detailed in Section 3.2.

### 3.2 Numerical scheme for the computation of \( \langle D \rangle \)

For simplicity, the scheme is presented in the two dimensional setting \( m = 2 \), but it extends easily to any dimension \( m \geq 3 \). Several examples are given for \( m = 4 \) in Section 3.3. The spatial domain will be a square \( C = [-R, R] \times [-R, R] \), for \( R > 0 \). Consider \( S > 0, N_s \in \mathbb{N}^* \) and \( I_s = \{0, \ldots, N_s\} \). We introduce a regular discretization \((s^k)_{k \in I_s}\) of the interval \([0, S]\) with a step \( \Delta s = S/N_s \), thus \( s^k = k\Delta s \) for any \( k \in I_s \). Moreover, we defined \( s^{k+1/2} = (k+1/2)\Delta s \) for any \( k \in \{0, \ldots, N_s-1\} \). Consider \( N \in \mathbb{N}^* \) and \( I = \{0, \ldots, N\} \). Assume that \((y_{ij})_{(i,j) \in I^2}\) is a regular cartesian discretization of the square \( C \), with \( i, j \in I \). The step of the spatial discretization is \( \Delta y = 2R/N \), and \( y_{ij} = (-R + i\Delta y, -R + j\Delta y) \) for any \((i, j) \in I^2\).

#### Resolution of the system (3.2)

For the approximation of \( B(s^k, y_{ij}) \), for \( k \in I_s \) and \((i,j) \in I^2 \), we introduce the matrices \( B^k_{ij} \in \mathcal{M}_2(\mathbb{R}) \). We solve numerically the system (3.2) at any point \( y_{ij}, i, j \in I \), with a Runge-Kutta 4 solver. We define the application \( F_{y_{ij}} : \mathbb{R} \times \mathcal{M}_2(\mathbb{R}) \rightarrow \mathcal{M}_2(\mathbb{R}), (s, M) \mapsto -\partial_y b(Y(-s; y_{ij})) M - M^t\partial_y b(Y(-s; y_{ij})) \). The scheme writes

\[
\begin{align*}
B^0_{ij} &= \begin{pmatrix} D_{11}(y_{ij}) & D_{12}(y_{ij}) \\ D_{21}(y_{ij}) & D_{22}(y_{ij}) \end{pmatrix} \\
B^{k+1}_{ij} &= B^k_{ij} + \frac{\Delta s}{6} \left( k_{1,ij} + 2k_{2,ij} + 2k_{3,ij} + k_{4,ij} \right)
\end{align*}
\]

(3.4)

where

\[
\begin{align*}
k_{1,ij} &= F_{y_{ij}}(s^k, B^k_{ij}) \\
k_{2,ij} &= F_{y_{ij}}(s^{k+1/2}, B^k_{ij} + \frac{\Delta s}{2}k_{1,ij}) \\
k_{3,ij} &= F_{y_{ij}}(s^{k+1/2}, B^k_{ij} + \frac{\Delta s}{2}k_{2,ij}) \\
k_{4,ij} &= F_{y_{ij}}(s^{k+1}, B^k_{ij} + \Delta s k_{3,ij})
\end{align*}
\]

At each step of the scheme, the computation of the flow \( Y(s; \cdot) \) associated to the vector field \( b(\cdot) \) needs to be evaluated at times \( s = -s^k, s = -s^{k+1/2} \) and \( s = -s^{k+1} \).

#### Semi-Lagrangian step

We introduce the matrices \( A^k_{ij} \in \mathcal{M}_2(\mathbb{R}) \) for the approximation of the matrices \( A(s^k, y_{ij}) \) for \( k \in I_s \) and \((i,j) \in I^2 \). We know that \( A(s^k, y_{ij}) = B(s^k, Y(s^k; y_{ij})) \), we first compute the flow \( Y(s; \cdot) \) at time \( s = s^k \), at any point \( y_{ij}, (i,j) \in I^2 \) by a Runge-Kutta 4 solver. The approximations \( B^k_{ij} \) of \( B(s^k, y_{ij}) \) are used for the reconstruction of \( B(s^k, Y(s^k; y_{ij})) \) by a Lagrangian interpolation. More exactly, cubic Lagrangian interpolation is performed by
using the values of 16 points surrounding \( Y(s^k; y_{ij}) \). We name \( \mathcal{S} \) the associated stencil, see Figure 1:
More precisely, the interpolation of the function \( B(s^k, \cdot) \) at the point \( Y(s^k; y_{ij}) \) will be done
by a polynomial function \( P(y_1, y_2) = \sum_{0 \leq \alpha, \beta \leq 3} a_{\alpha\beta} y_1^\alpha y_2^\beta \). The computation of the coefficients
\( a_{\alpha\beta} \), for \( 0 \leq \alpha, \beta \leq 3 \), is based on the 16 values of \( B^k_{ij} \), such that \( y_{ij} \in \mathcal{S} \), by solving the
linear system associated to the equations
\[
\sum_{0 \leq \alpha, \beta \leq 3} a_{\alpha\beta}(y_{ij})^\alpha (y_{ij})^\beta = B^k_{ij}, \quad y_{ij} \in \mathcal{S}.
\]
This Lagrangian interpolation provides a fourth order space approximation for regular data.

**Computation of \( \langle D \rangle \)**

The computation of \( \langle D \rangle \) is performed by a numerical integration of \( s \mapsto G(s)D \) on \([0, S]\). Actually, a four points Newton-Cotes quadrature method is used, which is five order accurate in time, for more details on these methods see [14]. Consider \( \tilde{D}_{ij} \), for \( i, j \in \mathcal{I} \), an element of \( \mathcal{M}_2(\mathbb{R}) \) which approximates \( \langle D \rangle (y_{ij}) \). The quadrature method, with the values \( A^k_{ij} \) computed in Section 3.2, writes
\[
\tilde{D}_{ij} = \frac{1}{S} \sum_{k=0}^{N_s/4-1} 4\Delta s \sum_{l=0}^{4} \omega_l A^{4k+l}_{ij},
\]
where the coefficients of quadrature are given by \( \omega_0 = \omega_4 = \frac{7}{90}, \omega_1 = \omega_3 = \frac{16}{45} \) and \( \omega_2 = \frac{2}{15} \).

### 3.3 Numerical computations and examples

In this section, we test the previous numerical method, for computing the average matrix field. Let \( \langle D \rangle (y) \) be the average matrix field associated to \( D(y) \) and \( \tilde{D} \) be the numerical approximation given by the numerical scheme. The error analysis between these two quantities is localized to a domain \( \mathcal{S} \subset \mathcal{C} \) which is left invariant by the flow associated to the vector field \( b \), i.e \( Y(s; \mathcal{S}) = \mathcal{S} \) for any \( s \in \mathbb{R} \). For any matrix \( A \in \mathcal{M}_2(\mathbb{R}) \), \( |A| = \sqrt{\text{tr} A \cdot A} \), we introduce the relative error based on the discrete \( L^2 \) norm
\[
\text{Error } L^2 = \sqrt{\frac{\sum_{(i,j) \in \mathcal{S}} |\langle D \rangle (y_{ij}) - \tilde{D}_{ij}|^2}{\sum_{(i,j) \in \mathcal{S}} |\langle D \rangle (y_{ij})|^2}}. \tag{3.5}
\]
Ellipsoidal flow

We consider the Hamiltonian vector field $b(y_1, y_2) = (\partial_{y_2} H(y), -\partial_{y_1} H(y))$, for $y = (y_1, y_2) \in \mathbb{R}^2$, with

$$H(y) = \frac{1}{2} y_1^2 + \frac{1}{2} y_2^2 + \frac{1}{2} y_1 y_2, \quad y = (y_1, y_2) \in \mathbb{R}^2.$$ 

The function $H$ is a coercive prime integral associated to $b$. We denote by $Y$ the flow associated to the vector field $b$. The characteristic curves are ellipses of the plane, the flow $Y(s; y) = \mathcal{E}(s) y$ is $4\pi/\sqrt{3}$-periodic, and we have

$$\mathcal{E}(s) = \left( \begin{array}{c} \cos \left( \frac{\sqrt{3}}{2} s \right) + \frac{1}{\sqrt{3}} \sin \left( \frac{\sqrt{3}}{2} s \right) \\ -\frac{2}{\sqrt{3}} \sin \left( \frac{\sqrt{3}}{2} s \right) \cos \left( \frac{\sqrt{3}}{2} s \right) \end{array} \right).$$

Thanks to (2.1), we have

$$\langle D \rangle = \frac{\sqrt{3}}{4\pi} \int_0^{4\pi/\sqrt{3}} G(s) D \, ds = \frac{\sqrt{3}}{4\pi} \int_0^{4\pi/\sqrt{3}} \mathcal{E}(-s) D(Y(s; y)) \mathcal{E}(-s) \, ds = \left( \begin{array}{c} \langle D \rangle_{11} \\ \langle D \rangle_{21} \\ \langle D \rangle_{22} \end{array} \right)$$

where

$$\langle D \rangle_{11} = \frac{1}{2} \left( \begin{array}{c} \langle D_{11}[1 + \cos(\sqrt{3} \cdot)] \rangle - \frac{1}{\sqrt{3}} \langle (D_{11} + D_{21} + D_{12}) \sin(\sqrt{3} \cdot) \rangle \\ + \frac{1}{6} \langle (D_{11} + 2(D_{21} + D_{12}) + 4D_{22})[1 - \cos(\sqrt{3} \cdot)] \rangle \end{array} \right)$$

$$\langle D \rangle_{21} = \frac{1}{2} \left( \begin{array}{c} \langle D_{21}[1 + \cos(\sqrt{3} \cdot)] \rangle + \frac{1}{\sqrt{3}} \langle (D_{11} - D_{22}) \sin(\sqrt{3} \cdot) \rangle \\ - \frac{1}{6} \langle (2D_{11} + D_{21} + 4D_{12} + 2D_{22})[1 - \cos(\sqrt{3} \cdot)] \rangle \end{array} \right)$$

$$\langle D \rangle_{12} = \frac{1}{2} \left( \begin{array}{c} \langle D_{12}[1 + \cos(\sqrt{3} \cdot)] \rangle + \frac{1}{\sqrt{3}} \langle (D_{11} - D_{22}) \sin(\sqrt{3} \cdot) \rangle \\ - \frac{1}{6} \langle (2D_{11} + 4D_{21} + D_{12} + 2D_{22})[1 - \cos(\sqrt{3} \cdot)] \rangle \end{array} \right)$$

$$\langle D \rangle_{22} = \frac{1}{2} \left( \begin{array}{c} \langle D_{22}[1 + \cos(\sqrt{3} \cdot)] \rangle + \frac{1}{\sqrt{3}} \langle (D_{21} + D_{12} + D_{22}) \sin(\sqrt{3} \cdot) \rangle \\ + \frac{1}{6} \langle (4D_{11} + 2(D_{21} + D_{12}) + D_{22})[1 - \cos(\sqrt{3} \cdot)] \rangle \end{array} \right)$$

and for any function $h$, we denote $\langle D_{ij} h(\cdot) \rangle = \frac{\sqrt{3}}{4\pi} \int_0^{4\pi/\sqrt{3}} D_{ij}(Y(s; y)) h(s) \, ds, \ (i, j) \in \{1, 2\}^2$. Finally, if $D_{11}, D_{21}, D_{12}, D_{22}$ are constant along the flow $Y(s; \cdot)$ (i.e $D_{11}, D_{21}, D_{12}, D_{22}$ only depend on the quantity $y_1^2 + y_2^2 + y_1 y_2$), the explicit expression of $\langle D \rangle$ reduces to

$$\langle D \rangle = \left( \begin{array}{ccc} \frac{2}{3}(D_{11} + D_{22}) + \frac{1}{3}(D_{21} + D_{12}) & -\frac{1}{3}(D_{11} + D_{22}) + \frac{1}{3}(D_{21} - 2D_{22}) & \frac{4}{3}(D_{11} + D_{22}) + \frac{2}{3}(D_{21} + D_{12}) \\ -\frac{1}{3}(D_{11} + D_{22}) + \frac{1}{3}(D_{21} - 2D_{22}) & \frac{2}{3}(D_{11} + D_{22}) + \frac{2}{3}(D_{21} + D_{12}) & \frac{4}{3}(D_{11} + D_{22}) + \frac{2}{3}(D_{21} + D_{12}) \end{array} \right).$$

(3.6)

We consider the two following matrix fields

$$D_1 = \left( \begin{array}{cc} 3 & 1 \\ 2 & 1 \end{array} \right) \quad \text{and} \quad D_2(y) = \left( \begin{array}{cc} 3 + \cos(\kappa(y_1^2 - y_2^2)) & \cos(y_1^2 - 2y_2) \\ \sin(2y_1 - y_2) & 3 + \sin(\kappa(y_1^2 - y_2)) \end{array} \right) \quad \text{with} \ \kappa = 25.$$
The explicit expression of $D_2$ can be determined by the above formula and the average of $D_1$ is given by

$$\langle D_1 \rangle = \begin{pmatrix} 11/3 & -7/3 \\ -4/3 & 11/3 \end{pmatrix}.$$ 

We check that the global space-time error committed for the computation of $\langle D \rangle$ is $O(\Delta s^4) + O(\Delta y^4)$. We choose $C = [-1; 1]^2$ and $\Delta s = \Delta y$. The Figure 2 shows the relative errors (3.5) committed when using the method presented in Section 3.2. The graphic on the left emphasizes a $O(\Delta y^4)$ error. In this example only the time error appears due to the resolution of the ordinary differential equation (3.2) by the Runge-Kutta 4 scheme (3.4). Indeed, the matrix field $D_1$ is constant and the Jacobian matrix associated to $b$ is also constant. The solution of (3.2) does not depend on the variable $y$. In this case, the interpolation step presented in Section 3.2 is exact. The graphic on the right presents the relative error in non constant, but regular, case. The interpolation error is order $O(\Delta y^4)$ and the global time-space error is $O(\Delta s^4) + O(\Delta y^4)$.

Non explicit central flow

We consider the Hamiltonian vector field $b(y_1, y_2) = (\partial_{y_2} H(y), -\partial_{y_1} H(y))$, defined for $y = (y_1, y_2) \in \mathbb{R}^2$, with $H$ a homogeneous function of degree two, i.e $H(\lambda y_1, \lambda y_2) = \lambda^2 H(y_1, y_2)$ for any $\lambda \in \mathbb{R}$ and $(y_1, y_2) \in \mathbb{R}^2$.

$$H(y_1, y_2) = \frac{1}{2} y_1^2 + \frac{1}{2} y_2^2 + \frac{1}{2} y_1 y_2 \frac{(y_1^2 - y_2^2)}{y_1^2 + y_2^2}, \quad (y_1, y_2) \in \mathbb{R}^2/\{(0, 0)\}, \quad \text{and} \quad H(0, 0) = 0. \quad (3.7)$$

The function $H$ is $C^2$ on $\mathbb{R}^2/\{(0, 0)\}$ and is a coercive prime integral of $b$. We denote by $Y$ the flow associated to the vector field $b$. The characteristic curves are closed and the flow $Y(s; \cdot)$ is periodic. A representation of these curves are given by the Figure 3. In polar coordinates, the function $\overline{H}$ defined by $H(r \cos(\theta), r \sin(\theta)) = \overline{H}(r, \theta)$, for $(r, \theta) \in \mathbb{R}_+ \times [0, 2\pi[$, writes

$$\overline{H}(r, \theta) = r^2 \left( \frac{1}{2} + g(\theta) \right) \quad \text{with} \quad g(\theta) = \frac{1}{4} \sin(4\theta).$$
The period $T(l)$ associated with each closed integral curve $H = l$, $l \geq 0$ because $\min_{\mathbb{R}^2} H = 0$, is constant $T(l) = T$. Indeed, we can compute $T$, see [20], by the following formula

$$T = \int_0^{2\pi} \frac{d\theta}{1 + 2g(\theta)} = \int_0^{2\pi} \frac{d\theta}{1 + \frac{1}{2} \sin(4\theta)} = \frac{4\pi}{\sqrt{3}}.$$  

The average matrix field associated to a matrix field $D$ is given, thanks to (2.1), by

$$\langle D \rangle = \frac{\sqrt{3}}{4\pi} \int_0^{4\pi/\sqrt{3}} G(s)D \, ds = \begin{pmatrix} \langle D \rangle_{11} & \langle D \rangle_{12} \\ \langle D \rangle_{21} & \langle D \rangle_{22} \end{pmatrix}.$$  

In this case, we do not have an explicit expression for the flow $Y$, and thus for the matrix field $G(s)D$. If the matrix field $D$ is constant, we can obtain some informations on the average matrix field. The Hamiltonian (3.7) is homogeneous of degree two, we deduce that $b(\lambda y) = \lambda b(y)$, for any $\lambda \in \mathbb{R}$ and $y \in \mathbb{R}^2$. Thus, we have

$$Y(s; \lambda y) = \lambda Y(s; y), \text{ for any } \lambda \in \mathbb{R} \text{ and } (s, y) \in \mathbb{R} \times \mathbb{R}^2. \quad (3.8)$$

By differentiation of the equality (3.8) with respect to $y$, we obtain

$$\partial Y(s, \lambda y) = \partial Y(s, y), \text{ for any } \lambda \neq 0, \ y \in \mathbb{R}^2.$$  

If $D(\lambda y) = D(y)$, for any $\lambda \neq 0$ and $y \in \mathbb{R}^2$, then, the formula (2.1) yields : $\langle D \rangle(\lambda y) = \langle D \rangle(y)$ for any $\lambda \neq 0$ and $y \in \mathbb{R}^2$. Thus, we expect that the average with respect to $b$ of a constant matrix field is constant along the straight lines passing through the origin of the plane, with a discontinuity at $y = (0,0)$. Indeed, the Hamiltonian $H$ is not $C^2$ at the origin, thus the average matrix field $\langle D \rangle$ is not continuous at the point $y = (0,0)$. We test the method of Section 3.2 for the matrix field $D = I_2$. We choose $C = [-1; 1] \times [-1; 1]$ as a numerical domain. The Figure 4 represents the coefficients of the matrix field $\langle I_2 \rangle$ localized to an invariant domain with respect to the flow of $b$. Each of these coefficients is constant along the straight lines passing to the origin with a discontinuity at $y = (0,0)$. In Figure 5, we observe the order of accuracy of the method with $\Delta s = \Delta y$. The reference solution is obtained by the average computation method and a spatial resolution $N = 512$. The default of regularity at the origin causes a degradation of the order of convergence. If we compute the error outside a small ball around the origin we find the expected accuracy $O(\Delta s^4 + \Delta y^4)$. 

Figure 3: Level set of the function (3.7)
Figure 4: Coefficients of the average matrix field $\langle I_2 \rangle$, from left to right and top to bottom, we have $\langle I_2 \rangle_{11}$, $\langle I_2 \rangle_{12}$, $\langle I_2 \rangle_{21}$ and $\langle I_2 \rangle_{22}$.

Figure 5: $L^2$ error for the approximation of $\langle I_2 \rangle$
Two dimensional Fokker-Planck equation

In this example, we approximate the effective diffusion matrix field associated to a model which describe the evolution of a density of charged particles under the action of high magnetic field by taking into account the collision effects. We assume that the magnetic field $B^c$ is uniform, defined by $B^c = (0, 0, B/\varepsilon)$, $B > 0$, and that the electric field is given by $E(t, x) = (E_1(t, x), E_2(t, x), 0)$ with $t \geq 0$ and $x = (x_1, x_2) \in \mathbb{R}^2$. We choose the asymptotic regime with finite Larmor radius that is the typical length in the perpendicular directions (with respect to the magnetic lines) is of the same order as the Larmor radius and the typical length in the parallel direction is much larger. The presence density of a population of charged particles $f^c$ satisfies the two dimensional Fokker-Planck equation

$$\partial_t f^c + \frac{1}{\varepsilon} (v_1 \partial_{x_1} + v_2 \partial_{x_2}) f^c + \frac{q}{m} E \cdot \nabla_v f^c + \frac{qB}{m \varepsilon} (v_2 \partial_{v_1} - v_1 \partial_{v_2}) f^c = \nu \text{div}_v \{ \Theta \nabla_v f^c + vf^c \}. \tag{3.9}$$

Here $m$ is the particle mass, $q$ is the particle charge, $\nu$ is the collision frequency and $\Theta$ is the temperature. The transport operator associated to the stiff part of the equation (3.9) is

$$b(x, v) \cdot \nabla_{x,v} = v_1 \partial_{x_1} + v_2 \partial_{x_2} + \omega_c (v_2 \partial_{v_1} - v_1 \partial_{v_2}), \quad \text{with} \quad \omega_c = \frac{qB}{m}, \quad (x, v) \in \mathbb{R}^4.$$ 

The flow of $b$ is denoted

$$(x, v) = (x_1, x_2, v_1, v_2) \in \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow Y(s; x, v) = (X(s; x, v), V(s; x, v)) \in \mathbb{R}^2 \times \mathbb{R}^2,$$

and can be determined explicitly

$$X(s; x, v) = x + \frac{v}{\omega_c} - \frac{\mathcal{R}(-\omega_c s)}{\omega_c} \frac{v}{\omega_c} V(s; x, v) = \mathcal{R}(-\omega_c s)$$

where $\mathcal{R}(\theta)$ is the two dimensional rotation $\mathbb{R}^2$ of angle $\theta \in \mathbb{R}$. We want to compute numerically the effective diffusion matrix field associated to the diffusion operator $\text{div}_v (\nabla_v \cdot) = \text{div}_{x,v} (D \nabla_{x,v})$ of the equation (3.9), where the diffusion field $D$ is defined by

$$D = \sum_{i=1}^2 e_{v_i} \otimes e_{v_i} = \begin{pmatrix} 0_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & I_2 \end{pmatrix}. \tag{3.10}$$

For more details on the asymptotic model related to the equation (3.9) see [9]. The Jacobian matrix associated to the flow writes

$$\partial_{x,v} Y(s; x, v) = \begin{pmatrix} I_2 & \frac{I_2 - \mathcal{R}(\omega_c s)}{\omega_c} \mathcal{R}(\omega_c s) \\ 0_{2 \times 2} & I_2 \end{pmatrix}$$

where $0_{m \times n}$ is the zero matrix with $m$ rows and $n$ columns. The flow $Y$ is $\frac{2\pi}{\omega_c}$-periodic, and a direct computation shows that

$$\langle D \rangle (x, v) = \lim_{S \rightarrow +\infty} \frac{1}{S} \int_0^S (G(s)D)(x, v) \, ds$$

$$= \frac{\omega_c}{2\pi} \int_0^{2\pi/\omega_c} \partial_y Y(-s; Y(s; x, v)) \begin{pmatrix} 0_{2 \times 2} & 0_{2 \times 2} \\ 0_{2 \times 2} & I_2 \end{pmatrix} \partial_y Y(-s; Y(s; x, v)) \, ds$$

$$= \frac{1}{\omega_c^2} \begin{pmatrix} 2I_2 & -\omega_c \mathcal{R}(\pi/2) \\ \omega_c \mathcal{R}(\pi/2) & \omega_c I_2 \end{pmatrix}. \tag{3.11}$$
Remark 3.1 Thanks to the Proposition 2.1, the kernel of $Q$ constant in front of the term $1$.

The numerical simulations, we have to localize the error to a ball $B$. Thus, at least in the periodic case, the committed theoretical error on $\langle A \rangle$ is $O\left( \frac{1}{S} \right)$. For the numerical simulations, we have to localize the error to a ball $B_r = \{ (x_1, x_2, v_1, v_2) \in \mathbb{R}^4 : x_1^2 + x_2^2 + v_1^2 + v_2^2 \leq r^2 \}$ of radius $r > 0$. We introduce the notation $\| A \|_{H_Q, r} := \| 1_{B_r} A \|_{H_Q}$ for any matrix field $A \in L^\infty(\mathbb{R}^m, \mathcal{M}_m(\mathbb{R}))$. Thus, we study numerically the error between $A, B \in H_Q$. The infinitesimal generator $L$ associated to $(G(s))_{s \in \mathbb{R}}$ is skew-adjoint in $H_Q$ and its kernel coincides with $\{ A \in H_Q \subset L^1_{\text{loc}}(\mathbb{R}^m) : [b, A] = 0 \in \mathcal{D}'(\mathbb{R}^m) \}$, see [8, 3].

Remark 3.1 Thanks to the Proposition 2.1, the kernel of $L$ can be interpreted as the set of matrix fields $A$ which ensure the commutation property between the operators $b \cdot \nabla_y$ and $\text{div}_y(A \nabla_y)$.

Moreover, we have the following decomposition $H_Q = \text{Ker} L \overline{\oplus} \text{Range} L$. Actually, the uniform boundedness of the flow periods implies the closure of the range of $L$, see [4]. Thus, for any matrix field $A \in H_Q$, there exists $C \in H_Q$ such that

$$A = \langle A \rangle + L(C).$$

Replacing $C$ by $C - \langle C \rangle$, we can also assume that $\langle C \rangle = 0$. Recall that $G(s) \langle A \rangle = \langle A \rangle$, for any $s \in \mathbb{R}$, and therefore, by the unitarity of the group $(G(s))_s$ in $H_Q$, we have

$$\left\| \frac{1}{S} \int_0^S G(s) A \, ds - \langle A \rangle \right\|_{H_Q} = \left\| \frac{1}{S} \int_0^S G(s) (L(C)) \, ds \right\|_{H_Q} = \left\| \frac{1}{S} \int_0^S \frac{d}{ds} G(s) C \, ds \right\|_{H_Q} = \left\| \frac{G(S) C - C}{S} \right\|_{H_Q} \leq \frac{2 \| C \|_{H_Q}}{S}.$$

Thus, at least in the periodic case, the committed theoretical $H_Q$ error on $\langle A \rangle$ is $O\left( \frac{1}{S} \right)$. For the numerical simulations, we have to localize the error to a ball $B_r = \{ (x_1, x_2, v_1, v_2) \in \mathbb{R}^4 : x_1^2 + x_2^2 + v_1^2 + v_2^2 \leq r^2 \}$ of radius $r > 0$. We introduce the notation $\| A \|_{H_Q, r} := \| 1_{B_r} A \|_{H_Q}$ for any matrix field $A \in L^\infty(\mathbb{R}^m, \mathcal{M}_m(\mathbb{R}))$. Thus, we study numerically the error between the quantities $S \mapsto \frac{1}{S} \int_0^S G(s) A \, ds$ and $\langle A \rangle$ for $A = 1_{B_r} D$. In this case, the multiplicative constant in front of the term $1/S$ can be specified if we can compute the matrix field $C$ and $Q$. We have

$$Q = \langle D \rangle^{-1} = \begin{pmatrix} I_2 & \mathcal{R}(-\pi/2) \\ -\mathcal{R}(-\pi/2) & 2I_2 \end{pmatrix}$$
For the matrix field $D$ defined by (3.10), a straightforward computation leads to the matrix field

$$C = \begin{pmatrix} 0_{2 \times 2} & I_2 \\ I_2 & 0_{2 \times 2} \end{pmatrix}$$

(3.15)
such that $D = \langle D \rangle + L(C)$ and $\langle C \rangle = 0$. The Figure 6 shows the relative numerical $L^2$ and $H_{Q,r}$ errors committed for the computation of (3.11) by a long time average of the matrix field (3.10). The time resolution is chosen equal to $N_s = 10^3$ with $S = 500$. The semi-Lagrangian part of the scheme is realized by a linear interpolation. The volume of $B_r$ is denoted $\text{mes}(B_r)$.

In this case, the expressions (3.11), (3.14) and (3.15) lead to

$$\| C \|_{H_{Q,r}} = \sqrt{\int_{B_r} QC : CQ \, dx \, dv} = \sqrt{\int_{B_r} 4 \, dx \, dv} = 2 \sqrt{\text{mes}(B_r)}$$

and

$$\| \langle D \rangle \|_{H_{Q,r}} = \sqrt{\int_{B_r} \langle Q \rangle : \langle D \rangle \, Q \, dx \, dv} = \sqrt{\int_{B_r} 4 \, dx \, dv} = 2 \sqrt{\text{mes}(B_r)}.$$ 

Thus

$$\frac{\frac{1}{S} \int_0^S G(s) D \, ds - \langle D \rangle}{\| \langle D \rangle \|_{H_{Q,r}}} \leq \frac{2}{S},$$

for any $S > 0$.

We retrieved the expected error for the relative $H_{Q,r}$ error, cf. Figure 6.

**Almost periodic flow**

We consider the vector field $b(y) = (y_2, -\omega_1^2 y_1, y_4, -\omega_2^2 y_3)$, defined for $y = (y_1, y_2, y_3, y_4) \in \mathbb{R}^4$, with $\omega_1, \omega_2 \in \mathbb{R}$ incommensurable, i.e $\omega_1/\omega_2 \notin \mathbb{Q}$. The function $\psi(y) = \omega_1^2 y_1^2 + y_2^2 + \omega_2^2 y_3^2 + y_4^2$, with $y \in \mathbb{R}^4$, is a coercive prime integral associated to $b$. We denote $Y(s; y)$ the flow associated...
to the vector field \( b \). We consider a constant matrix field \( D \in \mathcal{M}_4(\mathbb{R}) \). The flow \( Y(s; y) = R(-s; \omega_1, \omega_2) y \), \( (s, y) \in \mathbb{R} \times \mathbb{R}^4 \), with

\[
R(s; \omega_1, \omega_2) = \begin{pmatrix}
\cos(s\omega_1) & -\frac{1}{s} \sin(s\omega_1) & 0 & 0 \\
\omega_1 \sin(s\omega_1) & \cos(s\omega_1) & 0 & 0 \\
0 & 0 & \cos(s\omega_2) & -\frac{1}{s} \sin(s\omega_2) \\
0 & 0 & \omega_2 \sin(s\omega_2) & \cos(s\omega_2)
\end{pmatrix}.
\]

The incommensurability condition ensures that the flow \( Y(s; \cdot) \) is not periodic with respect to \( s \), but almost periodic. For more details on almost periodic functions see [11]. We have

\[
\langle D \rangle = \lim_{s \to \pm \infty} \frac{1}{S} \int_0^S \partial Y(-s; Y(s; \cdot)) D(Y(s; \cdot))^\dagger \partial Y(-s; Y(s; \cdot)) \, ds
\]

\[
= \lim_{s \to \pm \infty} \frac{1}{S} \int_0^S R(s; \omega_1, \omega_2) D(Y(s; \cdot))^\dagger R(s; \omega_1, \omega_2) \, ds
\]

\[
\begin{pmatrix}
\frac{1}{2} D_{11} + \frac{1}{2} D_{22} & \frac{1}{2} D_{12} - \frac{1}{2} D_{21} & 0 & 0 \\
\frac{1}{2} D_{21} - \frac{1}{2} D_{12} & \frac{1}{2} D_{11} + \frac{1}{2} D_{22} & 0 & 0 \\
0 & 0 & \frac{1}{2} D_{33} + \frac{1}{2} D_{44} & \frac{1}{2} D_{34} - \frac{1}{2} D_{43} \\
0 & 0 & \frac{1}{2} D_{43} - \frac{1}{2} D_{34} & \frac{1}{2} D_{33} + \frac{1}{2} D_{44}
\end{pmatrix}.
\]

For this flow \( Y \), the ergodic mean can not be reduced to an average over one period as in the periodic case. We need to compute a long time average. We study the error committed with respect to this long time average, when we use the method in Section 3.2, for the matrix field \( D \) defined by

\[
D = \begin{pmatrix}
2 & -1 & 0 & -2 \\
-1 & 1 & 2 & 0 \\
0 & 2 & 3 & 1 \\
1 & 0 & -1 & 1
\end{pmatrix}.
\]

In the figure 7, we observe that the error is \( O\left(\frac{1}{s}\right) \) as in the periodic case. Indeed, the matrix field \( D \) is constant and the computation of a matrix \( C \) which satisfies the equality (3.13) can be provided by solving the linear system \( L(C) = D - \langle D \rangle \).

### 3.4 Shear flow

In this example, we provide a two dimensional vector field such that the associated average matrix field does not exist. Actually, sufficient conditions for the existence of an average matrix field are given in [3]. These conditions are based on the existence of a basis \((b_i)_{1 \leq i \leq 2}\) of vector fields in involution with the vector field \( b(y) \), i.e when the operators \( b(y) \cdot \nabla_y \) and \( b_i(y) \cdot \nabla_y \) are commuting, for any \( 1 \leq i \leq 2 \). We define the vector field \( b(y) = (y_2, -y_1) \) for \( y = (y_1, y_2) \in \mathbb{R}^2 \). In this case, the flow \( Y \) associated to \( b \) is given by \( Y(s; y) = R(-s) y \), for any \( s \in \mathbb{R} \) and \( y \in \mathbb{R}^2 \). Moreover, we consider a smooth even function \( f : \mathbb{R} \to \mathbb{R}_+ \) such that \( f(0) = 1 \), \( f(x) = 0 \) for any \( x \in [1; +\infty[ \) and strictly decreasing on \([0, 1]\). Finally, we introduce the radial function \( T(y) = f(|y|) \) for \( y \in \mathbb{R}^2 \). We denote by \( Z \) the flow associated to the vector field \( Tb \). We have \( Z(s; y) = R(-sT(y)) y \) for any \( s \in \mathbb{R} \) and \( y \in \mathbb{R}^2 \). The flow \( Z \) is a rotating shear flow, indeed the rotating period associated at each characteristic is different. If \( y \) is a point of the characteristic \( Z(s; y) \), for \( s \in \mathbb{R} \), the associated period is \( T(y) \). The function \( T \) is constant along the flows \( Y \) and \( Z \). We claim that the average matrix field associated to \( D = I_2 \), with respect to the vector field \( Tb \) is not well defined, in the sense (2.4), on \( B(0, 1)/(\{(0, 0)\}) \) where \( B(0, 1) \) is the unit open ball of \( \mathbb{R}^2 \). Indeed, thanks to the
we obtain

Thus

We integrate (3.19) with respect to

Finally, we combine (3.16) and (3.18), and a straightforward computation leads to

A direct computation shows that, for any \( s \in \mathbb{R} \) and \( y \in \mathbb{R}^2 \), we have

\[
G(s)I_2 = \partial Z^{-1}(s; y) \partial Z^{-1}(s; y). \tag{3.16}
\]

On the other hand, thanks to the relation \( \partial Z^{-1}(s; y) = \partial Z(-s; Z(s; y)) \) which is available for any \( s \in \mathbb{R} \) and \( y \in \mathbb{R}^2 \), we obtain

\[
\partial Z^{-1}(s; y) = s \mathcal{R}(\pi/2) y \otimes \nabla_y T(y) + \mathcal{R}(sT(y)). \tag{3.17}
\]

Moreover, thanks to the equality \( \nabla_y T(y) = \frac{f'(|y|)}{|y|} y \), we can write (3.17) in the following form

\[
\partial Z^{-1}(s; y) = \frac{s f'(|y|)}{|y|} \mathcal{R}(\pi/2) y \otimes Z(s; y) + \mathcal{R}(sT(y)). \tag{3.18}
\]

Finally, we combine (3.16) and (3.18), and a straightforward computation leads to

\[
G(s)I_2 = s^2 f'(|y|)^2 (b \otimes b)(y) + s f'(|y|) \left( \frac{-2y_1y_2}{|y|^2} \frac{y_1^2 - y_2^2}{|y|^2} \right) + I_2. \tag{3.19}
\]

We integrate (3.19) with respect to \( s \) over the interval \([0, S]\) with \( S > 0 \), for any \( y \in \mathbb{R}^2 \), and we obtain

\[
\frac{1}{S} \int_0^S (G(s)I_2)(y) \, ds = \frac{S^2}{3} f'(|y|)^2 (b \otimes b)(y) + \frac{S}{2} f'(|y|) \left( \frac{-2y_1y_2}{|y|^2} \frac{y_1^2 - y_2^2}{|y|^2} \right) + I_2. \tag{3.20}
\]

Thus \( \langle I_2 \rangle (0, 0) = I_2 \) and \( \langle I_2 \rangle (y) = I_2 \) for any \( y \in B(0, 1)^c \). But, for \( y \in B(0, 1)/\{(0, 0)\} \), the expression (3.20) does not have a limit when \( S \to +\infty \). The average matrix field associated to \( D = I_2 \) with respect to \( Tb \) is not well defined.
4 Asymptotic behavior of the solutions of a parabolic problem with stiff transport terms

In this section, we study numerically the asymptotic behavior of the family \((u^\varepsilon)_{\varepsilon>0}\), solutions of (1.1), when \(\varepsilon\) goes to 0, in the two dimensional setting \(m = 2\). The behavior of \(u^\varepsilon\) can be described, when \(\varepsilon\) goes to 0, as a composition product of a profile \(v\), which does not depend of \(\varepsilon\), with the flow associated to the vector field \(-b/\varepsilon\). Moreover, the profile \(v\) solves the effective diffusion problem (2.3) with the diffusion matrix field \(\langle D\rangle\) (2.4). Thanks to the method in Section 3 for the computation of the effective diffusion field, we solve the system (2.3), and we study the error between a reference solution \(u^\varepsilon(t, \cdot)\) and \(v(t, Y(-t/\varepsilon; \cdot))\). The anisotropic diffusion equation, with \(T > 0\) and \(y \in \mathbb{R}^2\),

\[
\begin{align*}
\frac{\partial v}{\partial t} - \text{div}_y(\langle D\rangle \nabla_y v) &= 0, & (t, y) &\in [0, T] \times \mathbb{R}^2 \\
v(0, y) &= u^0(y), & y &\in \mathbb{R}^2
\end{align*}
\]

is solved by an implicit method in time and finite difference method in space, see [24]. As in Section 3.2, we introduce a time discretization \((t^k)\) of \([0, T]\), with \(k \in I_t = \{0, \ldots, N_t\}\) and \(\Delta t = T/N_t\). We consider also a spatial discretization \((y_{ij})\), with a step \(\Delta y\), for the square \(\mathcal{C} = [-R, R] \times [-R, R]\), with \(R > 0\), and we add the points \(y_{i+1/2,j}\) and \(y_{i,j+1/2}\) for any \(i, j \in I = \{0, \ldots, N - 1\}\), for the flux computation. We introduce the notation \(W = -\langle D\rangle \nabla_y v\). The operator \(\text{div}_y(W)\) at the point \(y_{ij}\) is approximated by

\[
(\text{div}_y(W))_{ij} \approx \frac{W^1_{i+1/2,j} - W^1_{i-1/2,j}}{\Delta y} + \frac{W^2_{i,j+1/2} - W^2_{i,j-1/2}}{\Delta y}
\]

where

\[
\begin{align*}
W^1_{i+1/2,j} &= -\langle D\rangle_{11} \frac{\partial v}{\partial y_1}
\end{align*}
\]

\[
\begin{align*}
W^2_{i,j+1/2} &= -\langle D\rangle_{21} \frac{\partial v}{\partial y_2}
\end{align*}
\]

The derivatives are approximated by the following expressions

\[
\begin{align*}
\frac{\partial v}{\partial y_1}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v}{\partial y_2}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v}{\partial y_1}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v}{\partial y_2}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v}{\partial y_1}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial v}{\partial y_2}
\end{align*}
\]

and the diffusion coefficients \(\langle D\rangle_{i+1/2,j}, \langle D\rangle_{i,j+1/2}\) by

\[
\begin{align*}
\langle D\rangle_{i+1/2,j} &= \frac{\langle D\rangle_{i+1,j} + \langle D\rangle_{i,j}}{2} \\
\langle D\rangle_{i,j+1/2} &= \frac{\langle D\rangle_{i+1,j} + \langle D\rangle_{i,j}}{2}
\end{align*}
\]

We are led to the semi-discrete scheme in space, where we denote by \(v_{ij}(t)\) the approximations of the unknowns \(v(t, y_{ij})\) for any \((i, j) \in I^2\)

\[
\begin{align*}
\frac{\partial v_{ij}(t)}{\partial t} + \frac{W^1_{i+1/2,j}(t) - W^1_{i-1/2,j}(t)}{\Delta y} + \frac{W^2_{i,j+1/2}(t) - W^2_{i,j-1/2}(t)}{\Delta y} &= 0.
\end{align*}
\]
The time resolution is done by an implicit Crank-Nicolson scheme, see [17] for more details. If we introduce the vector $V^k$ of discrete variables $v_{ij}^k$ which approximate $v(t^k, y_{ij})$ for $k \in \mathcal{I}_t$ and $(i, j) \in \mathcal{I}_d^2$, the Crank-Nicolson scheme writes

$$V^{k+1} = \left(I - \frac{\Delta t}{2} \mathcal{W}\right)^{-1} \left(I + \frac{\Delta t}{2} \mathcal{W}\right) V^k$$

where $\mathcal{W}$ is the discretization matrix associated to the operator (4.1) and obtained by combining (4.2), (4.3) and (4.4). The order of this scheme is two in time and space for smooth data. A reference solution for the stiff convection diffusion problem (1.1) is computed (4.2), (4.3) and (4.4). The solution $u^\varepsilon$ of the system (1.1) can be written in semigroup form:

$$u^\varepsilon(t, \cdot) = e^{-t(D+\frac{1}{\varepsilon}T)}u_{\text{in}}$$

for any $t \in [0, T]$. We approach this solution at the time $t^k$, for $k \in \mathcal{I}_t$, with a Strang splitting, see [21]

$$u^\varepsilon(t^k, \cdot) = \left[e^{-\frac{\Delta t}{2}D} e^{-\frac{\Delta t}{2}T} e^{-\frac{\Delta t}{2}D}\right]^k u_{\text{in}}.$$

This method provides a second order accuracy approximation in time if the data of the problem are smooth. The semigroup associated to $\mathcal{D}$ is computed by solving the associated diffusion equation by the finite difference scheme presented above. A numerical approximation of the group associated to the transport operator $\frac{1}{\varepsilon}T$ is performed by a semi-Lagrangian scheme, which consists in the computation of the flow $Y(t/\varepsilon, \cdot)$ and the interpolation step, see Section 3.2. A splitting method associated to a semi-Lagrangian scheme for the transport, leads us to solve separately the group associated to the stiff operator and to choose an adapted time discretization $(\hat{y}^k_\varepsilon)_{k \in \mathcal{I}_t}$ of the interval $[0, \frac{\Delta t}{\varepsilon}]$ with $\mathcal{I}_t = \{0, \ldots, N^t_\varepsilon\}$, for solving the flow $Y(\Delta t/\varepsilon, \cdot)$ even when $\varepsilon$ is small. In practice, we choose $N^t_\varepsilon = 200\left[\frac{\Delta t}{\varepsilon}\right]$.

**Examples**

We study numerically the error committed when we approach the solution $u^\varepsilon$ of the system (1.1) by the quantity $v(t, Y(-t/\varepsilon, \cdot))$, where $v$ is solution of (2.3). The average diffusion field is computed by the method presented in Section 3. For any $k \in \mathcal{I}_t$ and $(i, j) \in \mathcal{C}$, we denote by $v^k_{ij}$ the numerical approximation of $v(t^k, y_{ij})$. As in Section 3.3, the spatial error is localized to a set $\mathcal{S} \subset \mathcal{C}$ invariant by the flow of $b$. The $L^2([0, T], L^2)$ error is computed in the following way

$$\|v\|_{L^\infty([0, T], L^2)} = \max_{k \in \mathcal{I}_t} \sqrt{\sum_{(i,j) \in \mathcal{S}^2} \Delta y^2 |v^k_{ij}|^2}.$$

For the numerical tests, we assumed that : $\mathcal{C} = [-2, 2] \times [-2, 2]$, $T = 0.01$ and

$$v_{\text{in}}(y) = 10 \exp \left(-\frac{y_1^2 + (y_2 - 0.5)^2}{0.02}\right), \quad y \in \mathbb{R}^2.$$

The solutions of the problems (1.1) and (2.3) are computed with a spatial resolution $N = 512$ and time resolution $N_t = 100N$. We assume that the vector field $b$ is the ellipsoidal vector field defined in Section 3.3, and we pick a diffusion field

$$D = \begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}.$$
The average diffusion field associated to $D$ is also symmetric and positive definite, see [3]. By the formula (3.6), we have

$$\langle D \rangle = \begin{pmatrix} 10/3 & -5/3 \\ -5/3 & 10/3 \end{pmatrix}.$$ 

Figure 8 represents the time evolution of the $L^2$ norm $t \mapsto \|u^\varepsilon(t, \cdot) - v(t, Y(-t/\varepsilon, \cdot))\|_{L^2}$ and the error $L^\infty([0, T], L^2)$ with respect to $\varepsilon$. Figure 8 confirms numerically the expected rate of convergence given by (2.6). In Figure 9, we analyze the example of the non explicit central flow, see Section 3.3, with the diffusion field $D = I_2$. The coefficients of the associated average matrix field are represented in Figure 4. In this case, the expected convergence rate is not reached, this is due to the regularity default of the averaged matrix field $\langle I_2 \rangle$ at the origin.

The results of the Figures 8 and 9 confirm the asymptotic result (2.6) and, at least in the case where the transport vector field $b$ and the diffusion matrix field $D$ are smooth, the expected rate is obtained. Thus, at least for smooth data, we have proposed a numerical method which consists in computing the effective diffusion field (2.4) and the function $v$ solution of
the associated system (2.3), then providing the approximation $v(t, Y(-t/\varepsilon; \cdot))$ at the order one, with respect to $\varepsilon$, of the solution $u^\varepsilon$ of the stiff system (1.1).

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References


