Micro-macro discretizations for collisional kinetic equations of Boltzmann-BGK type in the diffusive scaling

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Outline

Numerical simulation of particle systems

We are interested in

- the numerical simulation of kinetic Problems$_\varepsilon$,
- different scales: collisions parameterized by the Knudsen number ε,
- the development of schemes that are efficient in both kinetic and fluid regimes.

There are two main strategies for multiscale problems:

- domain decomposition methods,
- asymptotic preserving (AP) schemes[5].

[5] Jin, SISC 1999.

Our first Problem$_\varepsilon$

1D radiative transport equation in the diffusive scaling

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

- distribution function $f(t, x, v)$,
- $x \in [0, L_x] \subset \mathbb{R}$, $v \in V = [-1, 1]$,
- charge density $\rho(t, x) = \frac{1}{2} \int_V f \mathrm{d}v$,
- $M(v) = 1$,
- periodic conditions in 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

$$\partial_t \rho - \frac{1}{3} \partial_{xx} \rho = 0. \tag{2}$$

Objectives

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

Tools

- Micro-macro decomposition[6,7] for this model. Previous work with a grid in v for the micro part[8], cost was constant w.r.t. ε.

Idea

- Use particles for the micro part since few information in v is necessary at the limit.

[6] Liu, Yu, CMP 2004.
[7] Lemou, Mieussens, SIAM JSC 2008.
[8] Crouseilles, Lemou, KRM 2011.

Micro-macro decomposition

- Micro-macro decomposition:

$$f = \rho M + g$$

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

$$\Pi h := \langle h \rangle M, \quad \langle h \rangle := \frac{1}{2} \int h \,\mathrm{d}v.$$

- Hypothesis: first moment of g must be zero:

$$\langle g \rangle = 0, \quad \text{since} \quad \langle f \rangle = \rho = \langle \rho M \rangle.$$

  True at the numerical level? If not, we have to work on it[9,10].

[9] Degond, Dimarco, Pareschi, IJNMF 2011.

[10] C., Crouseilles, Lemou, KRM 2012.

- 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

$$\partial_t g + \frac{1}{\varepsilon}[v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M] = -\frac{1}{\varepsilon^2} g. \tag{4}$$

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

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

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

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 $\Longrightarrow$ transport term (of order $1/\varepsilon$) stabilized.

But here:

- use of particles for the micro part

$\Rightarrow$ splitting between the transport term and the source term,

$\Rightarrow$ not possible to use the same strategy.

Idea?

- Suitable reformulation of the model.

[11] Lemou, Mieussens, SIAM SISC 2008.
[12] Crouseilles, Lemou, KRM 2011.

- Strategy of Lemou[13]:
  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 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 the initial micro eq. (4).

[13] Lemou, CRAS 2010.

New micro-macro model

The new micro-macro model writes

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

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

with $\mathcal{F}\left(\rho, g\right) = v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M$.

We propose the following hybrid discretization:

- macro equation (6): Finite Volume method,
- micro equation (7): Particle method.

First algorithm

Reformulated system

$$\begin{cases} \partial_t \rho + \dfrac{1}{\varepsilon}\partial_x \langle vg \rangle = 0, \\ \partial_t g = \dfrac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \dfrac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t}[v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M]. \end{cases}$$

Algorithm

1. Solving the micro part by a Particle-In-Cell (PIC) method.
2. Projection step to numerically force to zero the first moment of g (matching procedure[14]).
3. Solving the macro part by a Finite Volume (FV) scheme (mesh on x), with a source term dependent on g.

1-3 coupling: similarities with the δf method[15].

[14] Degond, Dimarco, Pareschi, IJNMF 2011.

[15] Brunner, Valeo, Krommes, Phys. of Plasmas 1999.

PIC method with evolution of weights

- Model: having N_p particles, with position $x_k(t)$, velocity $v_k(t)$ and weight $\omega_k(t)$, $k = 1, \ldots, N_p$, 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: positions and velocities of particles uniformly distributed in phase space (x, v), weights initialized to

$$\omega_k(0) = g(0, x_k, v_k) \frac{L_x L_v}{N_p},$$

(L_x x-length of the domain, L_v v-length).

Splitting between transport and source part

- Equation on g

$$\partial_t g + \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t}[v \partial_x g] = S_g$$

where

$$S_g := \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t}[v \partial_x \rho M - \partial_x \langle vg \rangle M].$$

- Solve transport part $\partial_t g + \varepsilon \frac{1-e^{-\Delta t/\varepsilon^2}}{\Delta t}[v \partial_x g] = 0$ thanks to motion equation

$$\frac{dx_k}{dt}(t) = \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} v_k(t).$$

For example

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

- Solve source part $\partial_t g = S_g$ by evolution of weights ω_k:

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

with

$$S_g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} [v\partial_x \rho M - \partial_x \langle vg \rangle M].$$

In practice:

$$\frac{\omega_k^{n+1} - \omega_k^n}{\Delta t} = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t}\omega_k^n - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t}\left[\alpha_k^n + \beta_k^n\right],$$

$$\text{with} \quad \alpha_k^n = v_k \partial_x \rho^n(x_k^{n+1}) M(v_k) \frac{L_x L_v}{N_p}$$

$$\text{and} \quad \beta_k^n = -\partial_x \langle vg \rangle (x_k^{n+1}) M(v_k) \frac{L_x L_v}{N_p}.$$

Macro part

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

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

discretized by a Finite Volume method:

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

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

- 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

- Write

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

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

$$\langle vg^{n+1}\rangle_i = -\varepsilon(1 - e^{-\Delta t/\varepsilon^2})\frac{1}{3}\partial_x \rho_i^n + h_i^n.$$

- Inject it in the macro equation

$$\rho_i^{n+1} = \rho_i^n + \Delta t(1 - e^{-\Delta t/\varepsilon^2})\frac{1}{3}\partial_{xx}\rho_i^n - \frac{\Delta t}{\varepsilon}\partial_x h_i^n.$$

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

Correction of the macro discretization

- Write

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

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$$\langle vg^{n+1}\rangle_i = -\varepsilon(1 - e^{-\Delta t/\varepsilon^2})\frac{1}{3}\partial_x\rho_i^n + h_i^n.$$

- Inject it in the macro equation and take the diffusion term implicit

$$\rho_i^{n+1} = \rho_i^n + \Delta t(1 - e^{-\Delta t/\varepsilon^2})\frac{1}{3}\partial_{xx}\rho_i^{n+1} - \frac{\Delta t}{\varepsilon}\partial_x h_i^n.$$

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

Properties

- For fixed $\varepsilon > 0$, the scheme is a first-order (in time) approximation of the reformulated micro-macro system.
- For fixed $\Delta t > 0$, the scheme degenerates into an implicit first-order (in time) scheme of the diffusion equation (2).

$$\Rightarrow \text{AP property}$$

- No parabolic CFL condition of type $\Delta t \leq C \Delta x^2$.
- No more stiffness, the numerical noise does not damage ρ.
- We only need a few particles at the limit to represent g: cost reduced.

Asymptotic behaviour

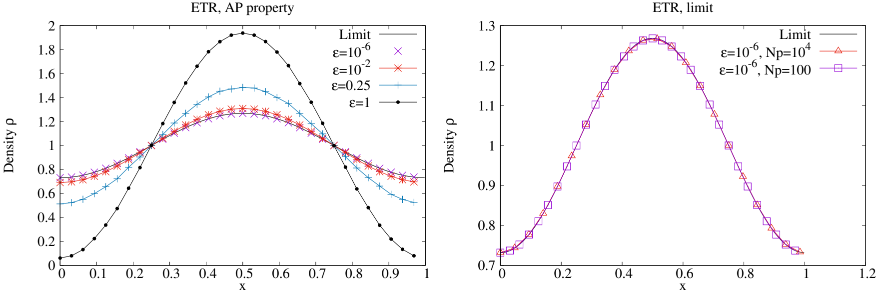
Initial distribution function

$f\,(t=0,x,v) = 1 + \cos\left(2\pi\left(x + \frac{1}{2}\right)\right), \quad x \in [0,1], v \in [-1,1].$

Density $\rho(t,x) = \frac{1}{2}\int_{-1}^{1} f(t,x,v)\mathrm{d}v,$ and $M(v) = 1.$

Left: $T = 0.1,\ N_x = 64,\ N_p = 10^4,\ \Delta t = 10^{-3},$

Right: $T = 0.1,\ N_x = 64,\ \varepsilon = 10^{-6},\ \Delta t = 10^{-2}.$



How to...

- How to derive a second-order in time scheme?
- How to consider a Problem$_\varepsilon$ with an electric field?
  Details in [C., Crouseilles, Lemou, CMS 2018].

- How to consider $d_x = d_v = 2$ or $d_x = d_v = 3$ testcases?
- How to automatically reduce the number of particles?
  Details in [C., Crouseilles, Dimarco, Lemou, JCP 2019].

How to derive a second-order in time scheme?

- Work on the micro-macro model.
- Work, of course, on the time scheme.
- Insure the order of the time scheme at the limit too.

New reformulation of the micro-macro system

- When integrating in time $\partial_t(e^{t/\varepsilon^2}g) = -\frac{e^{t/\varepsilon^2}}{\varepsilon}\mathcal{F}(\rho, g)$, use a midpoint method for the right-hand side

$$g^{n+1} = e^{-\Delta t/\varepsilon^2} g^n - \frac{\Delta t e^{-\Delta t/2\varepsilon^2}}{\varepsilon}\mathcal{F}\left(\rho^{n+1/2}, g^{n+1/2}\right) + \mathcal{O}\left(\Delta t^3\right).$$

- Make appear a discrete time derivative

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

- Perform Taylor expansions at $t^{n+1/2}$

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

- New second-order micro-macro system:

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

$$\partial_t g = \frac{2}{\Delta t}\frac{e^{-\Delta t/\varepsilon^2} - 1}{e^{-\Delta t/\varepsilon^2} + 1} g - \frac{2}{\varepsilon}\frac{e^{-\Delta t/2\varepsilon^2}}{e^{-\Delta t/\varepsilon^2} + 1}\left[v\partial_x \rho M + v\partial_x g - \partial_x \langle vg \rangle M\right].$$

- Time scheme of second order: $\rightarrow$ Prediction step on $\Delta t/2$:

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

$$\rho^{n+1/2} = \rho^n - \frac{\Delta t}{2\varepsilon}\partial_x \langle v g^{n+1/2} \rangle,$$

$\rightarrow$ Correction step on Δt:

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

$$\rho^{n+1} = \rho^n - \frac{\Delta t}{\varepsilon}\partial_x \langle v g^{n+1/2} \rangle.$$

- Choice of $\widetilde{g}$ in order to have a second-order in time scheme and the right asymptotic limit: $\widetilde{g} = \frac{g^n + g^{n+1}}{2}$.
- Correct the macro equation:

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\varepsilon}\partial_x \langle v g^{n+1/2} \rangle_i + \Delta t (1 - e^{-\Delta t/\varepsilon^2})^2 \frac{1}{3} \partial_{xx} \left(\frac{\rho_i^{n+1} + \rho_i^n}{2}\right).$$

- Same PIC/FV discretization in space as for the first-order scheme.

Properties

- For fixed $\varepsilon > 0$, the scheme is a second-order (in time) approximation of the reformulated micro-macro system.
- For fixed $\Delta t > 0$, the scheme degenerates into an implicit second-order (in time) scheme of the diffusion equation (2).

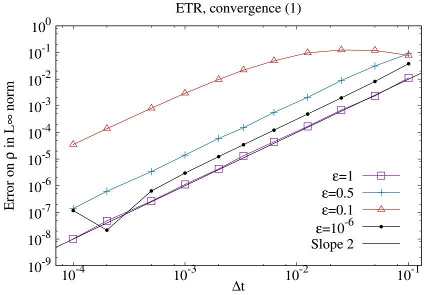
$\Rightarrow$ 2nd-order in time + AP property

Convergence - 2nd-order in time

Initial distribution function

$$f(t=0,x,v)=1+\cos\left(2\pi\left(x+\frac{1}{2}\right)\right),\quad x\in[0,1]\,,v\in[-1,1]\,.$$

Parameters: $T=0.1,\ N_x=16,\ N_p=100.$



How to consider a Problem$_\varepsilon$ with an electric field?

1D Vlasov-BGK equation in the diffusive scaling

$$\partial_t f + \frac{1}{\varepsilon} v \partial_x f + \frac{1}{\varepsilon} E \partial_v f = \frac{1}{\varepsilon^2}(\rho M - f) \tag{8}$$

- $x \in [0, L_x] \subset \mathbb{R}$, $v \in V = \mathbb{R}$,
- 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 may be of order 1 or tend to 0 at the drift-diffusion limit

$$\partial_t \rho - \partial_x \left(\partial_x \rho - E\rho\right) = 0. \tag{9}$$

Not any more difficult

- Change the definition of $\mathcal{F}(\rho, g)$:

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

- Same reformulation of the micro-macro system with this $\mathcal{F}$.
- Evolve positions and velocity of particles by considering

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

- Solve Poisson equation $\partial_x E = \rho - 1$ thanks to FFT or finite differences.

Landau damping

- Initial distribution function:

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

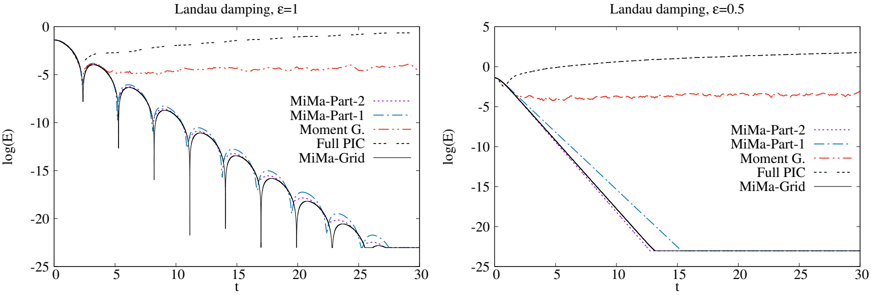
- Micro-macro initializations:

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

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

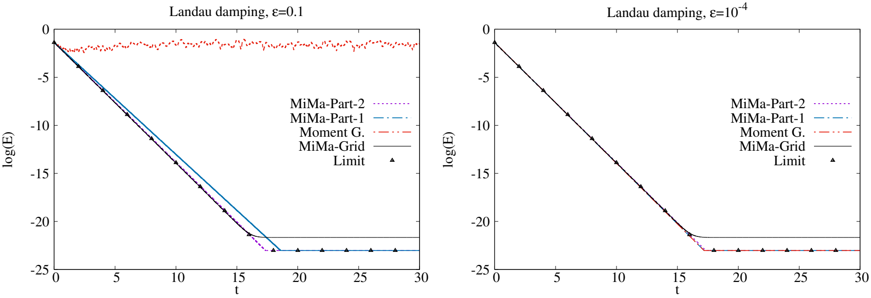
Evolution in time of the electrical energy

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



Two stream instability

- Initial distribution function:

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

- Micro-macro initializations:

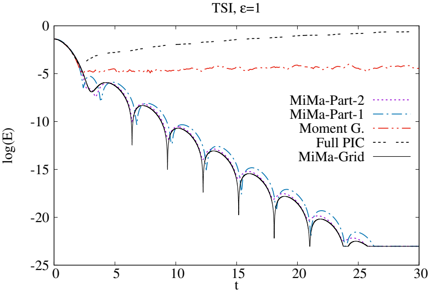
$$\rho(t=0,x)=1+\alpha\cos(kx)$$

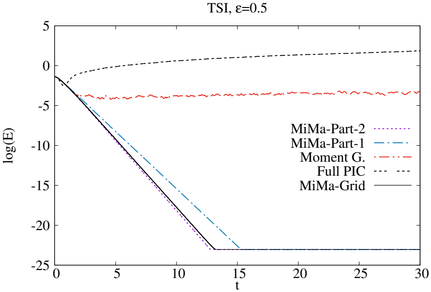
$$g\,(t=0,x,v)=\frac{1}{\sqrt{2\pi}}\left(v^2-1\right)\exp\left(-\frac{v^2}{2}\right)\left(1+\alpha\cos\left(kx\right)\right).$$

- Parameters: $\alpha=0.05$, $k=0.5$.

Evolution in time of the electrical energy

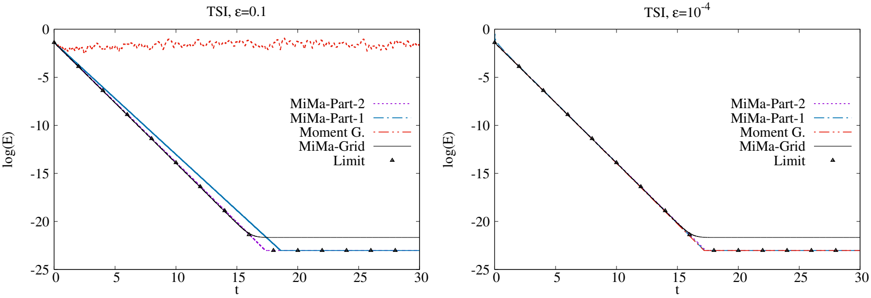
Kinetic and intermediate regimes
Left: $\varepsilon = 1$, $N_x = 128$, $N_p = 10^5$, $\Delta t = 0.1$.
Right: $\varepsilon = 0.5$, $N_x = 256$, $N_p = 10^5$, $\Delta t = 0.01$.





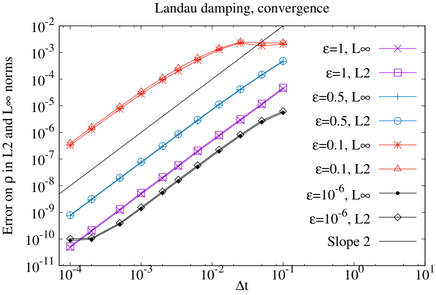
Evolution in time of the electrical energy

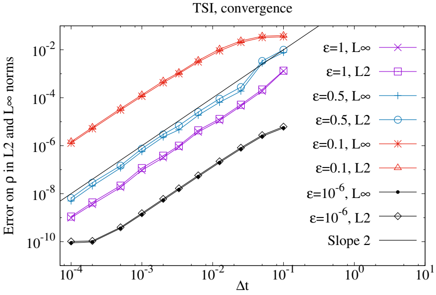
Limit regime
Left: $\varepsilon = 0.1$, $N_x = 128$, $N_p = 10^4$, $\Delta t = 0.001$.
Right: $\varepsilon = 10^{-4}$, $N_x = 128$, $N_p = 100$, $\Delta t = 0.01$.



Convergence - 2nd-order in time

Left: Landau damping case.
Right: two stream instability case.
Parameters: $T = 0.1$, $N_x = 16$, $N_p = 100$.





How to consider $d_x = d_v = 2$ or $d_x = d_v = 3$ testcases?

- In the radiative transport equation case (no electric field), use Monte Carlo techniques[16,17] for the particles discretization.
- Since the cost will be smaller, we can consider multi-dimensional frameworks: $(d_x, d_v) = (2, 2)$ or $(3, 3)$.

$$\partial_t f + \frac{1}{\varepsilon}\mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon^2}(\rho M - f) \tag{10}$$

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

The asymptotic diffusion equation being

$$\partial_t \rho - \Delta_{\mathbf{x}} \rho = 0. \tag{11}$$

[16] Degond, Dimarco, Pareschi, IJNMF 2011.

[17] Dimarco, Pareschi, Samaey, SISC 2018.

How to automatically reduce the number of particles?

- Same reformulation of the micro-macro system.
- Consider that the number of particles depends on t and that the weights are constant:

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

- Initially, sample particles corresponding to $g\left(t = 0, \mathbf{x}, \mathbf{v}\right)$.
- Solve transport part of the micro equation as previously (motion equations).

- Solve source part of the micro equation

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

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

with Monte Carlo techniques:

  - with probability $e^{-\Delta t/\varepsilon^2}$, the distribution g^{n+1} does not change,
  - with probability $(1 - e^{-\Delta t/\varepsilon^2})$, the distribution g^{n+1} is replaced by a new distribution given by $\varepsilon\Big[-\mathbf{v}\cdot\nabla_{\mathbf{x}}\rho^n M + \nabla_{\mathbf{x}}\cdot\langle\mathbf{v}\tilde{g}\rangle^n M\Big]$.

- Solve source part of the micro equation

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

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

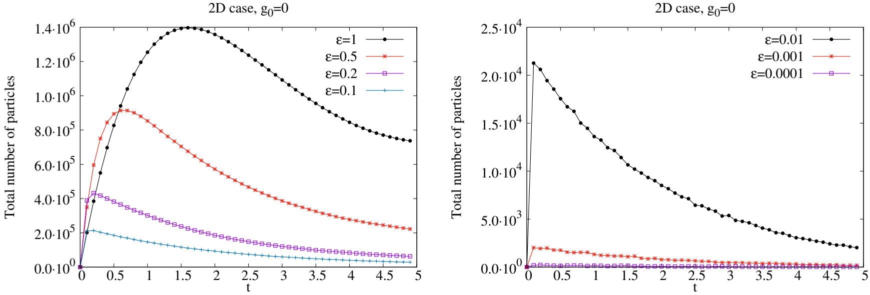
with Monte Carlo techniques:

  - keep $e^{-\Delta t/\varepsilon^2}N^n$ particles unchanged (uniformly taken in each cell) and delete the others,
  - create new particles by sampling

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

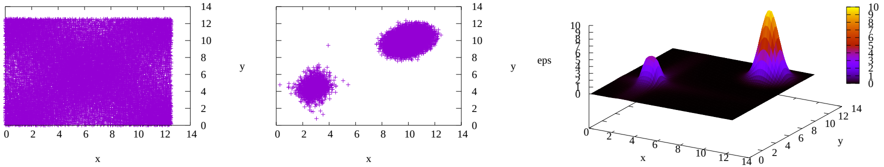
Time evolution of the number of particles

Time evolution of the number of particles in a $d_x = d_v = 2$ case.

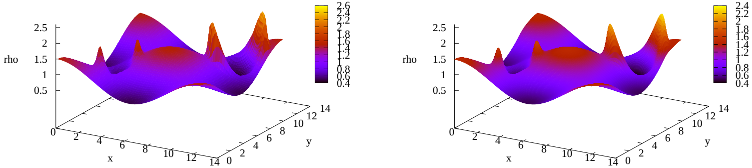


Slightly different model with $\varepsilon(\mathbf{x})$

Position of particles.
Left: particles at $T = 0$. Middle: particles at $T = 1$. Right: $\varepsilon(\mathbf{x})$.



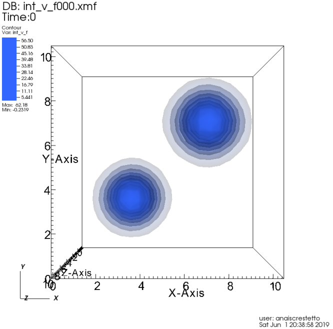
Density profile $\rho(T = 1, x, y)$.
Left: micro-macro Monte Carlo. Right: reference micro-macro grid.

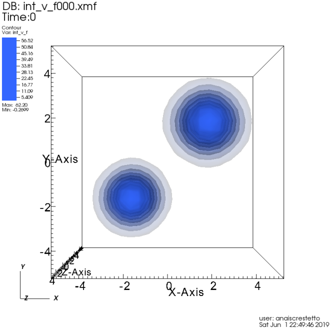


Full $d_x = d_v = 3$ case

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

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





Conclusions

- Right asymptotic behaviour: AP schemes.
- Possible to extend to a 2nd-order in time scheme.
- Computational cost reduces 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.

Future works

- More 3D-3D testcases, more physical relevance.
- Boltzmann operator.
- Add an electromagnetic field in the Monte Carlo / FV strategy.

Thank you for your attention!