A particle-based micro-macro decomposition for Boltzmann-BGK-like equations in the diffusion scaling

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IPP Garching, NumKin 2017
October 26, 2017

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Outline

1. Problem and objectives
2. Micro-macro model
3. Particle-In-Cell / FV scheme
4. Numerical results

1 Problem and objectives
- Introduction
- Our problem
- Objectives

2 Micro-macro model

3 Particle-In-Cell / FV scheme

4 Numerical results

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 Asymptotic Preserving (AP) schemes[4],
- the reduction of the cost at the limit $\varepsilon \to 0$.

[4] Jin, SIAM JSC 1999.

Our 1st Problem$_\varepsilon$

1D Vlasov-BGK equation, diffusion 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 $\rho = \int_V f \, \mathrm{d}v$,
- electric field E 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.

Main difficulty:

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

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

Our 2nd Problem$_\varepsilon$

1D radiative transport equation, diffusion scaling

$$\partial_t f + \frac{1}{\varepsilon} v \partial_x f = \frac{1}{\varepsilon^2}(\rho M - f) \tag{3}$$

- $x \in [0, L_x] \subset \mathbb{R}$, $v \in V = [-1, 1]$,
- charge density $\rho = \frac{1}{2}\int_V f \, \mathrm{d}v$,

- $M(v) = 1$,
- periodic conditions in x and initial conditions.

Main difficulty:

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

$$\partial_t \rho - \frac{1}{3}\partial_{xx}\rho = 0. \tag{4}$$

Objectives

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

Tools

- Micro-macro decomposition[5,6] for these models. Previous work with a grid in v for the micro part[7], cost was constant w.r.t. ε.

Idea

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

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

1 Problem and objectives

2 Micro-macro model
- Derivation of the micro-macro system
- First-order reformulation

3 Particle-In-Cell / FV scheme

4 Numerical results

Micro-macro model for the 2nd Problem$_\varepsilon$ (3)

- Micro-macro decomposition[5,7]: $f = \rho M + g$ with g the rest.
- $\mathcal{N} = \mathrm{Span}\{M\} = \{f = \rho M\}$ null space of the BGK operator $Q(f) = \rho M - f$.
- Π orthogonal projection in $L^2\left(M^{-1}\mathrm{d}v\right)$ onto $\mathcal{N}$:

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

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

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

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

[5] M. Lemou, L. Mieussens, SIAM JSC 2008.
[7] N. Crouseilles, M. Lemou, KRM 2011.

- Applying Π to (3) $\Longrightarrow$ macro equation on ρ

$$\partial_t \rho + \frac{1}{\varepsilon}\partial_x \langle vg \rangle = 0. \tag{5}$$

- Applying $(I - \Pi)$ to (3) $\Longrightarrow$ micro equation on g

$$\partial_t g + \frac{1}{\varepsilon}[v\partial_x \rho + v\partial_x g - \partial_x \langle vg \rangle] = -\frac{1}{\varepsilon^2} g. \tag{6}$$

Equation (3) $\Leftrightarrow$ micro-macro system:

$$\begin{cases} \partial_t \rho + \dfrac{1}{\varepsilon}\partial_x \langle vg \rangle = 0, \\ \partial_t g + \dfrac{1}{\varepsilon}\mathcal{F}(\rho, g) = -\dfrac{1}{\varepsilon^2} g, \end{cases} \tag{7}$$

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

Difficulties

- Stiff terms in the micro equation (6) on g.
- In previous works[5,7], 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

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

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

Idea?

- Suitable reformulation of the model.

[5] M. Lemou, L. Mieussens, SIAM JSC 2008.
[7] N. Crouseilles, M. Lemou, KRM 2011.

- Strategy of Lemou[8]:
  1. rewrite (6) $\partial_t g + \frac{1}{\varepsilon}\mathcal{F}(\rho, g) = -\frac{1}{\varepsilon^2} g$ as

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

  2. integrate in time between t^n and t^{n+1} and multiply by $e^{-t^{n+1}/\varepsilon^2}$:

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

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

$$\partial_t g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t}\mathcal{F}(\rho, g). \tag{8}$$

- No more stiff terms and consistent with the initial micro equation (6).

[8] Lemou, CRAS 2010.

1 Problem and objectives

2 Micro-macro model

3 Particle-In-Cell / FV scheme
- PIC method
- Finite volumes scheme
- Properties
- Second-order in time

4 Numerical results

Algorithm

Reformulated system

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

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[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].

[9] P. Degond, G. Dimarco, L. Pareschi, IJNMF, 2011
[10] S. Brunner, E. Valeo, J.A. Krommes, Phys. of Plasmas, 1999

1. PIC method with evolution of weights

- Equation

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

$$\Longleftrightarrow$$

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

where

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

- 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

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

Solving $\partial_t g + \varepsilon \frac{1-e^{-\Delta t/\varepsilon^2}}{\Delta t}[v\partial_x g] = 0$

1. Initialization:
   - mesh in space $X_i = i\Delta x$ for macroscopic quantities such as $\rho(t,x) \approx \rho_i(t)$ and $\langle vg \rangle(t,x) \approx \langle vg \rangle_i(t)$,
   - particles uniformly distributed in phase space (x, v), independently of the mesh,
   - 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.)
2. Movement of particles thanks to motion equations:

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

For example

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

Solving $\partial_t g = S_g$

3. Deposition and interpolation for communications between macro mesh and particles.
4. 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
$$S_g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} [v\partial_x \rho - \partial_x \langle vg \rangle].$$

In practice:

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

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

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

2. Projection step

- We now have

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

- Nothing ensures $\langle g^{n+1} \rangle = 0$ at the numerical level. We have to impose it.
- How? By applying a discrete approximation of $(I - \Pi)$ to each weight ω_k.
  In the case of no regularization (Dirac masses):

$$\forall k \in \mathcal{I}_i := \left\{ k \ / \ x_k \in [X_{i-1/2}, X_{i+1/2}] \right\}, \ \omega_k \leftarrow \omega_k - \Delta x \frac{\langle g \rangle_i}{\sum_{k \in \mathcal{I}_i} p_k} p_k,$$

  where $p_k := \rho(x_k) M(v_k) \frac{L_x L_v}{N_p}$ is the weight associated to the Maxwellian.

3. Macro part

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

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\varepsilon} \frac{\langle vg^{n+1} \rangle_{i+1} - \langle vg^{n+1} \rangle_{i-1}}{2\Delta x}.$$

Numerical limit

- Micro equation is discretized as

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

- When $\varepsilon \to 0$, $\beta_k^n = \mathcal{O}(\varepsilon)$ thus $\omega_k^{n+1} = -\varepsilon\alpha_k^n + \mathcal{O}(\varepsilon^2)$ and

$$\langle vg^{n+1}\rangle_i = -\varepsilon \underbrace{\langle v^2\rangle_i^n}_{\underset{N_p\to\infty}{\longrightarrow} 1/3} \partial_x\rho_i^n + \mathcal{O}(\varepsilon^2).$$

- Injecting in the macro equation $\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\varepsilon}\partial_x\langle vg^{n+1}\rangle_i$ gives

$$\rho_i^{n+1} = \rho_i^n + \frac{\Delta t}{3}\partial_{xx}\rho_i^n,$$

$\Longrightarrow$ we recover a discretization of the limit equation (4).

Correction of the macro discretization

- Aim: use this idea to implicit the diffusion term.
- Write $\omega_k^{n+1} = e^{-\Delta t/\varepsilon^2}\omega_k^n - \varepsilon(1-e^{-\Delta t/\varepsilon^2})\left[\underbrace{v\partial_x\rho}_{\alpha_k^n} + \underbrace{-\partial_x\langle vg\rangle}_{\beta_k^n}\right]$.
- Let $h_i^n := e^{-\Delta t/\varepsilon^2}\langle g^n\rangle_i - \varepsilon(1-e^{-\Delta t/\varepsilon^2})\langle -\partial_x\langle vg\rangle\rangle$ 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 and take the diffusion term implicit

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

AP property

- 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 (4).

$\Longrightarrow$ AP property.

Second-order scheme in time: new reformulation

- 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:

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

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

- Time scheme: RK2 $\rightarrow$ Prediction step on $\Delta t/2$:

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

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

$\rightarrow$ Correction step on Δt:

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

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

- Choice of $\widetilde{g}$ in order to have a second-order scheme in time 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.
- Use only B-splines of order $\ell \geq 1$ for depositions and interpolations.

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 (4).

$\Longrightarrow$ AP property.

- Both schemes of order 1 and 2 in time can be (and have been) extended to the Vlasov-BGK-Poisson case.

1 Problem and objectives

2 Micro-macro model

3 Particle-In-Cell / FV scheme

4 Numerical results
- Radiative Transport Equation case
- Vlasov-BGK-Poisson cases

Radiative Transport Equation case

- Initial distribution function:

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

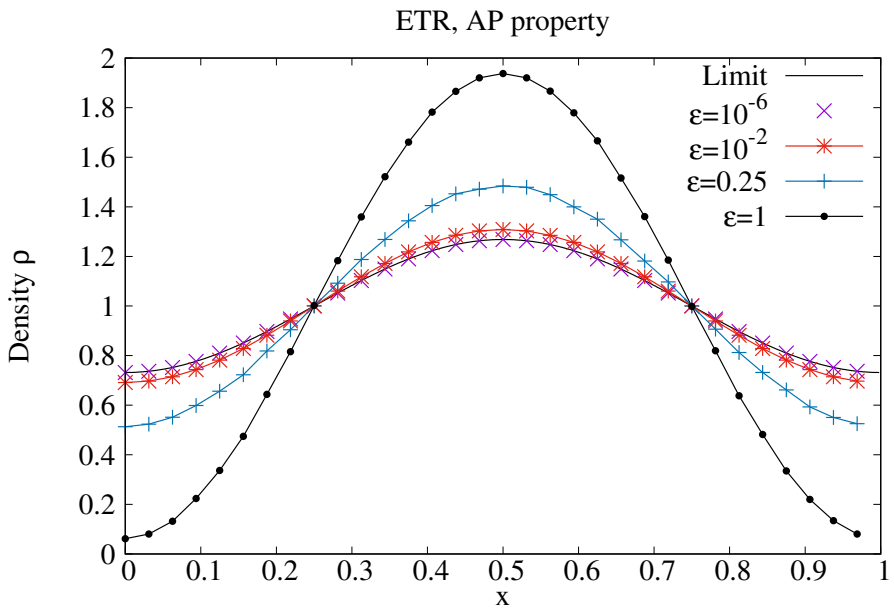
- Micro-macro initializations:

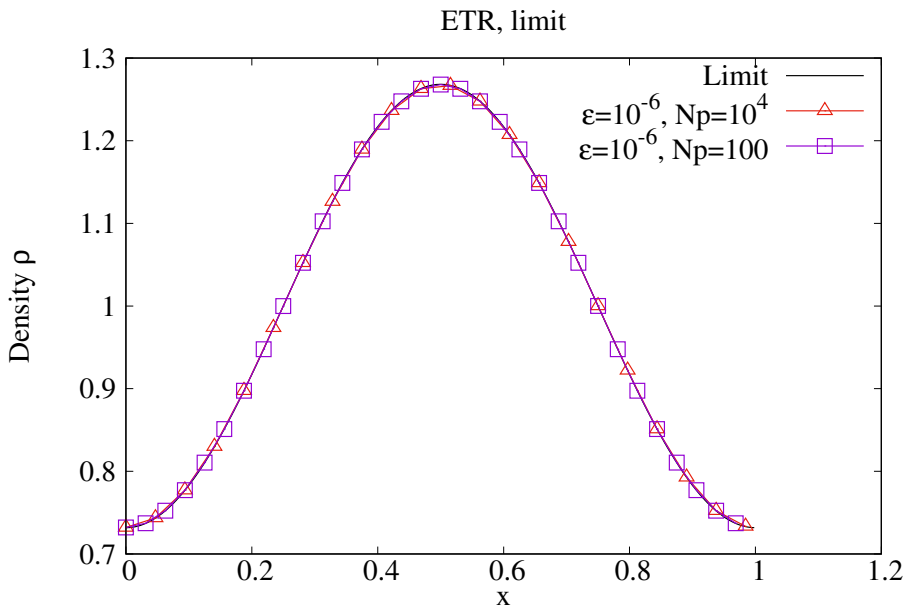
$$\rho(t=0,x)=1+\cos\left(2\pi\left(x+\frac{1}{2}\right)\right)\quad\text{and}\quad g(t=0,x,v)=0.$$

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

Asymptotic behaviour

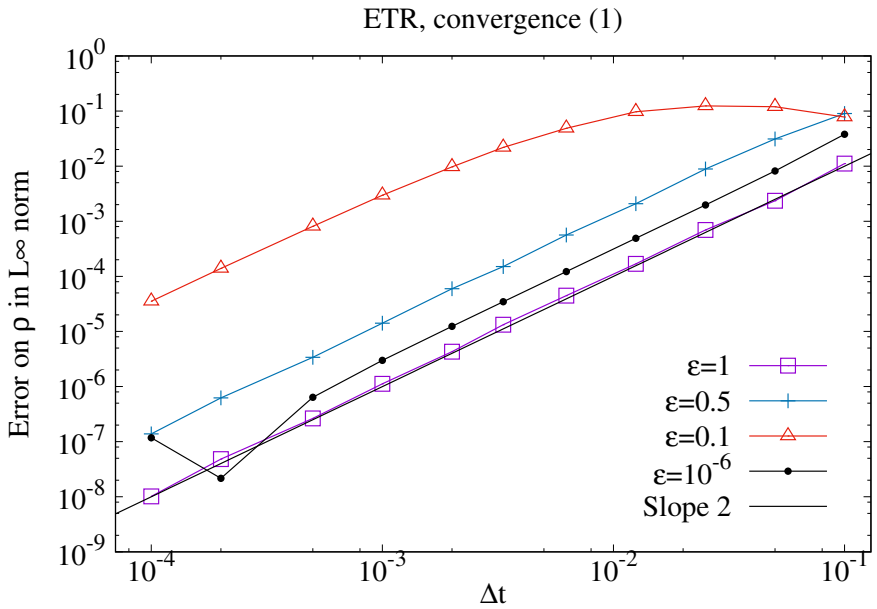
$T = 0.1$, $N_x = 64$, $N_p = 10^4$, $\Delta t = 10^{-3}$ (left),
$T = 0.1$, $N_x = 64$, $\varepsilon = 10^{-6}$, $\Delta t = 10^{-2}$ (right).





Convergence

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



Landau damping

- Initial distribution function:

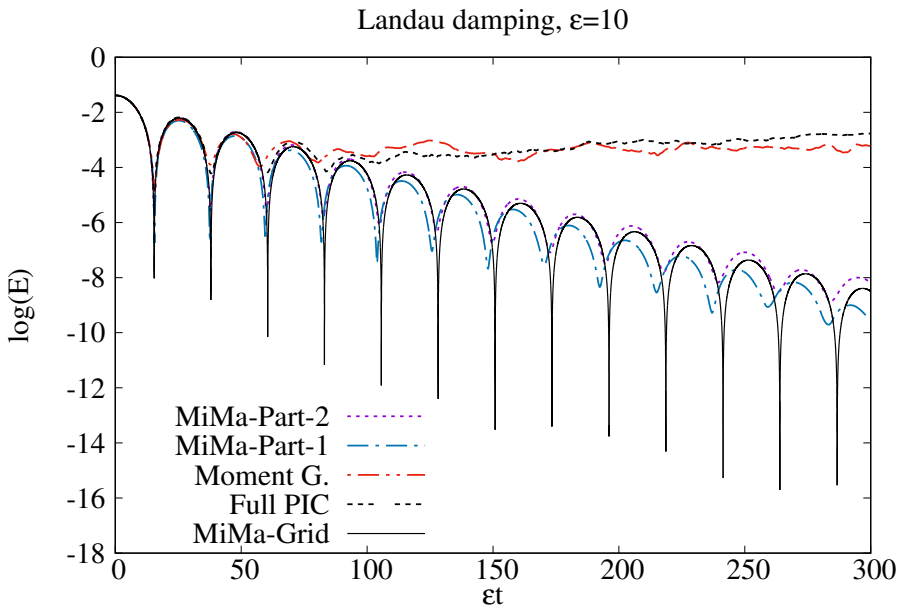
$$f\,(t=0,x,v)=\frac{1}{\sqrt{2\pi}}\exp(-\frac{v^2}{2})(1+\alpha\cos(kx)),\quad x\in[0,\frac{2\pi}{k}],v\in\mathbb{R}.$$

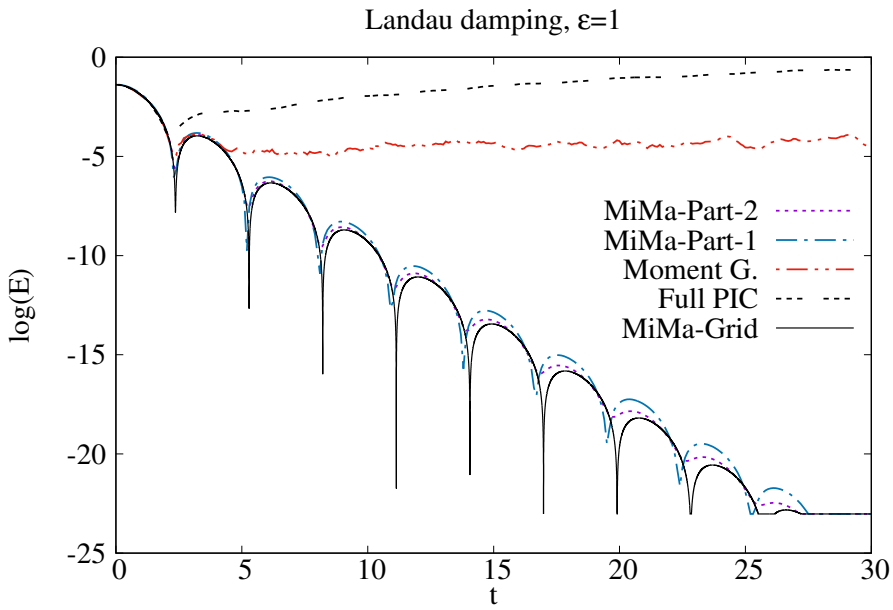
- Micro-macro initializations:

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

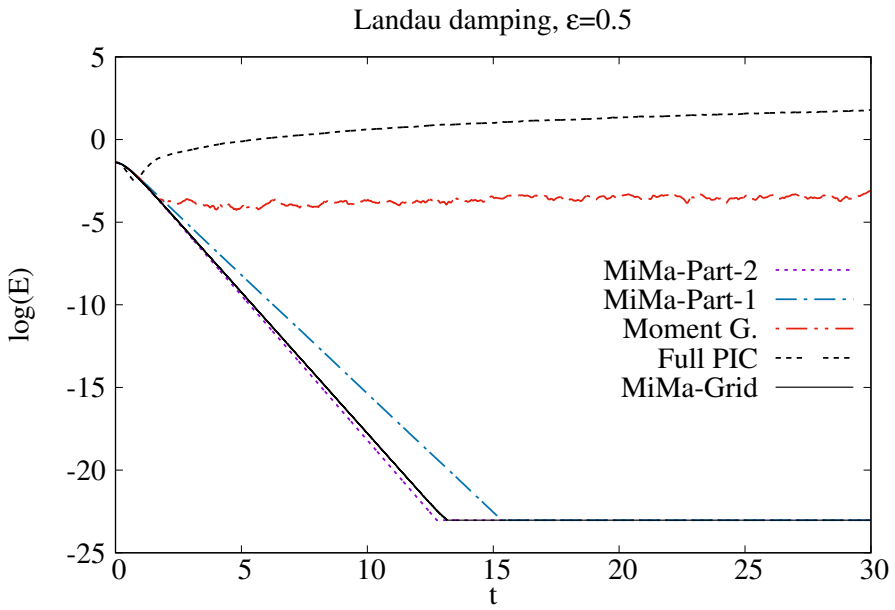
- Parameters: $\alpha=0.05$, $k=0.5$.
- Electrical energy $\mathcal{E}(t)=\sqrt{\int E(t,x)^2dx}$.

Kinetic regime,
$N_x = 128$, $N_p = 10^5$, $\Delta t = 0.1$.

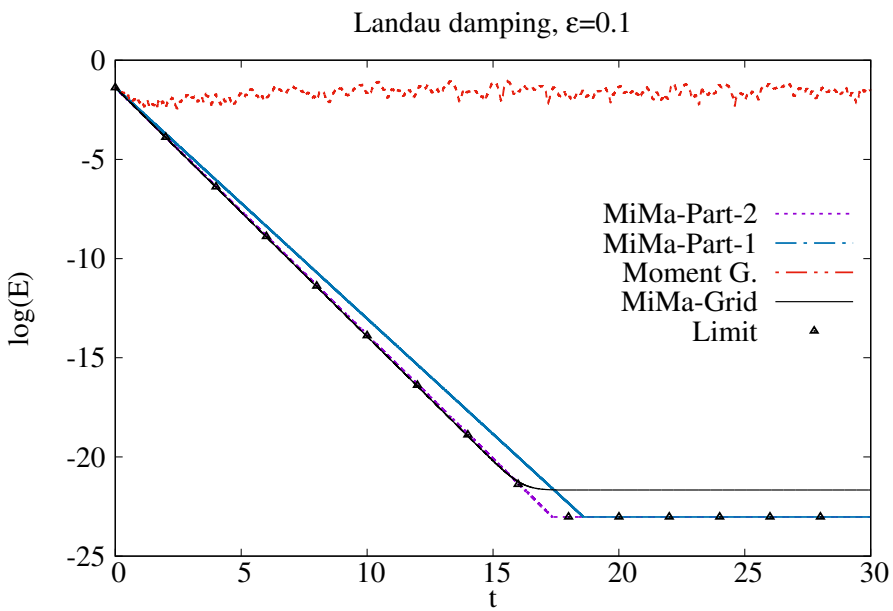


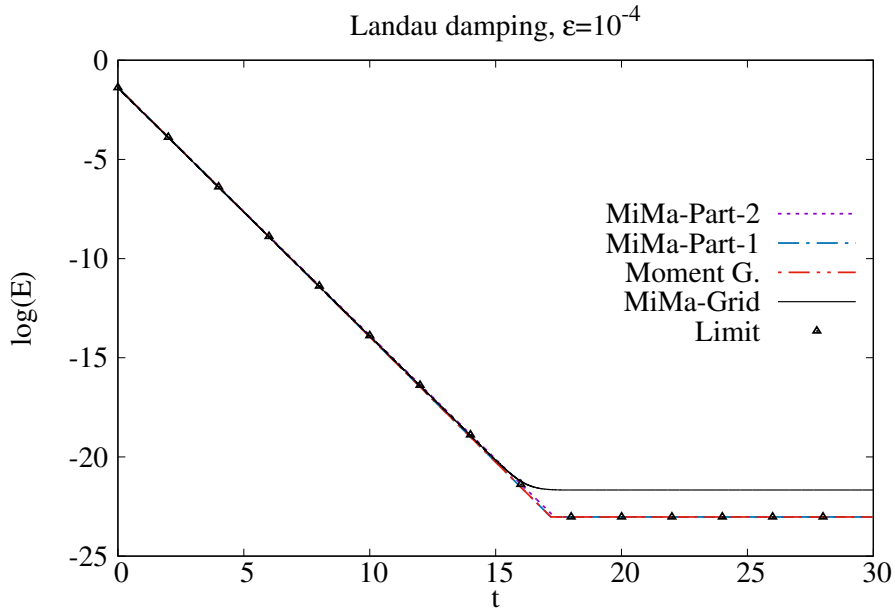


Intermediate regime,
$N_x = 256$, $N_p = 10^5$, $\Delta t = 0.01$.



Limit regime,
$N_x = 128$, $N_p = 10^4$, $\Delta t = 0.001$ (left),
$N_x = 128$, $N_p = 100$, $\Delta t = 0.01$ (right).





Two stream instability

- Initial distribution function:

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

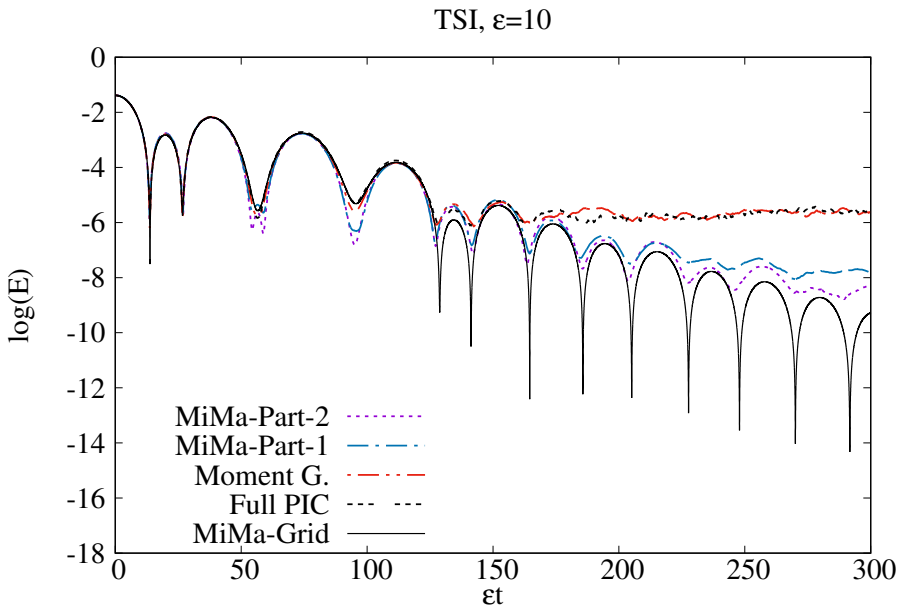
- Micro-macro initializations:

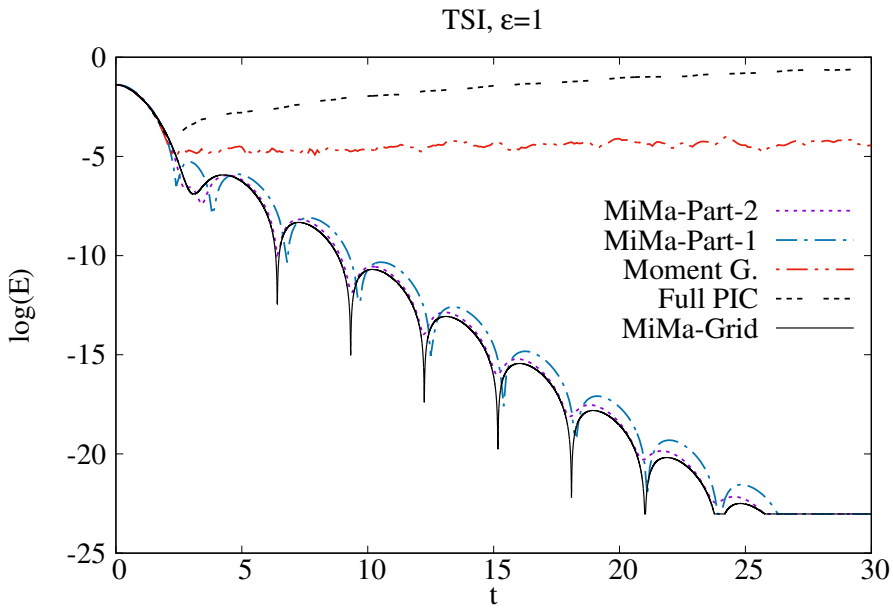
$$\rho(t=0,x)=1+\alpha\cos(kx)$$

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

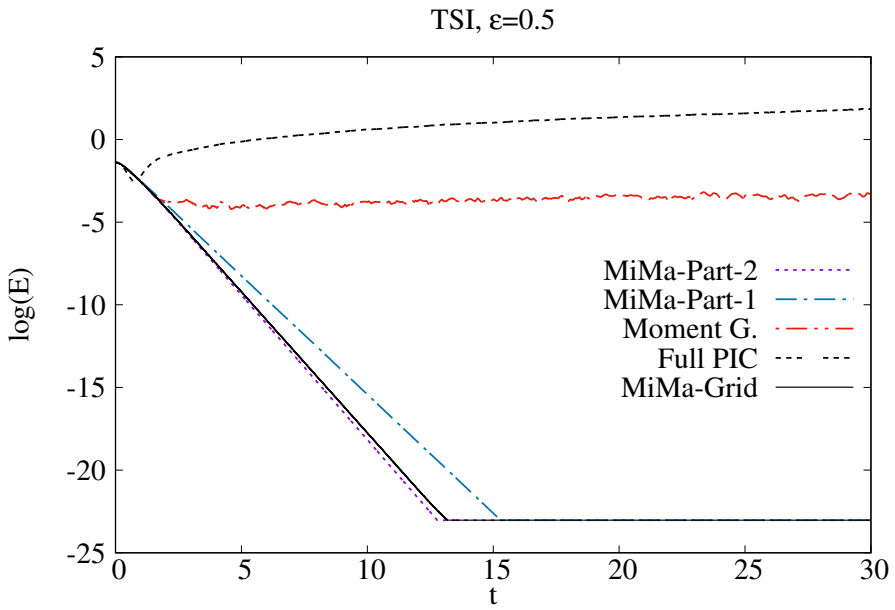
- Parameters: $\alpha=0.05$, $k=0.5$.

Kinetic regime,
$N_x = 128$, $N_p = 10^6$, $\Delta t = 0.1$ (left),
$N_x = 128$, $N_p = 10^5$, $\Delta t = 0.1$ (right).

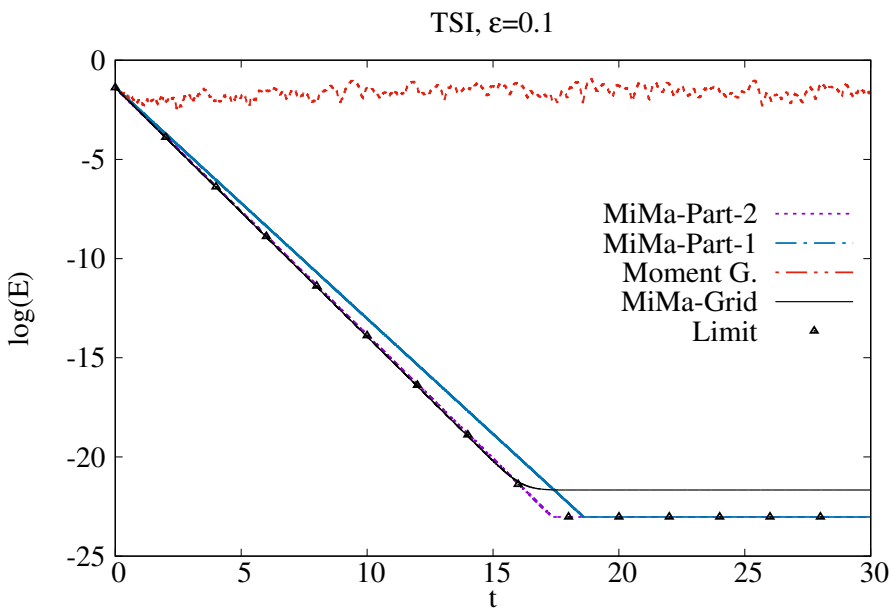


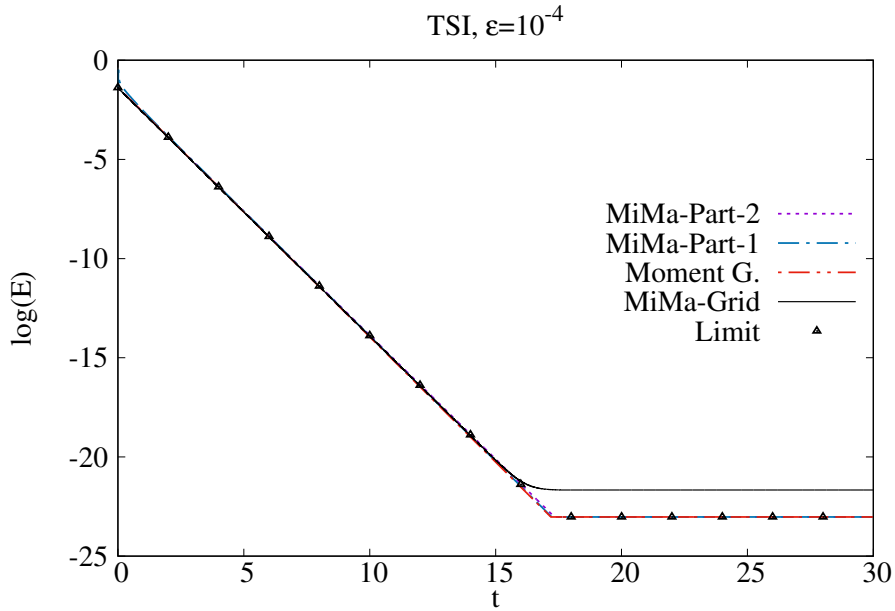


Intermediate regime,
$N_x = 256$, $N_p = 10^5$, $\Delta t = 0.01$.



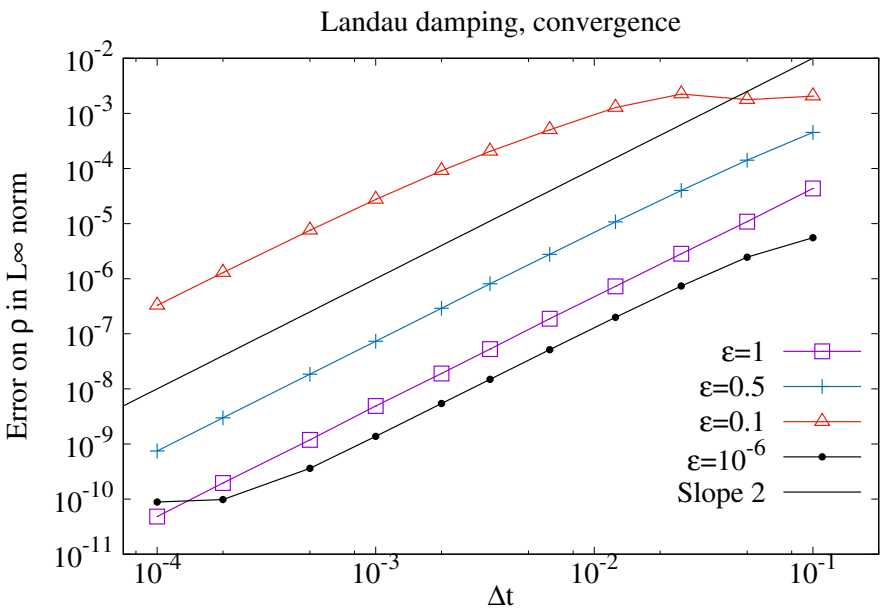
Limit regime,
$N_x = 128$, $N_p = 10^4$, $\Delta t = 0.001$ (left),
$N_x = 128$, $N_p = 100$, $\Delta t = 0.01$ (right).

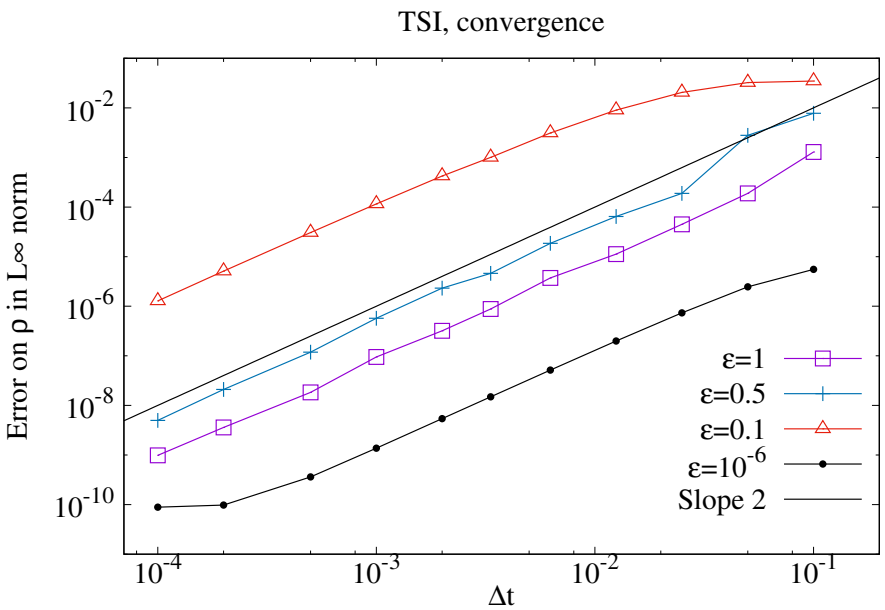




Convergence

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





Conclusions

- Diffusion (resp. drift-diffusion) limit recovered when $\varepsilon \to 0$.

  ☺ AP scheme.

- $g \to 0$ 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.

- Second-order in time.

Future works

- Monte-Carlo method for adapting the number of particles automatically.
- Models where $\varepsilon = \varepsilon(x)$.
- Extension to a Vlasov-BGK-Maxwell model: 1D in x / 2D in v.
- ...

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Thank you for your attention!