Monte Carlo methods for kinetic equations

Giacomo Dimarco

Department of Mathematics and Computer Sciene &
Center for Modeling Computing and Statistics CMCS
University of Ferrara, Italy

Main collaborators: L. Pareschi (Ferrara, Italy), N. Crouseilles (INRIA, France),
M. Lemou (CNRS, France), A. Crestetto (University of Nantes, France)

Workshop PRIN:
Innovative numerical methods for evolutionary partial differential equations and applications
Catania, February 20-22, 2023

Outline

Outline

Monte Carlo integration

Consider the simple integral

$$I[f] = \int_{[0,1]^d} f(x)dx, \quad d \geq 1,$$

if x is a random vector uniformly distributed in $[0,1]^d$ we have $I[f] = E[f(x)]$, where $E[\cdot]$ denotes the *expectation*. If $\{x_n\}$ is a sequence of pseudo-random vectors uniform in $[0,1]^d$ then

$$I_N[f] = \frac{1}{N}\sum_{n=1}^{N} f(x_n), \quad E[I_N[f]] = I[f].$$

For the law of large numbers it converges in probability[1]

$$\lim_{N\to\infty} I_N[f] = I[f],$$

and

$$I[f] - I_N[f] \approx \sigma_f N^{-1/2} w, \quad E[(I[f] - I_N[f])^2] = \sigma_f N^{-1/2},$$

where σ_f^2 is the variance of f and w is a normal random variable. Note that there is no dependence on the dimension.
Remark: The convergence rate for a deterministic grid based quadrature is $O(N^{-k/d})$ for an order k method. Thus Monte Carlo is "better" if $k/d \leq 1/2$.

[1] W.Feller '71, R.E.Caflisch '98

Reconstruction

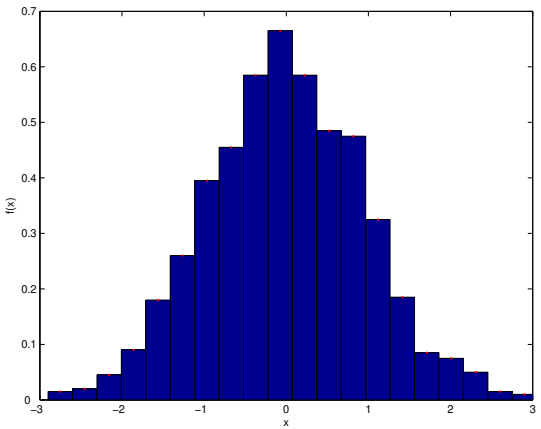
Given a set of N samples $\xi_1, \xi_2, \ldots, \xi_N$ the probability density is defined by

$$f(x) = \frac{1}{N} \sum_{k=1}^{N} \delta(x - \xi_k).$$

The simplest method, which produces a piecewise constant reconstruction, is based on evaluating the histogram of the samples at the cell centers of a grid

$$f(x_{j+1/2}) = \frac{1}{N} \sum_{k=1}^{N} \Psi(\xi_k - x_{j+1/2}), \quad j = \ldots, -2, -1, 0, 1, 2, \ldots$$

where $\Psi(x) = 1/\Delta x$ if $|x| \leq \Delta x/2$ and $\Psi(x) = 0$ elsewhere.



The kinetic model

In the Boltzmann description of RGD, the density $f = f(x, v, t)$ of particles follows the equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f), \quad x \in \Omega \subset \mathbb{R}^3, v \in \mathbb{R}^3,$$

The parameter $\varepsilon > 0$ is called *Knudsen number* and it is proportional to the mean free path between collisions. The bilinear *collisional operator* $Q(f, f)$ is given by

$$Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(|v - v_*|, \omega)(f(v')f(v'_*) - f(v)f(v_*))dv_* d\omega,$$

where ω is a vector of the unitary sphere $S^2 \subset \mathbb{R}^3$ and for simplicity the dependence of f on x and t has been omitted.
The *collisional velocities* (v', v'_*) are given by the relations

$$v' = \frac{1}{2}(v + v_* + |q|\omega), \quad v'_* = \frac{1}{2}(v + v_* + |q|\omega),$$

where $q = v - v_*$ is the relative velocity.

Collision details

The kernel B characterizes the details of the binary interactions. The classical *Variable Hard Spheres* (VHS) model used for RGD simulations is

$$B(|q|, \omega) = K|q|^{\alpha}, \quad 0 \leq \alpha < 1,$$

where K is a positive constant. The case $\alpha = 0$ corresponds to a *Maxwellian gas*, while $\alpha = 1$ is called a *Hard Sphere Gas*.
The collisional operator is such that the *H-Theorem* holds

$$\int_{\mathbb{R}^3} Q(f, f) \log(f) dv \leq 0.$$

This condition implies that each function f in equilibrium (i.e. $Q(f, f) = 0$) has locally the form of a *Maxwellian distribution*

$$M(\rho, u, T)(v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|u - v|^2}{2T}\right),$$

where ρ, u, T are the *density*, the *mean velocity* and the gas *temperature*

$$\rho = \int_{\mathbb{R}^3} f dv, \quad \rho u = \int_{\mathbb{R}^3} f v dv, \quad T = \frac{1}{3\rho} \int_{\mathbb{R}^3} (v - u)^2 f dv.$$

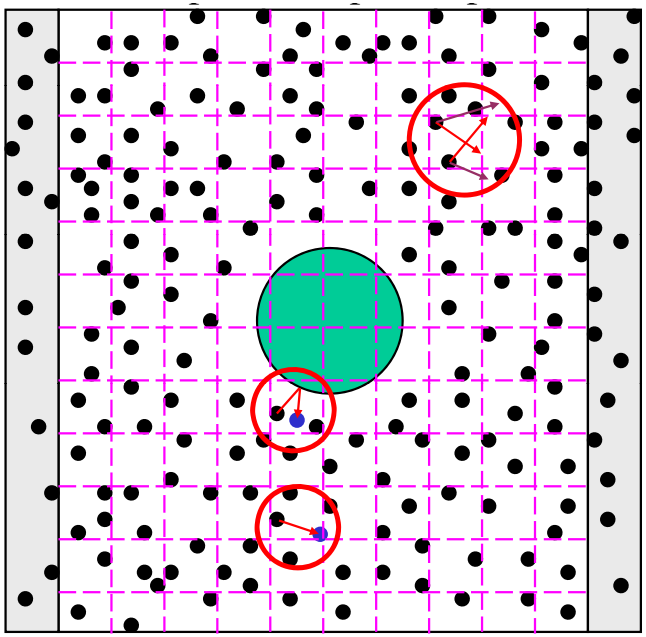
Hydrodynamic equations

- If we consider the Boltzmann equation and multiply it for the elementary *collisional invariants* $1, v, |v|^2$ and integrate in v we obtain a system of conservation laws corresponding to conservation of mass, momentum and energy.
- Clearly the differential system is not closed since it involves higher order moments of the function f.
- Formally as $\varepsilon \to 0$ the function f is locally replaced by a Maxwellian. In this case it is possible to compute f from its low order moments thus obtaining to leading order the closed system of *compressible Euler equations*

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i) = 0, \\
\frac{\partial}{\partial t}(\rho u_j) &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i u_j) + \frac{\partial}{\partial x_j} p = 0, \quad j = 1, 2, 3 \\
\frac{\partial E}{\partial t} &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(E u_i + p u_i) = 0,
\end{aligned}$$

where $p = \rho T$.

DSMC basics



- Initialize system with particles (x_i, v_i), $i = 1, \ldots, N$ (*sampling*).
- Loop over time steps of size Δt.
- Create particles at open boundaries.
- Move all the particles $x_i = x_i + v_i \Delta t$ (*transport step)*.
- Process any interactions of particle and boundaries (*Maxwell's b.c.*).
- Sort particles into cells.
- Select and execute random collisions (*collision step*).
- Compute average statistical values.

DSMC for the collision step

- We will describe the *classical DSMC methods* due to Nanbu in the case of spatially homogeneous Boltzmann equations[2].
- We assume that the kinetic equations can be written in the form

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon}[P(f,f) - \mu f],$$

where $\mu > 0$ is a constant and $P(f,f)$ is a non negative bilinear operator s.t.

$$\frac{1}{\mu}\int_{\mathbb{R}} P(f,f)(v)\phi(v)\,dv = \int_{\mathbb{R}} f(v)\phi(v)\,dv, \quad \phi(v) = 1, v, v^2.$$

- For the BGK equation $P(f,f) = \mu M(\rho,u,T)(v)$, for the Boltzmann equation in the Maxwellian case

$$P(f,f) = Q^+(f,f)(v) = \int_{\mathbb{R}^3}\int_{S^2} b_0(\cos\theta) f(v') f(v'_*)\,d\omega\,dv_*,$$

and $\mu = 4\pi\rho$.

- The case of general VHS kernels is different and it will not discussed.

[2] G.Bird '63, K.Nanbu '83

Nanbu's method (DSMC no time counter)

- We assume that f is a probability density, i.e. $\rho = \int_{-\infty}^{+\infty} f(v,t)\,dv = 1$.
- Consider a time interval $[0, t_{\max}]$, and discretize it in n_{TOT} intervals of size Δt.
- Let $f^n(v)$ be an approximation of $f(v, n\Delta t)$. The forward Euler scheme writes

$$f^{n+1} = \left(1 - \frac{\mu \Delta t}{\epsilon}\right) f^n + \frac{\mu \Delta t}{\epsilon} \frac{P(f^n, f^n)}{\mu}.$$

- Clearly if f^n is a probability density both $P(f^n, f^n)/\mu$ and f^{n+1} are probability densities. Thus the equation has the following probabilistic interpretation.
- *Physical level*: a particle with velocity v_i will not collide with probability $(1 - \mu\Delta t/\epsilon)$, and it will collide with probability $\mu\Delta t/\epsilon$, according to the collision law described by $P(f^n, f^n)(v)$.
- *Monte Carlo level*: to sample v_i from f^{n+1} with probability $(1 - \mu\Delta t/\epsilon)$ we sample from f^n, and with probability $\mu\Delta t/\epsilon$ we sample from $P(f^n, f^n)(v)/\mu$.

Note that $\Delta t \leq \epsilon/\mu$ to have the probabilistic interpretation. For the BGK model the algorithm is straightforward since sampling from $P(f,f)/\mu$ is simply sampling from a Maxwellian.

Outline

Decomposition of the collision operator

Let us rewrite the collision step as

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon}\left[P(f,f) - \mu f\right],$$

where $P(f,f) = Q(f,f) + \mu f$ and $\mu > 0$ is such that $P(f,f) \geq 0$.
By construction we have

$$\frac{1}{\mu}\int_{\mathbb{R}^3} \phi(v) P(f,f)\, dv = \int_{\mathbb{R}^3} \phi(v) f\, dv.$$

Thus $P(f,f)/\mu$ is a density function and we take the *micro-macro* decomposition

$$P(f,f)/\mu = M + g.$$

Inserting the above decomposition into the collision step leads to

$$\partial_t f = \frac{\mu}{\varepsilon} g + \frac{\mu}{\varepsilon}(M - f) = \frac{\mu}{\varepsilon}\left(\frac{P(f,f)}{\mu} - M\right) + \frac{\mu}{\varepsilon}(M - f).$$

Exponential Runge-Kutta methods

Let us consider a system of ODEs of the type

$$y' = G(y) + \lambda(E - y), \quad y(t_0) = y_0,$$

where $G(y) = 0 \Leftrightarrow y = E$ and $E' = 0$.
The general form of an explicit exponential Runge-Kutta method is

Exponential Runge-Kutta

$$\begin{aligned} Y^{(i)} &= e^{-c_i\lambda\Delta t} y_n + (1 - e^{-c_i\lambda\Delta t}) E_n + \Delta t \sum_{j=1}^{i-1} A_{ij}(\lambda\Delta t) G(Y^{(j)}),\ i = 1, \dots, \nu \\ y_{n+1} &= e^{-\lambda\Delta t} y_n + (1 - e^{-\lambda\Delta t}) E_n + \Delta t \sum_{i=1}^{\nu} W_i(\lambda\Delta t) G(Y^{(i)}), \end{aligned}$$

where $c_i \geq 0$, and the coefficients A_{ij} and the weights W_i are such that

$$A_{ij}(0) = a_{ij}, \quad W_i(0) = w_i, \quad i, j = 1, \dots, \nu$$

with a_{ij} and w_i given by a standard explicit Runge-Kutta method called the *underlying method*.

IF-RK methods

- The two most popular approaches to get exponential schemes are the integrating factor (IF) and the exponential time differencing (ETD) methods.
- For the so-called *Integrating Factor* methods we have

$$\begin{aligned} A_{ij}(\lambda\Delta t) &= a_{ij}e^{-(c_i-c_j)\lambda\Delta t}, \quad i,j=1,\dots,\nu, \quad j>i \\ W_i(\lambda\Delta t) &= w_i e^{-(1-c_i)\lambda\Delta t}, \quad i=1,\dots,\nu. \end{aligned}$$

- The underlying Runge-Kutta schemes are characterized by the matrice $A=(a_{ij})$ such that the resulting scheme is explicit and the coefficient vector $w=(w_1,..,w_\nu)^T$. The schemes described can be represented by the so-called Butcher tableau

c	A
	ω^T

where the coefficients c used for the treatment of non autonomous systems, are given by the usual relation $c_i=\sum_{j=1}^{i} a_{ij}$

Exponential schemes for the Boltzmann equation

- When applied to the Boltzmann equation the first order IF-RK scheme gives

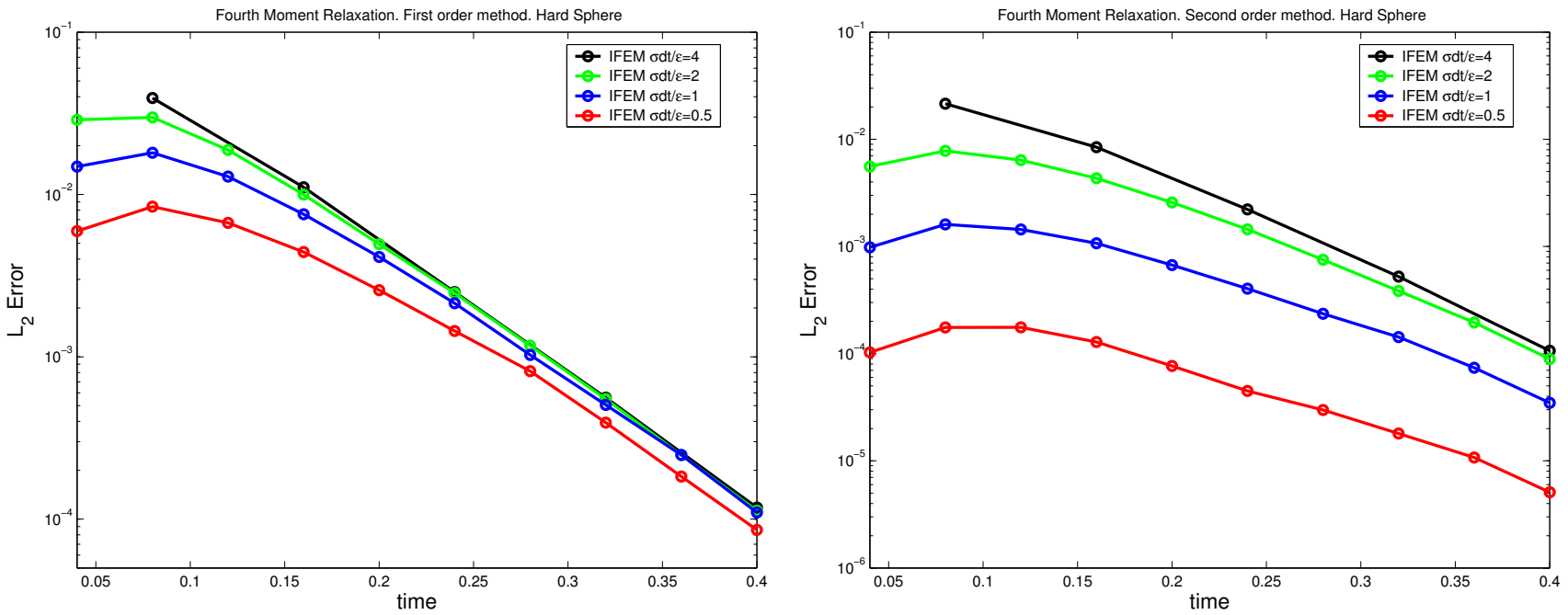
$$f^{n+1} = e^{-\mu\Delta t/\varepsilon} f^n + \frac{\mu\Delta t}{\varepsilon} e^{-\mu\Delta t/\varepsilon} \frac{P(f^n, f^n)}{\mu} + \left(1 - e^{-\mu\Delta t/\varepsilon} - \frac{\mu\Delta t}{\varepsilon} e^{-\mu\Delta t/\varepsilon}\right) M.$$

- Note that again the scheme is a convex combination of particle densities independently of $\Delta t/\varepsilon$ and satisfies conservations, nonnegativity and asymptotic preservation.
- Higher order schemes can be constructed in the same way. For instance a second order IF-RK scheme based on midpoint is given by

$$\begin{aligned} f^* &= e^{-\frac{\mu\Delta t}{2\varepsilon}} f^n + \frac{\mu\Delta t}{2\varepsilon} e^{-\frac{\mu\Delta t}{2\varepsilon}} \frac{P(f^n, f^n)}{\mu} + \left(1 - e^{-\frac{\mu\Delta t}{2\varepsilon}} - \frac{\mu\Delta t}{2\varepsilon} e^{-\frac{\mu\Delta t}{2\varepsilon}}\right) M \\ f^{n+1} &= e^{-\frac{\mu\Delta t}{\varepsilon}} f^n + \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{2\varepsilon}} \frac{P(f^*, f^*)}{\mu} + \left(1 - e^{-\frac{\mu\Delta t}{\varepsilon}} - \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{2\varepsilon}}\right) M. \end{aligned}$$

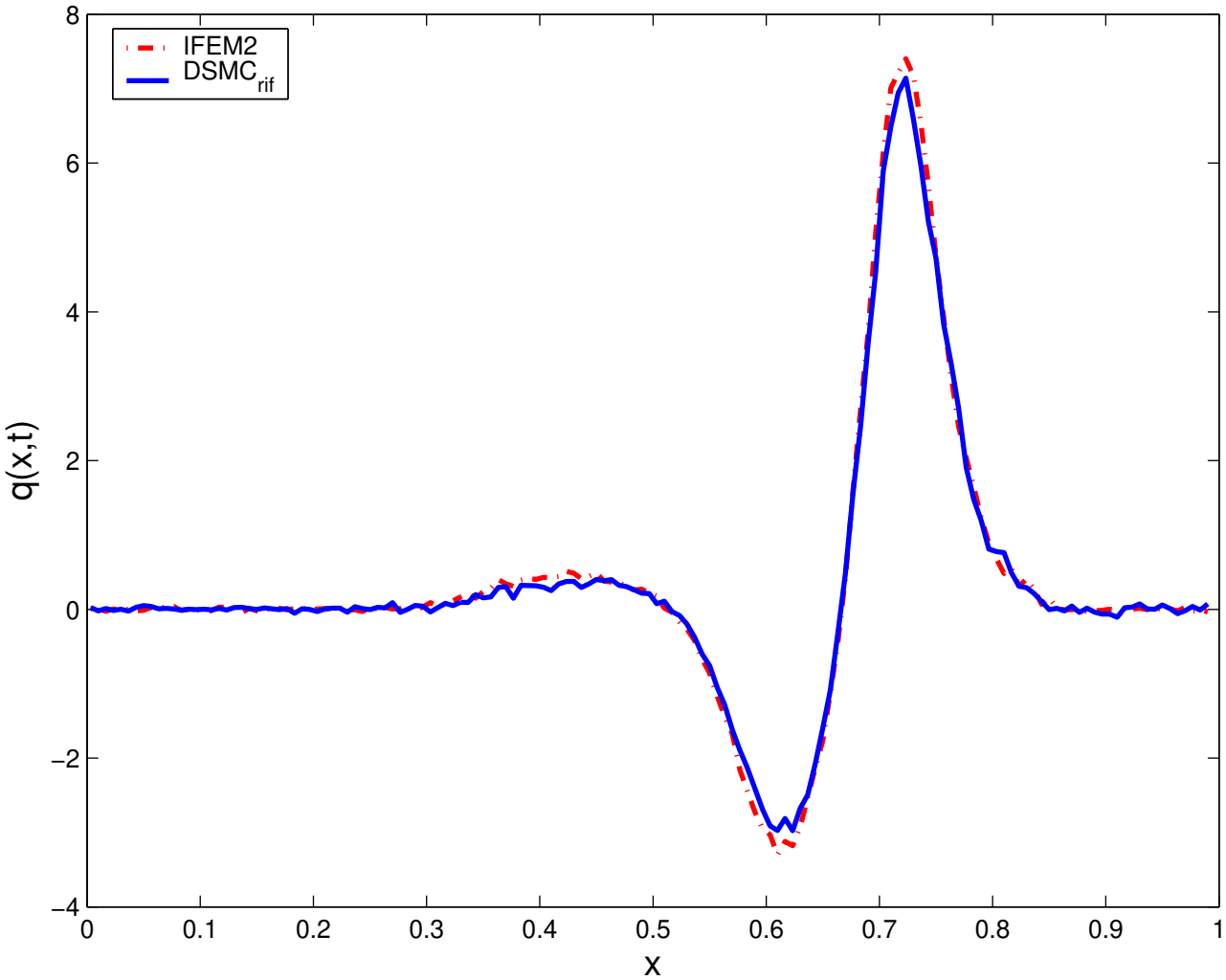
- It is easy to verify that even this scheme is convex independently of $\Delta t/\varepsilon$. So it satisfies conservations, nonnegativity and asymptotic preservation.

Boltzmann equation: 4th order moment



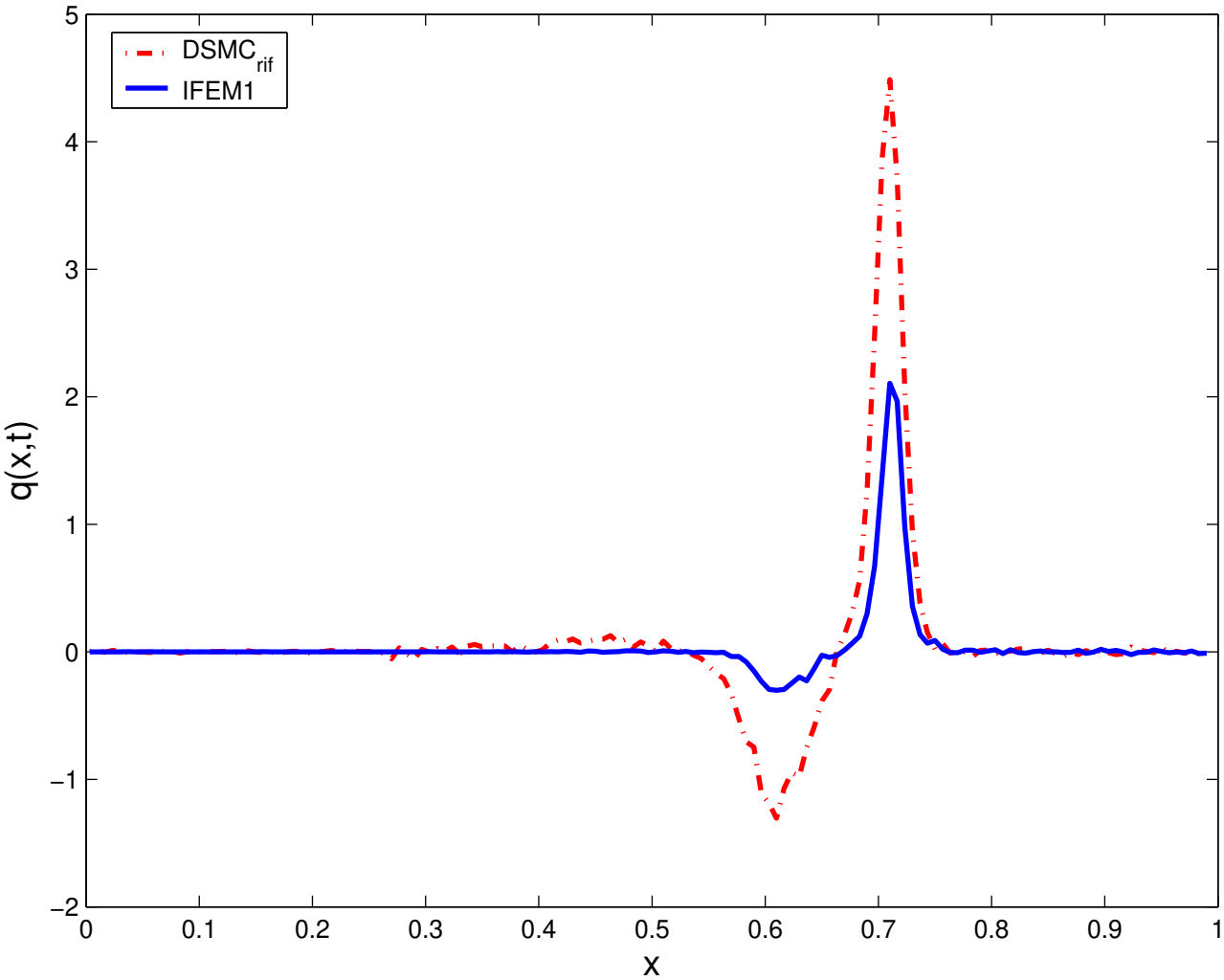
L2-error for first and second order IF scheme.

Sod test: heat flux for $\varepsilon = 5 \times 10^{-4}$



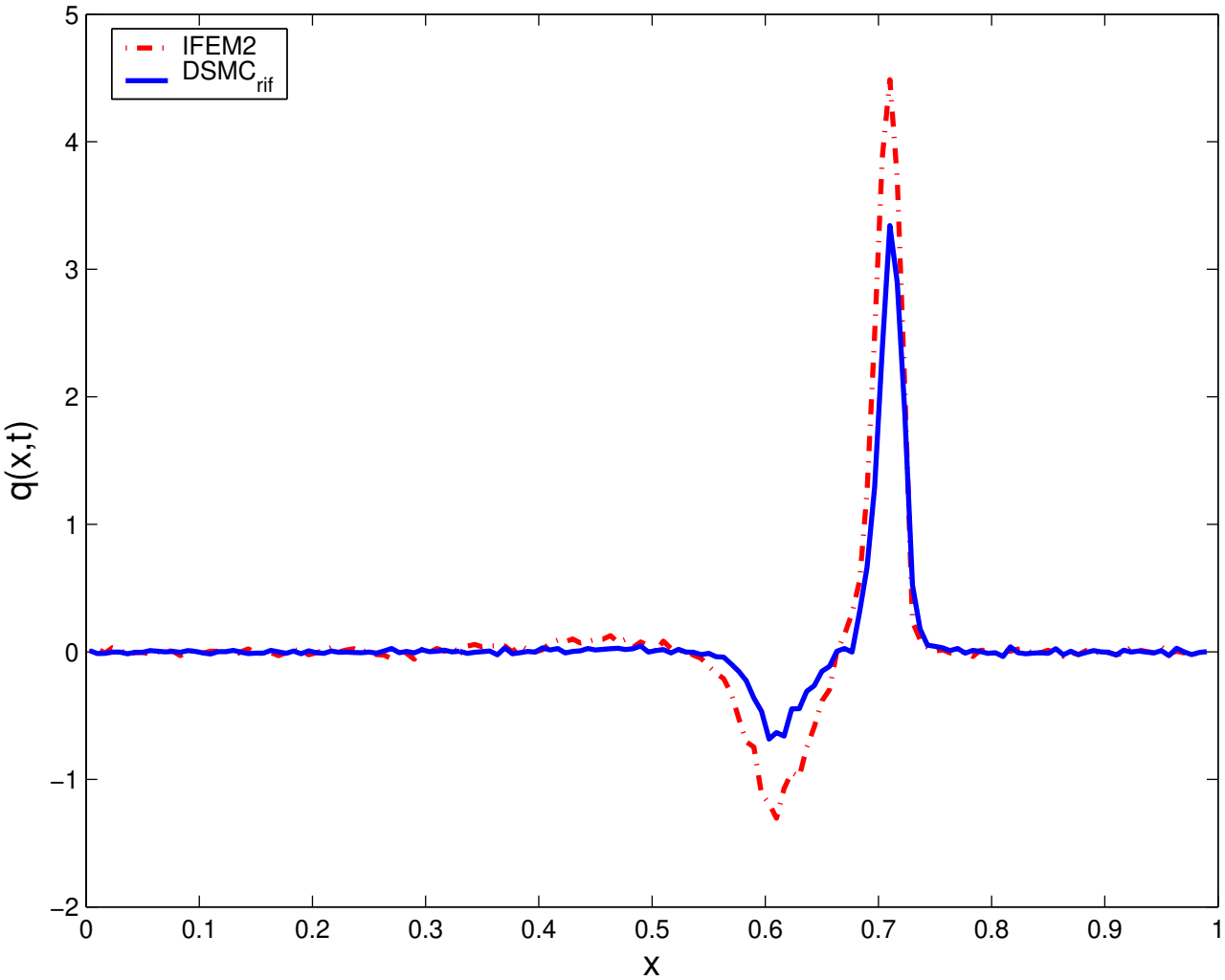
Heat flux at $t = 0.05$ for Strang splitting and IF-2 with $\Delta t/\Delta t_E = 2$.

Sod test: heat flux for $\varepsilon = 10^{-4}$



Heat flux at $t = 0.05$ for simple splitting and IF-1 with $\Delta t/\Delta t_E = 10$.

Sod test: heat flux for $\varepsilon = 10^{-4}$



Heat flux at $t = 0.05$ for Strang splitting and IF-2 with $\Delta t/\Delta t_E = 10$.

Outline

Derivation of the micro-macro model

- The distribution function f is rewritten accordingly to the following decomposition

$$f = M + g, \quad \text{with } M = \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|v-u|^2}{2T}\right).$$

- Now, since $M[U]$ and f shares the same first three moments, we have

$$U(t,x) = \int_{\mathbb{R}^d} m(v) f(t,x,v) dv = \int_{\mathbb{R}^d} m(v) M(t,x,v) dv,$$

- Then the kinetic equation writes

$$\partial_t M + \partial_t g + v \cdot \nabla_x M + v \cdot \nabla_x g = -\frac{\nu}{\varepsilon} g.$$

- Denoting by Π_M the orthogonal projection in $\mathcal{N}(L_Q) = \text{Span}\left\{M, vM, |v|^2 M\right\}$ the null space of the operator Q

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

The micro-macro model for the Navier-Stokes equation

- The micro-macro model for the unknowns (g, U), equivalent to the kinetic BGK equation, can be written as follows with $\mathscr{T}\phi = v \cdot \nabla_x \phi$

$$\partial_t g + (I - \Pi_M)\mathscr{T} g = \frac{\nu}{\varepsilon}\left[-g - \frac{\varepsilon}{\nu}(I - \Pi_M)\mathscr{T} M\right],$$
$$\partial_t U + \nabla_x \cdot F(U) + \nabla_x \cdot \langle v m(v) g \rangle = 0,$$

- Let us consider now a second decomposition

$$f = f_0 + \varepsilon f_1 + g, \text{ with } f_0 = M, \text{ and } f_1 = -(I - \Pi_M)\mathscr{T} M.$$

- Injecting the above decomposition into the kinetic equation and applying the projection operator Π_M gives

$$\partial_t M + \Pi_M(v \cdot \nabla_x M) + \Pi_M(v \cdot \nabla_x (f_1 + g)) = 0$$

- This is equivalent to the following equation on the moments U

$$\partial_t U + \nabla_x \cdot F(U) + \varepsilon \mathscr{D} U + \nabla_x \cdot \langle v m(v) g \rangle = 0,$$

with $\mathscr{D} U = \nabla_x \cdot \langle v m(v)(I - \Pi_M)\mathscr{T} M \rangle$.

A new Time Diminishing Asymptotic Preserving class of methods for kinetic equations II

With the previous decomposition the microscopic part reads

$$\partial_t g + (I - \Pi_M)(v \cdot \nabla_x g) = -\frac{\nu}{\varepsilon}(g + \varepsilon(I - \Pi_M)(\partial_t f_1 + v \cdot \nabla_x f_1)).$$

The scheme can be summarized by the following steps, at each time step t^n

- Solve the kinetic equation for the perturbation part using a particle method. This will give the perturbation values at time $(n+1)$.
- Solve the macroscopic part with a finite volume method where particles are used to evaluate the perturbation terms. This gives the moments value U^{n+1}.
- Modify the perturbation g at time $n+1$ to ensure the zero-moments property at the particle level.
- Eliminate particles with same speed and different sign in order to reduce the global computational cost.

Solving the kinetic equation for the perturbation

We consider the solution in a time interval $[0, \Delta t]$ by an operator splitting between transport

$$\partial_t g + \mathscr{T} g = 0,$$

and the source terms respectively for the first and the second decompositions

$$\partial_t g = -\frac{\nu g}{\varepsilon} + \Pi_M \mathscr{T} g - (I - \Pi_M)\mathscr{T} M,$$

$$\partial_t g = \Pi_M \mathscr{T} g - \frac{\nu}{\varepsilon}(g + \varepsilon(I - \Pi_M)(\partial_t f_1 + v \cdot \nabla_x f_1)).$$

The distribution g is approximated by a finite set of N particles

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

where $x_k(t)$ represents the position, $v_k(t)$ the velocity and $\omega_k = \pm m_p$ the weight of each particle.

Solving the kinetic equation II

The transport step solves the characteristic equations, which corresponds to push the particles: $x_k^{n+1} = x_k^n + \Delta t\, v_k^n$. The second part reads, for the first decomposition

$$g^{n+1} = g^* - \frac{\Delta t \nu}{\varepsilon} g^{n+1} + \Delta t \left[\Pi_M \mathscr{T} g^n - (I - \Pi_M) \mathscr{T} M^n \right],$$

which gives

$$g^{n+1} = \frac{\varepsilon/\nu}{\varepsilon/\nu + \Delta t} g^* + \frac{\Delta t}{\varepsilon/\nu + \Delta t} \mathscr{P}[g^n, M^n].$$

and for the second decomposition

$$g^{n+1} = g^* - \frac{\Delta t \nu}{\varepsilon} g^{n+1} + \Delta t \left[\Pi_M \mathscr{T} g^n - \varepsilon (I - \Pi_M)(\partial_t f_1 + v \cdot \nabla_x f_1) \right],$$

which gives

$$g^{n+1} = \frac{\varepsilon/\nu}{\varepsilon/\nu + \Delta t} g^* + \frac{\Delta t}{\varepsilon/\nu + \Delta t} \mathscr{P}_1[g^n, f_1^n].$$

where g^* represents the solution after the transport step.

Monte Carlo vs Time Diminishing scheme : density profile

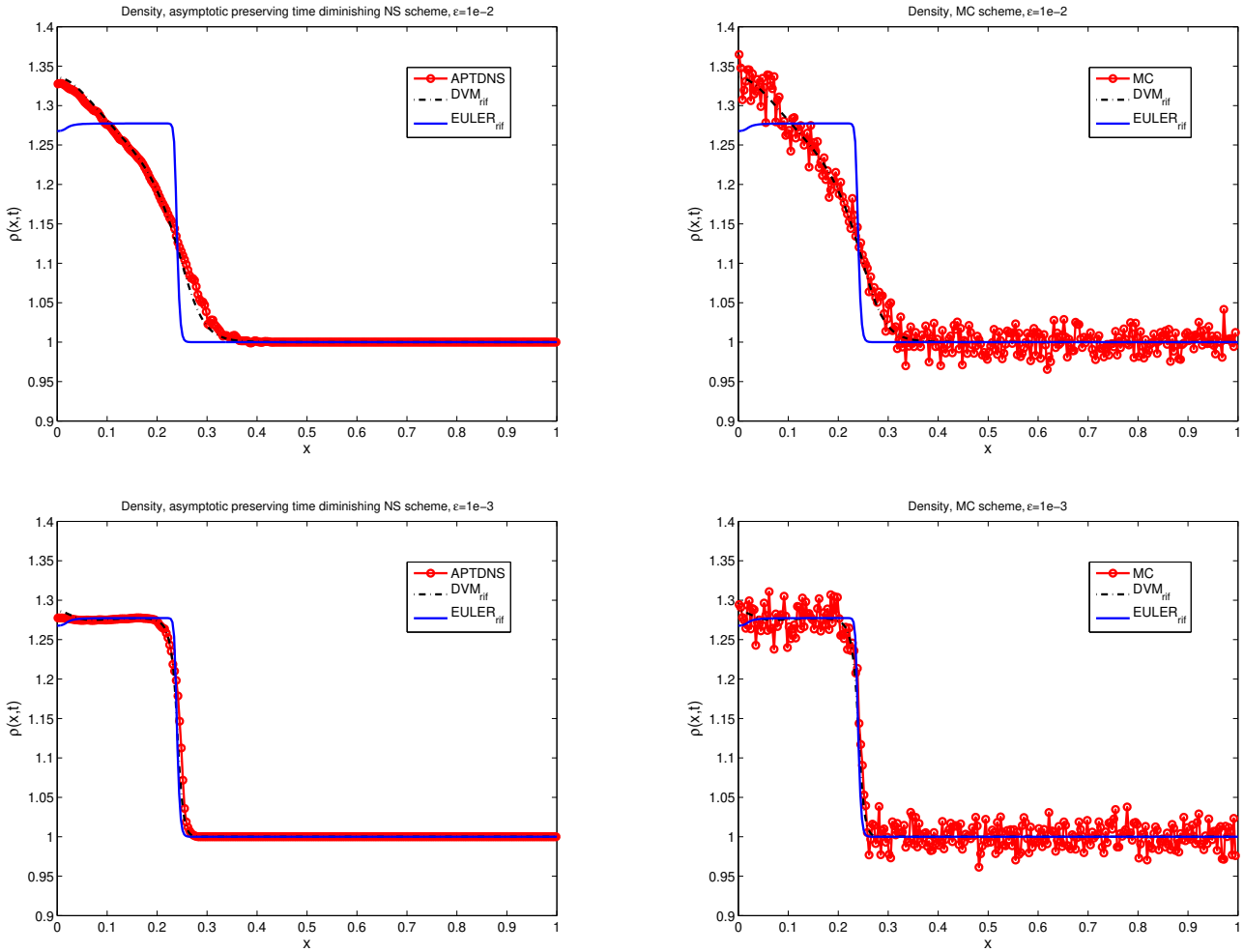
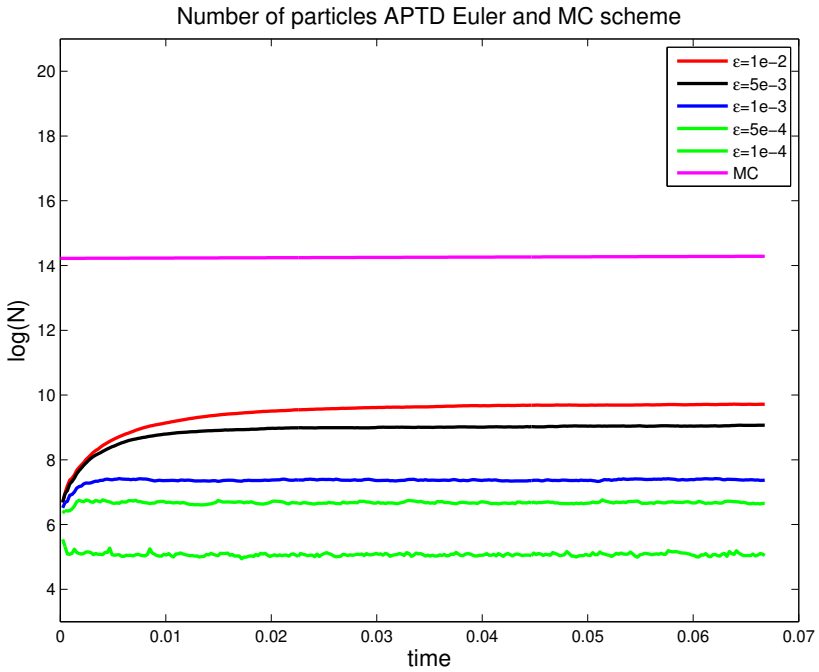
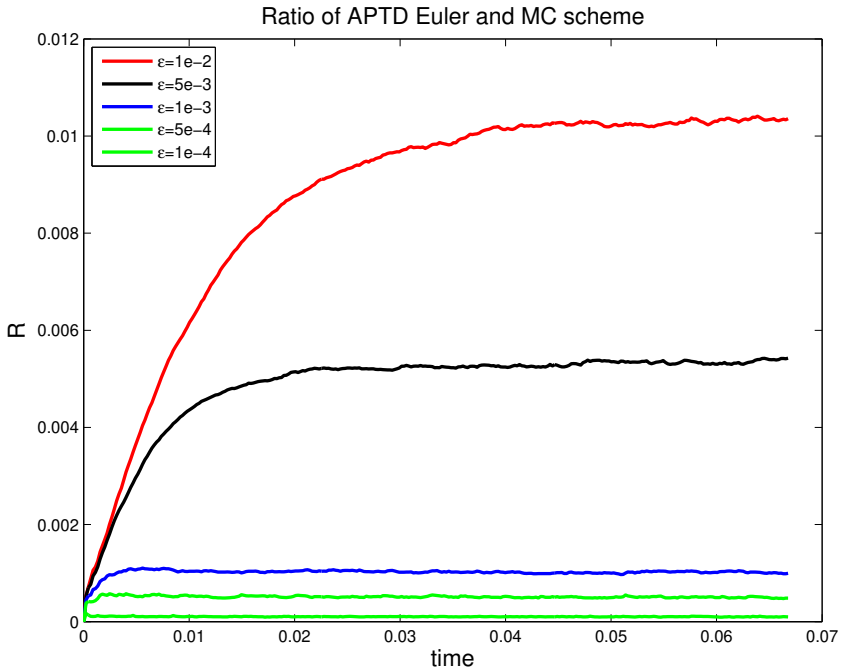


Figure: Right Monte Carlo, Left Time Diminishing scheme, $\varepsilon = 10^{-2}$ and $\varepsilon = 10^{-3}$.

Number of particles employed for the solution





Outline

A deviational Monte Carlo for the Boltzmann equation

- The starting point is again the following decomposition

$$f(v,t) = M(v) + g(v,t)$$

with $\int_{\mathbb{R}^{d_v}} \phi(v) g(v,t) dv = 0$.

- We rewrite the space homogeneous Boltzmann using this new variable $g(v,t)$ as

$$\begin{aligned}\frac{\partial\Big(ge^{\mu t/\varepsilon}\Big)}{\partial t} &= \frac{1}{\varepsilon}\Big(P(M+g,M+g) - \mu M\Big)e^{\mu t/\varepsilon} \\ &= \frac{1}{\varepsilon}\Big(P(M,M) + P(g,g) + P(M,g) + P(g,M) - \mu M\Big)e^{\mu t/\varepsilon}\end{aligned}$$

where we used the bilinearity property of the gain operator P.

- By noticing that $P(M,M) = \mu M$, we finally have

$$\frac{\partial\Big(ge^{\mu t/\varepsilon}\Big)}{\partial t} = \frac{1}{\varepsilon}\Big(P(g,g) + P(M,g) + P(g,M)\Big)e^{\mu t/\varepsilon}.$$

A deviational Monte Carlo for the Boltzmann equation II

- Now by applying a first order explicit Runge-Kutta method we get

$$g^{n+1} = e^{-\frac{\mu\Delta t}{\varepsilon}} g^n + \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} \left(\frac{P(g^n, g^n) + P(g^n, M) + P(M, g^n)}{\mu} \right).$$

- We divide the perturbation g into a difference of two positive parts:

$$g(v,t) = g_p(v,t) - g_m(v,t)$$

  where $g_p(v,t) := \max(g(v,t), 0)$ and $g_m(v,t) := -\min(g(v,t), 0)$.
- In the above decomposition, both parts are positive, $g_p(v,t) \geq 0$ and $g_m(v,t) \geq 0, \ \forall v \in \mathbb{R}^{d_v}$.
- Consequently they can then be reinterpreted as probability distributions once suitably normalized.

A deviational Monte Carlo for the Boltzmann equation III

Now, we can write

$$g_p^{n+1} - g_m^{n+1} = e^{-\frac{\mu\Delta t}{\varepsilon}}(g_p^n - g_m^n) + \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} \left(\frac{P(g_p^n, g_p^n) + P(g_p^n, M) + P(M, g_p^n) + P(g_m^n, g_m^n)}{\mu} \right) - \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} \left(\frac{P(g_p^n, g_m^n) + P(g_m^n, M) + P(M, g_m^n) + P(g_m^n, g_p^n)}{\mu} \right).$$

Then, since P is positive, one deduces the equations for the g_p^{n+1} and g_m^{n+1}

$$g_p^{n+1} = e^{-\frac{\mu\Delta t}{\varepsilon}} g_p^n + \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} \left(\frac{P(g_p^n, g_p^n) + P(g_p^n, M) + P(M, g_p^n) + P(g_m^n, g_m^n)}{\mu} \right),$$

and

$$g_m^{n+1} = e^{-\frac{\mu\Delta t}{\varepsilon}} g_m^n + \frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} \left(\frac{P(g_p^n, g_m^n) + P(g_m^n, M) + P(M, g_m^n) + P(g_m^n, g_p^n)}{\mu} \right).$$

We now approximate the two distributions $g_p(v,t)$ and $g_m(v,t)$ by a finite set of N_p and N_m particles

$$g_p(v,t) \approx m \sum_{k=1}^{N_p(t)} \delta_{v_{p,k}(t)}(v),$$

$$g_m(v,t) \approx m \sum_{k=1}^{N_m(t)} \delta_{v_{m,k}(t)}(v),$$

A deviational Monte Carlo for the Boltzmann equation IV

- Compute the initial velocities of the particles belonging to the approximation of $g_p(v, t=0)$ and $g_m(v, t=0)$: $\{v_{p,1}(t=0), .., v_{p,N_p}(t=0)\}$, $\{v_{m,1}(t=0), .., v_{m,N_m}(t=0)\}$.
- from $n=1$ to $n=n_{fin}$
  - discard $ND_p = \text{Iround}\left((1-e^{-\frac{\mu\Delta t}{\varepsilon}} - \frac{\mu\Delta t}{\varepsilon}e^{-\frac{\mu\Delta t}{\varepsilon}})N_p(t)\right)$.
  - discard $ND_m = \text{Iround}\left((1-e^{-\frac{\mu\Delta t}{\varepsilon}} - \frac{\mu\Delta t}{\varepsilon}e^{-\frac{\mu\Delta t}{\varepsilon}})N_m(t)\right)$.
  - sampling of $P(g,g)/\mu_g$: keep a fraction $NC_1 = \text{Iround}\left(\frac{\mu_g\Delta t}{\varepsilon}e^{-\frac{\mu\Delta t}{\varepsilon}}(N_p(t)+N_m(t))\right)$.
  - sampling of $P(g,M)/\mu$: keep a fraction $NC_2 = \text{Iround}\left(\frac{\mu\Delta t}{\varepsilon}e^{-\frac{\mu\Delta t}{\varepsilon}}(N_p(t)+N_m(t))\right)$.
  - sampling of $P(M,g)/\mu$: keep a fraction $NC_3 = \text{Iround}\left(\frac{\mu\Delta t}{\varepsilon}e^{-\frac{\mu\Delta t}{\varepsilon}}(N_p(t)+N_g(t))\right)$.
- end loop over time

The number of particles increases with time. Remedy have to be studied.

Discarding particles

- In details, the collisional step causes the introduction of the following number of particles

$$NC(t) = \text{Iround}\left(\frac{\mu\Delta t}{\varepsilon} e^{-\frac{\mu\Delta t}{\varepsilon}} (N_p(t) + N_g(t))(2 + \mu_g/\mu)\right).$$

- The total number of particles after one time step is consequently given by

$$N_p(t+\Delta t) + N_g(t+\Delta t) = \text{Iround}\left(e^{-\frac{\mu\Delta t}{\varepsilon}} (N_p(t) + N_g(t))\right) + NC(t).$$

  This means that the total number of samples may increase after one time step.

- A method which reduces the number of samples at a cost which is close to linear with respect to the number of samples is a density kernel estimate procedure which employ only a subset of $NC(t)$.
- This density estimate is then used in an acceptance-rejection technique to decide which samples can be eliminated without losing information in the solution.

$$\hat{g}_p(v,t) = \frac{1}{\tilde{N}_p(t) h^{d_v}} \sum_{k=1}^{\tilde{N}_p(t)} K_h\left(\frac{v - v_k(t)}{h}\right), \quad \hat{g}_m(v,t) = \frac{1}{\tilde{N}_m(t) h^{d_v}} \sum_{k=1}^{\tilde{N}_m(t)} K_h\left(\frac{v - v_m(t)}{h}\right),$$

where $K_h(v)$ is the kernel.

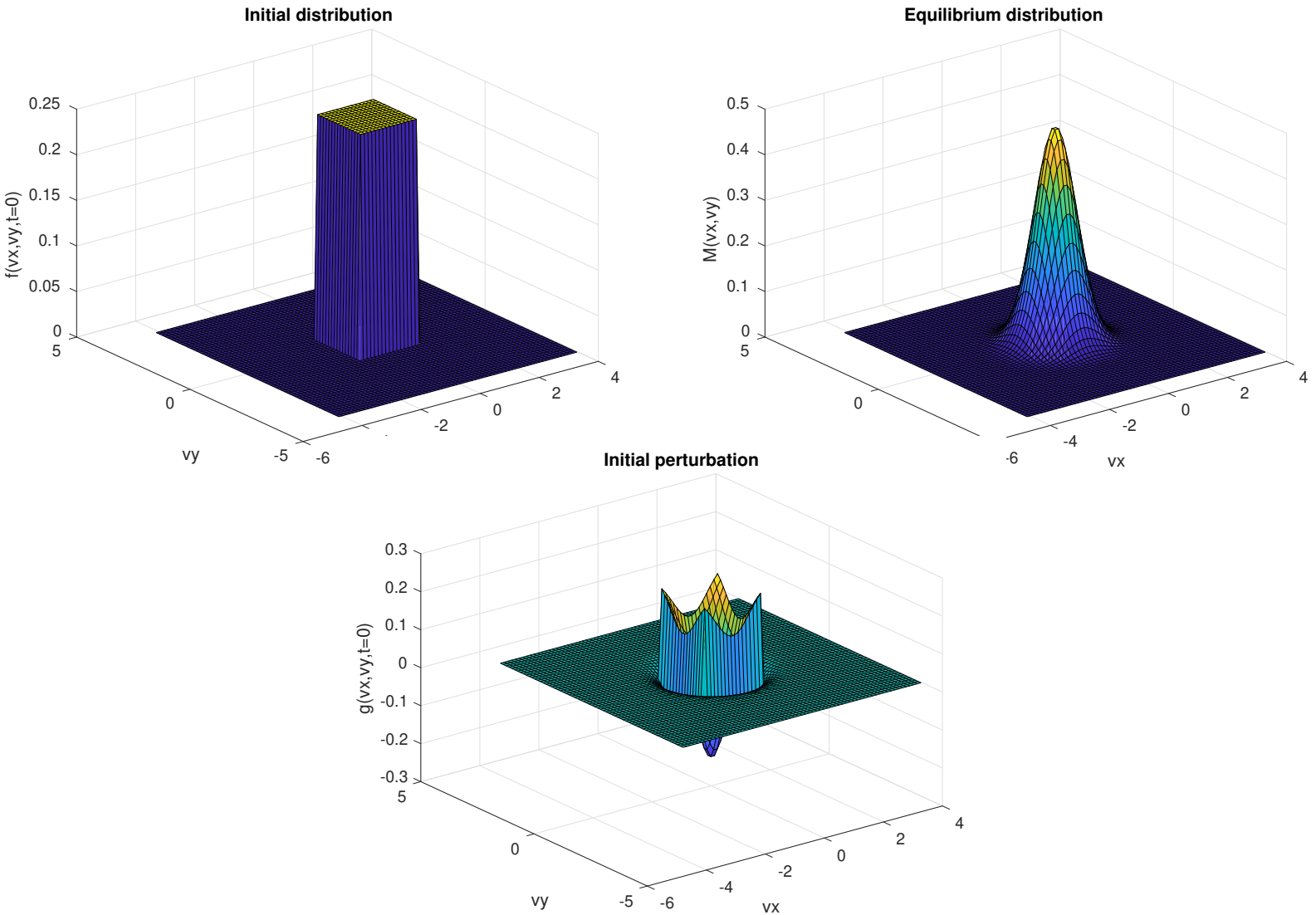


Figure: Left image: shape of the initial distribution $f(v_x, v_y, t = 0)$. Right image: Shape of the equilibrium distribution $M(v_x, v_y)$. Bottom image: Shape of the initial perturbation $g(v_x, v_y, t = 0)$.

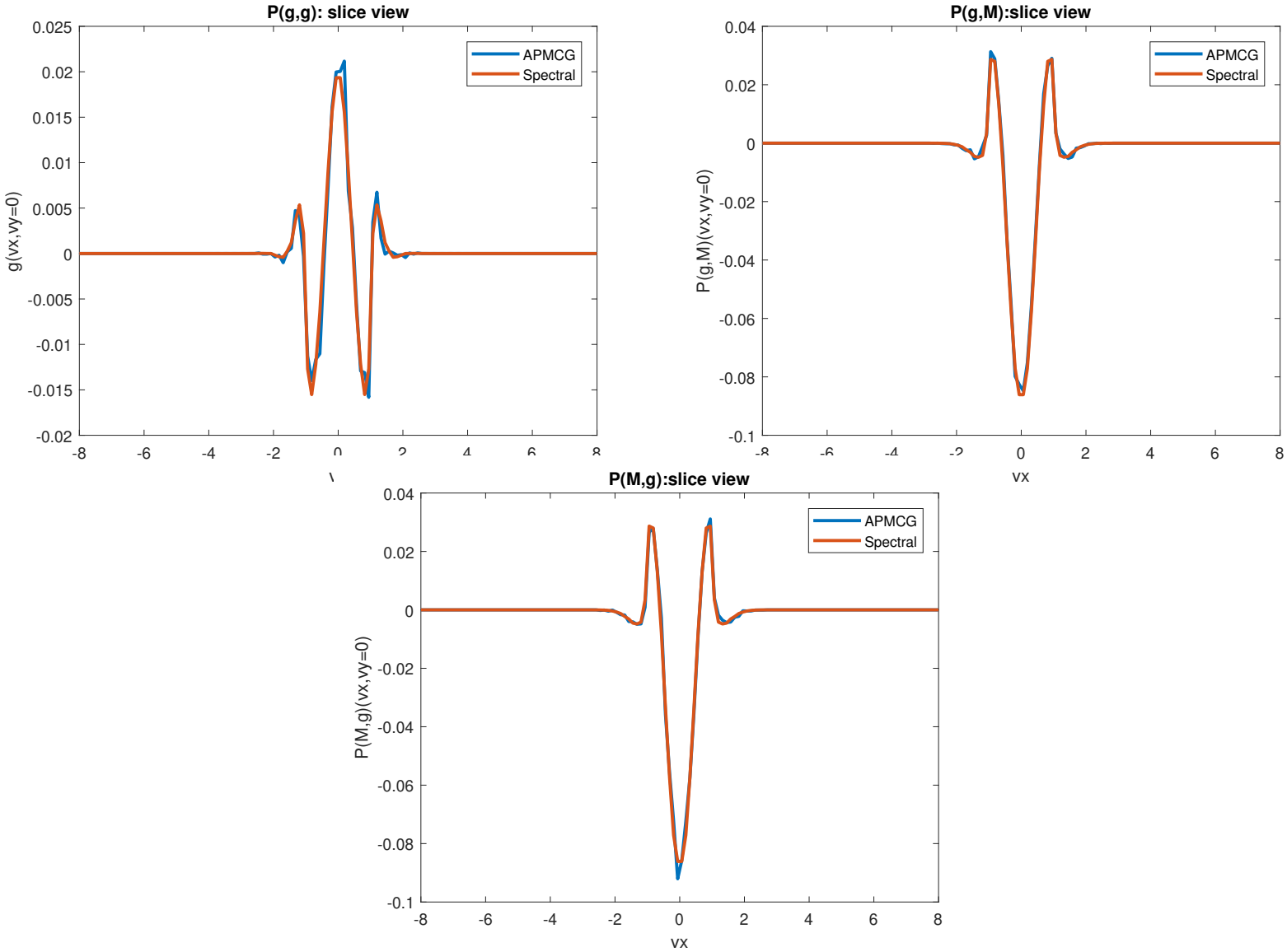
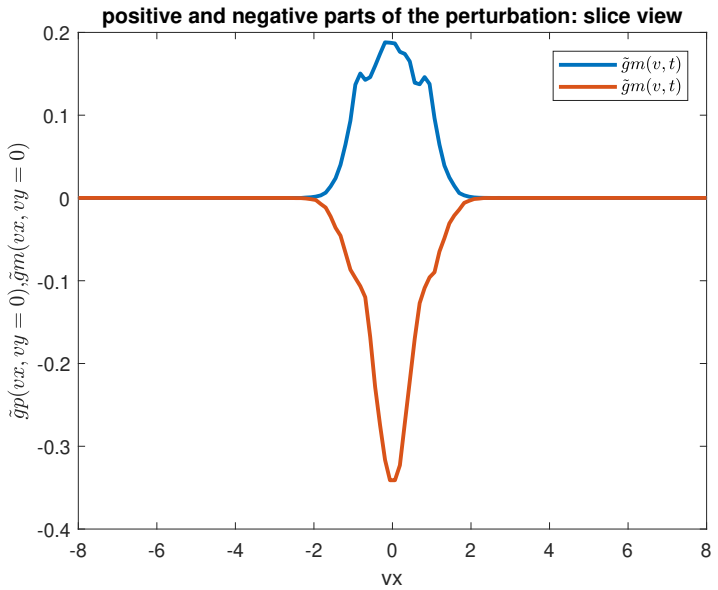
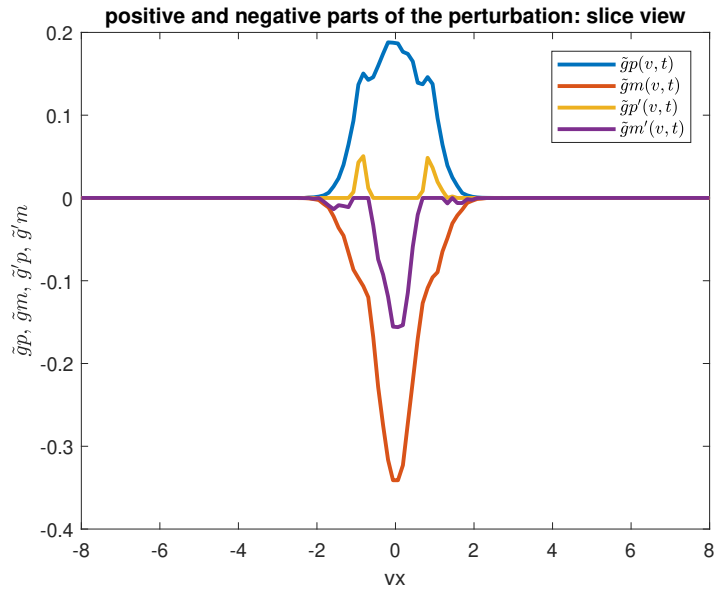
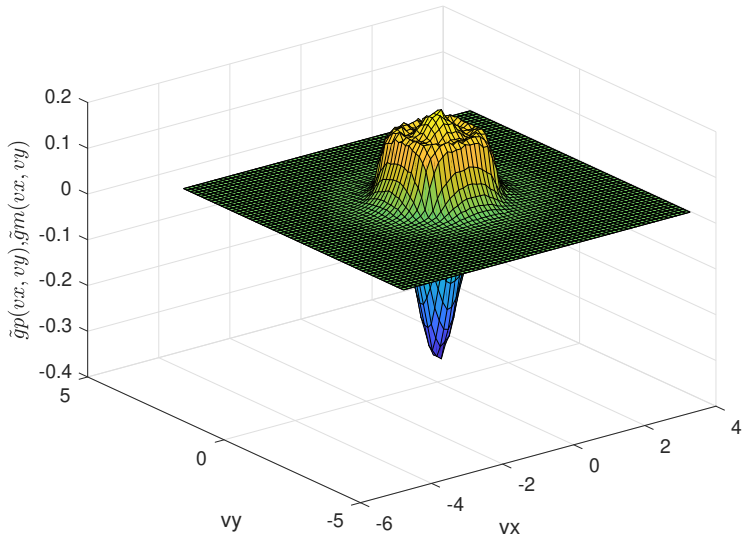


Figure: Computation of the integrals $P(g,g)(v_x,v_y)$, $P(M,g)(v_x,v_y)$,$P(g,M)(v_x,v_y)$ by the deviational and the spectral methods.





positive and negative parts of the perturbation: $\tilde{g}p(vx, vy), \tilde{g}m(vx, vy)$



Outline

Conclusions

- We have presented a series of Monte Carlo strategies to solve kinetic type equations.
- Exponential Runge-Kutta methods represent a very powerful technique which well adapts to particle discretizations and preserve many properties of the original equation.
- Time diminishing methods are based on a suitable merging between Monte Carlo approach and a finite volume methods.
- Their statistical noise is smaller and it diminishes when the scaling parameter ε decreases. They are uniformly stable with respect to the scaling parameter as well as with respect to the space mesh size.
- Their computational cost as well as their variance diminish as the equilibrium is approached. They not need artificial transitions to pass from the microscopic description to the macroscopic one.