Monte Carlo methods for integro-differential equations

Lecture 2: Kinetic equations

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Course Outline

1. Lecture #1: Monte Carlo methods
   (a) Introduction to Monte Carlo methods
   (b) Integration and applications to PDEs
2. Lecture #2: Kinetic equations
   (a) Direct Simulation Monte Carlo
   (b) Asymptotic Preserving Monte Carlo

Outline

Introduction

Finally let us consider more generally the group of problems which gave rise to the development of the method to which this article is devoted.... The problem of the behavior of such a system is formulated by a set of integro-differential equations. Such equations are known in the kinetic theory of gases as the Boltzmann equation. In the theory of probability one has a somewhat similar situation described by the Fokker-Planck equation.

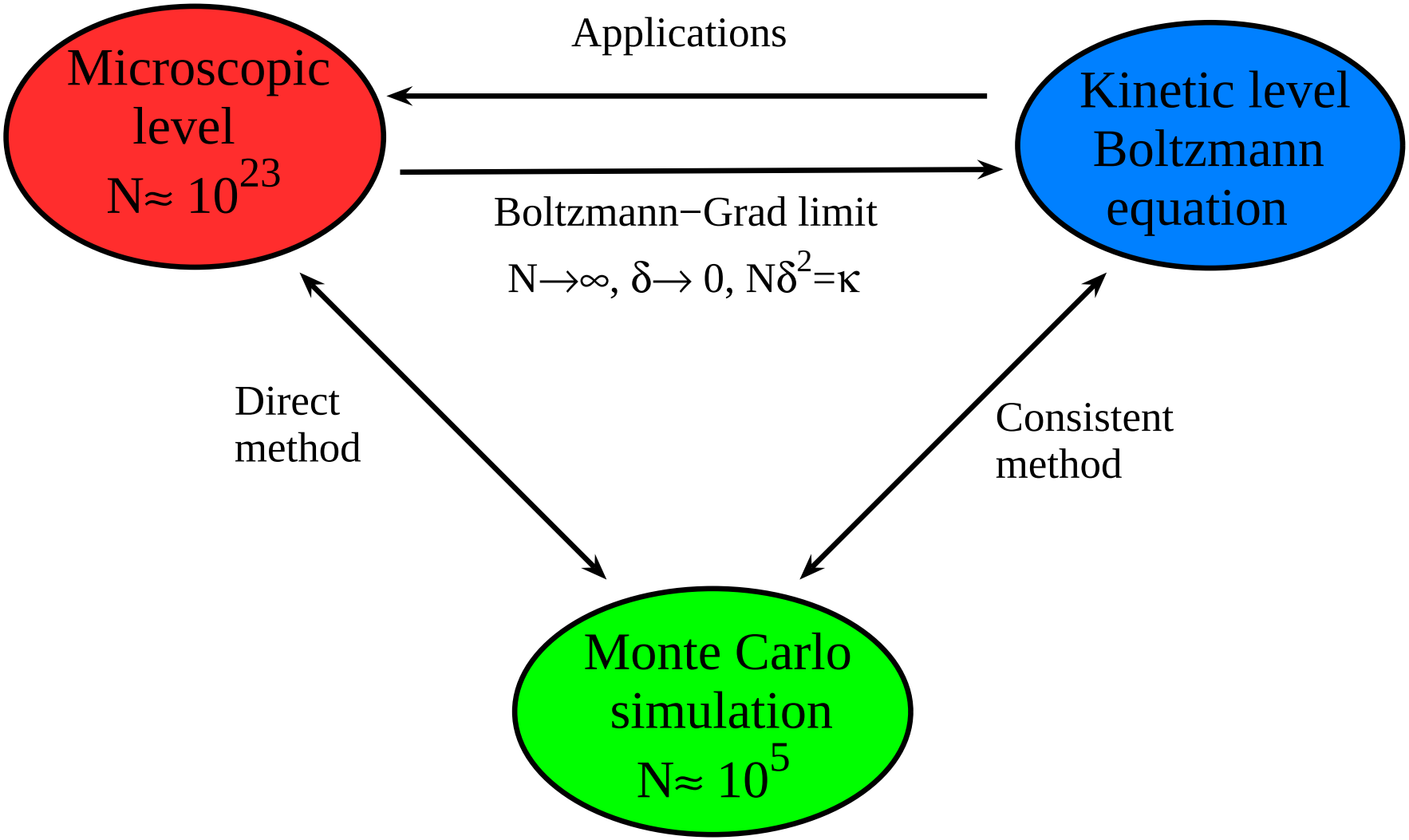
(N.Metropilis, S.Ulam, "The Monte Carlo method", J. Am. Stat. Ass., 1949.)

Levels of representation

- Interacting particle systems are ubiquitous in nature: gases, fluids, plasmas, solids (metals, semiconductors or insulators), vehicles on a road, economic agents can be considered as interacting particle systems.
- Particle systems can be described at the microscopic level by particle dynamics (*Newton's equations*) describing the individual motions of the particles. However, particle dynamic is impossible to use in most practical cases, due to the extraordinary large number of equations that must be solved simultaneously.
- At the macroscopic level fluid models (such as the *Euler or Navier-Stokes equations*) describe averaged quantities, local density, momentum, energy... However, fluid models involve constants (viscosity, heat conductivity, diffusion) which depend on the microscopic properties of the elementary particles interactions.

- There is a need to bridge the gap between particle dynamics and fluid models. This question of how to pass from microscopic properties of matters to macroscopic properties of systems is one of the most fundamental ones in physics. It is also one of the most difficult.
- The problem is slightly simplified by introducing an intermediate step between particle systems and fluid models: the so-called kinetic level. These models, characterized by *Boltzmann equations*, deal with a quantity, the distribution function, which is the density of particles in phase-space (say position and velocity).
- The essential idea of *Monte Carlo* or *particle* simulations for the Boltzmann equation is to return to the particle description with a number of particles small enough to make the situation computationally treatable but "sufficiently close" to the physical situation. As we will see this will involve evaluations of high dimensional integrals for which Monte Carlo methods arise quite naturally.

Microscopic, kinetic and computational levels



The kinetic model

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

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

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

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

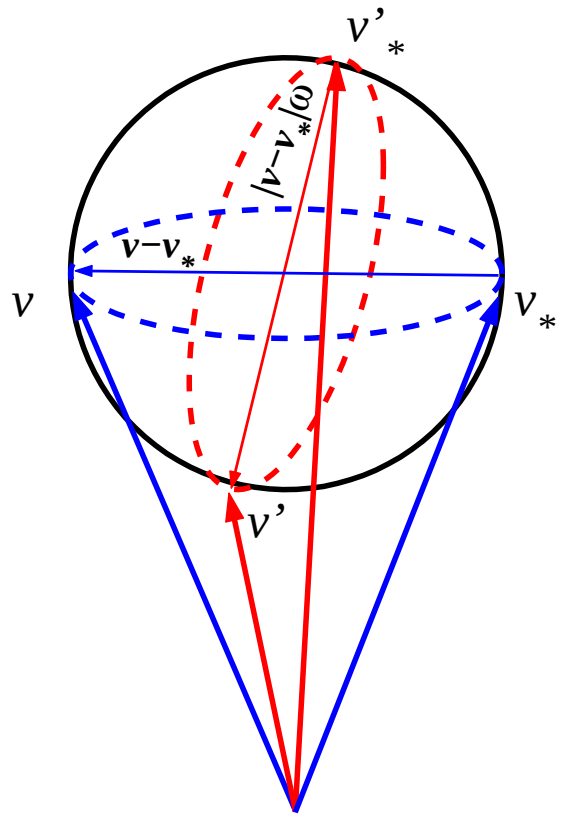
where σ is a vector of the unitary sphere $S^2 \subset I\!R^3$ and the dependence of f on x and t has been omitted.The kernel B characterizes the binary interactions. The *Variable Hard Spheres*[1] (VHS) model used for RGD simulations is

$$B(|q|, |q \cdot \sigma|) = C|q|^\alpha, \quad 0 \leq \alpha \leq 1,$$

where C is a positive constant. The case $\alpha = 0$ corresponds to a *Maxwellian gas*, while $\alpha = 1$ is called a *Hard Sphere Gas*.

[1] G.Bird, 1976

The collision sphere



The collisional velocities (v', v'_*) are associated to the velocities (v, v_*) and to the parameter σ by the relations

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

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

Main properties

The collision operator preserves mass, momentum and energy

$$\int_{\mathbb{R}^3} Q(f,f)\phi(v)\,dv = 0, \quad \phi(v) = 1, v^x, v^y, v^z, |v|^2,$$

and in addition is such that the *H-Theorem* holds

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

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

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

Fluid limit

The most natural method to derive fluid equations is the *moment method*. Let us multiply the Boltzmann equation by its collision invariants and integrate

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} f\phi(v)\,dv + \nabla_x\left(\int_{\mathbb{R}^3} vf\phi(v)\,dv\right) = 0, \quad \phi(v) = 1, v_1, v_2, v_3, |v|^2.$$

These equations descrive the balance of mass, momentum and energy. The system is not closed since it involves higher order moments of f.
As $\varepsilon \to 0$ we have formally $Q(f,f) \to 0$ and thus $f \to M$. Higher order moments of f can be computed as function of ρ, u, and T and we obtain the compressible Euler equations

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho u) = 0$$
$$\frac{\partial \rho u}{\partial t} + \nabla_x \cdot (\rho u \otimes u + p) = 0$$
$$\frac{\partial E}{\partial t} + \nabla_x \cdot (Eu + pu) = 0, \quad p = \rho T = \frac{2}{3}E - \frac{1}{3}\rho u^2.$$

Splitting approach

A common approach to solve a kinetic equation is operator splitting. The solution in one time step Δt may be obtained by the sequence of two steps.
First integrate the space homogeneous equation for all $x \in \Omega$,

$$\begin{aligned} \frac{\partial \tilde{f}}{\partial t} &= \frac{1}{\varepsilon} Q(\tilde{f}, \tilde{f}), \\ \tilde{f}(x, v, 0) &= f_0(x, v), \end{aligned}$$

for a time step Δt (*collision step*) to obtain $\tilde{f} = C_{\Delta t}(f_0)$.
Then solve the transport equation using the output of the previous step as initial condition,

$$\begin{aligned} \frac{\partial f}{\partial t} + v \cdot \nabla_x f &= 0, \\ f(x, v, 0) &= \tilde{f}(x, v, \Delta t). \end{aligned}$$

for a time step Δt (*transport step*) to get $f = T_{\Delta t}(\tilde{f}) = T_{\Delta t}(C_{\Delta t}(f_0))$.
After this splitting the major numerical difficulties are in the collision step. Note that the transport step corresponds to simple free flow of particles.

Splitting approach

- The splitting scheme described above is first order accurate in time. The accuracy in time may be improved by a more sophisticated splitting. For example Strang splitting[2] is second order accurate (provided both steps are at least second order). It can be written as

$$f = C_{\Delta t/2}(T_{\Delta t}(C_{\Delta t/2}(f_0))),$$

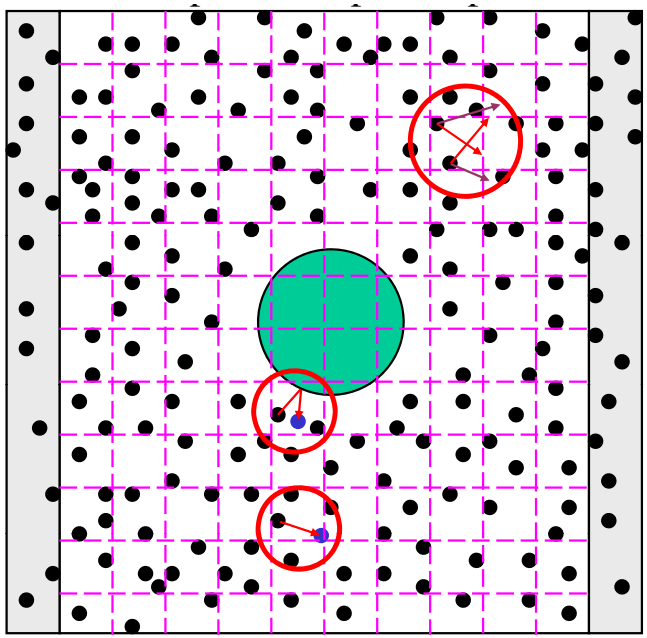
or equivalently as

$$f = T_{\Delta t/2}(C_{\Delta t}(T_{\Delta t/2}(f_0))).$$

- Note that, if the initial data is in local equilibrium and both steps are solved exactly, then simple splitting and Strang splitting does not differ. So simple splitting becomes second order accurate.
- Both splitting methods for vanishingly small values of ε becomes a first order *kinetic scheme* for the underlying fluid dynamic limit. The collision step becomes a projection towards the local Maxwellian $C_{\Delta t}(f_0) = M(f_0)$ which is then transported by the transport step $f = T_{\Delta t}(M(f_0))$. Thus Strang splitting reduces its accuracy to first order in time in this regime.

[2] G.Strang, 1968

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

In this paragraph we will describe the *classical DSMC methods* due to Bird and Nanbu in the case of spatially homogeneous Boltzmann equations[3].
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 Boltzmann equation in the Maxwellian case

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

and $\mu = 4\pi\rho$. The case of general VHS kernels will be discussed later.

[3] 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.

Maxwellian case

First we consider the case where the collision kernel does not depend on the relative velocity.

Algorithm[Nanbu for Maxwell molecules]:

1. *compute the initial velocity of the particles,* $\{v_i^0, i = 1, \ldots, N\}$, *by sampling them from the initial density* $f_0(v)$
2. for $n = 1$ to n_{TOT}
   for $i = 1$ to N
   with probability $1 - \mu\Delta t/\epsilon$
   - *set* $v_i^{n+1} = v_i^n$

   with probability $\mu\Delta t/\epsilon$
   - *select a random particle* j
   - *compute* v_i' *by performing the collision between particle* i *and particle* j
   - *assign* $v_i^{n+1} = v_i'$

   end for
   end for

Nanbu's algorithm is not conservative, i.e. momentum and energy are conserved only in the mean, but not at each collision. A conservative algorithm is obtained selecting independent particle pairs, instead of single particles.

Nanbu-Babovsky for the Maxwellian case

The expected number of collision pairs in a time step Δt is $N\mu\Delta t/(2\epsilon)$.

Algorithm[Nanbu-Babovsky for Maxwell molecules]:

1. *compute the initial velocity of the particles,* $\{v_i^0, i = 1, \dots, N\}$, *by sampling them from the initial density* $f_0(v)$
2. for $n = 1$ to n_{TOT}
   given $\{v_i^n, i = 1, \dots, N\}$
   - *set* $N_c = \mathrm{Iround}(\mu N \Delta t/(2\epsilon))$
   - *select* N_c *pairs* (i, j) *uniformly among all possible pairs, and for those*
     - *perform the collision between* i *and* j, *and compute* v_i' *and* v_j' *according to the collision law*
     - *set* $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$
   - *set* $v_i^{n+1} = v_i^n$ *for all the particles that have not been selected*

   end for

Here by $\mathrm{Iround}(x)$ we denote

$$\mathrm{Iround}(x) = \begin{cases} \lfloor x \rfloor + 1 & \text{with probability} \quad x - \lfloor x \rfloor \\ \lfloor x \rfloor & \text{with probability} \quad \lfloor x \rfloor + 1 - x \end{cases}$$

where $\lfloor x \rfloor$ denotes the integer part of x.

Collisional velocities

The collisional velocities are

$$v_i' = \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2}\omega, \quad v_j' = \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2}\omega,$$

where ω is chosen uniformly in the unit sphere.
More precisely we have:
Two-dimension:

$$\omega = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \quad \theta = 2\pi\xi,$$

Three-dimension:

$$\omega = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix}, \quad \theta = \arccos(2\xi_1 - 1), \quad \phi = 2\pi\xi_2,$$

where ξ_1, ξ_2 are uniformly distributed random variables in $[0, 1]$.

Variable Hard Sphere case

The extend the algorithm to non constant scattering cross section we shall assume that the collision kernel satisfies some *cut-off hypothesis*.
We will denote by $Q_\Sigma(f,f)$ the collision operator with kernel

$$B_\Sigma(|v-v_*|) = \min\left\{B(|v-v_*|), \Sigma\right\}, \quad \Sigma > 0.$$

and, for a fixed Σ, consider the homogeneous problem

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} Q_\Sigma(f,f).$$

The operator $Q_\Sigma(f,f)$ can be written in the form $P(f,f) - \mu f$ taking

$$P(f,f) = Q_\Sigma^+(f,f) + f(v) \int_{\mathbb{R}^3} \int_{S^2} [\Sigma - B_\Sigma(|v-v_*|)] f(v_*)\, d\omega\, dv_*,$$

with $\mu = 4\pi\Sigma\rho$ and

$$Q_\Sigma^+(f,f) = \int_{\mathbb{R}^3} \int_{S^2} B_\Sigma(|v-v_*|) f(v') f(v'_*)\, d\omega\, dv_*.$$

In this case, a simple scheme is obtained by using the acceptance-rejection technique to sample the collisional velocity according to $P(f,f)/\mu$.

Nanbu-Babovsky for VHS

The conservative DSMC algorithm for VHS collision kernels can be written as

Algorithm[Nanbu-Babovsky for VHS molecules]:

1. *compute the initial velocity of the particles,* $\{v_i^0, i = 1, \dots, N\}$, *by sampling them from the initial density* $f_0(v)$
2. for $n = 1$ to n_{TOT}
   given $\{v_i^n, i = 1, \dots, N\}$
   - *compute an upper bound* Σ *of the cross section*
   - *set* $N_c = \mathrm{Iround}(N\rho\Sigma\Delta t/(2\epsilon))$
   - *select* N_c *dummy collision pairs* (i, j) *uniformly among all possible pairs, and for those*
     - *compute the relative cross section* $B_{ij} = B(|v_i - v_j|)$
     - if $\Sigma\,\mathrm{Rand} < B_{ij}$
       perform the collision between i *and* j, *and compute* v_i' *and* v_j' *according to the collisional law*
       set $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$
   - *set* $v_i^{n+1} = v_i^n$ *for all the particles that have not collided*

   end for

Evaluation of Σ

The upper bound Σ should be chosen as small as possible, to avoid inefficient rejection, and it should be computed fast. It is be too expensive to compute Σ as

$$\Sigma = B_{\max} \equiv \max_{ij} B(|v_i - v_j|),$$

since this computation would require an $O(N^2)$ operations.
An upper bound of $B_{\max}$ is obtained by taking $\Sigma = B(2\Delta v)$, where

$$\Delta v = \max_i |v_i - \bar{v}|, \quad \bar{v} := \frac{1}{N}\sum_i v_i.$$

Remarks:

- The probabilistic interpretation breaks down if $\Delta t/\epsilon$ is too large. This implies that the time step becomes extremely small when approaching the fluid dynamic limit.
- The cost of the method is proportional to the number of dummy collision pairs, that is $\mu N \Delta t/2$. Thus for a fixed final time T the total cost is independent of the choice of $\Delta t = T/n$. However this is true only if we do not had to compute Σ (like in the Maxwellian case).

Bird's method (DSMC time counter)

The method is currently the most popular method for the numerical solution of the Boltzmann equation. It has been derived accordingly to physical considerations (as a simplified molecular dynamics) for the simulation of particle collisions.
Let us consider first the Maxwellian case. The number of collisions in a short time step Δt is given by

$$N_c = \frac{N\mu\Delta t}{2\varepsilon}, \quad \mu = 4\pi\rho.$$

This means that the average time between collisions Δt_c is given by

$$\Delta t_c = \frac{\Delta t}{N_c} = \frac{2\varepsilon}{\mu N}.$$

The method is then based on selecting randomly a particle pair, compute the collision result and update the local time counter by Δt_c.

Bird for Maxwellian case

It is possible to set a time counter, t_c, and to perform the calculation as follows

Algorithm[Bird for Maxwell molecules]:

1. *compute the initial velocity of the particles,* $\{v_i^0, i = 1, \ldots, N\}$, *by sampling them from the initial density* $f_0(v)$
2. *set time counter* $t_c = 0$
3. *set* $\Delta t_c = 2\varepsilon/(\mu N)$
4. for $n = 1$ to n_{TOT}
   - repeat
     - *select a random pair* (i, j) *uniformly within all possible pairs*
     - *perform the collision and produce* v_i', v_j'
     - *set* $\tilde{v}_i = v_i', \tilde{v}_j = v_j'$
     - *update the time counter* $t_c = t_c - \Delta t_c$

     until $t_c \geq (n+1)\Delta t$
   - *set* $v_i^{n+1} = \tilde{v}_i, i = 1, \ldots, N$

   end for

The algorithm is similar to the Nanbu-Babovsky (NB) scheme for Maxwellian molecules. The main difference is that in NB scheme the particles can collide only once per time step, while in Bird's scheme multiple collisions are allowed.

Variable Hard Sphere case

For a more general kernel, Bird's scheme is modified to take into account that the average number of collisions in a given time interval is not constant, and that the collision probability on all pairs is not uniform. This can be done as follows.
The expected number of collisions in a time step Δt is given by

$$N_c = \frac{N\rho\overline{B}\Delta t}{2\varepsilon},$$

where $\overline{B}$ denotes the *average collision frequency*.
Then the mean collision time can be computed as

$$\Delta t_c = \frac{\Delta t}{N_c} = \frac{2\varepsilon}{N\rho\overline{B}}.$$

The N_c collisions have to be performed with probability proportional to $B_{ij} = B(|v_i - v_j|)$. In order to do this one can use the same acceptance-rejection technique as in Nanbu-Babovsky scheme. The drawback of this procedure is that computing $\overline{B}$ is too expensive. To avoid this one computes a local time counter as follows. First select a collision pair (i, j) using rejection. Then compute

$$\Delta t_{ij} = \frac{2\varepsilon}{N\rho B_{ij}}.$$

Bird for VHS

Bird's algorithm for general VHS molecules can therefore be summarized as:

Algorithm[Bird for VHS molecules]:

1. *compute the initial velocity of the particles,* $\{v_i^0, i = 1, \ldots, N\}$, *by sampling them from the initial density* $f_0(v)$
2. *set time counter* $t_c = 0$
3. for $n = 1$ to n_{TOT}
   - *compute an upper bound* Σ *of the cross section*
   - repeat
     - *select a random pair* (i, j) *uniformly*
     - *compute the relative cross section* $B_{ij} = B(|v_i - v_j|)$
     - if $\Sigma\,\xi < B_{ij}$
       - *perform the collision between* i *and* j, *and compute* v_i' *and* v_j' *according to the collisional law*
       - *set* $\tilde{v}_i = v_i', \tilde{v}_j = v_j'$
       - *set* $\Delta t_{ij} = 2\varepsilon/(N\rho B_{ij})$
       - *update the time counter* $t_c = t_c + \Delta t_{ij}$

     until $t_c \geq (n+1)\Delta t$
   - *set* $v_i^{n+1} = \tilde{v}_i, i = 1, \ldots, N$

   end for

Final remarks

- The presence of *multiple collisions* per time step in Bird's method has a profound influence on the time accuracy. While Nanbu scheme converges in probability to the time discrete Boltzmann equation, Bird's method converges to the space homogeneous Boltzmann equation[4].
- Numerical tests confirm that in space non homogeneous situations Bird's method with simple splitting can achieve *second order accuracy* in time whereas Nanbu's is always first order[5].
- In the original nonconservative form one can show that Nanbu's method gives the wrong expectation for the temperature[6].
- Exact conservation of moments forces the velocity domain to remain bounded during relaxation $|v_i| \leq \sqrt{2EN}$. As a consequence steady state particles are never "true" Maxwellian samples.
- Similarly to Nanbu's method also Bird's method becomes very expensive and practically unusable near the *fluid regime*. Infact, the collision time between the particles Δt_{ij} becomes very small, and a huge number of collisions is needed in order to reach a fixed final time $t_{\max}$.

[4] R.Illner, H.Babovski '89, W.Wagner '92
[5] A.Garcia, W.Wagner '00
[6] C.Greengard, L.G.Reyna '91

Main goal

The goal is to construct simple and efficient Monte Carlo methods for the solution of RGD problems in regions with a large variation in the mean free path.
As a consequence the methods should have the following features

- for large Knudsen numbers, the methods behave as classical DSMC methods;
- for intermediate Knudsen numbers the methods are capable to speed up the computation time without degradation of accuracy;
- in the limit of the very small Knudsen number, the collision step replaces the distribution function by a local Maxwellian with the same moments. The methods will behave as a stochastic kinetic scheme for the underlying Euler equations of gas dynamics (asymptotic preserving (AP) property);
- mass, momentum, and energy are preserved.

Exponential methods

Let us rewrite the homogeneous equation in the form[7]

$$\partial_t f = \frac{1}{\varepsilon}(P(f,f) - \mu f) = \frac{\mu}{\varepsilon}\left(\frac{P(f,f)}{\mu} - M\right) + \frac{\mu}{\varepsilon}(M - f).$$

Note that the above system is is composed by a linear part $\mu(M-f)/\varepsilon$ which characterizes the asymptotic behavior of f and a nonlinear part $(P(f,f)/\mu - M)/\varepsilon$ which describes the deviations of $P(f,f)/\mu$ from M, or equivalently the deviations of the Boltzmann operator from the BGK model. The system has the general structure

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

where $\lambda > 0$, and E is a local equilibrium value.

[7] F.Filbet, S.Jin '09, G.Dimarco, L.Pareschi '09

Exponential Runge-Kutta

We can apply an explicit exponential Runge-Kutta method to the above system in the form [8]

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

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*. So when $G = 0$ the method is exact and when $\lambda = 0$ the method reduces to an explicit one-step method for ODEs.

[8] M.Hochbruck, C.Lubich, H.Selhofer '98. S.Maset, M.Zennaro '09

IF and ETD methods

Various schemes come from the different choices of the coefficients and the weights. The two most popular approaches are the integrating factor (IF) and the exponential time differencing (ETD) methods.
For the so-called *Integrating Factor* methods we have[9]

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

For the *Exponential Time Differencing* the weights $W_i(\lambda\Delta t)$ are linear combinations of the functions $\phi_l(\lambda\Delta t)$, $l=1,\dots,\nu$ and the coefficients $A_{ij}(\lambda\Delta t)$ are linear combinations of the functions $\phi_l(c_i\lambda\Delta t)$, $l=1,\dots,\nu$ where the functions ϕ_l are defined recursively from[10]

$$\phi_l(z)=\frac{\phi_{l-1}(z)-\frac{1}{(l-1)!}}{z}, \quad \phi_0(z)=e^z.$$

[9] J. Lawson, '67
[10] A. Friedli, '78

Application to the Boltzmann equation

When applied to the Boltzmann equation the first order IF scheme takes the form

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

whereas the ETD scheme becomes

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

Note that both schemes are of the general form

$$f^{n+1} = A_1\left(\frac{\mu\Delta t}{\varepsilon}\right) f^n + A_2\left(\frac{\mu\Delta t}{\varepsilon}\right) \frac{P(f^n, f^n)}{\mu} + A_3\left(\frac{\mu\Delta t}{\varepsilon}\right) M^n,$$

with $A_1, A_2, A_3 \in [0, 1]$ and $A_1 + A_2 + A_3 = 1$ independently of $\mu\Delta t/\epsilon$. The above property assures that they are unconditionally stable, preserve nonnegativity and the main physical conservations properties.

It can be shown that the general class of methods can be written in the following form

$$f^{n+1}(v) = \sum_{k=0}^{m} A_k f_k^n(v) + A_{m+1} M(v),$$

where the functions f_k are given by the recurrence formula

$$f_{k+1}(v) = \frac{1}{k+1} \sum_{h=0}^{k} \frac{1}{\mu} P(f_h, f_{k-h}), \quad k = 0, 1, \dots.$$

We require the weights $A_k = A_k(\mu \Delta t/\varepsilon)$ to be nonnegative function (eventually under a time step restriction) that satisfy the following properties

- *conservation :*

$$\sum_{k=0}^{m+1} A_k(\mu \Delta t/\varepsilon) = 1 \quad \tau \in [0, 1],$$

- *asymptotic preserving :*

$$\lim_{\mu \Delta t/\varepsilon \to \infty} A_{m+1}(\mu \Delta t/\varepsilon) = 1.$$

Remarks

- Note that the AP property is not satisfied by the standard first order ETD whereas it is satisfied by the first order IF scheme. This remains true also for higher order methods. A modification of ETD methods that satisfy AP property can be derived using the so called time relaxed methods[11] corresponding to

$$A_k = e^{-\mu\Delta t/\varepsilon}(1 - e^{-\mu\Delta t/\varepsilon})^k, \quad A_{m+1} = (1 - e^{-\mu\Delta t/\varepsilon})^{m+1}.$$

- An important property of the coefficients $f_k(v)$ appearing in the expansion is that they are nonnegative and that

$$\int_{\mathbb{R}^3} f_k(v)\phi(v)\,dv = \int_{\mathbb{R}^3} f_0(v)\phi(v)\,dv, \qquad \phi(v) = 1, v, |v|^2, \quad \forall\ k.$$

- The schemes have a nice probabilistic interpretation. In fact, if f^n is a probability density function so are f_k^n for all k and then the schemes describe the next time level f^{n+1} as a convex combination of probability density functions which makes them suitable for Monte Carlo simulations.

[11] E.Gabetta, L.P., G.Toscani, '97. L.P., G.Russo, '01

Asymptotic Preserving Monte Carlo (APMC) Methods

First order scheme (APMC1):
Form $m = 1$ the generalized AP schemes give

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 M$$

The probabilistic interpretation of the above equation is the following.
A particle extracted from f^n

- does not collide with probability A_0, (i.e. it is sampled from f^n)
- collides with another particle extracted from f^n with probability A_1 (i.e. it is sampled from the function f_1)
- is replaced by a particle sampled from a Maxwellian with probability A_2.

Remarks: In this formulation the probabilistic interpretation holds uniformly in $\mu\Delta t$, at variance with NB, which requires $\mu\Delta t < 1$. Furthermore, as $\mu\Delta t \to \infty$, the distribution at time $n+1$ is sampled from a Maxwellian.
In a space non homogeneous case, this would be equivalent to a particle method for Euler equations.

Second order APMC scheme

Form $m = 2$ the generalized AP schemes give

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 f_2 + A_3 M,$$

with $f_1 = P(f^n, f^n)/\mu, f_2 = P(f^n, f_1)/\mu$.

The probabilistic interpretation of the scheme is the following. Given N particles distributed according to f^n:

- NA_0 particles do not collide,
- NA_1 are sampled from f_1, as in the first order scheme,
- NA_2 are sampled from f_2, i.e. $NA_2/2$ particles sampled from f^n will undergo dummy collisions with $NA_2/2$ particles sampled from f_1,
- NA_3 particles are sampled from a Maxwellian.

Remarks: Previous MC schemes can be made exactly conservative. This goal is achieved by using a suitable algorithm for sampling a set of particles with prescribed momentum and energy from a Maxwellian.
Higher order APMC methods can be constructed similarly.

Numerical results

Space homogeneous case

- Comparison between: NB and APMC1 with the IF coefficients.
- Test problem: Asymmetric bimodal distribution in 2D.
- Number of particles: $N = 5 \times 10^5$

1D Shock wave profiles

- Comparison between: NB, APMC1, APMC2, APMC3 with the time relaxed coefficients.
- Initial data $f(x, v, t) = M(\rho, u, T)$, with

$$\rho = 1.0, \quad T = 1.0, \quad Ma = 3.0, \qquad x > 0,$$

where Ma is the Mach number. The mean velocity is

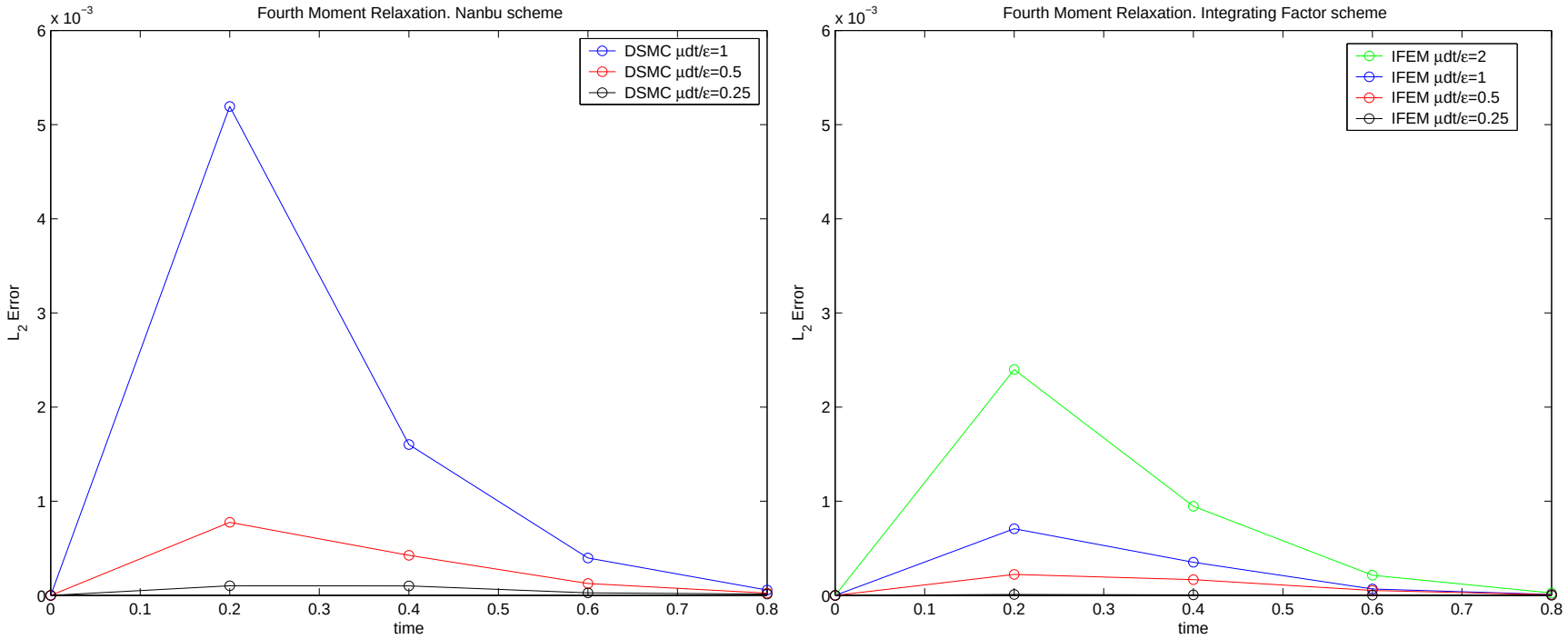
$$u_x = -Ma\sqrt{(\gamma T)}, \quad u_y = 0,$$

with $\gamma = 5/3$. The values for ρ, u and T for $x < 0$ are given by the Rankine-Hugoniot conditions.

- Test problem : Hard sphere gas with $50 - 100$ space cells and 500 particles in each cell on $x > 0$.
- For stationary shocks the accuracy of the methods can be increased by computing averages on the solution for $t \gg$.

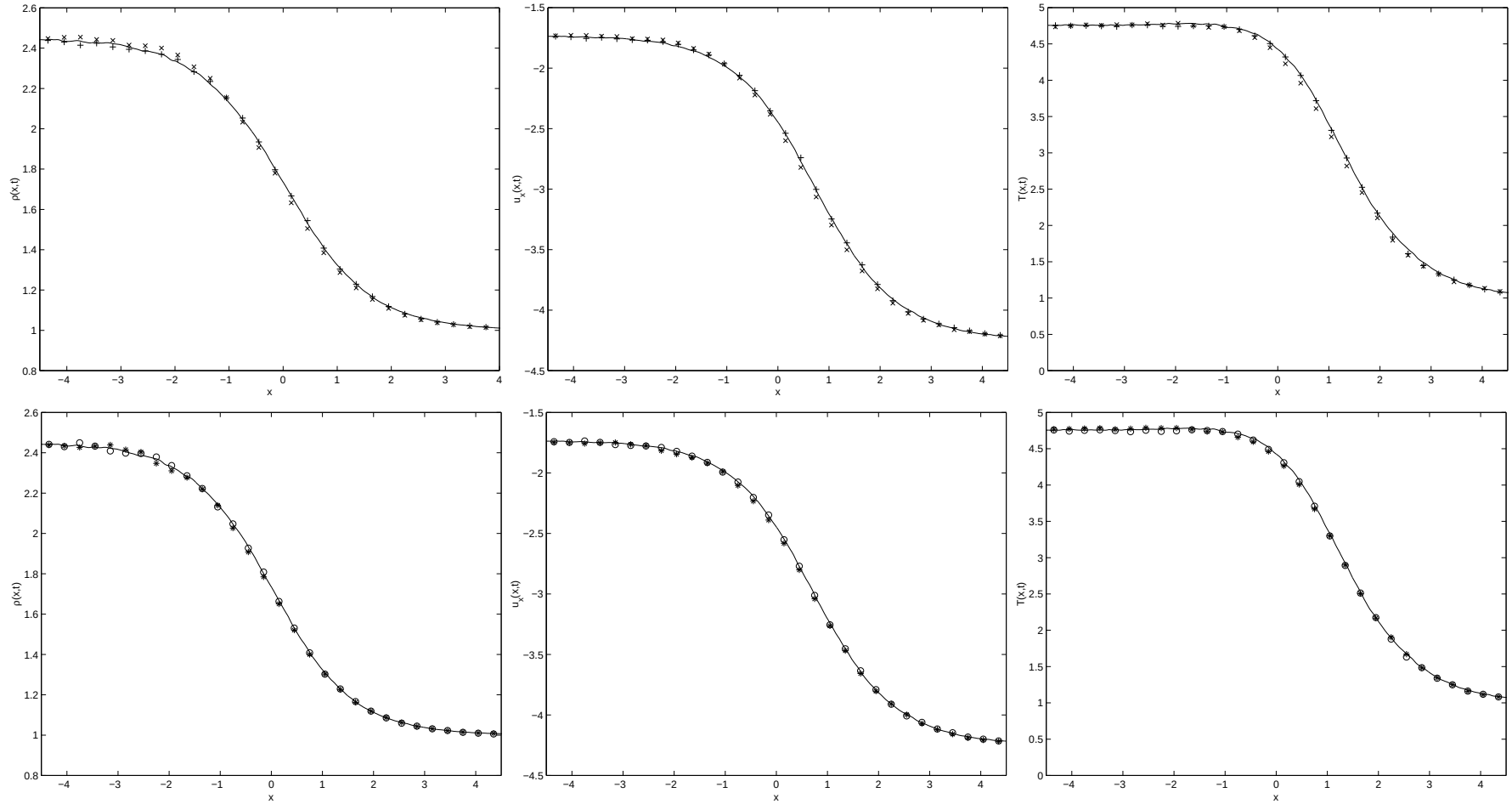
Homogeneous case

Maxwellian case: L^2 norm of the error vs time for the 4-th order moment. DSMC (left) and first order APMC (right) with different time steps.



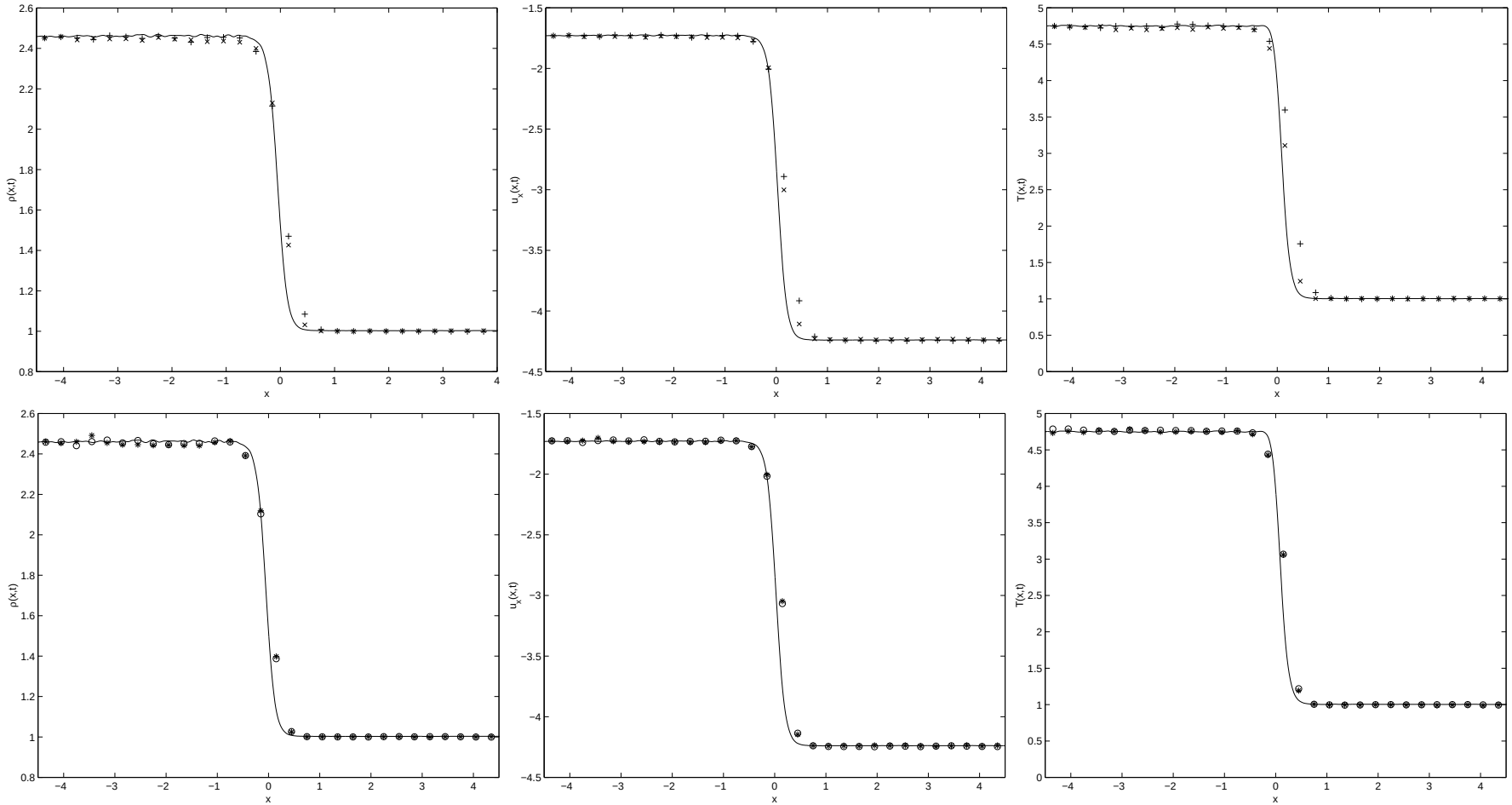
Shock profile rarefied regime

1D shock profile: DSMC($+$) and first order APMC ($\times$) (top), second order ($*$) and third order ($\circ$) APMC (bottom) for $\epsilon = 1.0$ and $\Delta t = 0.025$. From left to right: ρ, u, T. The line is the reference solution.



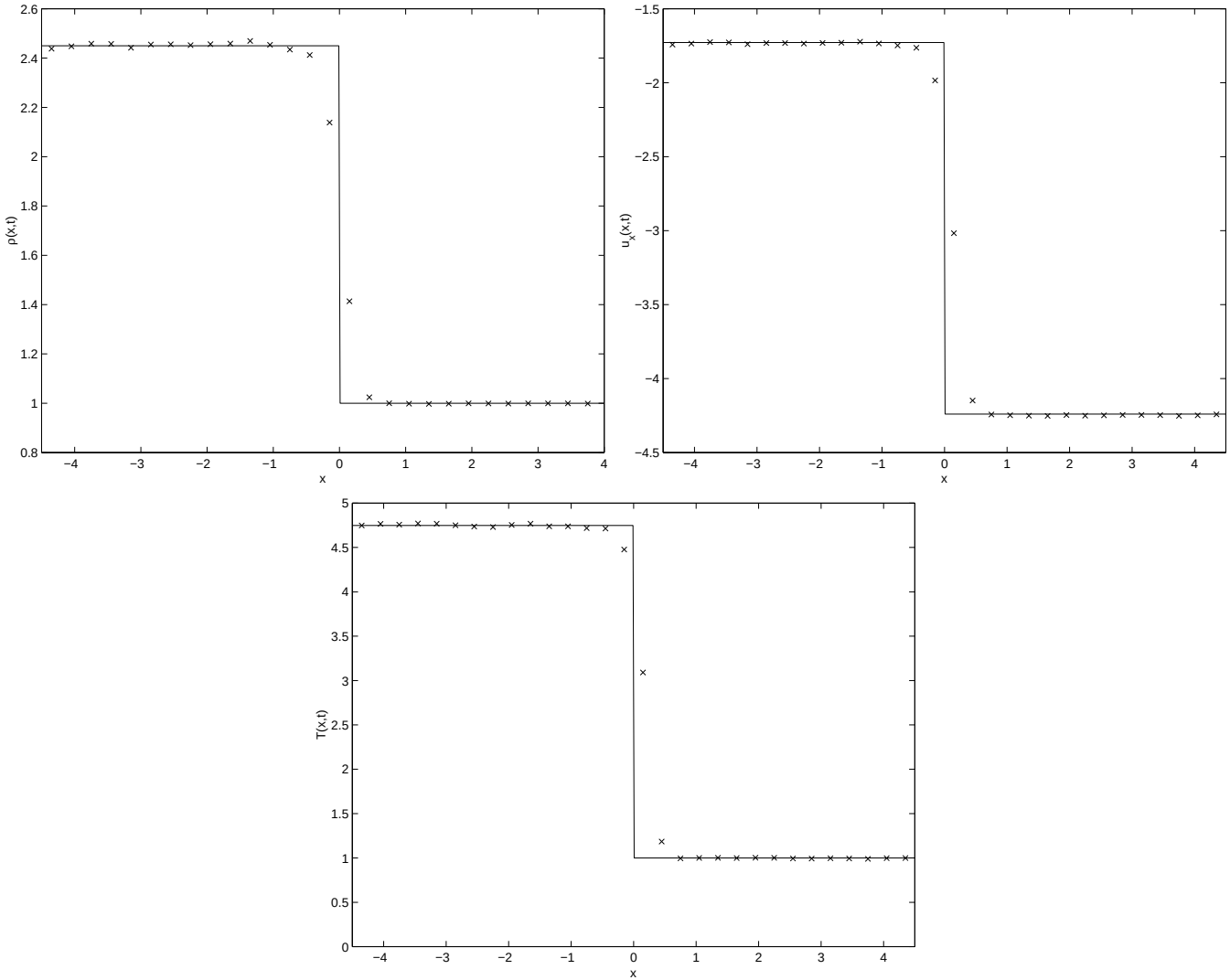
Shock profile intermediate regime

1D shock profile: DSMC($+$) and first order APMC ($\times$) (top), second order ($*$) and third order ($\circ$) APMC (bottom) for $\epsilon = 0.1$ and $\Delta t = 0.0025$ for DSMC, $\Delta t = 0.025$ for APMC. From left to right: ρ, u, T. The line is the reference solution.

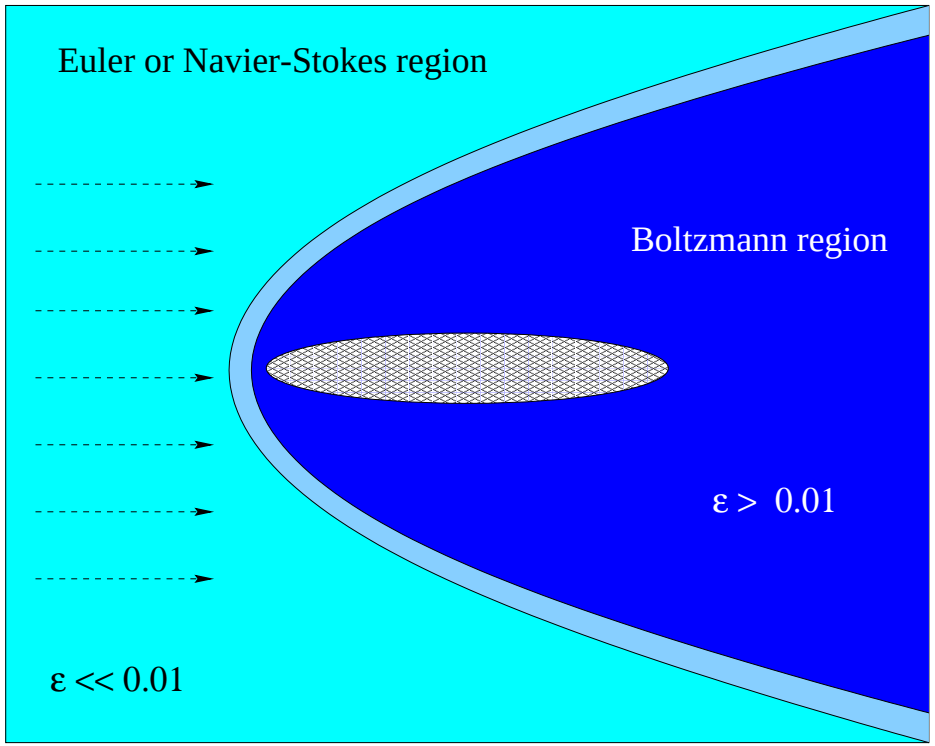


Shock profile fluid regime

1D shock profile: First order APMC ($\times$) for $\epsilon = 10^{-6}$ and $\Delta t = 0.025$. From left to right: ρ, u, T.



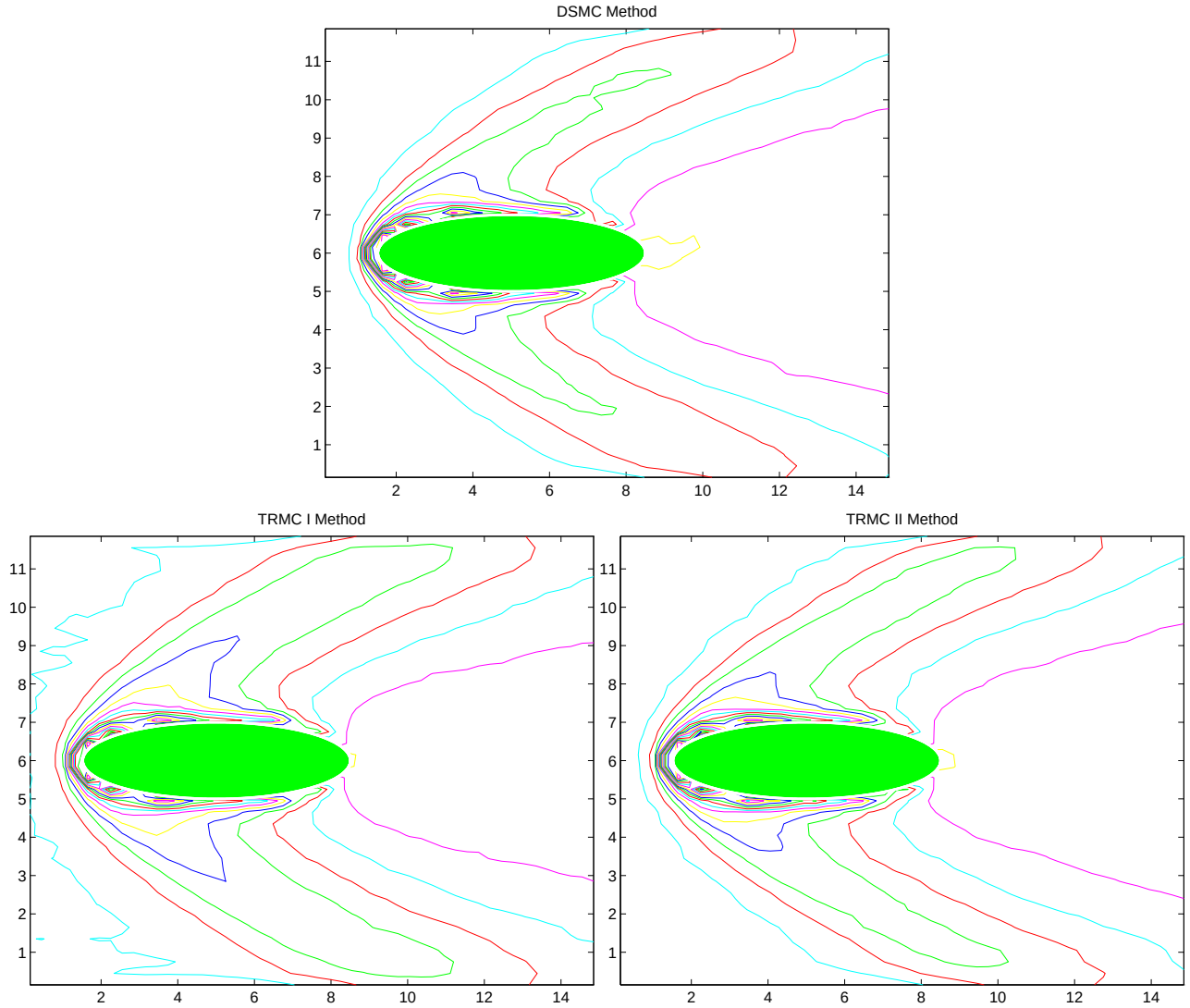
2D Flow past an ellipse



- NB, APMC1 and APMC2 schemes
- $Ma = 20$, $\rho_{inf} = 0.01$, $T_{inf} = 200$, $T_{obj} = 1000$, $\epsilon = 0.1, 0.01, 10^{-6}$
- Test problem : Hard spheres with 75×60 space cells and 100 particles in each cell at 'infinity'. Full accomodation boundary condition.

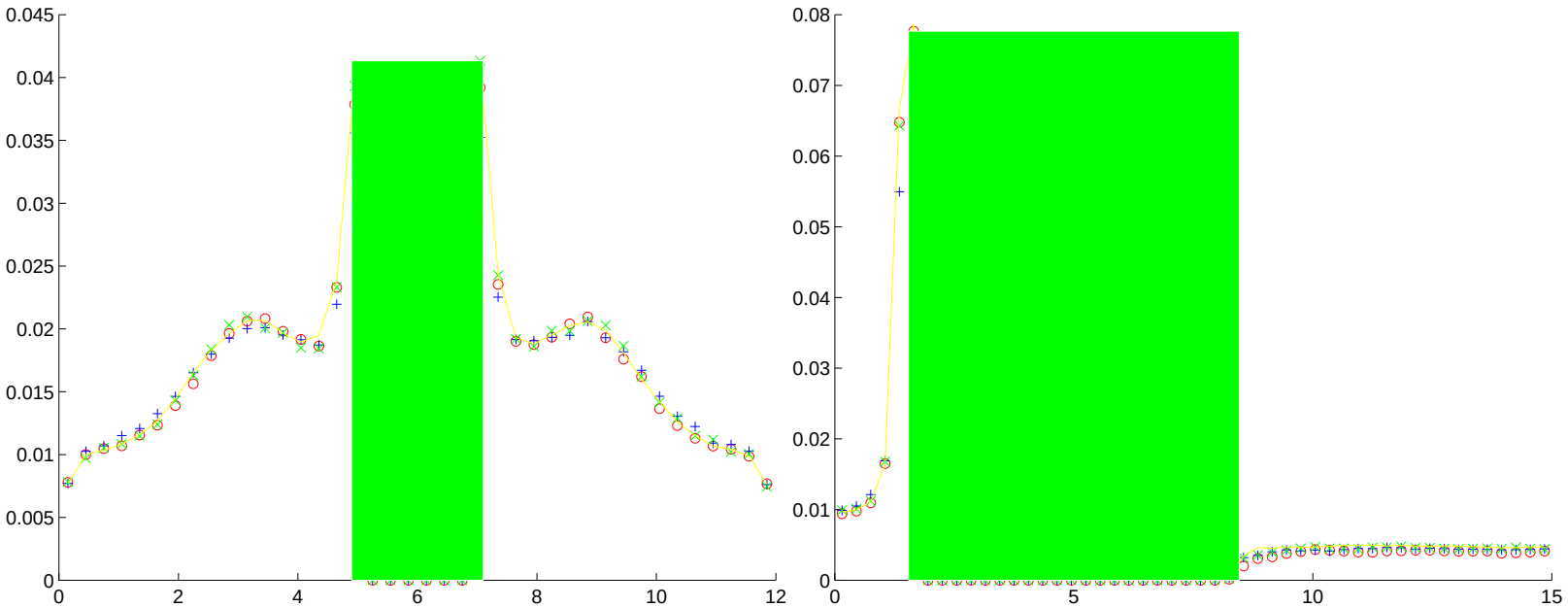
2D flow: $\varepsilon = 0.1$

NB, APMC1 and APMC2 solution for the mass ρ.



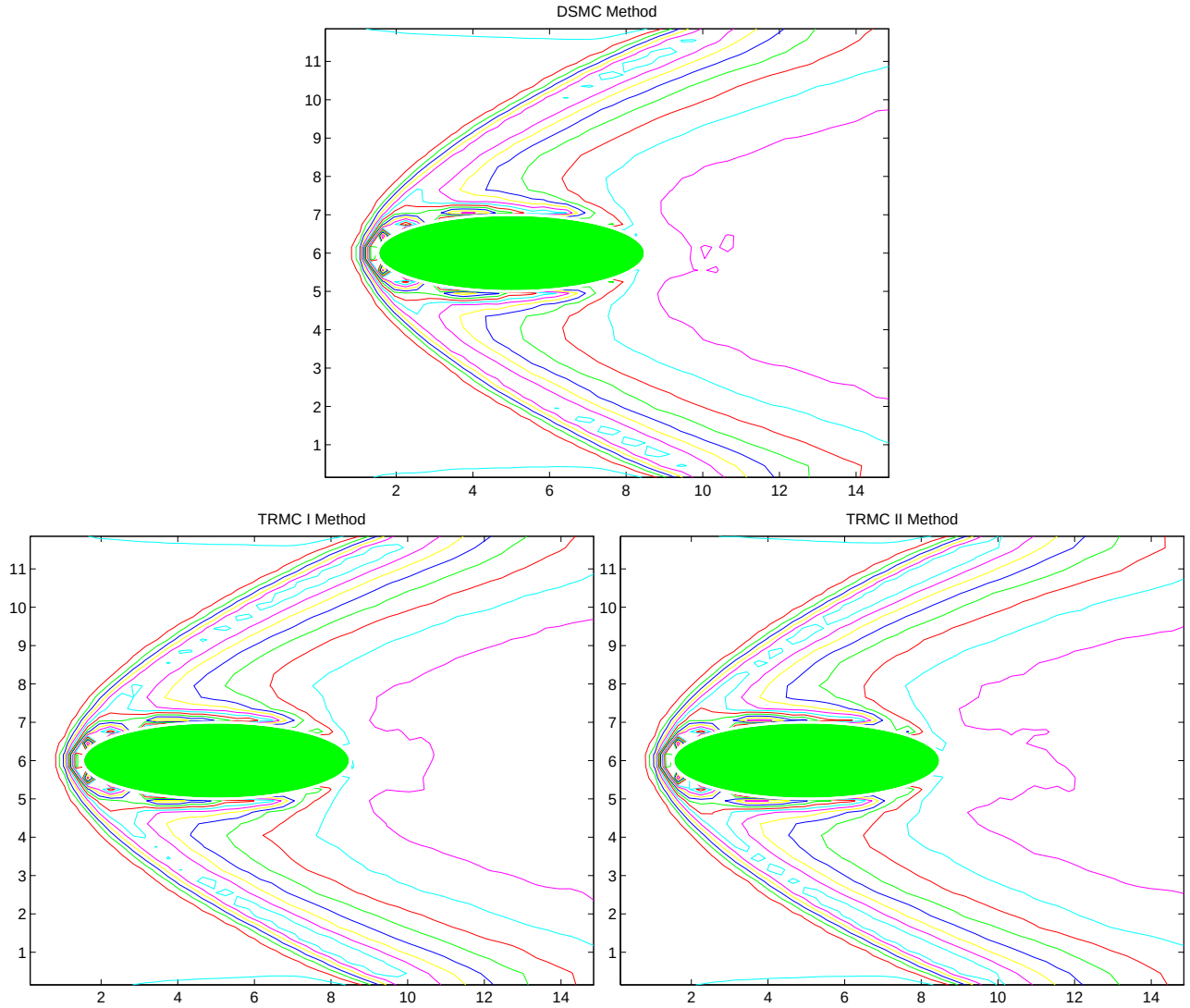
2D flow: $\varepsilon = 0.1$

Transversal and longitudinal sections for the mass ρ at $y = 6$ and $x = 5$ respectively for $\epsilon = 0.1$ and $M = 20$; DSMC-NB ($\circ$), APMC I ($+$), APMC II ($\times$).



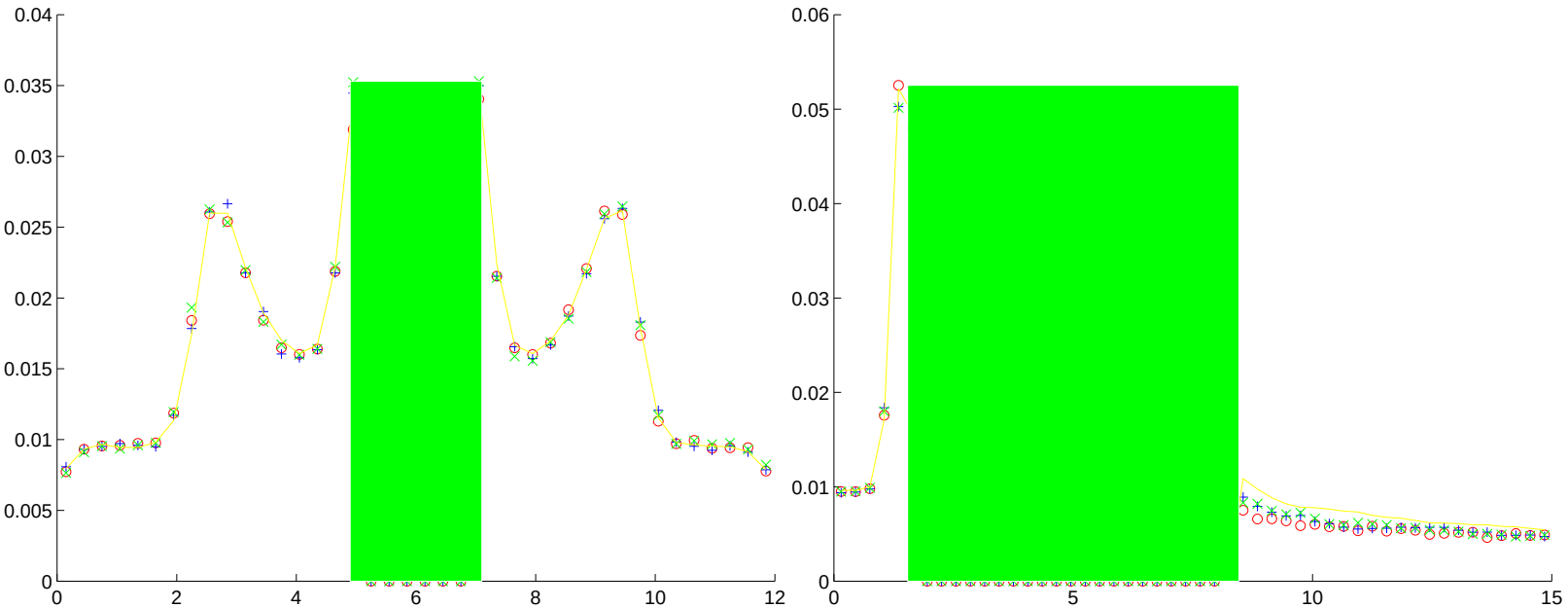
2D flow: $\varepsilon = 0.01$

NB, APMC1 and APMC2 solution for the mass ρ.



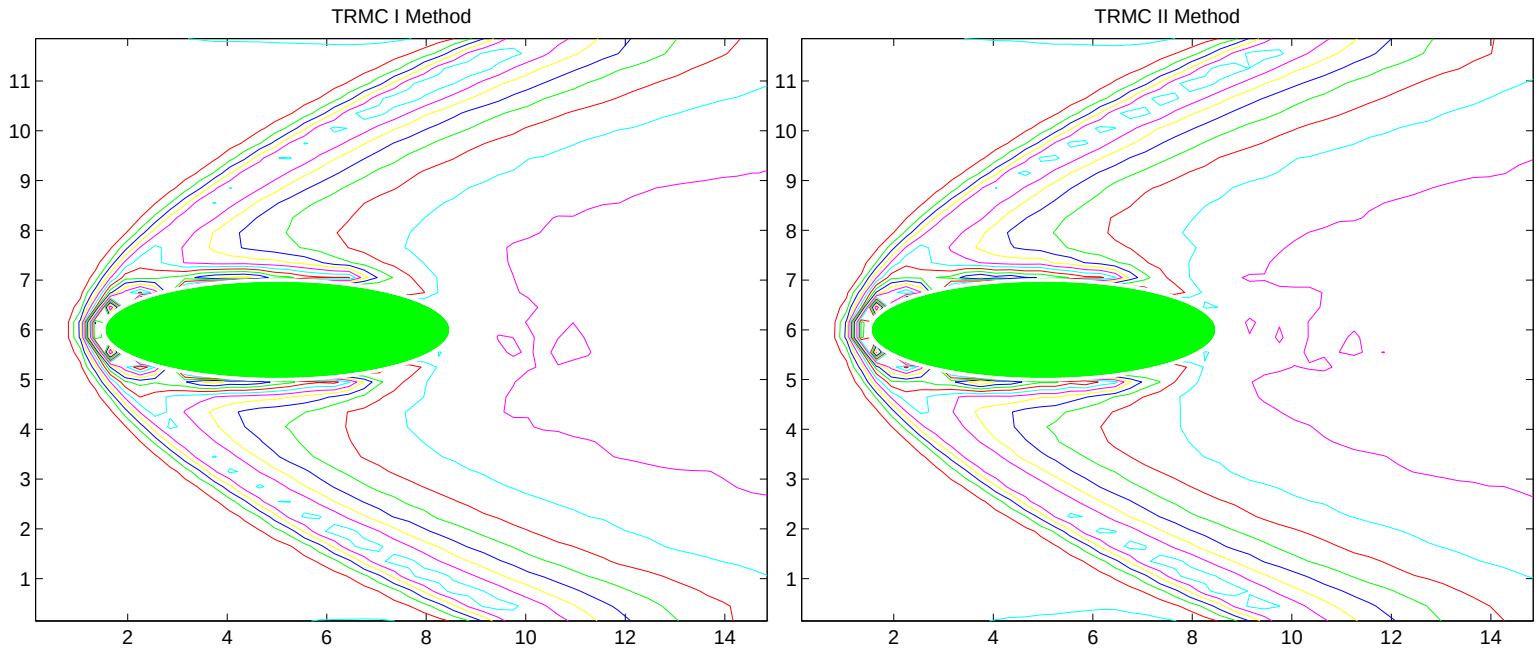
2D flow: $\varepsilon = 0.01$

Transversal and longitudinal sections for the mass ρ at $y = 6$ and $x = 5$ respectively for $\epsilon = 0.1$ and $M = 20$; DSMC-NB ($\circ$), APMC I ($+$), APMC II ($\times$).



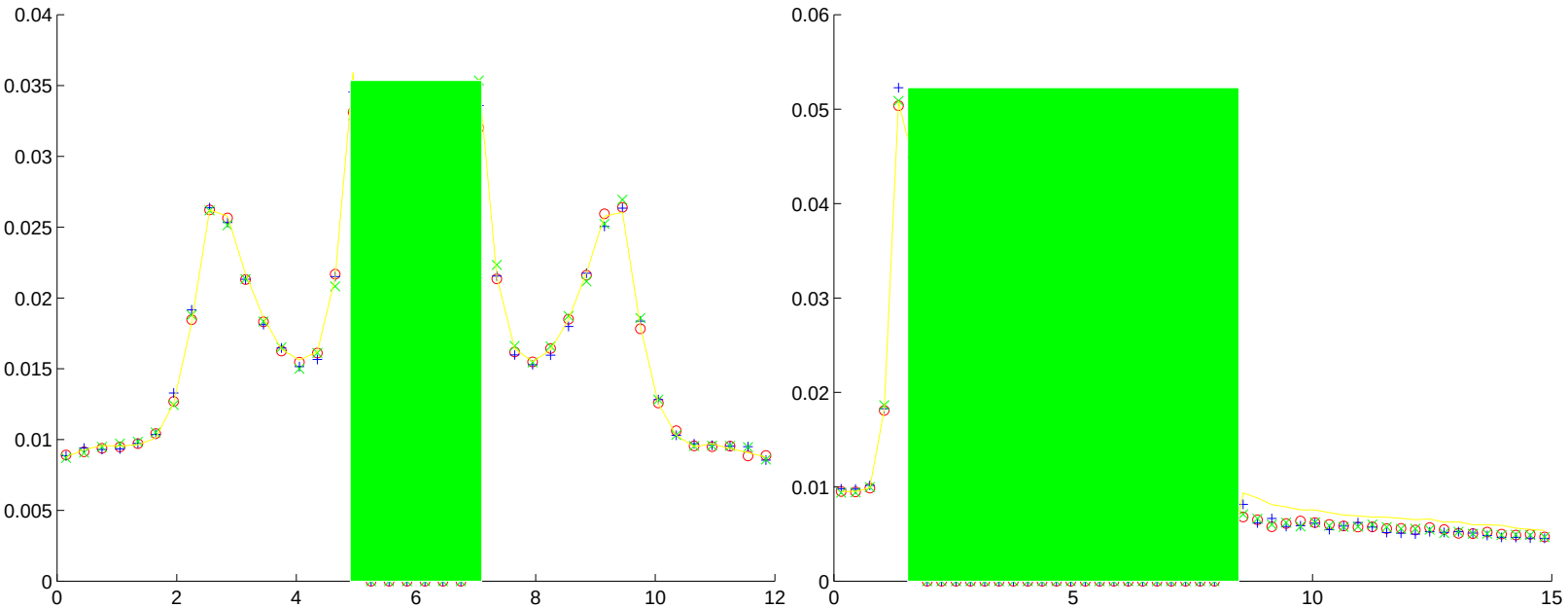
2D flow: $\varepsilon = 10^{-6}$

NB, APMC1 and APMC2 solution for the mass ρ.



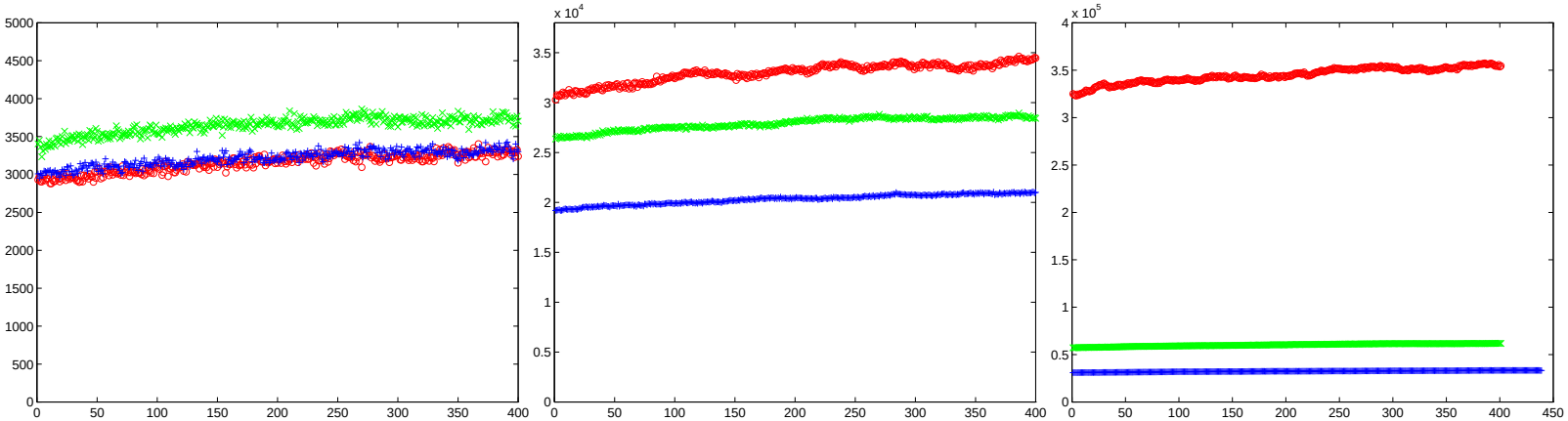
2D flow: $\varepsilon = 10^{-6}$

Transversal and longitudinal sections for the mass ρ at $y = 6$ and $x = 5$ respectively for $\epsilon = 0.1$ and $M = 20$; DSMC-NB ($\circ$), APMC I ($+$), APMC II ($\times$).



2D flow: Number of "Collisions"

From left to right $\epsilon = 0.1, 0.01, 0.001$; NB ($\circ$), APMC1 ($+$), APMC2 ($\times$).



Further developments

- There are many different possible improvements of DSMC methods. Typically these methods tackle particular situations like the case of low Mach number flows[12] and simulation of rare events (Stochastic Weighted Particle methods). [13]
- Hybrid Monte Carlo methods: Couplings of microscopic stochastic models to macroscopic deterministic models is highly desirable in many applications. Similar arguments apply also to numerical methods[14]. Main advantages are reduced variance and improved efficiency close to fluid regimes.
- Hydro-guided Monte Carlo: The basic idea consists in obtaining reduced variance Monte Carlo methods forcing particles to match prescribed sets of moments given by the solution of deterministic macroscopic fluid equations[15]. A similar idea has been used in Information Preserving Monte Carlo. [16]

[12] N. Hadjiconstantinou, T. Homolle, '07
[13] S.Rjasanow, W.Wagner, '05
[14] W.E, B.Engquist '03, L.P. '05, L.P., G.Dimarco '06, '08
[15] P.Degond, G.Dimarco, L.P., '09
[16] Q.Sun, D.Boyd, '02.