Examples of issues in the numerical simulation of collisional kinetic equations

Anaïs Crestetto[1]
joint works with Nicolas Crouseilles[2], Giacomo Dimarco[3] and Mohammed Lemou[4]

Conférence itinérante du GDR Analyse des EDP
February 2nd, 2022

[1]Nantes Université, LMJL.
[2]Inria & University of Rennes 1, IRMAR.
[3]University of Ferrara, Dept of Mathematics and Computer Science.
[4]University of Rennes 1, IRMAR & CNRS & Inria.

Numerical simulation of particle systems

We are interested in

- the numerical simulation of collisional kinetic problems,
- different scales: collisions, parameterized by the Knudsen number $\varepsilon(t, \mathbf{x})$, bring the system closer to a thermodynamical (fluid) equilibrium,
- 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 $f\left(t,\mathbf{x},\mathbf{v}\right)$.
- Solving a (rescaled) Boltzmann or Vlasov-type equation

$$\partial_t f + \frac{1}{\varepsilon^\alpha}\mathbf{v}\cdot\nabla_\mathbf{x} f + \frac{1}{\varepsilon^\beta}\left(\mathbf{E}+\mathbf{v}\wedge\mathbf{B}\right)\cdot\nabla_\mathbf{v} f = \frac{1}{\varepsilon^{1+\alpha}}Q\left(f,f\right),$$

  with $Q\left(f,f\right)$ a collisional operator.
- Example of scalings:
  - $\alpha=\beta=0$: hydrodynamic limit,
  - $\alpha=0$, $\beta=1$: high-field limit,
  - $\alpha=\beta=1$: diffusive limit.
- Coupling with Maxwell (or Poisson) equations.

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

- Collisions bring the system closer to a thermodynamical equilibrium: in $\mathbf{v}$, $f(t, \mathbf{x}, \mathbf{v})$ approaches a Gaussian function.
- System is described by moment equations on macroscopic quantities linked to f, for example:
  - density ρ: $\rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$,
  - mean velocity $\mathbf{u}$: $\rho(t, \mathbf{x})\mathbf{u}(t, \mathbf{x}) = \int f(t, \mathbf{x}, \mathbf{v})\mathbf{v} d\mathbf{v}$.

  :-(Lost of precision compared to a kinetic description.

  :-) Smaller cost.

  :-) Good enough at thermodynamical equilibrium.
- We approach the limit when
  - $\varepsilon \to 0$,
  - $t \to +\infty$.

Outline

About the kinetic description

- Kinetic description is necessary when system is far from equilibrium.

:-) Very accurate.

:-(Some issues:

  - $(t, \mathbf{x}, \mathbf{v})$: 7 variables, numerical simulation is costly (memory and computational time).
  - Nonlinear coupling with Maxwell equations: computation of density and current.
  - Complicated expression of the collisional operator: how to discretize it?
  - Multiscale problem: how to let $\varepsilon \to 0$ in a numerical scheme?

Strategies to deal with multiscale problems

First strategy: domain decomposition approach.

- When $\varepsilon(t, \mathbf{x})$ is large in some parts of the domain and small in others.
- Use the suitable model in the appropriate region.
  - :-) Very efficient in each region.
  - :-(How to determine the validity of each model and let both models communicate?
- Non exhaustive list of interesting papers on this subject:
  - Klar, SISC 1998.
  - Golse, Jin, Levermore, M2AN 2003.
  - Degond, Jin, SINUM 2005.
  - Tiwari, Klar, Hardt, JCP 2009.
  - Degond, Dimarco, Mieussens, JCP 2010.
  - Filbet, Rey, SISC 2015.
  - Li, Lu, Sun, JCP 2015.
  - Xiong, Qiu, JCP 2017.

Second strategy: Asymptotic Preserving (AP) approach.

- Develop a model/scheme suitable in any region.
  - :-) Only one model/scheme.
  - :-(A priori has the less favorable cost.
- Some examples of papers on AP schemes:
  - Jin, SISC 1999.
  - Klar, SINUM 1998.
  - Degond, Deluzet, Sangam, Vignal, JCP 2009.
  - Filbet, Jin, JCP 2010.
  - Crouseilles, Lemou, KRM 2011.
  - Lemou, Méhats, SISC 2012.
  - Besse, Carles, Méhats, MMS 2013.
  - Krycki, Berthon, Frank, Turpault, M2AS 2013.
  - Buet, Després, Franck, JSC 2015.
  - Degond, Deluzet, JCP 2017.
  - Dimarco, Pareschi, Samaey, SISC 2018.
  - + Works of Badsi, Besse, Ottaviani, Schratz, Seguin, Vignal, *etc.*

Asymptotic Preserving approach[5]

$$
\begin{tikzcd}
\boxed{\text{Problem}_\varepsilon} \arrow[d, "\varepsilon \to 0"] & \boxed{\text{Discretized Problem}_{h,\varepsilon}} \arrow[l, "h \to 0"'] \arrow[d, dashed, "\varepsilon \to 0"] \\
\boxed{\text{Limit}} & \boxed{\text{Discretized limit}_h} \arrow[l, "h \to 0"']
\end{tikzcd}
$$

h: space step Δx or time step Δt.

Properties of an AP scheme:
Stability and consistency $\forall \varepsilon$, in particular when $\varepsilon \to 0$.

[5] Jin, SISC 1999.

Problem of classical schemes: stability constraint $h = \mathcal{O}(\varepsilon)$.
Example:

- Stiff EDO:
$$y'(t) = -\frac{1}{\varepsilon} y(t),$$
$\varepsilon > 0$, approximation $y^n \approx y(t^n)$, where $t^n = n\Delta t$, $n \in \mathbb{N}$ and $\Delta t > 0$.
- Explicit Euler scheme: $y^{n+1} = y^n - \frac{\Delta t}{\varepsilon} y^n$ leads to
$$y^{n+1} = \left(1 - \frac{\Delta t}{\varepsilon}\right)^{n+1} y^0.$$
Stable under the constraint $\Delta t < 2\varepsilon$.
- Implicit Euler scheme: $y^{n+1} = y^n - \frac{\Delta t}{\varepsilon} y^{n+1}$ leads to
$$y^{n+1} = \left(\frac{1}{1 + \frac{\Delta t}{\varepsilon}}\right)^{n+1} y^0.$$
Unconditionally stable.

Our kinetic Problem$_\varepsilon$

1D Vlasov-BGK equation in the diffusive scaling

$$\partial_t f + \frac{1}{\varepsilon} v \partial_x f + \frac{1}{\varepsilon} E \partial_v f = \frac{1}{\varepsilon^2}(\rho M - f) \tag{1}$$

- $x \in [0, L_x] \subset \mathbb{R}$, $v \in V = \mathbb{R}$,
- charge density $\rho(t,x) = \int_V f \mathrm{d}v$,
- electric field $E(t,x)$ given by Poisson equation $\partial_x E = \rho - 1$,
- $M(v) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{v^2}{2}\right)$,
- periodic conditions in x and initial conditions.

Multiscale framework:

- Knudsen number ε can be of order 1 or tend to 0 at the drift-diffusion limit

$$\partial_t \rho - \partial_x \left(\partial_x \rho - E\rho\right) = 0. \tag{2}$$

Objective: AP scheme

To have a chance to construct an AP scheme, we work on the model.

- Main tool: Micro-macro decomposition.
- Examples of previous works:
  - Liu, Yu, CMP 2004.
  - Lemou, Mieussens, SIAM SISC 2008.
  - Crouseilles, Lemou, KRM 2011.

Micro-macro decomposition

- Micro-macro decomposition:

$$f = \rho M + g$$

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

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

- Hypothesis: $\langle g \rangle = 0$ since $\langle f \rangle = \rho$.
- Properties: $\partial_v M = -vM$, $\langle vM \rangle = 0$, $\langle v^2 M \rangle = 1$.

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

$$\partial_t \rho + \frac{1}{\varepsilon}\partial_x \langle vg \rangle = 0. \tag{3}$$

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

$$\partial_t g + \frac{1}{\varepsilon}\left(v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M - vME\rho + E\partial_v g\right) = -\frac{1}{\varepsilon^2} g. \tag{4}$$

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

$$\begin{cases} \partial_t \rho + \dfrac{1}{\varepsilon}\partial_x \langle vg \rangle = 0, \\ \partial_t g + \dfrac{1}{\varepsilon}\mathcal{F}(\rho, g) = -\dfrac{1}{\varepsilon^2} g, \end{cases} \tag{5}$$

where $\mathcal{F}(\rho, g) = v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M - vME\rho + E\partial_v g$.

AP Eulerian scheme

:-(We have stiff terms in the micro equation (4) on g.

- If we consider a Eulerian scheme in (x, v): $g_{ij}^n \approx g(t^n, x_i, v_j)$ and take the stiffest term implicit [6,7]:

$$g_{ij}^{n+1} = g_{ij}^n - \frac{\Delta t}{\varepsilon} \mathcal{F}\left(\rho_i^n, g_{ij}^n\right) - \frac{\Delta t}{\varepsilon^2} g_{ij}^{n+1}$$

we obtain

$$g_{ij}^{n+1} = \frac{\varepsilon^2}{\varepsilon^2 + \Delta t} g_{ij}^n - \frac{\varepsilon \Delta t}{\varepsilon^2 + \Delta t} \mathcal{F}\left(\rho_i^n, g_{ij}^n\right).$$

:-) Right asymptotic behavior:

$$g = -\varepsilon\left(v \partial_x \rho M - v M E \rho\right) + \mathcal{O}\left(\varepsilon^2\right)$$

injected into the equation on ρ gives at the limit $\varepsilon \to 0$

$$\partial_t \rho - \partial_x \langle v^2 \partial_x \rho M - v^2 M E \rho \rangle = 0.$$

By using $\langle v^2 M \rangle = 1$, we get the drift-diffusion equation.

[6] Lemou, Mieussens, SIAM SISC 2008.

[7] Crouseilles, Lemou, KRM 2011.

AP particle method

:-(Eulerian schemes are costly in 3Dx-3Dv...

- We would like to use a particle method for g, especially since g is small when approaching equilibrium.
- But in particle methods
  - we have a splitting between the transport term and the interaction term,
  - it will not be possible to stabilize the transport term by taking the collisional term implicit.
- We propose to reformulate the model.

- Strategy [8]:
  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 $t^{n+1} = t^n + \Delta t$:
  $$e^{t^{n+1}/\varepsilon^2} g^{n+1} = e^{t^n/\varepsilon^2} g^n + \int_{t^n}^{t^{n+1}} -\frac{e^{t/\varepsilon^2}}{\varepsilon}\mathcal{F}(\rho, g)\mathrm{d}t,$$
  3. use 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).

[8] Lemou, CRAS 2010.

New micro-macro model

The new micro-macro model writes

$$\partial_t \rho + \frac{1}{\varepsilon}\partial_x \langle v g \rangle = 0, \tag{6}$$

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

We propose [9] the following hybrid discretization:

- macro equation (6): Finite Volume (FV) method,
- micro equation (7): Particle-In-Cell (PIC) method.

[9] C., Crouseilles, Lemou, CMS 2018.

1) PIC method for g

- Model: having N_p particles, with position x_k, velocity v_k and weight ω_k, $k = 1, \ldots, N_p$, g is approximated by

$$g_{N_p}(t,x,v) = \sum_{k=1}^{N_p} \omega_k(t)\,\delta(x - x_k(t))\,\delta(v - v_k(t))\,.$$

- Initialization:
  - $x_k(t=0)$ and $v_k(t=0)$ uniformly distributed in phase space domain (x,v),
  - weights initialized to $\omega_k(t=0) = g(t=0, x_k, v_k)\,\frac{L_x L_v}{N_p}$ (L_x x-length of the domain, L_v v-length.).
- Solve equation on g by splitting the transport and the interaction terms.

Solving the transport part

- Transport part of equation on g is

$$\partial_t g + \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} (v\partial_x g + E\partial_v g) = 0.$$

- Evolution of positions and velocities of particles with motion equations:

$$\frac{dx_k}{dt}(t) = \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} v_k(t) \text{ and } \frac{dv_k}{dt}(t) = \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} E(t, x_k(t)).$$

For example

$$x_k^{n+1} = x_k^n + \varepsilon(1 - e^{-\Delta t/\varepsilon^2}) v_k^n \text{ and } v_k^{n+1} = v_k^n + \varepsilon(1 - e^{-\Delta t/\varepsilon^2}) E^n(x_k^n).$$

Solving the interaction part

- Interaction part of equation on g is

$$\partial_t g = S_g$$

with

$$S_g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \left(v \partial_x \rho M - \partial_x \langle v g \rangle M - v M E \rho \right).$$

- Evolution of weights ω_k:

$$\frac{d\omega_k}{dt}(t) = S_g \left(t, x_k(t), v_k(t) \right) \frac{L_x L_v}{N_p}.$$

In practice:

$$\omega_k^{n+1} = \omega_k^n + \Delta t S_g \left(x_k^n, v_k^n \right) \frac{L_x L_v}{N_p}.$$

2) FV method for ρ

- Equation $\partial_t \rho + \frac{1}{\varepsilon}\partial_x \langle vg \rangle = 0$.
- First proposition:

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\varepsilon}\partial_x \langle v g^{n+1} \rangle_i,$$

discretized by a Finite Volume method:

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

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

- 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

- Study equation on weights to write

$$\omega_k^{n+1} = e^{-\Delta t/\varepsilon^2}\omega_k^n - \varepsilon(1-e^{-\Delta t/\varepsilon^2})\left[\overbrace{\alpha_k^n}^{v\partial_x\rho M - vME\rho} + \overbrace{\beta_k^n}^{-\partial_x\langle vg\rangle M}\right].$$

- Approximate

$$\langle vg^{n+1}\rangle_i = -\varepsilon(1-e^{-\Delta t/\varepsilon^2})\left(\partial_x\rho_i^n - E_i^n\rho_i^n\right) + h_i^n,$$

where $h_i^n := e^{-\Delta t/\varepsilon^2}\langle vg^n\rangle_i - \varepsilon(1-e^{-\Delta t/\varepsilon^2})\langle -v\partial_x\langle vg\rangle M\rangle_i$.

- Inject it in the macro equation

$$\rho_i^{n+1} = \rho_i^n + \Delta t(1-e^{-\Delta t/\varepsilon^2})\partial_x\left(\partial_x\rho_i^n - E_i^n\rho_i^n\right) - \frac{\Delta t}{\varepsilon}\partial_x h_i^n.$$

- Remark: when $\varepsilon \to 0$, $h_i^n = \mathcal{O}(\varepsilon^2)$.

Nice properties of the PIC / FV discretization

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

$$\rho_i^{n+1} = \rho_i^n + \Delta t(1 - e^{-\Delta t/\varepsilon^2})\partial_x \left(\partial_x \rho_i^{n+1} - E_i^n \rho_i^n\right) - \frac{\Delta t}{\varepsilon}\partial_x h_i^n.$$

- No more stiffness, the numerical noise does not damage ρ.
- AP property: for fixed $\Delta t > 0$, the scheme degenerates when $\varepsilon \to 0$ to an implicit discretization of the drift-diffusion equation $\partial_t \rho - \partial_x \left(\partial_x \rho - E\rho\right) = 0$.

Moreover

- Easy coupling with Poisson equation $\partial_x E = \rho - 1$ since we have an approximation of ρ.
- We only need a few particles at the limit to represent g: cost reduced.

Landau damping

- Initial distribution function:

$$f\,(t=0,x,v) = \frac{1}{\sqrt{2\pi}}\exp(-\frac{v^2}{2})(1+\alpha\cos(kx)), \quad x \in \left[0, \frac{2\pi}{k}\right], v \in \mathbb{R}.$$

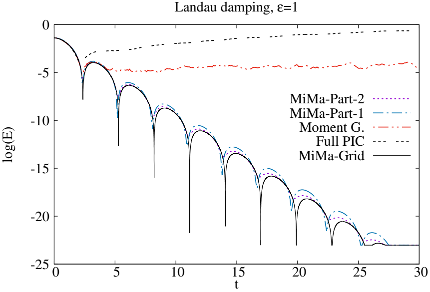
- Micro-macro initializations:

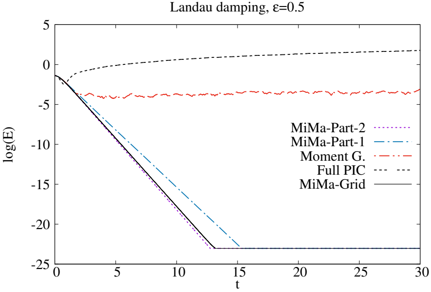
$$\rho(t=0,x) = 1+\alpha\cos(kx) \quad \text{and} \quad g(t=0,x,v) = 0.$$

- Parameters: $\alpha = 0.05$, $k = 0.5$.
- Electrical energy $\mathcal{E}(t) = \sqrt{\int E(t,x)^2 dx}$.

Evolution in time of the electrical energy

Kinetic and intermediate regimes
Left: $\varepsilon = 1$, $N_x = 128$, $N_p = 10^5$, $\Delta t = 0.1$.
Right: $\varepsilon = 0.5$, $N_x = 256$, $N_p = 10^5$, $\Delta t = 0.01$.



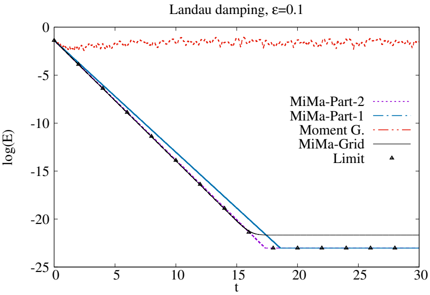


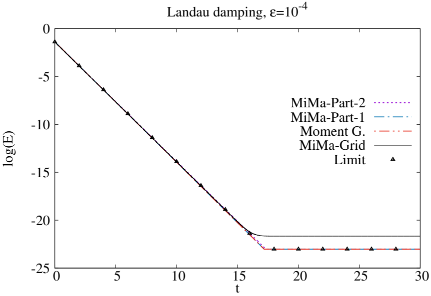
Evolution in time of the electrical energy

Limit regime

Left: $\varepsilon = 0.1$, $N_x = 128$, $N_p = 10^4$, $\Delta t = 0.001$,

Right: $\varepsilon = 10^{-4}$, $N_x = 128$, $N_p = 100$, $\Delta t = 0.01$.





3Dx-3Dv problem

To handle 3Dx-3Dv problem, such as the radiative transport equation in the diffusive scaling

$$\partial_t f + \frac{1}{\varepsilon}\mathbf{v}\cdot\nabla_{\mathbf{x}} f = \frac{1}{\varepsilon^2}Q(f,f), \quad Q(f,f) = (\rho M - f) \qquad (8)$$

we propose [10] to use a Monte Carlo approach for the particle method.

- Micro-macro model is the same but in 3Dx-3Dv and with $E = 0$.
- We will apply the same FV method for the macro equation on ρ.

[10] C., Crouseilles, Dimarco, Lemou, JCP 2019.

- Particle discretization of g is slightly different: we consider at each time step N^n particles, with position $\mathbf{x}_k^n$, velocity $\mathbf{v}_k^n$ and constant weight ω_k, $k = 1, \ldots, N^n$, g is approximated by [11]

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

- We solve the transport part by evolving the positions with motion equation.
- We solve the interaction part with a Monte Carlo approach.

[11] Crouseilles, Dimarco, Lemou, KRM 2017.

Monte Carlo approach for the interaction part

- Solve interaction part by writing

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

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

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

In practice

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

- We choose randomly $\lfloor e^{-\Delta t/\varepsilon^2} N^n \rfloor$ particles and keep them unchanged,
- we discard the others.

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

- We sample a number $\tilde{N}^n$ of new particles representing $\varepsilon\big[-\mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v}\tilde{g} \rangle^n M \big]$.
- $\tilde{N}^n$ is of order of ε.

Asymptotically Complexity Diminishing Property

- At the end of the time step, we have

$$N^{n+1} = \lfloor e^{-\Delta t/\varepsilon^2} N^n \rfloor + \tilde{N}^n$$

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

2Dx-2Dv, constant ε, $g(t=0,\mathbf{x},\mathbf{v})=0$

Initialization:

$$f(t=0,\mathbf{x},\mathbf{v}) = \rho_0(\mathbf{x})M(\mathbf{v}),\ \ \mathbf{x}\in[0,4\pi]^2,\ \ \mathbf{v}\in\mathbb{R}^2$$

with

$$\rho_0(\mathbf{x}) = 1+\frac{1}{2}\cos\left(\frac{\mathrm{x}}{2}\right)\cos\left(\frac{\mathrm{y}}{2}\right),$$

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

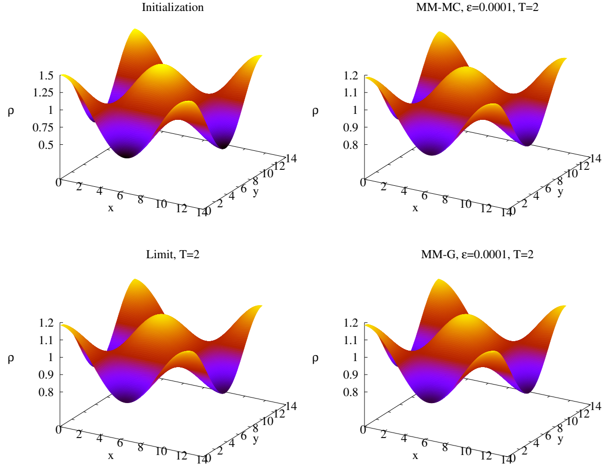
so that

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

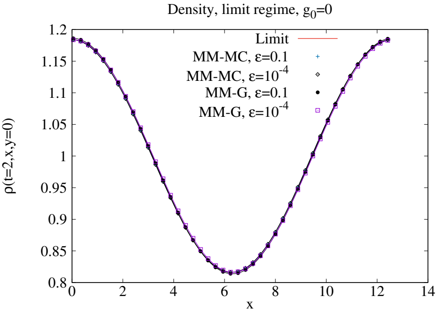
Periodic boundary conditions in space.

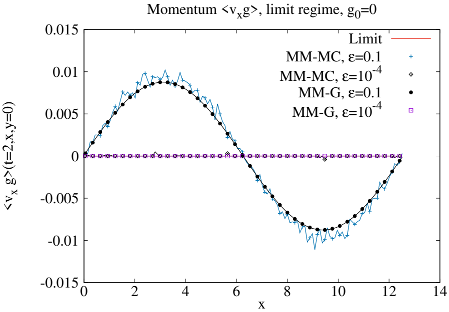
Asymptotic behaviour, $\varepsilon = 10^{-4}$

MM-MC: the presented Micro-Macro Monte Carlo scheme.
MM-G: a Micro-Macro Grid code, considered as reference.



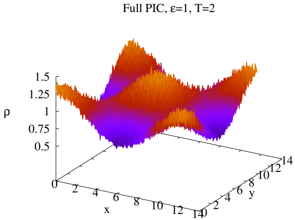
Slices of the density $\rho(T=2,\mathrm{x},\mathrm{y}=0)$ and of the momentum $\langle \mathrm{v_x} g\rangle(T=2,\mathrm{x},\mathrm{y}=0)$.

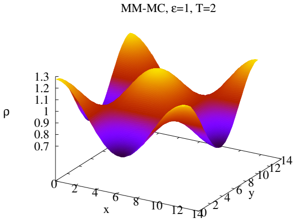


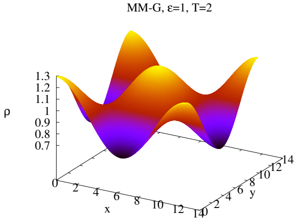


Kinetic regime, $\varepsilon = 1$

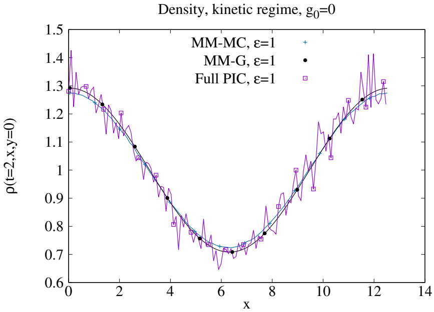
Full PIC: standard particle method on f.

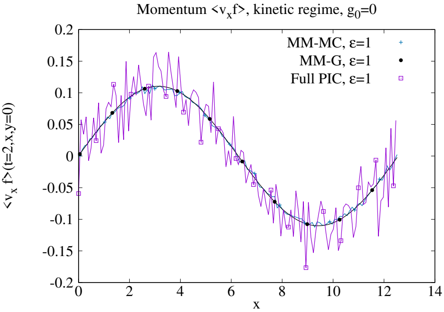




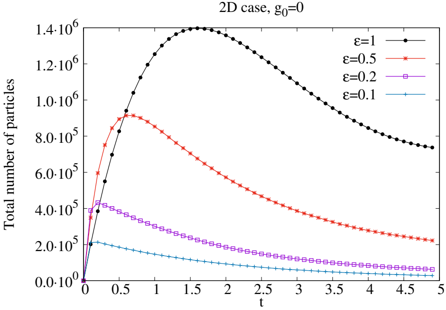


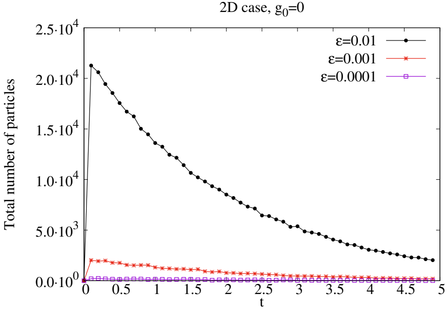
Slices of the density $\rho(T = 2, \mathrm{x}, \mathrm{y} = 0)$ and of the momentum $\langle \mathrm{v_x} f \rangle (T = 2, \mathrm{x}, \mathrm{y} = 0)$.





Time evolution of the number of particles





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

Initialization:

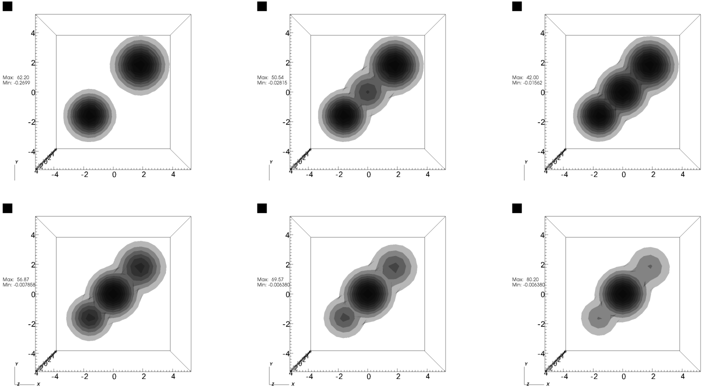
$$f(0,\mathbf{x},\mathbf{v}) = \frac{1}{2\,(2\pi)^{3/2}} \left[\exp\left(-\frac{|\mathbf{v}-\mathbf{u}|^2}{2} \right) + \exp\left(-\frac{|\mathbf{v}+\mathbf{u}|^2}{2} \right) \right] \rho_0(\mathbf{x}),$$

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

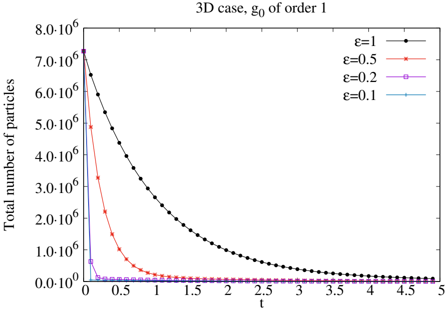
$$\rho_0(\mathbf{x}) = 1 + \frac{1}{2} \cos\left(\frac{\mathrm{x}}{2}\right) \cos\left(\frac{\mathrm{y}}{2}\right) \cos\left(\frac{\mathrm{z}}{2}\right),$$

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

Integral of the distribution function in space $\int_{\mathbf{x}} f(T, \mathbf{x}, \mathbf{v}) d\mathbf{x}$ for $\varepsilon = 1$ and different times (T=0, 0.2, 0.4, 0.6, 0.8, 1).



Time evolution of the number of particles



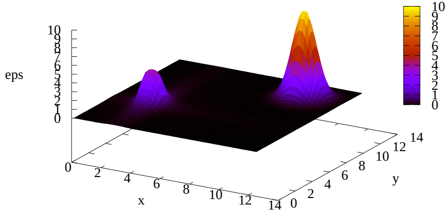
2Dx-2Dv, $\varepsilon(\mathbf{x})$, $g(t=0,\mathbf{x},\mathbf{v}) \neq 0$

Modified model:

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

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

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



Initialization:

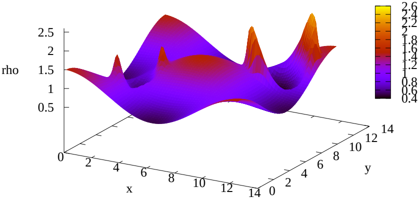
$$f(t=0,\mathbf{x},\mathbf{v}) = \frac{1}{4\pi}\left(\exp\left(-\frac{|\mathbf{v}-\mathbf{u}|^2}{2}\right) + \exp\left(-\frac{|\mathbf{v}+\mathbf{u}|^2}{2}\right)\right)\rho_0(\mathbf{x}),$$

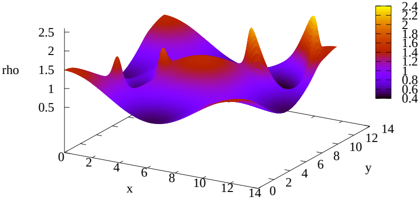
with

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

$$\rho_0(\mathbf{x}) = 1 + \frac{1}{2}\cos\left(\frac{\mathrm{x}}{2}\right)\cos\left(\frac{\mathrm{y}}{2}\right).$$

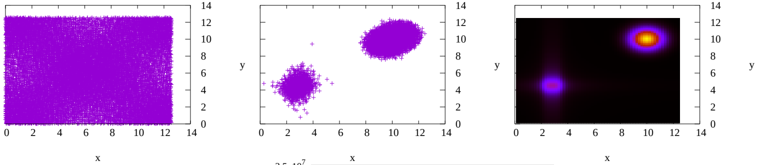
Density profile $\rho(T=1,\mathrm{x},\mathrm{y})$. Left: MM-MC, right: MM-G.

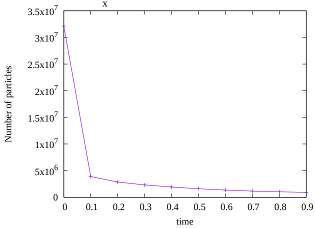




Asymptotically Complexity Diminishing Property

Top: position of the particles in $\mathbf{x}$.
Left: at $T = 0$; middle: at $T = 1$. Right: $\varepsilon(\mathrm{x}, \mathrm{y})$.





Bottom: time evolution of the number of particles.

Conclusions

- Micro-macro model is a tool to develop AP schemes.
- With particle method, you can reduce the cost when the equilibrium is approached.
- Monte Carlo approach helps optimizing the number of particles and then simulating 3Dx-3Dv problems.
- We somehow developed an automatic domain decomposition method without imposing any artificial transition to pass from the microscopic to the macroscopic model.

Extensions

- More complex collisional operator?
  - You have to be able to discretize the operator...
  - We were able to deal with the Boltzmann collisional operator in the space homogeneous case [12].
- Boundary conditions?
  - Difficult with particle methods.
- Solving efficiently Maxwell equations is not straightforward.
- Our next objective? Combining Monte Carlo approach with electromagnetic field and Boltzmann operator.

[12] C., Crouseilles, Dimarco, Lemou, CMS 2020.

Thank you for your attention!