An asymptotic-preserving scheme based on a finite volume/particle-in-cell coupling for Boltzmann-BGK-like equations

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Outline

Numerical simulation of particles systems

Different scales, for example collisions parameterized by the Knudsen number $\varepsilon \Rightarrow$ different models.

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

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

  coupled to Maxwell or Poisson equations.

  ☺ Accurate and necessary far from thermodynamical equilibrium.

  ☹ In 3D $\Longrightarrow$ 7 variables $\Longrightarrow$ heavy computations.

- Fluid model
  - 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.

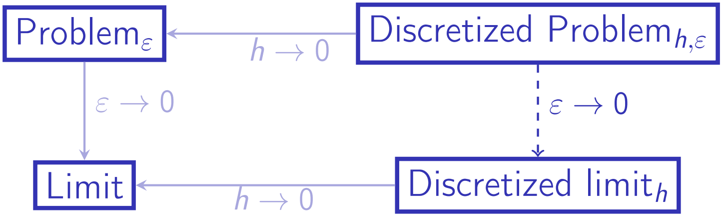
General difficulties

- Find a well adapted model for the problem, with a good precision/cost ratio.
- If two scales in the same simulation, develop a numerical scheme efficient in each regime:
  - $\rightarrow$ spatial coupling of two schemes, with an interface,

    or
  - $\rightarrow$ asymptotic-preserving (AP) scheme[4].

[4] Jin, SIAM JSC 1999.

AP scheme



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

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

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

Our Problem$_\varepsilon$: 1D Vlasov-BGK equation

- Vlasov with collisions $\Longrightarrow$ Vlasov-BGK equation:

$$\partial_t f + v\partial_x f + E\partial_v f = \frac{1}{\varepsilon} Q(f)$$

coupled to Poisson equation:

$$\partial_x E(x,t) = \rho(x,t) - 1 = \int f(x,v,t)\, dv - 1.$$

\+ Periodic boundary conditions.
\+ Initial conditions.

- $\rho(x,t) := \int f(x,v,t)\, dv$ the density, $E(x,t)$ the electric field.
- $Q(f)$ BGK (Bhatnagar-Gross-Krook) collision operator:

$$Q(f) = M(U) - f,$$

$M(U)$ being the Maxwellian having the same first three moments than f, denoted by U.

- $M(U) = \frac{\rho}{\sqrt{2\pi T}} \exp\left(-\frac{|v-u|^2}{2T}\right)$.
- $T(x,t)$ the temperature, $u(x,t)$ the mean velocity.
- $U = \int \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} f \, dv = \int \begin{pmatrix} 1 \\ v \\ \frac{v^2}{2} \end{pmatrix} M(U) \, dv$

  $\Longrightarrow U = \begin{pmatrix} \rho \\ \rho u \\ \frac{1}{2}(\rho u^2 + \rho T) \end{pmatrix}$.

- Remarks:
  - $M(U) \in \mathcal{N}(L_Q) = Span\left\{M, vM, |v|^2 M\right\}$, the null space of the linearized operator L_Q of Q,
  - $f - M(U) \to 0$ when $\varepsilon \to 0$: collisions move f closer to its Maxwellian,

  $\to$ a fluid description is sufficient when f is close to $M(U)$.

Micro-macro model

- Decomposition[5,6] $f = M(U) + g$:

$$\partial_t M(U) + v\partial_x M(U) + E\partial_v M(U) + \partial_t g + v\partial_x g + E\partial_v g = -\frac{1}{\varepsilon} g.$$

Transport operator $\mathcal{T} \cdot = v\partial_x \cdot + E\partial_v \cdot$:

$$\partial_t M(U) + \mathcal{T} M(U) + \partial_t g + \mathcal{T} g = -\frac{1}{\varepsilon} g.$$

- Hypothesis: first three moments of g must be zero $\Longrightarrow$

$$\langle mf \rangle := \int m(v) f(x,v,t)\, dv = U(x,t),$$

where $m(v) = \left(1, v, \frac{v^2}{2}\right)^t$.

True at the numerical level? If not, we have to impose it.

[5] M. Lemou, L. Mieussens, SIAM JSC 2008.

[6] N. Crouseilles, M. Lemou, KRM 2010.

Micro-macro equations

Let Π_M the orthogonal projection in $L^2(M^{-1}dv)$ onto $\mathcal{N}(L_Q)$[7] :

$$\Pi_M(\varphi) = \frac{1}{\rho} \left[\langle \varphi \rangle + \frac{(v-u)\langle (v-u)\varphi \rangle}{T} + \left(\frac{|v-u|^2}{2T} - \frac{1}{2} \right) \left\langle \left(\frac{|v-u|^2}{T} - 1 \right) \varphi \right\rangle \right] M.$$

- Properties: $(I - \Pi_M)(\partial_t M) = \Pi_M(g) = \Pi_M(\partial_t g) = 0$.
- Applying $(I - \Pi_M)$ to Vlasov-BGK $\Longrightarrow$ micro equation on g

$$\partial_t g + (I - \Pi_M)\mathcal{T}(M + g) = -\frac{1}{\varepsilon} g.$$

[7] M. Bennoune, M. Lemou, L. Mieussens, JCP 2008.

- Applying Π_M to Vlasov-BGK $\Longrightarrow$ macro equation on $M(U)$

$$\partial_t M + \Pi_M \mathcal{T}(M+g) = 0$$

or by taking his first three moments

$$\partial_t U + \partial_x F(U) + \partial_x \langle v m(v) g \rangle = S(U),$$

$$F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + \rho T \\ \rho u \left(\frac{u}{2} + \frac{3}{2} T \right) \end{pmatrix} : \text{ Euler flux}$$

$$S(U) = \begin{pmatrix} 0 \\ \rho E \\ \rho u E \end{pmatrix} : \text{ source term.}$$

Algorithm

System
$$\begin{cases} \partial_t g + (I - \Pi_M)\mathcal{T}(M+g) = -\frac{1}{\varepsilon} g \\ \partial_t U + \partial_x F(U) + \partial_x \langle v m(v) g \rangle = S(U) \end{cases}$$

equivalent to Vlasov-BGK.

Algorithm:[8]

1. Solving the micro part by a Particle-In-Cell (PIC) method.
2. Projection step to numerically force to zero the first three moments of g (matching procedure[9]).
3. Solving the macro part by a finite volume scheme (mesh on x), with a source term dependent on g.

1-3 coupling: similarities with the δf method[10] but here: AP scheme.

[8] A. C., N. Crouseilles, M. Lemou, KRM, 2012

[9] P. Degond, G. Dimarco, L. Pareschi, IJNMF, 2011

[10] S. Brunner, E. Valeo, J.A. Krommes, Phys. of Plasmas, 1999

1. PIC method

- Equation

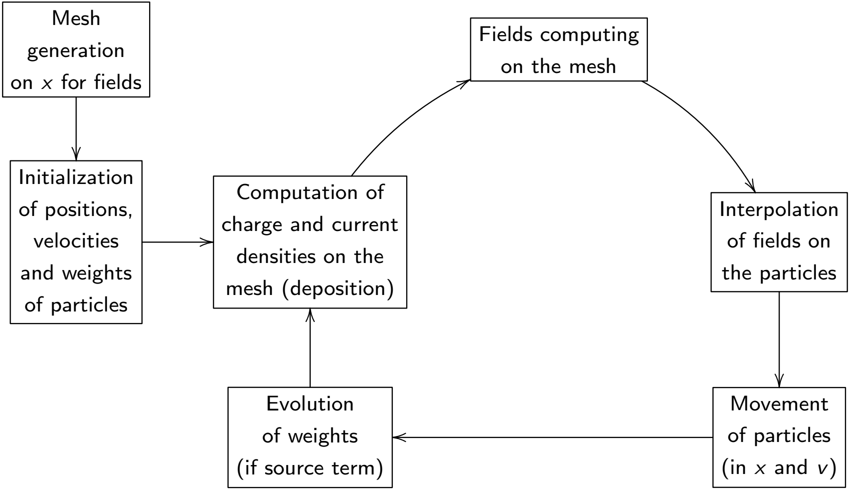
$$\partial_t g + (I - \Pi_M)\mathcal{T}(M+g) = -\frac{1}{\varepsilon}g$$

$$\Longleftrightarrow$$

$$\partial_t g + \mathcal{T}g = -(I - \Pi_M)\mathcal{T}M + \Pi_M \mathcal{T}g - \frac{g}{\varepsilon} =: S_g.$$

- Model: having N_p particles, with position x_k, velocity v_k and weight ω_k, g is approximated by

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


Mesh generation on x for fields
Initialization of positions, velocities and weights of particles
Computation of charge and current densities on the mesh (deposition)
Fields computing on the mesh
Interpolation of fields on the particles
Movement of particles (in x and v)
Evolution of weights (if source term)

Regularization using shape functions

Use of shape functions such as B-spline of order ℓ

$$B_\ell(x) = (B_0 * B_{\ell-1})(x),$$

with

$$B_0(x) = \begin{cases} \frac{1}{\Delta x} & \text{if} \quad |x| < \Delta x/2, \\ 0 & \text{else.} \end{cases}$$

In particular

$$B_1(x) = \frac{1}{\Delta x} \begin{cases} 1 - |x|/\Delta x, & \text{if} \quad |x| < \Delta x, \\ 0 & \text{else.} \end{cases}$$

- Order 0: Nearest Grid Point.
- Order 1: Cloud In Cell.

Deposition and interpolation

Deposition:

computation of the moment $\mathcal{M}$ of order p on the cell i:

$$\begin{aligned}\mathcal{M}_{p,i}(t) &= \int_{\mathbb{R}} \mathcal{M}_p(x,t)\, B_\ell(x_i - x)\; dx \\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} v^p g(x,v,t)\; dv\; B_\ell(x_i - x)\; dx \\ &= \sum_{k=1}^{N_p} \omega_k(t)\, v_k^p(t)\, B_\ell(x_i - x_k(t))\,.\end{aligned}$$

Interpolation:

evaluation of the electric field on particle k:

$$E(x_k,t) = \sum_{i=1}^{N_x} E(x_i,t)\, B_\ell(x_i - x_k(t))\,.$$

1. Initialization:
    - particles randomly (or quasi) distributed in phase space (x, v),
    - weights initialized to $\omega_k(0) = g(x_k, v_k, 0)\frac{L_x L_v}{N_p}$.
      (L_x x-length of the domain, L_v v-length.)
2. Deposition $\to \rho_i(t^n)$.
3. Solving the Poisson equation $\partial_x E(x,t) = \rho(x,t) - 1$ on the mesh:

$$\frac{E_{i+1}(t^n) - E_i(t^n)}{\Delta x} = \rho_i(t^n) - 1 \quad \text{(for example)}$$

   $\to E_i(t^n)$.
4. Interpolation on the particles $\to E(x_k, t^n)$.

Solving $\partial_t g + \mathcal{T} g = 0$

5. Movement of particles thanks to motion equations:

$$\frac{dx_k}{dt}(t) = v_k(t) \quad \text{and} \quad \frac{dv_k}{dt}(t) = E(x_k, t).$$

Verlet scheme (for example):

$$\begin{cases} v_k^{n+\frac{1}{2}} = v_k^n + \dfrac{\Delta t}{2} E^n(x_k^n) \\ x_k^{n+1} = x_k^n + \Delta t v_k^{n+\frac{1}{2}} \\ v_k^{n+1} = v_k^{n+\frac{1}{2}} + \dfrac{\Delta t}{2} E^{n+1}(x_k^{n+1}) \end{cases}.$$

Solving $\partial_t g = S_g$

6. Evolution of weights ω_k (step specific to kinetic equations with source term):

$$\frac{d\omega_k}{dt}(t) = s_k(t),$$

where

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

is the weight associated to the source term

$$S_g = -(I - \Pi_M)\mathcal{T}M + \Pi_M \mathcal{T} g - \frac{g}{\varepsilon}.$$

In our case:

$$\frac{d\omega_k}{dt}(t) = \alpha_k(t) - \frac{\omega_k(t)}{\varepsilon},$$

where $\alpha_k(t)$ is associated to $-(I - \Pi_M)\mathcal{T}M + \Pi_M \mathcal{T} g$.

$-(I - \Pi_M)\mathcal{T}M + \Pi_M \mathcal{T} g$ is constituted of moments of g, their derivatives and M.

- Moments of g are computed by deposition, derived by finite differences and evaluated on (x_k, v_k) by interpolation.
- ρ, u and T are evaluated on (x_k, v_k) by interpolation.
- $M = \frac{\rho}{\sqrt{2\pi T}} \exp\left(-\frac{|v-u|^2}{2T}\right)$ is now easily evaluated on (x_k, v_k).

$\rightarrow$ α_k computed.

Key point to ensure the AP property

- To have an AP scheme, we make the stiff term $\frac{\omega_k(t)}{\varepsilon}$ implicit:

$$\omega_k^{n+1} = \frac{\omega_k^n + \Delta t \alpha_k^n}{1 + \frac{\Delta t}{\varepsilon}}.$$

2. Projection step

- We now have

$$g^{n+1}(x,v,t) \approx \sum_{k=1}^{N_p} \omega_k^{n+1} \delta\left(x - x_k^{n+1}\right) \delta\left(v - v_k^{n+1}\right).$$

We want to ensure $\langle m g^{n+1} \rangle = 0$.

- How? By correcting the weights.
- We compute $U_g := \langle m g^{n+1} \rangle \neq 0$,

$$U_g(x_i) = \langle m g^{n+1} \rangle |_{x_i} = \sum_{k=1}^{N_p} \omega_k m(v_k) B_\ell (x_i - x_k).$$

- We seek $h \in \mathcal{N}(L_Q)$ of the form $h(x,v) = \lambda(x) \cdot m(v) M(x,v)$ s.t. $U_g(x_i) = \langle m h(x_i, v)\rangle$.
- We expand $\lambda(x)$ on the basis of B-splines of degree ℓ

$$\lambda(x) = \sum_{j=1}^{N_x} \lambda_j B_\ell(x - \mathrm{x}_j), \qquad \lambda_j \in \mathbb{R}^3.$$

  For example $\ell = 0$ ($\ell = 1$ is also computed).
- Let p_k the weights associated to M, we compute

$$\langle m h\rangle|_{\mathrm{x}_i} \approx \frac{1}{\Delta x^2} \left(\sum_{k/|x_k - \mathrm{x}_i| \leq \Delta x/2} m(v_k) \otimes m(v_k) p_k \right) \lambda_i.$$

- We solve the 3×3 linear system

$$U_g(\mathrm{x}_i) = A_i \lambda_i,$$

with

$$A_i = \frac{1}{\Delta x} \begin{pmatrix} M_{0,i} & M_{1,i} & M_{2,i} \\ M_{1,i} & M_{2,i} & M_{3,i} \\ M_{2,i} & M_{3,i} & M_{4,i} \end{pmatrix},$$

and $M_{j,i} = \frac{1}{\Delta x} \sum_{k/|x_k - \mathrm{x}_i| \leq \Delta x/2} p_k v_k^j$.

- We compute the weights γ_k of h

$$\gamma_k = \sum_{j=1}^{N_x} \lambda_j B_0(x_k - \mathrm{x}_j) \cdot m(v_k) p_k = \frac{1}{\Delta x} \lambda_{j_k} \cdot m(v_k) p_k,$$

where j_k is such that $|x_k - \mathrm{x}_{j_k}| < \Delta x/2$.

- We correct the weights of g

$$\omega_k^{new} \leftarrow \omega_k - \gamma_k,$$

to obtain

$$\langle m g^{n+1,new} \rangle |_{x_i} = \frac{1}{\Delta x} \sum_{k/|x_k - x_i| \leq \Delta x/2} \omega_k^{new} m(v_k)$$

$$= \frac{1}{\Delta x} \sum_{k/|x_k - x_i| \leq \Delta x/2} \omega_k m(v_k) - \frac{1}{\Delta x} \sum_{k/|x_k - x_i| \leq \Delta x/2} \gamma_k m(v_k) = 0.$$

- Remark: order 1 $\Longrightarrow$ $(3N_x \times 3N_x)$ system.

3. Macro part

- Equation $\partial_t U + \partial_x F(U) = \tilde{S}(U, g) \ (= S(U) - \partial_x \langle vm(v)g \rangle)$.
- Finite volume method

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1/2}^n - F_{i-1/2}^n\right) - \Delta t \tilde{S}_i^n,$$

with Rusanov flux

$$F_{i+1/2}^n = \frac{1}{2}\left(F\left(U_{i+1}^n\right) + F\left(U_i^n\right) - a_{i+1/2}(U_{i+1} - U_i)\right),$$

where $a_{i+1/2} = max_{j=i,i+1}\left(abs\ R\left(J_F\left(x_j\right)\right)\right)$, $R\left(J_F\right)$ being the eigenvalues of the Jacobian of F.

$$\tilde{S}_i^n = S\left(U_i^n\right) - \left(\frac{\langle vmg^{n+1}\rangle|_{x_{i+1/2}} - \langle vmg^{n+1}\rangle|_{x_{i-1/2}}}{\Delta x}\right)$$

where

$\langle vmg^{n+1}\rangle|_{x_{i+1/2}} = \frac{1}{\Delta x}\sum_{k/|x_k - x_{i+1/2}| \leq \Delta x/2} \omega_k^{n+1} v_k m(v_k)$.

Analytical limit

$$\partial_t g + (I - \Pi_M)\mathcal{T}(M+g) = -\frac{1}{\varepsilon} g, \qquad (1)$$

$$\partial_t U + \partial_x F(U) + \partial_x \langle v m(v) g \rangle = S(U). \qquad (2)$$

- Limit $\varepsilon \to 0$ in (1): $g = \mathcal{O}(\varepsilon) \Longrightarrow$

$$\begin{aligned} g &= -\varepsilon(I - \Pi_M)\mathcal{T} M + \mathcal{O}(\varepsilon^2), \\ &= -\varepsilon(I - \Pi_M)(v\partial_x M + E\partial_v M) + \mathcal{O}(\varepsilon^2), \\ &= -\varepsilon(I - \Pi_M)(v\partial_x M) + \mathcal{O}(\varepsilon^2), \end{aligned}$$

  because $E\partial_v M \in \mathcal{N}(L_Q)$ and then $(I - \Pi_M)(E\partial_v M) = 0$.

- Injected into (2), we obtain the Navier-Stokes model

$$\partial_t U + \partial_x F(U) = S(U) + \varepsilon \partial_x \langle v m(v)(I - \Pi_M)(v\partial_x M)\rangle + \mathcal{O}(\varepsilon^2).$$

Numerical limit

- (1) can be discretized as

$$\frac{\omega_k^{n+1}-\omega_k^n}{\Delta t} = -\overbrace{\alpha_{1,k}^n}^{weight\ \ of\ \ (I-\Pi_M)\mathcal{T}M} - \overbrace{\alpha_{2,k}^n}^{weight\ \ of\ \ (I-\Pi_M)\mathcal{T}g} - \frac{\omega_k^{n+1}}{\varepsilon},$$

$$\omega_k^{n+1} = \frac{1}{1+\Delta t/\varepsilon}\left(\omega_k^n - \Delta t\alpha_{1,k}^n - \Delta t\alpha_{2,k}^n\right).$$

- But $\frac{1}{1+\Delta t/\varepsilon} = \frac{\varepsilon}{\Delta t} + \mathcal{O}(\varepsilon^2)$ when $\varepsilon \to 0$, $\omega_k^n = \mathcal{O}(\varepsilon)$ and $\alpha_{2,k}^n = \mathcal{O}(\varepsilon)$ thus

$$\omega_k^{n+1} = -\varepsilon\alpha_{1,k}^n + \mathcal{O}(\varepsilon^2).$$

- We obtain the diffusion term of the Navier-Stokes model

$$g^{n+1} = -\varepsilon(I-\Pi_M)\mathcal{T}M + \mathcal{O}(\varepsilon^2)$$

$\Longrightarrow$ AP property.

Landau damping

- Initial distribution function:

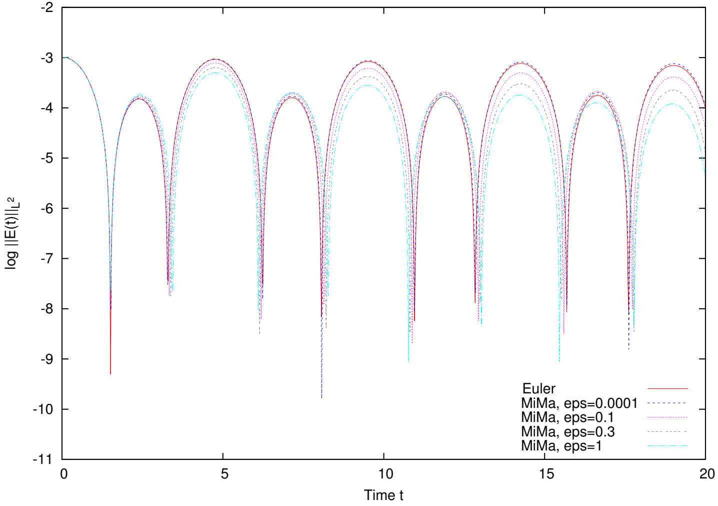
$$f(x, v, 0) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{v^2}{2})(1 + \alpha \cos(kx)), \qquad x \in [0, 2\pi/k]$$

- Micro-macro initializations:

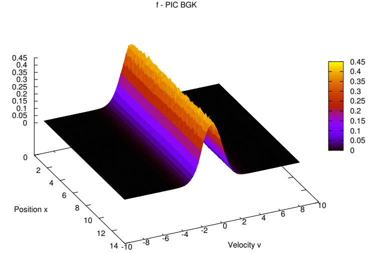
$$U(x) = \begin{pmatrix} 1 + \alpha \cos(kx) \\ 0 \\ 1 + \alpha \cos(kx) \end{pmatrix} \quad \text{and} \quad g(x, v, t = 0) = 0.$$

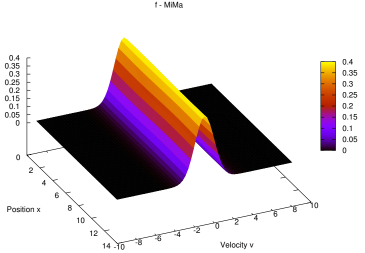
- Parameters: $\alpha = 0.01$, $k = 0.5$.
- Electrical energy $\mathcal{E}(t) = \sqrt{\int E(t, x)^2 dx}$.

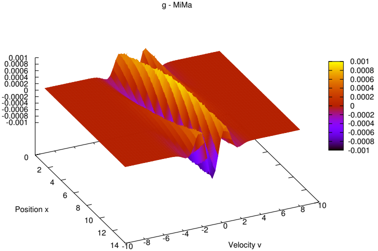
Convergence at the $\varepsilon \to 0$ limit, $N_x = 128$, $N_p = 5 \times 10^3$:

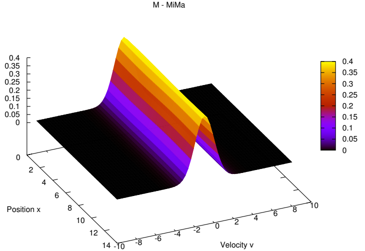


Distribution function f of PIC BGK, MiMa, g and M, at $t = 20$, $\varepsilon = 1$, $N_p = 5 \times 10^5$:

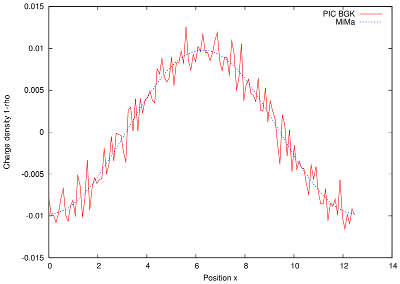


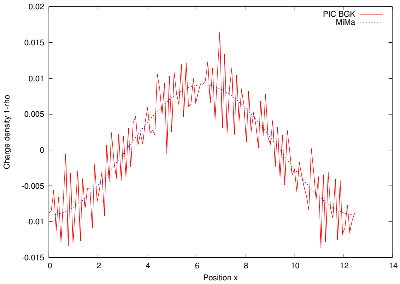




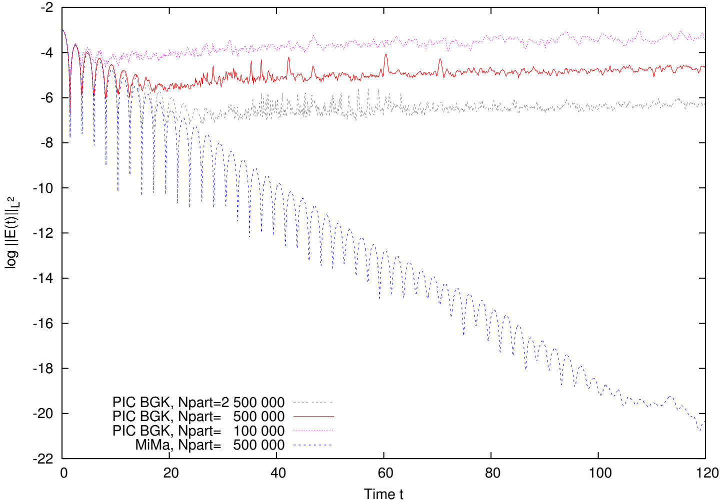


Noise reduction on ρ, $\varepsilon = 1$, $N_x = 128$, $N_p = 5 \times 10^5$, at $t = 0.2$ (left) and $t = 0.4$ (right):

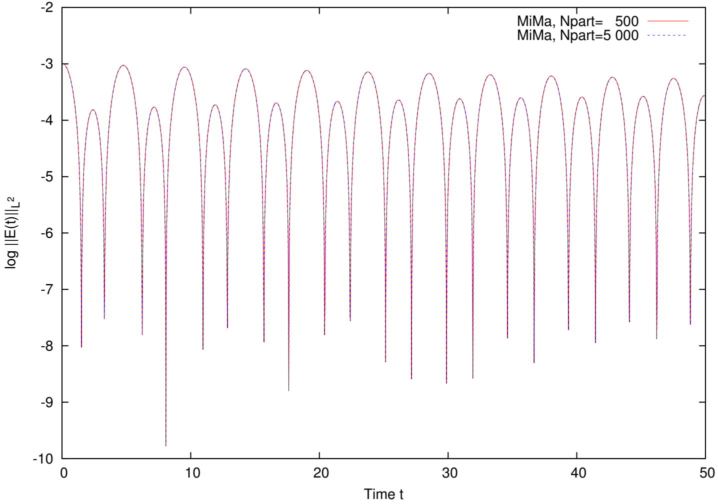




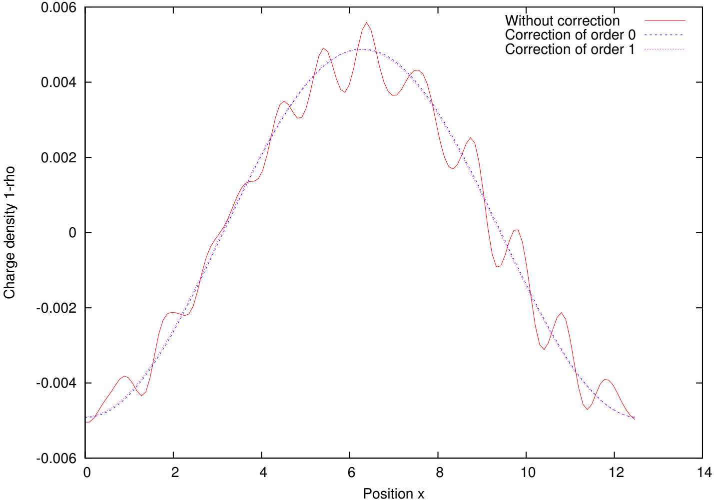
Necessary number of particles, $\varepsilon = 10$, $N_x = 128$:



Convergence in particles, $\varepsilon = 10^{-4}$, $N_x = 128$:



Importance of the projection step on ρ at $t = 5$, $\varepsilon = 1$, $N_p = 5 \times 10^5$:



Test 2

- Initial distribution function:

$$f\,(x,v,0) = \frac{v^4}{\sqrt{2\pi}}\exp(-\frac{v^2}{2})(1+\alpha\cos(kx)), \qquad x \in [0, 2\pi/k]$$

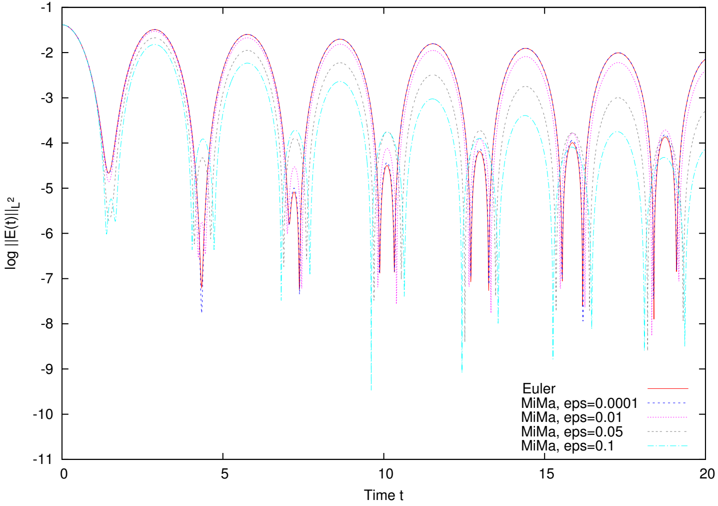
- Micro-macro initializations:

$$U(x) = \begin{pmatrix} 1+\alpha\cos(kx) \\ 0 \\ 5\,(1+\alpha\cos(kx)) \end{pmatrix}$$

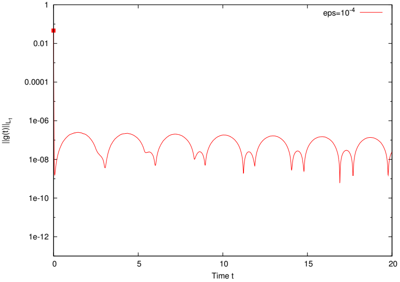
$$g_0\,(x,v) = \frac{1+\alpha\cos(kx)}{\sqrt{2\pi}}\left(\frac{v^4}{3}\exp(-v^2/2) - \frac{1}{\sqrt{5}}\exp(-v^2/10)\right).$$

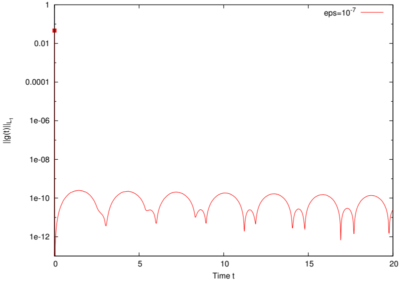
- Parameters: $\alpha = 0.05$, $k = 0.5$.

Convergence at the $\varepsilon \to 0$ limit, $N_x = 128$, $N_p = 5 \times 10^3$:



L1-norm of g, $\varepsilon = 10^{-4}$ (left) and $\varepsilon = 10^{-7}$ (right):

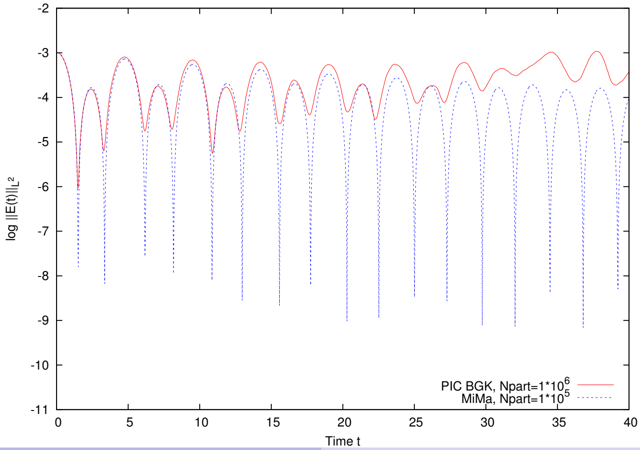




Computational cost

Landau damping, $\varepsilon = 0.1$:

MiMa	$N_p = 1 \times 10^5$	153 s.
PIC-BGK	$N_p = 1 \times 10^6$	694 s.



Conclusions

- Fluid limit recovered when $\varepsilon \to 0$.

☺ AP scheme.

- Projection step to numerically force the moments of g to zero.
- $g \to 0$ when $\varepsilon \to 0 \Longrightarrow$ few particles are sufficient at the limit, whereas grid methods have a constant cost, whatever the value of ε.
- Noise due to PIC method reduced (because only on g) $\Longrightarrow$ at equivalent results, fewer particles are necessary.

☺ Computational cost reduced at the limit.

Perspectives

- Extension to the diffusion limit:

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

- Consider Dirichlet boundary conditions.
- Consider more general collisions operators.
- Extension to two species: ions and electrons $\Rightarrow$ more complicated right-hand side.
- Extension to higher dimensions.

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Thank you for your attention!