Kinetic/Fluid micro-macro numerical scheme for Vlasov-Poisson-BGK equation using particles

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Outline

Numerical simulation of plasmas

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

$\rightarrow$ Kinetic models

- Particles represented by a distribution function $f(\mathbf{x}, \mathbf{v}, t)$.
- Solving the Vlasov equation (with source term $S(\varepsilon)$)

$$\partial_t f + \mathbf{v} \cdot \partial_\mathbf{x} f + \frac{q}{m}(\mathbf{E} + \mathbf{v} \wedge \mathbf{B}) \cdot \partial_\mathbf{v} f = S(\varepsilon)$$

  coupled to Maxwell equations or Poisson equation.
- In 3D $\Rightarrow$ 7 variables: 3 in space, 3 in velocity and the time $\Rightarrow$ heavy computations.

$\rightarrow$ Fluid models

- Moment equations on physical quantities linked to f (density, mean velocity, temperature, etc.).
- Smaller cost, but lost of precision.

General difficulties

- Find a well adapted model for our system, with a good precision/cost ratio.
- If two scales in the same simulation: two schemes with an interface? Difficult to deal with the interface!

Vlasov-Poisson-BGK system

Collisions between particles parameterized by the Knudsen number ε.

- The Vlasov-Poisson-BGK equations (on $[0, L_x] \times \mathbb{R} \times \mathbb{R}^+$, $L_x \in \mathbb{R}^{+\star}$)

$$\begin{aligned} \partial_t f + v\partial_x f + E\partial_v f &= \frac{1}{\varepsilon} Q(f), \\ \partial_x E &= -1 + \int f \, dv. \end{aligned}$$

- Periodic conditions on f and E.
- Zero mean condition on E and initial conditions

$$\begin{aligned} \int_0^{L_x} E(x,t)\,dx &= 0, & \forall\ t \geq 0, \\ f(x,v,0) &= f_0(x,v), & \forall\ x \in [0, L_x],\ v \in \mathbb{R}. \end{aligned}$$

- $Q(f)$ is the BGK collisions operator (Bhatnagar-Gross-Krook):

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

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

- We denote by $\mathcal{N}(L_Q) = Span\left\{M, vM, |v|^2 M\right\}$, the kernel of the linearized operator L_Q of Q.

Objectives

- Construction of a stable and consistent at the $\varepsilon \to 0$ limit scheme, of constant cost with respect to ε: an asymptotic preserving (AP) scheme[4].

- Reduction of the numerical cost: micro-macro decomposition with particles.
  Especially at the $\varepsilon \to 0$ limit since collisions bring f to its Maxwellian : $f - M(U) \to 0$ when $\varepsilon \to 0$.

[4] Jin, SIAM JSC 1999.

Micro-macro model

- Micro-macro 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 3 moments of g are zeros:

$$\langle mg \rangle := \int m(v)\, g(x,v,t)\, dv = \mathbf{0}, \quad \text{with} \quad m(v) := \left(1, v, \frac{|v|^2}{2}\right)^T.$$

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

[5] Lemou, Mieussens, SIAM JSC 2008.

[6] Liu, Yu, CMP 2004.

Micro-macro equations

Let Π_M the orthogonal projection in $L^2\left(M^{-1}dv\right)$ on $\mathcal{N}\left(L_Q\right)$:

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

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

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

- By applying Π_M to Vlasov-BGK $\Rightarrow$ macro equation on $M(U)$

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

And by taking its first 3 moments

$$\boxed{\partial_t U + \partial_x F(U) + \partial_x \langle vm(v)g \rangle = S(U),}$$

with $F(U)$ the Euler flux and $S(U)$ a source term.

Micro-macro system[7]

$$\boxed{\left\{ \begin{array}{c} \partial_t g + (I - \Pi_M)\mathcal{T}(M+g) = -\frac{1}{\varepsilon} g \\ \partial_t U + \partial_x F(U) + \partial_x \langle vm(v)g \rangle = S(U) \end{array} \right.}$$

equivalent to Vlasov-BGK.

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

Algorithm

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[8]).
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[9] but here: AP scheme.

[8] Degond, Dimarco, Pareschi, IJNMF, 2011
[9] Brunner, Valeo, Krommes, Phys. of Plasmas 1999.

1. PIC method on g

- Solving by a PIC method the equation

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

$$\Longleftrightarrow$$

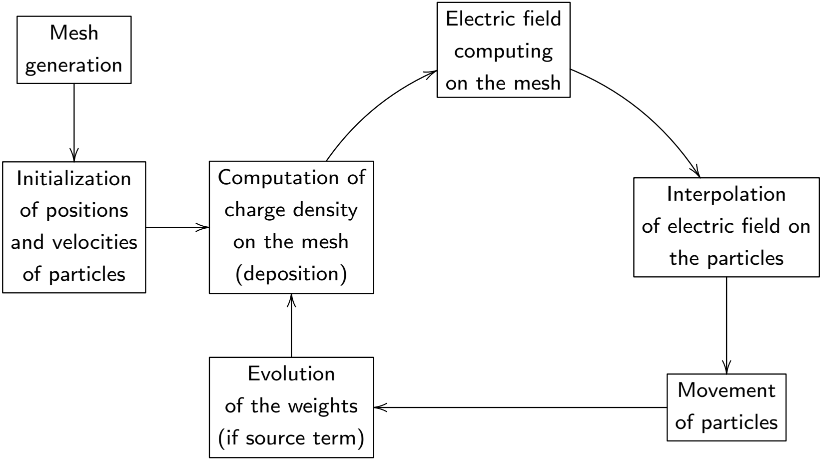
$$\partial_t g + \mathcal{T} g = -(I - \Pi_M)\mathcal{T} M + \Pi_M \mathcal{T} g - \frac{g}{\varepsilon} =: S_g,$$

coupled to the Poisson equation for the electric field.

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

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

PIC algorithm



Equation with source term $\rightarrow$ splitting.

1. Solving the transport part $\partial_t g + \mathcal{T} g = 0$.

$\rightarrow$ Displacement of particles thanks to the equations of motion

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

Second order Verlet scheme (for example):

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

2. Solving the source part

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

→ Equation on weights of the form

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

where α_k is the weight "associated" to

$$-(I - \Pi_M)(\mathcal{T} M) + \Pi_M(\mathcal{T} g).$$

→ To have an AP scheme, we make the stiff term implicit:

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

2. Projection step

At time $n+1$, we have

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

Micro-macro structure: $\langle mg\left(x, v, t^{n+1}\right)\rangle = 0$.

A priori not true for $g^{n+1}(x,v) \rightarrow$ correction[10].

1. We compute $U_g := \langle mg^{n+1}\rangle \neq 0$ on each cell x_i :

$$U_g(x_i) = \langle mg^{n+1}\rangle |_{x_i} = \sum_{k / x_k \in [x_i, x_{i+1}]} \omega_k m(v_k).$$

2. We seek $h \in \mathcal{N}(L_Q) = Span\left\{M, vM, |v|^2 M\right\}$

$$h(x,v) = \lambda(x) \cdot m(v) M(x,v) \quad \text{s.t.} \quad U_g(x_i) = \langle mh(x_i, v)\rangle.$$

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

$\rightarrow$ Solving N_x linear systems (3×3)

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

with A_i a matrix containing moments of M and $\lambda_i \approx \lambda\left(x_i\right)$.

$\rightarrow$ Computation of weights γ_k "associated" to h on each particle.

3. Correction of the weights in order to preserve the micro-macro structure

$$\boxed{\omega_k^{new} \leftarrow \omega_k - \gamma_k}.$$

$\rightarrow$ By construction : $\langle m g^{n+1,new} \rangle \,|_{x_i} = U_g\left(x_i\right) - \langle m h\left(x_i, v\right) \rangle = 0$.

Remark: correction "of order 1" (by using linear shape functions) $\Rightarrow$ $(3N_x \times 3N_x)$ system.

3. Macro part

- Solving the equation

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

- 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

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

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.

- Computation of the moments of g to evaluate

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

Landau damping

- Initial distribution function:

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

- Micro-macro initializations:

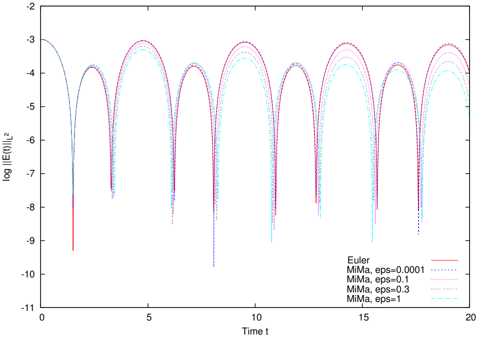
$$U\left(x\right)=\begin{pmatrix}1+\alpha\cos\left(kx\right)\\0\\1+\alpha\cos\left(kx\right)\end{pmatrix}\quad\text{and}\quad g\left(x,v,t=0\right)=0.$$

- Parameters: $\alpha=0.01$, $k=0.5$, $L_x=2\pi/k$.
- Observation: electrical energy $\mathcal{E}\left(t\right)=\sqrt{\int E\left(t,x\right)^2\,dx}$.

AP property

Convergence to Euler-Poisson at the $\varepsilon \to 0$ limit?

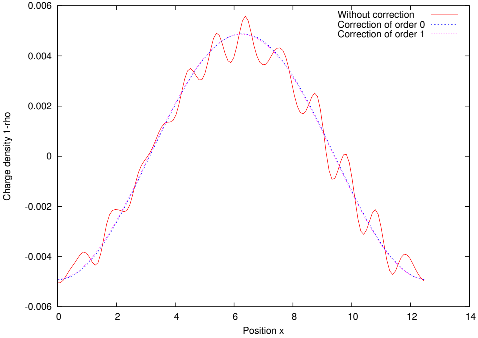
$\mathcal{E}(t)$, comparison with Euler-Poisson.
$N_x = 128,\ N_p = 5 \times 10^3$, different values of ε.



$\rightarrow$ Good convergence $\Rightarrow$ AP scheme.

Importance of the projection step

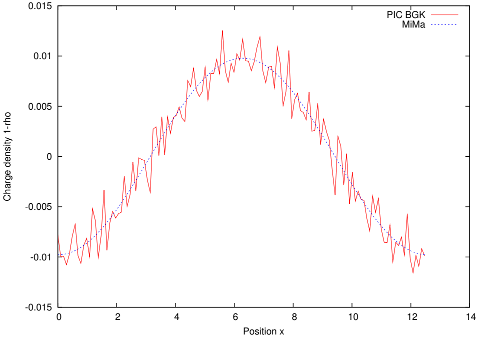
$\rho(x)$, with and without correction.
$\varepsilon = 1$, $N_p = 5 \times 10^5$ at $t = 5$.



$\rightarrow$ Correction $\Rightarrow$ the instabilities disappear.

Numerical-noise reduction

$\rho(x)$, comparison with a PIC method on the whole f.
$\varepsilon = 1$, $N_x = 128$, $N_p = 5 \times 10^5$, at $t = 0.2$.

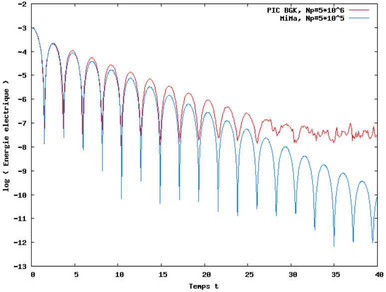


→ Micro-macro decomposition ⇒ noise due to the PIC method reduced.

Computational cost

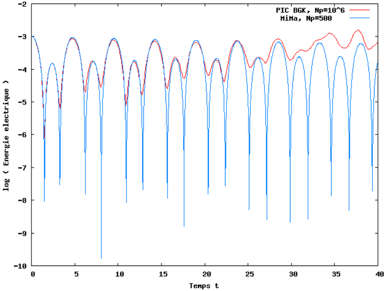
$\mathcal{E}(t)$, comparison with a PIC method on the whole f.

$\varepsilon = 10$



	N_p	Time
MiMa	5×10^5	768 s.
PIC-BGK	5×10^6	1391 s.

$\varepsilon = 10^{-4}$



	N_p	Time
MiMa	500	11 s.
PIC-BGK	10^6	230 s.

Conclusion

- Micro-macro decomposition for Vlasov-Poisson-BGK using a PIC method.
- Projection step to numerically force the first 3 moments of g to zero.

$\rightarrow$ AP scheme.

$\rightarrow$ Reduction of the numerical noise due to the PIC method because only on g.

$\rightarrow$ Reduction of the cost compared to grid methods at the $\varepsilon \rightarrow 0$ limit because few particles are sufficient.

$\rightarrow$ Also true when $g(x, v, 0) \neq 0$.

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Thank you for your attention!