

Particle Micro-Macro schemes for collisional kinetic equations in the diffusive scaling

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Outline

- 1 Problem and objectives
- 2 Micro-macro model
- 3 Monte Carlo / FV discretization
- 4 Numerical results

- 1 Problem and objectives
 - Introduction
 - Our problem
 - Objectives
- 2 Micro-macro model
- 3 Monte Carlo / FV discretization
- 4 Numerical results

Numerical simulation of particle systems

We are interested in

- the numerical simulation of collisional kinetic Problems $_{\varepsilon}$,
- different scales: collisions parameterized by the Knudsen number $\varepsilon(t, \mathbf{x})$,
- the development of schemes that are efficient in both kinetic and fluid regimes.

Kinetic regime $\varepsilon(t, \mathbf{x}) = \mathcal{O}(1)$

- Particles represented by a distribution function $f(t, \mathbf{x}, \mathbf{v})$.
- Solving a Boltzmann or Vlasov-type equation

$$\partial_t f + \mathcal{A}(\mathbf{v}, \varepsilon) \cdot \nabla_{\mathbf{x}} f + \mathcal{B}(\mathbf{v}, \mathbf{E}, \mathbf{B}, \varepsilon) \cdot \nabla_{\mathbf{v}} f = \mathcal{S}(\varepsilon).$$

:-) Accurate and necessary far from thermodynamical equilibrium.

:-(In 3D $\implies$ 7 variables $\implies$ heavy computations.

Fluid regime $\varepsilon(t, \mathbf{x}) \ll 1$

- Moment equations on physical quantities linked to f (density ρ , mean velocity u , temperature T , etc.).
- :- (Lost of precision.
- :-) Small cost and sufficient at thermodynamical equilibrium.

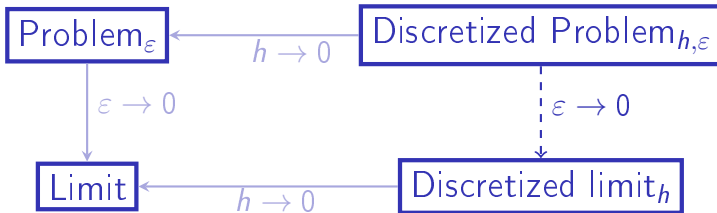
There are two main strategies for multiscale problems:

- domain decomposition methods,
- asymptotic preserving (AP) schemes.

- Domain decomposition approach: use the suitable model in the appropriate region.
 - :-) Very efficient in each region.
 - :-(How to determine the validity of each model and let them communicate?

- Domain decomposition approach: use the suitable model in the appropriate region.
 - :-) Very efficient in each region.
 - :- (How to determine the validity of each model and let them communicate?
- Asymptotic Preserving approach: develop a model suitable in any region.
 - :-) Only one model.
 - :- (Generally have the less favorable cost.

Asymptotic Preserving approach⁵



h : space step Δx or time step Δt .

Prop.: Stability and consistency $\forall \varepsilon$, particularly when $\varepsilon \rightarrow 0$.

:- (Standard schemes: constraint $h = \mathcal{O}(\varepsilon)$.

Aim: Construct a scheme for which h is independent of ε .

⁵Jin, SISC 1999.

Our Problem _{ε}

Radiative transport equation in the diffusive scaling

$$\partial_t f + \frac{1}{\varepsilon} \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon^2} (\rho M - f) \quad (1)$$

- $\mathbf{x} \in \Omega \subset \mathbb{R}^{d_x}$, $\mathbf{v} \in V = \mathbb{R}^{d_v}$,
- charge density $\rho(t, \mathbf{x}) = \int_V f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$,
- $M(\mathbf{v}) = \frac{1}{(2\pi)^{d_v/2}} \exp\left(-\frac{|\mathbf{v}|^2}{2}\right)$,
- periodic conditions in $\mathbf{x}$ and initial conditions.

Main difficulty:

- Knudsen number ε may be of order 1 or tend to 0 in the diffusive scaling. The **asymptotic diffusion equation** being

$$\partial_t \rho - \Delta_{\mathbf{x}} \rho = 0. \quad (2)$$

Objectives

- Construction of an AP scheme.
- Reduction of the numerical cost at the limit $\varepsilon \rightarrow 0$.

Tools

- Micro-macro decomposition^{6,7} for this model. Previous work with a grid in v for the micro part⁸, cost was constant w.r.t. ε .
- Particle method for the micro part since few information in v is necessary at the limit⁹.
- Monte Carlo techniques¹⁰.

⁶Lemou, Mieussens, SIAM SISC 2008.

⁷Liu, Yu, CMP 2004.

⁸Crouseilles, Lemou, KRM 2011.

⁹C., Crouseilles, Lemou, CMS 2018.

¹⁰Degond, Dimarco, Pareschi, IJNMF 2011.

- 1 Problem and objectives
- 2 **Micro-macro model**
 - Derivation of the micro-macro system
 - Reformulation of the micro-macro model
- 3 Monte Carlo / FV discretization
- 4 Numerical results

Micro-macro decomposition

- Micro-macro decomposition:

$$f = \rho M + g$$

with g the perturbation.

- $\mathcal{N} = \text{Span} \{M\} = \{f = \rho M\}$ null space of the BGK operator
 $Q(f) = \rho M - f$.
- Π orthogonal projection onto $\mathcal{N}$:

$$\Pi h := \langle h \rangle M, \quad \langle h \rangle := \int_V h \, d\mathbf{v}.$$

- Applying Π to (1) $\implies$ macro equation on ρ

$$\partial_t \rho + \frac{1}{\varepsilon} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle = 0. \quad (3)$$

- Applying $(I - \Pi)$ to (1) $\implies$ micro equation on g

$$\partial_t g + \frac{1}{\varepsilon} [\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M] = -\frac{1}{\varepsilon^2} g. \quad (4)$$

Equation (1) $\Leftrightarrow$ micro-macro system:

$$\begin{cases} \partial_t \rho + \frac{1}{\varepsilon} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle = 0, \\ \partial_t g + \frac{1}{\varepsilon} \mathcal{F}(\rho, g) = -\frac{1}{\varepsilon^2} g, \end{cases} \quad (5)$$

where $\mathcal{F}(\rho, g) = \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M$.

Difficulties

- Stiff terms in the micro equation (4) on g .
- In previous works^{11,12}, stiffest term (of order $1/\varepsilon^2$) considered implicit in time $\implies$ transport term (of order $1/\varepsilon$) stabilized.

But here:

- use of particles for the micro part
- $\implies$ splitting between the transport term and the source term,
 $\implies$ not possible to use the same strategy.

Idea?

- Suitable reformulation of the model.

¹¹Lemou, Mieussens, SIAM SISC 2008.

¹²Crouseilles, Lemou, KRM 2011.

• Strategy of Lemou¹³:

1. rewrite (4) $\partial_t g + \frac{1}{\varepsilon} \mathcal{F}(\rho, g) = -\frac{1}{\varepsilon^2} g$ as

$$\partial_t (e^{t/\varepsilon^2} g) = -\frac{e^{t/\varepsilon^2}}{\varepsilon} \mathcal{F}(\rho, g),$$

2. integrate in time between two times t^n and $t^{n+1} = t^n + \Delta t$:

$$e^{t^{n+1}/\varepsilon^2} g^{n+1} = e^{t^n/\varepsilon^2} g^n + \int_{t^n}^{t^{n+1}} -\frac{e^{t/\varepsilon^2}}{\varepsilon} \mathcal{F}(\rho, g) dt,$$

3. use left-rectangle method for $\mathcal{F}(\rho, g)$ and multiply by $e^{-t^{n+1}/\varepsilon^2} / \Delta t$:

$$\frac{g^{n+1} - g^n}{\Delta t} = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g^n - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathcal{F}(\rho^n, g^n) + \mathcal{O}(\Delta t),$$

4. approximate up to terms of order $\mathcal{O}(\Delta t)$ by:

$$\partial_t g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathcal{F}(\rho, g).$$

• No more stiff terms and consistent with initial micro equation (4).

¹³Lemou, CRAS 2010.

New micro-macro model

The new micro-macro model writes

$$\partial_t \rho + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} g \rangle = 0, \quad (6)$$

$$\partial_t g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathcal{F}(\rho, g), \quad (7)$$

with $\mathcal{F}(\rho, g) = \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M$.

We propose the following hybrid discretization:

- macro equation (6): Finite Volume method,
- micro equation (7): Monte Carlo technique.

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Discretization of the micro equation

- Model: considering at each time step N^n particles, with position $\mathbf{x}_k^n$, velocity $\mathbf{v}_k^n$ and constant weight ω_k , $k = 1, \dots, N^n$, g is approximated by¹⁴

$$g_{N^n}(t^n, \mathbf{x}, \mathbf{v}) = \sum_{k=1}^{N^n} \omega_k \delta(\mathbf{x} - \mathbf{x}_k^n) \delta(\mathbf{v} - \mathbf{v}_k^n).$$

- For the coupling with the macro equation, we need a grid in $\mathbf{x}$. For $d_x = 1$, we define for $i = 0, \dots, N_x - 1$

$$x_i = x_{\min} + i\Delta x, \quad x_{i\pm 1/2} = x_i \pm \frac{\Delta x}{2}.$$

- How to define/compute ω_k , N^n , $\mathbf{x}_k^n$, $\mathbf{v}_k^n$?

¹⁴Crouseilles, Dimarco, Lemou, KRM 2017.

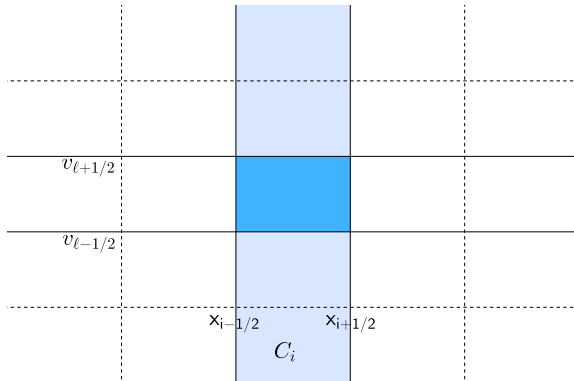
Initialization

- Choose the characteristic weight m_p or the characteristic number of particles N_p necessary to sample the full distribution function f , and link them with

$$m_p = \frac{1}{N_p} \int_{\mathbb{R}^{d_x}} \int_{\mathbb{R}^{d_v}} f(t=0, \mathbf{x}, \mathbf{v}) d\mathbf{v} d\mathbf{x}.$$

- Now, we want to sample $g(t=0, \mathbf{x}, \mathbf{v})$, that has no sign.
- We impose $\omega_k \in \{m_p, -m_p\}$.
- For velocities, we impose $\mathbf{v}_k^n$ on a cartesian grid in $\mathbb{R}^{d_v}$.
 For $d_v = 1$, it writes $v_k^n \in \{v_\ell, \ell = 0, \dots, N_v - 1\}$
 $\forall k = 1, \dots, N^n$, where $v_\ell = v_{\min} + \ell \Delta v$, $\ell = 0, \dots, N_v - 1$.

Let us introduce the notations in 1D...



Let us introduce the notations in 1D...

- The number of initial positive (resp. negative) particles having the velocity $v_k = v_\ell$ in the strip $C_i = [x_{i-1/2}, x_{i+1/2}] \times \mathbb{R}$ is given by

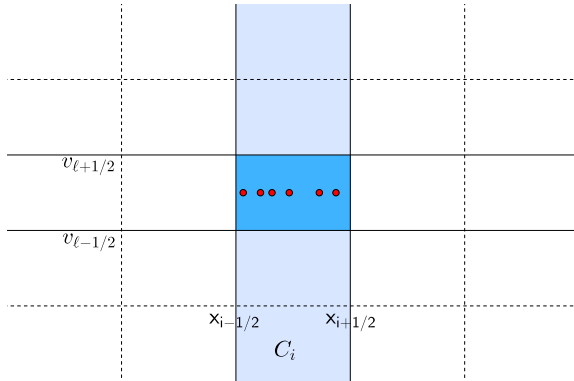
$$N_{i,\ell}^{0,\pm} = \lfloor \pm \frac{\Delta x \Delta v}{m_p} g^\pm(t=0, x_i, v_\ell) \rfloor,$$

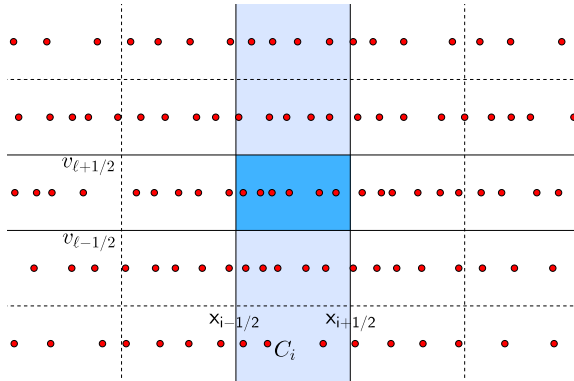
that is an approximation of

$$N_{i,\ell}^{0,\pm} = \pm \frac{1}{m_p} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \int_{v_\ell - \Delta v/2}^{v_\ell + \Delta v/2} g^\pm(t=0, x, v) dv dx,$$

with $g^\pm = \frac{g \pm |g|}{2}$ the positive (resp. negative) part of g .

- Positions of these $N_{i,\ell}^{0,\pm}$ particles are taken uniformly in $[x_{i-1/2}, x_{i+1/2}]$.
- At time $t=0$, we have $N^0 = \sum_i \left(\sum_\ell N_{i,\ell}^{0,+} + \sum_\ell N_{i,\ell}^{0,-} \right)$.





From t^n to t^{n+1}

Solve the micro equation (7) by Monte Carlo technique.

- **Splitting** between the transport part

$$\partial_t g + \varepsilon \frac{1 - e^{-\Delta t / \varepsilon^2}}{\Delta t} \mathbf{v} \cdot \nabla_{\mathbf{x}} g = 0,$$

and the interaction part

$$\partial_t g = \frac{e^{-\Delta t / \varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t / \varepsilon^2}}{\Delta t} (\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M).$$

- Solve the **transport part** thanks to motion equation:

$$\frac{d\mathbf{x}_k}{dt}(t) = \varepsilon \frac{1 - e^{-\Delta t / \varepsilon^2}}{\Delta t} \mathbf{v}_k, \quad \mathbf{x}_k^{n+1} = \mathbf{x}_k^n + \varepsilon (1 - e^{-\Delta t / \varepsilon^2}) \mathbf{v}_k^n.$$

Remark that $\mathbf{v}_k^{n+1} = \mathbf{v}_k^n$.

- Solve **interaction part** by writing

$$g^{n+1} = e^{-\Delta t/\varepsilon^2} \tilde{g}^n + (1 - e^{-\Delta t/\varepsilon^2}) \varepsilon \left[-\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \tilde{g} \rangle^n M \right]$$

where $\tilde{g}^n$ is the function after the transport part.

Apply a **Monte Carlo technique**:

- with probability $e^{-\Delta t/\varepsilon^2}$, the distribution g does not change,
- with probability $(1 - e^{-\Delta t/\varepsilon^2})$, the distribution g is replaced by a new distribution given by

$$\varepsilon \left[-\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \tilde{g} \rangle^n M \right].$$

In practice (1)

“With probability $e^{-\Delta t/\varepsilon^2}$, the distribution g does not change.”

→ In each strip C_i

- we choose randomly $e^{-\Delta t/\varepsilon^2} \tilde{N}_i^n$ particles and keep them unchanged (with $\tilde{N}_i^n$ the number of particles in C_i after the transport part),
- we discard the others.

In practice (2)

“With probability $(1 - e^{-\Delta t/\varepsilon^2})$, the distribution g is replaced by a new distribution given by $\varepsilon \left[-\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \tilde{g} \rangle^n M \right]$.”

→ We define the function

$$\mathcal{P}^{n,\pm}(\mathbf{x}, \mathbf{v}) = \varepsilon \left[-\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \tilde{g} \rangle^n M \right]^{\pm}.$$

→ In each strip C_i

- we sample a corresponding number $M_i^{n,\pm}$ of new particles with weights $\pm m_p$ from $(1 - e^{-\Delta t/\varepsilon^2}) \mathcal{P}^{n,\pm}(\mathbf{x}_i, \mathbf{v})$,
- in 1D, we have

$$M_{i,\ell}^{n,\pm} = \frac{1}{m_p} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \int_{v_\ell - \Delta v/2}^{v_\ell + \Delta v/2} \pm (1 - e^{-\Delta t/\varepsilon^2}) \mathcal{P}^{n,\pm}(x, v) dv dx,$$

- these $M_{i,\ell}^{n,\pm}$ created particles are such that $v_k^n = v_\ell$ and x_k^n are uniformly distributed in $[x_{i-1/2}, x_{i+1/2}]$.

Asymptotically Complexity Diminishing Property

- At the end of the time step, we have in each strip C_i

$$N_i^{n+1} = e^{-\Delta t/\varepsilon^2} \tilde{N}_i^n + \sum_{\ell} \left(M_{i,\ell}^{n,+} + M_{i,\ell}^{n,-} \right)$$

particles.

- The number of particles automatically diminishes with ε .
- Reduction of the computational complexity when approaching equilibrium: **Asymptotically Complexity Diminishing Property**.

Macro equation

- Equation $\partial_t \rho + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} g \rangle = 0$.
- First proposition:

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} g^{n+1} \rangle = 0,$$

discretized by a Finite Volume method. For example in 1D:

$$\rho_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \rho(t^n, x) dx,$$

$$\langle v g^n \rangle_i = \frac{1}{\Delta x} \sum_{x_k^n \in [x_{i-1/2}, x_{i+1/2}]} v_k \omega_k \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \langle v g \rangle(t^n, x) dx.$$

- Problem: g^{n+1} suffers from numerical noise inherent to particles method. This noise, amplified by $\frac{1}{\varepsilon}$, will damage ρ^{n+1} .

Correction of the macro discretization

- Use the expression of g^{n+1} and write

$$\begin{aligned}\langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g^{n+1} \rangle &= e^{-\Delta t / \varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle \\ &\quad - \varepsilon (1 - e^{-\Delta t / \varepsilon^2}) \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} (\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M) \rangle \\ &\quad + \varepsilon (1 - e^{-\Delta t / \varepsilon^2}) \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} (\langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g} \rangle^n M) \rangle,\end{aligned}$$

or after simplifications

$$\langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g^{n+1} \rangle = e^{-\Delta t / \varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - \varepsilon (1 - e^{-\Delta t / \varepsilon^2}) \Delta_{\mathbf{x}} \rho^n.$$

- Plug it into the macro equation

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{1}{\varepsilon} e^{-\Delta t / \varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - (1 - e^{-\Delta t / \varepsilon^2}) \Delta_{\mathbf{x}} \rho^n = 0.$$

- To avoid the parabolic CFL condition of type $\Delta t \leq C \Delta x^2$, take the **diffusion term implicit**:

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{1}{\varepsilon} e^{-\Delta t / \varepsilon^2} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \tilde{\mathbf{g}}^n \rangle - (1 - e^{-\Delta t / \varepsilon^2}) \Delta_{\mathbf{x}} \rho^{n+1} = 0.$$

- **No more stiffness**, the numerical noise does not damage ρ .
- **AP property**: for fixed $\Delta t > 0$, the scheme degenerates when $\varepsilon \rightarrow 0$ to an implicit discretization of the diffusion equation $\partial_t \rho - \Delta_{\mathbf{x}} \rho = 0$.

Space discretization

- Macro equation is solved between transport and source parts of micro scheme.
- In 1D, solve

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} + \frac{1}{\varepsilon} e^{-\Delta t / \varepsilon^2} \frac{\langle v \tilde{g}^n \rangle_{i+1} - \langle v \tilde{g}^n \rangle_{i-1}}{2\Delta x} - (1 - e^{-\Delta t / \varepsilon^2}) \frac{\rho_{i+1}^{n+1} - 2\rho_i^{n+1} + \rho_{i-1}^{n+1}}{\Delta x^2} = 0.$$

Space discretization in 2D

In 2D, we use an Alternating Direction Implicit (ADI) method¹⁵:

- 1) Starting from ρ^n , solve over a time step Δt

$$\partial_t \rho + \frac{1}{2\varepsilon} e^{-\Delta t/\varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - (1 - e^{-\Delta t/\varepsilon^2}) \partial_{xx} \rho = 0,$$

using a Crank-Nicolson time discretization to get ρ^* .

- 2) Starting from ρ^* , solve over a time step Δt

$$\partial_t \rho + \frac{1}{2\varepsilon} e^{-\Delta t/\varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - (1 - e^{-\Delta t/\varepsilon^2}) \partial_{yy} \rho = 0,$$

using a Crank-Nicolson time discretization to get ρ^{n+1} .

¹⁵Peaceman, Rachford, J. Soc. Indust. Appl. Math. 1955.

Nice properties

- Only 1D systems of size N_x or N_y .
- ADI method unconditionally stable in 2D.
- Straightforward extension in 3D: a priori conditionally stable, but better extensions have been derived¹⁶.
- Right asymptotic behaviour.

¹⁶Sharma, Hammett, JCP 2011.

1 Problem and objectives

2 Micro-macro model

3 Monte Carlo / FV discretization

4 Numerical results

- Test 1 - 2Dx2D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) = 0$
- Test 2 - 2Dx2D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$
- Test 3 - 3Dx3D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$
- Test 4 - 2Dx2D, $\varepsilon(\mathbf{x})$, $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$

Test 1 - 2Dx2D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) = 0$

Initialization:

$$f(t=0, \mathbf{x}, \mathbf{v}) = \rho(t=0, \mathbf{x})M(\mathbf{v}), \quad \mathbf{x} \in [0, 4\pi]^2, \quad \mathbf{v} \in \mathbb{R}^2$$

with

$$\rho(t=0, \mathbf{x}) = 1 + \frac{1}{2} \cos\left(\frac{x}{2}\right) \cos\left(\frac{y}{2}\right),$$

$$M(\mathbf{v}) = \frac{1}{2\pi} \exp\left(-\frac{|\mathbf{v}|^2}{2}\right),$$

so that

$$g(t=0, \mathbf{x}, \mathbf{v}) = 0.$$

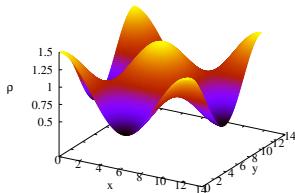
Periodic boundary conditions in space.

Asymptotic behaviour, $\varepsilon = 10^{-4}$

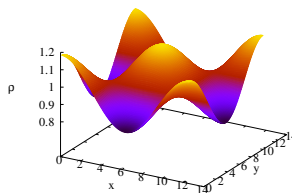
MM-MC: the presented Micro-Macro Monte Carlo scheme.

MM-G: a Micro-Macro Grid code, considered as reference.

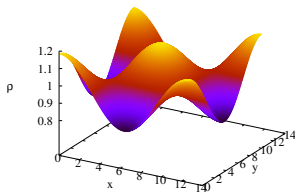
Initialization



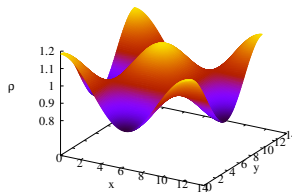
MM-MC, $\varepsilon=0.0001$, $T=2$



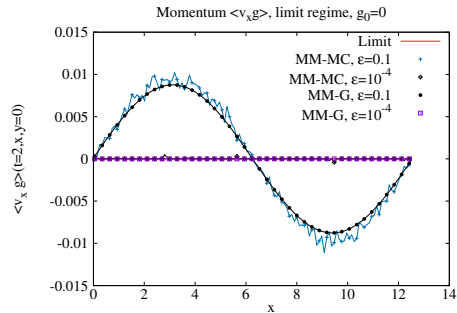
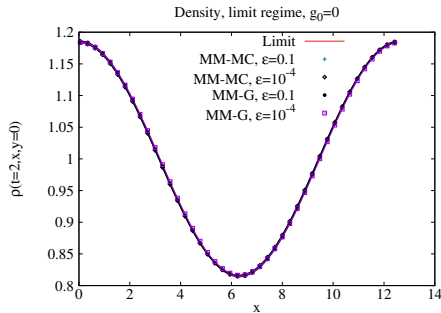
Limit, $T=2$



MM-G, $\varepsilon=0.0001$, $T=2$



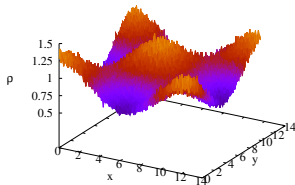
Slices of the density $\rho(T=2, x, y=0)$ and of the momentum $\langle v_x g \rangle(T=2, x, y=0)$.



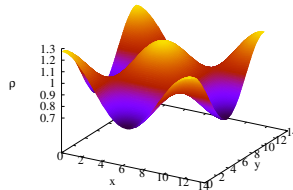
Kinetic regime, $\varepsilon = 1$

Full PIC: standard particle method on f .

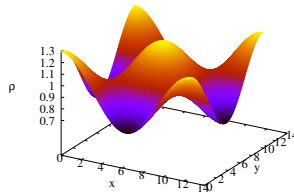
Full PIC, $\varepsilon=1$, $T=2$



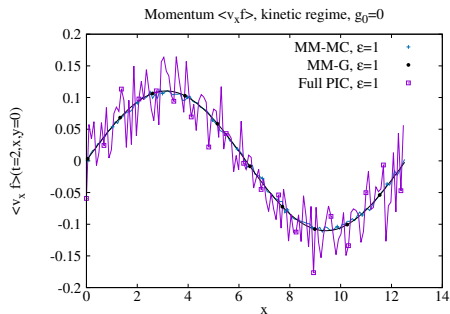
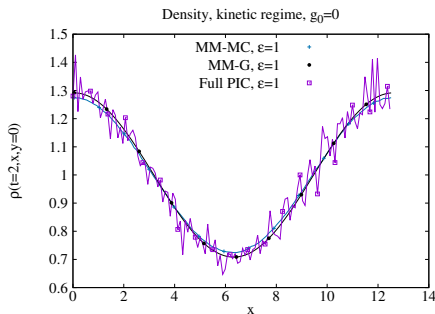
MM-MC, $\varepsilon=1$, $T=2$



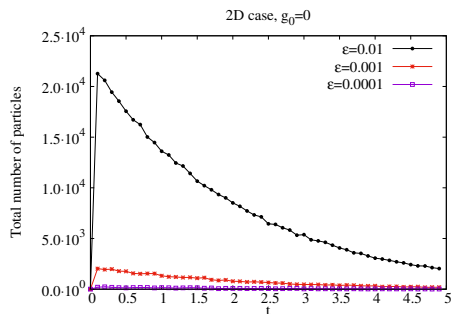
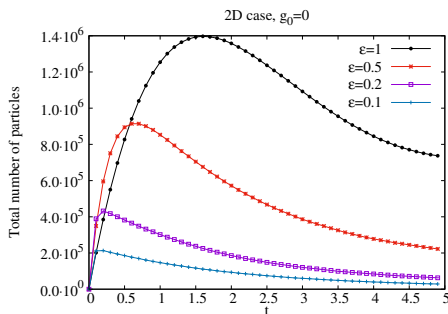
MM-G, $\varepsilon=1$, $T=2$



Slices of the density $\rho(T=2, x, y=0)$ and of the momentum $\langle v_x g \rangle(T=2, x, y=0)$.



Time evolution of the number of particles



Test 2 - 2Dx2D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$

Initialization:

$$f(t=0, \mathbf{x}, \mathbf{v}) = \frac{1}{4\pi} \left(\exp \left(-\frac{|\mathbf{v} - 2|^2}{2} \right) + \exp \left(-\frac{|\mathbf{v} + 2|^2}{2} \right) \right) \rho(t=0, \mathbf{x}),$$

with

$$\mathbf{x} \in [0, 4\pi]^2, \quad \mathbf{v} \in \mathbb{R}^2,$$

$$\rho(t=0, \mathbf{x}) = 1 + \frac{1}{2} \cos \left(\frac{x}{2} \right) \cos \left(\frac{y}{2} \right),$$

so that

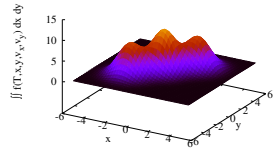
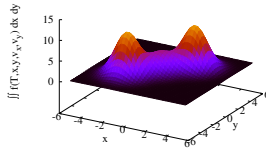
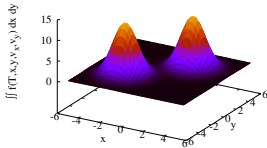
$$g(t=0, \mathbf{x}, \mathbf{v}) = \rho(t=0, \mathbf{x})M(\mathbf{v}) - f(t=0, \mathbf{x}, \mathbf{v}) \neq 0.$$

Integral of the distribution function in space $\int f(T, x, v) dx$.

MM-MC, $\varepsilon=1$, $T=0$

MM-MC, $\varepsilon=1$, $T=0.2$

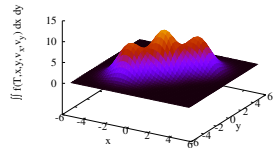
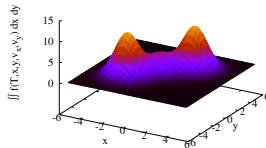
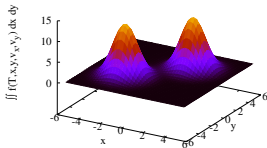
MM-MC, $\varepsilon=1$, $T=0.5$



MM-G, $\varepsilon=1$, $T=0$

MM-G, $\varepsilon=1$, $T=0.2$

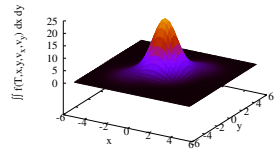
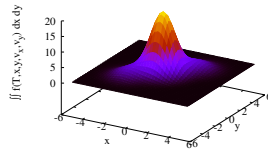
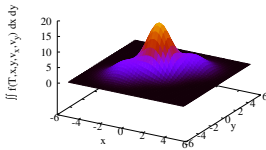
MM-G, $\varepsilon=1$, $T=0.5$



MM-MC, $\varepsilon=1$, $T=1$

MM-MC, $\varepsilon=1$, $T=1.5$

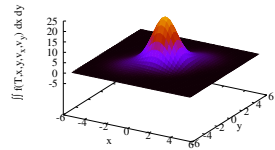
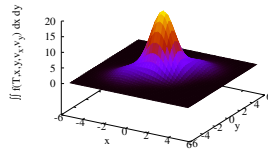
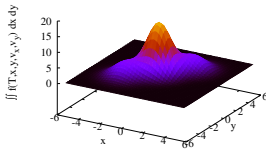
MM-MC, $\varepsilon=1$, $T=2$



MM-G, $\varepsilon=1$, $T=1$

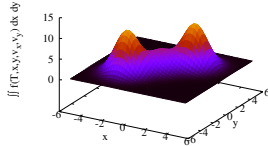
MM-G, $\varepsilon=1$, $T=1.5$

MM-G, $\varepsilon=1$, $T=2$

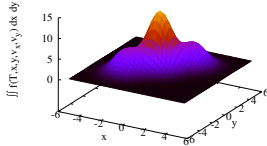


Influence of ε

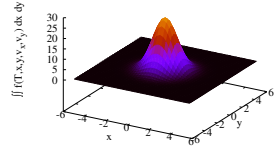
MM-MC, $\varepsilon=1$, $T=0.2$



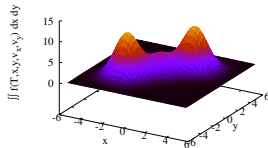
MM-MC, $\varepsilon=0.5$, $T=0.2$



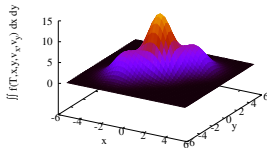
MM-MC, $\varepsilon=0.1$, $T=0.2$



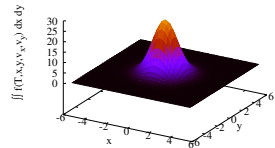
MM-G, $\varepsilon=1$, $T=0.2$



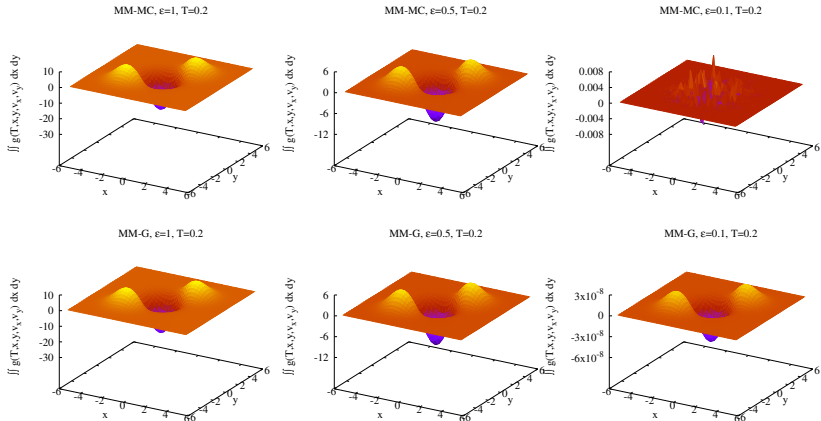
MM-G, $\varepsilon=0.5$, $T=0.2$



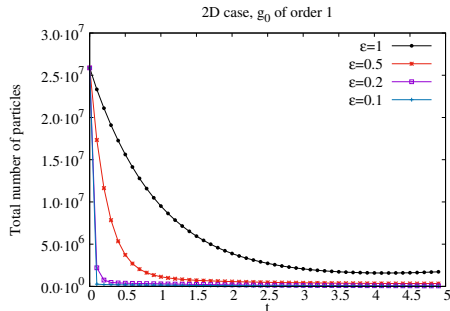
MM-G, $\varepsilon=0.1$, $T=0.2$



Integral of the perturbation in space $\int g(T=0.2, x, v) dx$ for different ε .



Time evolution of the number of particles



Test 3 - 3Dx3D, constant ε , $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$

Initialization:

$$f_0(\mathbf{x}, \mathbf{v}) = \frac{1}{2(2\pi)^{3/2}} \left[\exp\left(-\frac{|\mathbf{v} - \mathbf{u}|^2}{2}\right) + \exp\left(-\frac{|\mathbf{v} + \mathbf{u}|^2}{2}\right) \right] \rho(0, \mathbf{x}),$$

with $\mathbf{u} = (2, 2, 2)$,

$$\rho(0, \mathbf{x}) = 1 + \frac{1}{2} \cos\left(\frac{x}{2}\right) \cos\left(\frac{y}{2}\right) \cos\left(\frac{z}{2}\right),$$

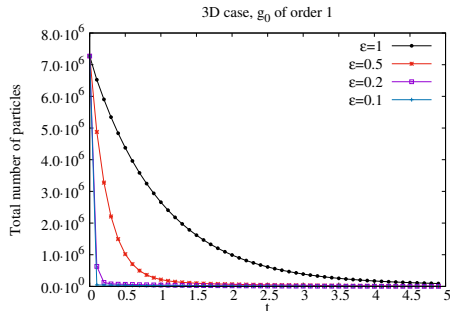
$$\mathbf{x} = (x, y, z) \in [0, 4\pi]^3, \quad \mathbf{v} = (v_x, v_y, v_z) \in \mathbb{R}^3.$$

Full $d_x = d_v = 3$ case

Integral of the distribution function in space $\int_{\mathbf{x}} f(T, \mathbf{x}, \mathbf{v}) d\mathbf{x}$

Left: $\varepsilon = 1$, right: $\varepsilon = 0.5$, $T = 1$.

Time evolution of the number of particles



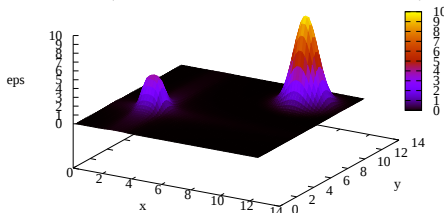
Test 4 - 2Dx2D, $\varepsilon(\mathbf{x})$, $g(t=0, \mathbf{x}, \mathbf{v}) \neq 0$

Modified model:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon^2(\mathbf{x})}(\rho M - f),$$

where $(\mathbf{x}, \mathbf{v}) \in [0, 4\pi]^2 \times \mathbb{R}^2$,

$$\varepsilon(\mathbf{x}) = 10 \left[\operatorname{atan}\left(2(y-5)\right) + \operatorname{atan}\left(-2(y-5)\right) \right] \\ \times \exp\left(- (x-10)^2 - (y-10)^2\right) + 10^{-3}.$$



Initialization:

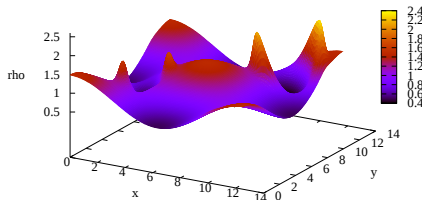
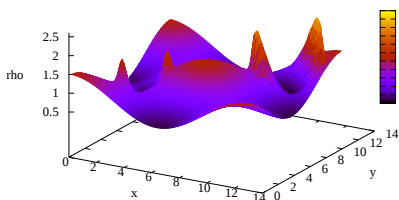
$$f(t=0, \mathbf{x}, \mathbf{v}) = \frac{1}{4\pi} \left(\exp \left(-\frac{|\mathbf{v} - 2|^2}{2} \right) + \exp \left(-\frac{|\mathbf{v} + 2|^2}{2} \right) \right) \rho(t=0, \mathbf{x}),$$

with

$$\mathbf{x} \in [0, 4\pi]^2, \quad \mathbf{v} \in \mathbb{R}^2,$$

$$\rho(t=0, \mathbf{x}) = 1 + \frac{1}{2} \cos \left(\frac{x}{2} \right) \cos \left(\frac{y}{2} \right).$$

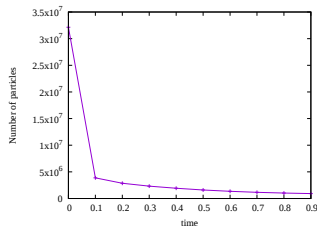
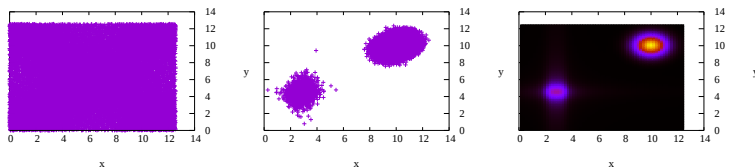
Density profile $\rho(T=1, x, y)$. Left: MM-MC, right: MM-G.



Asymptotically Complexity Diminishing Property

Top: position of the particles in x .

Left: at $T = 0$; middle: at $T = 1$. Right: $\varepsilon(x, y)$.



Bottom: time evolution of the number of particles.

Conclusions

- Right asymptotic behaviour.
- Computational cost diminishes as the equilibrium is approached.
- Numerical noise smaller than a standard particle method on f .
- Implicit treatment of the diffusion term.
- Suitable for multi-dimensional testcases.
- Somehow an automatic domain decomposition method without imposing any artificial transition to pass from the microscopic to the macroscopic model.

Possible extensions

- More 3D-3D testcases, more physical relevance.
- Boltzmann operator.
- Second-order in time scheme.
- Add an electromagnetic field $\Rightarrow v_k$ no constant anymore.

Thank you for your attention!