Un schéma micro-macro pour les équations cinétiques en limite de diffusion dont le coût diminue à l'approche de l'équilibre

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Workshop IPL FRATRES, 23 novembre 2018

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## Problem and objectives

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I**ntroduction** Our problem Objectives

## Numerical simulation of particle systems

We are interested in

- the numerical simulation of collisional kinetic Problems $_{\varepsilon}$ ,
- different scales: collisions parameterized by the Knudsen number ε(t, x),
- 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.

Asymptotic Preserving approach<sup>5</sup>: develop a model suitable in any region.



h: space step  $\Delta x$  or time step  $\Delta t$ .

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  $\varepsilon$ .

<sup>5</sup> Jin, SISC 1999.

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Introduction Our problem Objectives

## Our Problem $_{\varepsilon}$

Radiative transport equation in the diffusive scaling

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

•  $\mathbf{x} \in \Omega \subset \mathbb{R}^{d_x}$ ,  $\mathbf{v} \in V = \mathbb{R}^{d_v}$ ,

• charge density 
$$\rho(t, \mathbf{x}) = \int_V f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$$

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

• periodic conditions in x and initial conditions.

## Main difficulty:

 Knudsen number ε may be of order 1 or tend to 0 in the diffusive scaling. The asymptotic diffusion equation being

$$\partial_t \rho - \Delta_{\mathbf{x}} \rho = 0. \tag{2}$$

Introduction Our problem Objectives

# Objectives

• Construction of an AP scheme.

 ${\rm \bullet}\,$  Reduction of the numerical cost at the limit  $\varepsilon \rightarrow {\rm 0}.$  Tools

- Micro-macro decomposition<sup>6,7</sup> for this model. Previous work with a grid in v for the micro part<sup>8</sup>, cost was constant w.r.t.  $\varepsilon$ .
- Particle method for the micro part since few information in v is necessary at the limit<sup>9</sup>.
- Monte Carlo techniques<sup>10,11,12,13</sup>.

<sup>6</sup>Lemou, Mieussens, SIAM SISC 2008.
<sup>7</sup>Liu, Yu, CMP 2004.
<sup>8</sup>Crouseilles, Lemou, KRM 2011.
<sup>9</sup>C., Crouseilles, Lemou, CMS 2018.
<sup>10</sup>Degond, Dimarco, Pareschi, IJNMF 2011.
<sup>11</sup>Degond, Dimarco, JCP 2012.
<sup>12</sup>Crouseilles, Dimarco, Lemou, KRM 2017
<sup>13</sup>Dimarco, Pareschi, Samaey, SIAM SISC 2018.

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Derivation of the micro-macro system Reformulation of the micro-macro model



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  - Derivation of the micro-macro system
  - Reformulation of the micro-macro model

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Derivation of the micro-macro system Reformulation of the micro-macro model

## Micro-macro decomposition

- Micro-macro decomposition<sup>14,15</sup>:  $f = \rho M + g$  with g the rest.
- $\mathcal{N} = \text{Span} \{M\} = \{f = \rho M\}$  null space of the BGK operator  $Q(f) = \rho M f$ .
- $\Pi$  orthogonal projection onto  $\mathcal{N}$  :

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

<sup>14</sup>Lemou, Mieussens, SIAM JSC 2008.
 <sup>15</sup>Crouseilles, Lemou, KRM 2011.

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Derivation of the micro-macro system Reformulation of the micro-macro model

• Applying  $\Pi$  to (1)  $\Longrightarrow$  macro equation on  $\rho$ 

$$\partial_t \rho + \frac{1}{\varepsilon} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle = 0.$$
 (3)

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

$$\partial_t g + \frac{1}{\varepsilon} \left[ \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M \right] = -\frac{1}{\varepsilon^2} g. \quad (4)$$

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

$$\begin{cases} \partial_t \rho + \frac{1}{\varepsilon} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle = 0, \\ \partial_t g + \frac{1}{\varepsilon} \mathcal{F}(\rho, g) = -\frac{1}{\varepsilon^2} g, \end{cases}$$
(5)  
where  $\mathcal{F}(\rho, g) = \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M.$ 

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Derivation of the micro-macro system Reformulation of the micro-macro model

# Difficulties

- Stiff terms in the micro equation (4) on g.
- In previous works<sup>16,17</sup>, stiffest term (of order  $1/\varepsilon^2$ ) considered implicit in time  $\implies$  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.

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 <sup>&</sup>lt;sup>16</sup>Lemou, Mieussens, SIAM SISC 2008.
 <sup>17</sup>Crouseilles, Lemou, KRM 2011.

Derivation of the micro-macro system Reformulation of the micro-macro model

- Strategy of Lemou<sup>18</sup>:
  - 1. rewrite (4)  $\partial_t g + rac{1}{arepsilon} \mathcal{F}(
    ho,g) = -rac{1}{arepsilon^2} g$  as

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

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:

$$\partial_t g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathcal{F}(\rho, g).$$
(6)

No more stiff terms and consistent with the initial micro equation

 (4).

<sup>18</sup>Lemou, CRAS 2010.

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Derivation of the micro-macro system Reformulation of the micro-macro model

## New micro-macro model

The new micro-macro model writes

$$\partial_t \rho + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} g \rangle = 0, \tag{7}$$

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

with  $\mathcal{F}(\rho, g) = \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M + \mathbf{v} \cdot \nabla_{\mathbf{x}} g - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M$ .

We propose the following hybrid discretization:

- macro equation (7): Eulerian method,
- micro equation (8): Monte Carlo technique.

Monte Carlo approach Discretization of the macro part



Micro-macro model

## 3 Monte Carlo / Eulerian discretization

- Monte Carlo approach
- Discretization of the macro part

## 4 Numerical results

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Monte Carlo approach Discretization of the macro part

Discretization of the micro equation

• Model: considering at each time step  $N^n$  particles, with position  $\mathbf{x}_k^n$ , velocity  $\mathbf{v}_k^n$  and constant weight  $\omega_k$ ,  $k = 1, \ldots, N^n$ , g is approximated by<sup>19</sup>

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

• For the coupling with the macro equation, we need a grid in x. For  $d_x = 1$ , we define  $x_i = x_{\min} + i\Delta x$ ,  $i = 0, \dots, N_x - 1$ .

• How to define 
$$\omega_k$$
,  $N^n$ ,  $\mathbf{x_k^n}$ ,  $\mathbf{v_k^n}$  ?

<sup>19</sup>Crouseilles, Dimarco, Lemou, KRM 2017.

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Monte Carlo approach Discretization of the macro part

## Initialization

 Choose the characteristic weight m<sub>p</sub> or the characteristic number of particles N<sub>p</sub> necessary to sample the full distribution function f, and link them with

$$m_{p}=rac{1}{N_{p}}\int_{\mathbb{R}^{d_{x}}}\int_{\mathbb{R}^{d_{v}}}f(t=0,\mathbf{x},\mathbf{v})d\mathbf{v}d\mathbf{x}.$$

- Now, we want to sample  $g(t = 0, \mathbf{x}, \mathbf{v})$ , that has no sign.
- We impose  $\omega_k \in \{m_p, -m_p\}$ .
- For velocities, we impose  $\mathbf{v}_{\mathbf{k}}^{\mathbf{n}}$  on a cartesian grid in  $\mathbb{R}^{d_{\mathbf{v}}}$ . For  $d_{\mathbf{v}} = 1$ , it writes  $v_{k}^{n} \in \{v_{\ell}, \ \ell = 0, \dots, N_{\mathbf{v}} - 1\}$  $\forall k = 1, \dots, N^{n}$ , where  $v_{\ell} = v_{\min} + \ell \Delta v, \ \ell = 0, \dots, N_{\mathbf{v}} - 1$ .

Monte Carlo approach Discretization of the macro part

#### Let us introduce the notations in 1D...



Let us introduce the notations in 1D...

 The number of initial positive (resp. negative) particles having the velocity v<sub>k</sub> = v<sub>ℓ</sub> in the cell C<sub>i</sub> = [x<sub>i</sub>, x<sub>i+1</sub>] × ℝ is given by

$$N_{i,\ell}^{0,\pm} = \lfloor \pm \frac{\Delta x \Delta v}{m_p} g^{\pm}(t=0, \mathbf{x}_i, \mathbf{v}_\ell) \rfloor,$$

that is an approximation of

$$N_{i,\ell}^{0,\pm} = \pm \frac{1}{m_p} \int_{x_i}^{x_{i+1}} \int_{v_\ell}^{v_{\ell+1}} g^{\pm}(t=0,x,v) dv dx,$$

with  $g^{\pm} = \frac{g \pm |g|}{2}$  the positive (resp. negative) part of g.

• Positions of these  $N_{i,\ell}^{0,\pm}$  particles are taken uniformly in  $[x_i, x_{i+1}]$ .

• At time 
$$t=0$$
, we have  $N^0=\sum_i \left(\sum_\ell N^{0,+}_{i,\ell}+\sum_\ell N^{0,-}_{i,\ell}\right)$ .

Monte Carlo approach Discretization of the macro part



Monte Carlo approach Discretization of the macro part



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Monte Carlo approach Discretization of the macro part

From  $t^n$  to  $t^{n+1}$ 

Solve the micro equation (8) by Monte Carlo technique.

Splitting between the transport part

$$\partial_t g + \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathbf{v} \cdot \nabla_{\mathbf{x}} g = 0,$$

and the interaction part

$$\partial_t g = \frac{e^{-\Delta t/\varepsilon^2} - 1}{\Delta t} g - \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \left( \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho M - \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g \rangle M \right).$$

• Solve the transport part by shifting particles:

$$\frac{d\mathbf{x}_k}{dt}(t) = \varepsilon \frac{1 - e^{-\Delta t/\varepsilon^2}}{\Delta t} \mathbf{v}_k, \qquad \mathbf{x}_k^{n+1} = \mathbf{x}_k^n + \varepsilon (1 - e^{-\Delta t/\varepsilon^2}) \mathbf{v}_k^n.$$

Remark that  $\mathbf{v}_k^{n+1} = \mathbf{v}_k^n$ .

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Monte Carlo approach Discretization of the macro part

Solve interaction part by writing

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

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

• Solve interaction part by writing

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

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

In practice:

- In each cell  $C_i$ , we keep  $e^{-\Delta t/\varepsilon^2} \tilde{N}_i^n$  particles unchanged (with  $\tilde{N}_i^n$  the number of particles in  $C_i$  after the transport part) and discard the others.
- Create new particles to sample

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

as in the initialization stage. Let us denote by  $M_i^n$  the number of created particles in  $C_i$ .

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Monte Carlo approach Discretization of the macro part

Time-Diminishing Property

• At the end of the time step, we have in each cell C<sub>i</sub>

$$N_i^{n+1} = e^{-\Delta t/\varepsilon^2} \tilde{N}_i^n + M_i^n$$

particles.

- The number of particles automatically diminishes with  $\varepsilon$ .
- Reduction of the computational complexity when approaching equilibrium: Time-Diminishing Property.

Monte Carlo approach Discretization of the macro part

## Macro equation

• Equation 
$$\partial_t \rho + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} g \rangle = 0.$$

• First proposition:

$$\frac{\rho^{n+1}-\rho^n}{\Delta t}+\frac{1}{\varepsilon}\nabla_{\mathbf{x}}\cdot\langle\mathbf{v}g^{n+1}\rangle=0.$$

• Problem:  $g^{n+1}$  suffers from numerical noise inherent to particles method. This noise, amplified by  $\frac{1}{\varepsilon}$ , will damage  $\rho^{n+1}$ .

Monte Carlo approach Discretization of the macro part

Correction of the macro discretization

• Use the expression of  $g^{n+1}$  and write

$$\begin{split} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} g^{n+1} \rangle &= e^{-\Delta t/\varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle \\ &-\varepsilon (1 - e^{-\Delta t/\varepsilon^2}) \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \left( \mathbf{v} \cdot \nabla_{\mathbf{x}} \rho^n M \right) \rangle \\ &+\varepsilon (1 - e^{-\Delta t/\varepsilon^2}) \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \left( \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g} \rangle^n M \right) \rangle, \end{split}$$

or after simplifications

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

Plug it into the macro equation

$$\frac{\rho^{n+1}-\rho^n}{\Delta t}+\frac{1}{\varepsilon}e^{-\Delta t/\varepsilon^2}\langle \mathbf{v}\cdot\nabla_{\mathbf{x}}\tilde{g}^n\rangle-(1-e^{-\Delta t/\varepsilon^2})\Delta_{\mathbf{x}}\rho^n=0.$$

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

$$\frac{\rho^{n+1}-\rho^n}{\Delta t}+\frac{1}{\varepsilon}e^{-\Delta t/\varepsilon^2}\nabla_{\mathbf{x}}\cdot\langle\mathbf{v}\tilde{g}^n\rangle-(1-e^{-\Delta t/\varepsilon^2})\Delta_{\mathbf{x}}\rho^{n+1}=0.$$

• No more stiffness, the numerical noise does not damage  $\rho$ .

• As  $\varepsilon \to 0$ , implicit discretization of the diffusion equation  $\partial_t \rho - \Delta_{\mathbf{x}} \rho = 0$ .

Monte Carlo approach Discretization of the macro part

Space discretization in 2D

In 2D, we use an Alternating Direction Implicit (ADI) method<sup>20</sup>: 1) Starting from  $\rho^n$ , solve over a time step  $\Delta t$ 

$$\partial_t \rho + \frac{1}{2\varepsilon} e^{-\Delta t/\varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - (1 - e^{-\Delta t/\varepsilon^2}) \partial_{\mathbf{xx}} \rho = 0,$$

using a Crank-Nicolson time discretization to get  $\rho^*$ . 2) Starting from  $\rho^*$ , solve over a time step  $\Delta t$ 

$$\partial_t \rho + \frac{1}{2\varepsilon} e^{-\Delta t/\varepsilon^2} \langle \mathbf{v} \cdot \nabla_{\mathbf{x}} \tilde{g}^n \rangle - (1 - e^{-\Delta t/\varepsilon^2}) \partial_{yy} \rho = 0,$$

using a Crank-Nicolson time discretization to get  $\rho^{n+1}$ .

<sup>20</sup>Peaceman, Rachford, J. Soc. Indust. Appl. Math. 1955.

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Monte Carlo approach Discretization of the macro part

## Nice properties

- Only 1D systems of size  $N_x$  and  $N_y$ .
- ADI method unconditionally stable in 2D.
- Straightforward extension in 3D: a priori conditionally stable, but better extensions have been derived<sup>21</sup>.
- Right asymptotic behaviour.

<sup>21</sup>Sharma, Hammett, JCP 2011.

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Problem and objectives	Test 1 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) = 0$
Micro-macro model	Test 2 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Monte Carlo / Eulerian discretization	Test 3 - 3Dx3D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Numerical results	Test 4 - 2D×2D, $\varepsilon(\mathbf{x})$ , $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$

## Problem and objectives

Micro-macro model

## 3 Monte Carlo / Eulerian discretization

#### 4 Numerical results

- Test 1 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) = 0$
- Test 2 2Dx2D, constant arepsilon,  $m{g}(t=0, \mathbf{x}, \mathbf{v}) 
  eq 0$
- Test 3 3Dx3D, constant arepsilon,  $g(t=0,\mathbf{x},\mathbf{v})
  eq 0$
- Test 4 2Dx2D,  $\varepsilon(\mathbf{x})$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$

Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

Test 1 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) = 0$ 

Initialization:

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

with

$$\begin{split} \rho(t=0,\mathbf{x}) &= 1 + \frac{1}{2}\cos\left(\frac{x}{2}\right)\cos\left(\frac{y}{2}\right),\\ M(\mathbf{v}) &= \frac{1}{2\pi}\exp\left(-\frac{|\mathbf{v}|^2}{2}\right), \end{split}$$

so that

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

Periodic boundary conditions in space.

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Problem and objectives<br/>Micro-macro modelTest 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0<br/>Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Monte Carlo / Eulerian discretization<br/>Numerical resultsTest 4 - 2Dx2D, c(x),  $g(t = 0, x, v) \neq 0$ 

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



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Micro-Macro for kinetic eq. in the diffusive scaling

Problem and objectives	Test 1 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) = 0$
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Slices of the density 
$$\rho(T = 2, x, y = 0)$$
 and of the momentum  $\langle v_x g \rangle (T = 2, x, y = 0)$ .



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

## Kinetic regime, $\varepsilon = 1$

#### Full PIC: standard particle method on f.



Problem and objectives	Test 1 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) = 0$
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Slices of the density 
$$\rho(T = 2, x, y = 0)$$
 and of the momentum  $\langle v_x g \rangle (T = 2, x, y = 0)$ .



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

Time evolution of the number of particles



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Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$ 

#### Initialization:

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

with

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

$$\rho(t=0,\mathbf{x})=1+\frac{1}{2}\cos\left(\frac{x}{2}\right)\cos\left(\frac{y}{2}\right),$$

so that

$$g(t=0,\mathbf{x},\mathbf{v})=
ho(t=0,\mathbf{x})M(\mathbf{v})-f(t=0,\mathbf{x},\mathbf{v})
eq 0.$$

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### Integral of the distribution function in space $\int f(T, \mathbf{x}, \mathbf{v}) d\mathbf{x}$ .



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(\mathbf{x})$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$ 



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

# Integral of the perturbation in space $\int g(T = 0.2, \mathbf{x}, \mathbf{v}) d\mathbf{x}$ for different $\varepsilon$ .



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

Time evolution of the number of particles



Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ **Test 3 - 3Dx3D**, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 4 - 2Dx2D,  $\varepsilon(x)$ ,  $g(t = 0, x, v) \neq 0$ 

Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$ 

#### Initialization:

$$\begin{split} f_0(\mathbf{x}, \mathbf{v}) &= \frac{1}{2 \left(2\pi\right)^{3/2}} \left[ \exp\left(-\frac{|\mathbf{v}-u|^2}{2}\right) + \exp\left(-\frac{|\mathbf{v}+u|^2}{2}\right) \right] \rho(0, \mathbf{x}), \\ \text{with } u &= (2, 2, 2), \\ \rho(0, \mathbf{x}) &= 1 + \frac{1}{2} \cos(\frac{x}{2}) \cos(\frac{y}{2}) \cos(\frac{z}{2}), \end{split}$$

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

Problem and objectives	Test 1 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) = 0$
Micro-macro model	Test 2 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Monte Carlo / Eulerian discretization	Test 3 - 3Dx3D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Numerical results	Test 4 - 2Dx2D, $\varepsilon(\mathbf{x})$ , $g(t = 0, \mathbf{x}, \mathbf{v}) \neq 0$

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).



Problem and objectives Micro-macro model Monte Carlo / Eulerian discretization Numerical results Numeri

Top: integral of the distribution function in space  $\int_{\mathbf{x}} f(T, \mathbf{x}, \mathbf{v}) d\mathbf{x}$  for T = 0.2 and different  $\varepsilon$  (1, 0.5, 0.1).



Bottom: time evolution of the number of particles.

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Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ **Test 4 - 2Dx2D**,  $\varepsilon(\mathbf{x})$ ,  $g(t = 0, x, v) \neq 0$ 

Test 4 - 2Dx2D, 
$$\varepsilon(\mathbf{x})$$
,  $g(t=0,\mathbf{x},\mathbf{v}) 
eq 0$ 

Modified model:

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

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





Problem and objectives	Test 1 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) = 0$
Micro-macro model	Test 2 - 2Dx2D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Monte Carlo / Eulerian discretization	Test 3 - 3Dx3D, constant $\varepsilon$ , $g(t = 0, x, v) \neq 0$
Numerical results	Test 4 - 2D×2D $\varepsilon(\mathbf{x})$ $\varphi(t = 0, \mathbf{x}, \mathbf{y}) \neq 0$

Initialization:

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

with

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

$$ho(t=0,\mathbf{x})=1+rac{1}{2}\cos\left(rac{x}{2}
ight)\cos\left(rac{y}{2}
ight).$$

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



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Test 1 - 2Dx2D, constant  $\varepsilon$ , g(t = 0, x, v) = 0Test 2 - 2Dx2D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ Test 3 - 3Dx3D, constant  $\varepsilon$ ,  $g(t = 0, x, v) \neq 0$ **Test 4 - 2Dx2D**,  $\varepsilon(\mathbf{x})$ ,  $g(t = 0, x, v) \neq 0$ 

## Time-Diminishing Property

Top: position of the particles in x. Left: at T = 0; right: at T = 1.



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## Conclusions

- Right asymptotic behaviour.
- Computational cost diminishes 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.

## Possible extensions

- More 3D-3D testcases, more physical relevance.
- Boltzmann operator.
- Second-order in time scheme.
- Add an electromagnetic field  $\Rightarrow v_k$  no constant anymore.

# Merci pour votre attention !



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