Monte Carlo methods for kinetic equations

Lecture 3: Fluid-limit and TRMC methods

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Outline

Motivations

- One of the major computational challenges in *rarefied gas dynamic* (RGD) simulations is the difficulty to compute regimes where the collisional time becomes very small.
- A nondimensional measure of the significance of collisions is given by the *Knudsen number*, which is small in the fluid dynamic limit and large in the rarefied state. For small Knudsen numbers most numerical methods lose their efficiency because they are forced to operate on a very short time scale.
- This difficulty is present, at different levels, both in *deterministic* as well as in *stochastic methods* such as Nanbu and Bird's method.

Main goal

The goal of *time relaxed Monte Carlo* (TRMC) methods[1] is to construct simple and efficient numerical methods for the solution of RGD problems in regions with a large variation in the mean free path.
As a consequence TRMC methods have the following features

- for large Knudsen numbers, the TRMC 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;
- mass, momentum, and energy are preserved.

In the sequel we will present some recent advances in this direction based on the use of *recursivity* and *adaptivity*[2].

[1] L.Pareschi, G.Russo SISC '01
[2] L.Pareschi, S.Trazzi, B.Wennberg SISC '08

Exponential expansions

Let us consider a kinetic equation of the type

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

with initial condition $f(v,0) = f^0(v)$, and where $\mu > 0$ and P a bilinear operator. The solution of such equation admits the following *exponential expansion*[3]

$$f(v,t) = e^{-\mu t/\varepsilon} \sum_{k=0}^{\infty} (1 - e^{-\mu t/\varepsilon})^k f_k(v),$$

where the functions f_k are given by the recurrence formula

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

It is obtained from a Taylor expansion with respect to the *relaxed variables*

$$\tau = (1 - e^{-\mu t/\varepsilon}), \qquad F(v,\tau) = f(v,t)e^{\mu t/\varepsilon}.$$

[3] E. Wild '51

Application to the Boltzmann equation

The starting point of most numerical methods for the Boltzmann equation is a *first order splitting* in time, which consists of solving separately a purely convective step (i.e., $Q \equiv 0$) and a collision step characterized by a space homogeneous equation.
After this splitting, most of the main computational difficulties are contained in the *collision step*

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

Assuming that the collision kernel is bounded by Σ taking $P(f, f) = Q(f, f) + \mu f$, with $\mu \geq 4\pi\rho\Sigma$ then the solution can be written in the above exponential expansion form.
In this case, an important property of the coefficients $f_k(v)$ appearing in the expansion is that they are nonnegative and that

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

Thus the exponential expansion has the nice property of being a convex combination of nonnegative functions with the same moments of order $0, 1$ and 2.

Simple exponential schemes

In a time step Δt a simple truncation at the order m of the series is given by

$$f^{n+1}(v) = (1 - A(\Delta t)) \sum_{k=0}^{m-1} A(\Delta t)^k f_k^n(v) + A(\Delta t)^m f_m^n(v),$$

where $f^n = f(n\Delta t)$ and $A(\Delta t) = 1 - e^{-\mu \Delta t/\varepsilon}$. The methods can be seen as a particular class of *exponential integrators*[4] and are exact for any linear operator

$$Q(f, f) = \mu(G - f),$$

with $G = G(v)$ an arbitrary given function.
If we define the function $\varphi(\Delta t) = \frac{A(\Delta t)}{\mu \Delta t/\varepsilon}$, the first order scheme reads

$$f^{n+1}(v) \quad = \quad f^n(v) + \varphi(\Delta t) \frac{\Delta t}{\varepsilon} Q(f^n, f^n),$$

which is the *explicit exponential Euler method*. Note that, if μ is a sufficiently accurate estimate of the Jacobian of $Q(f, f)$ then the method is of order 2.

[4] M.Hochbruck, C.Lubich, H.Selhofer '98, M.Banda, G.Dimarco, L.Pareschi '08

Time relaxed schemes

Since the coefficients f_k in the exponential expansion are characterized by successive applications of the collision operator, it is natural to expect that

$$\lim_{k\to\infty} f_k(v) = \lim_{t\to\infty} f(v,t) = M(v),$$

where $M(v) = M[f](v)$ is the local Maxwellian equilibrium[5].
Using this remark, we consider a *Maxwellian truncation* for $k > m \geq 1$ to get[6]

$$f^{n+1}(v) = (1 - A(\Delta t)) \sum_{k=0}^{m} A(\Delta t)^k f_k^n(v) + A(\Delta t)^{m+1} M(v).$$

Since M has the same moments of f^n then f^{n+1} is a convex combination of density functions. The schemes are *conservative* and *asymptotic preserving* ($f^{n+1}(v) \to M(v)$ as $\varepsilon \to 0$).
Moreover they are exact for linear problems like

$$Q(f,f) = \mu(M - f).$$

[5] E.Carlen, M.Carvalho, E.Gabetta, '00
[6] E.Gabetta, L.Pareschi, G.Toscani '97

Generalized TR schemes

Generalized schemes can be derived, of the following form

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

The weights $A_k = A_k(\tau)$ are nonnegative function that satisfy the following properties

- i)*conservation :*

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

- ii)*asymptotic preserving :*

$$\lim_{\tau \to 1} A_k(\tau) = 0, \quad k = 0, \dots, m$$

- iii)*consistency :*

$$\lim_{\tau \to 0} A_1(\tau)/\tau = 1, \quad \lim_{\tau \to 0} A_k(\tau)/\tau = 0, \quad k = 2, \dots, m+1$$

Remarks

- For both classes of methods we have the *monotonicity property* $H(f^{n+1}) \leq H(f^n)$ (where H is for example the entropy functional) at any order m of the numerical schemes provided that[7]

$$H\left(\frac{P(f,f)}{\mu}\right) \leq H(f).$$

  In fact, using the recursive representation of the coefficients it follows that

$$H(f_{k+1}) \leq H(f_k), \quad \forall\, k$$

  and hence since $H(M) \leq H(f_k), \forall\, k$ by convexity we obtain the monotonicity property.

- 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.

[7] A.Bobylev, G.Toscani '92

Time Relaxed Monte Carlo Methods

First order TR scheme (TRMC1):
Form $m = 1$ the generalized TR 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 TRMC scheme

Form $m = 2$ the generalized TR 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 TRMC methods can be constructed similarly.

Numerical results

1D Shock wave profiles

Comparison between:
NB, TRMC1, TRMC2, TRMC2
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

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

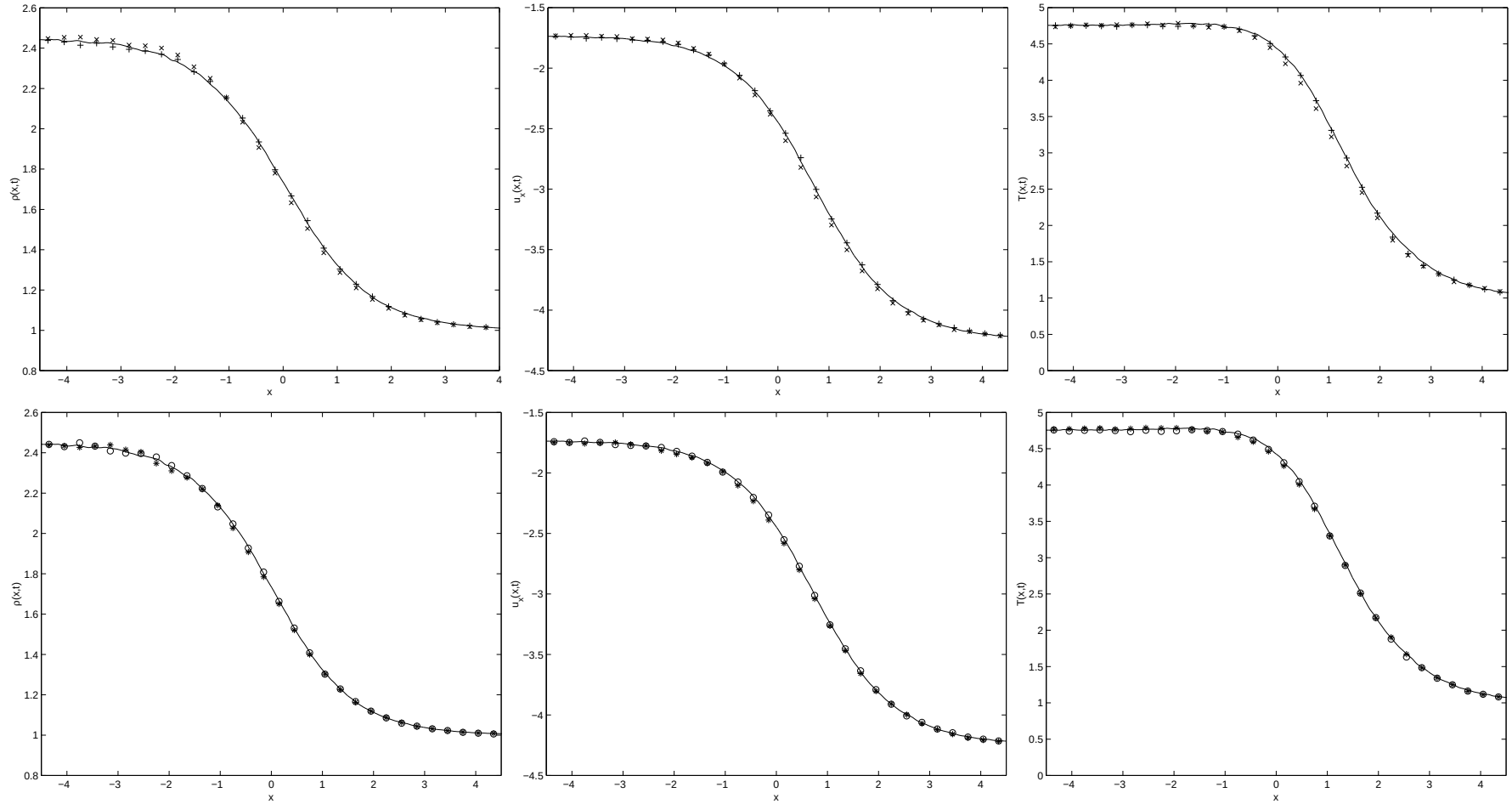
with $\gamma = 5/3$
The values for ρ, u and T for $x < 0$ are given by the Rankine-Hugoniot conditions.
Test problem :

- *Hard spheres*: $50 - 100$ space cells and 500 particles in each cell on $x > 0$. The reference solution is obtained with 200 space cells and 500 particles in each cell on $x > 0$.

Remark: Since we have a stationary shock wave the accuracy of the methods can be increased by computing averages on the solution for $t \gg$.

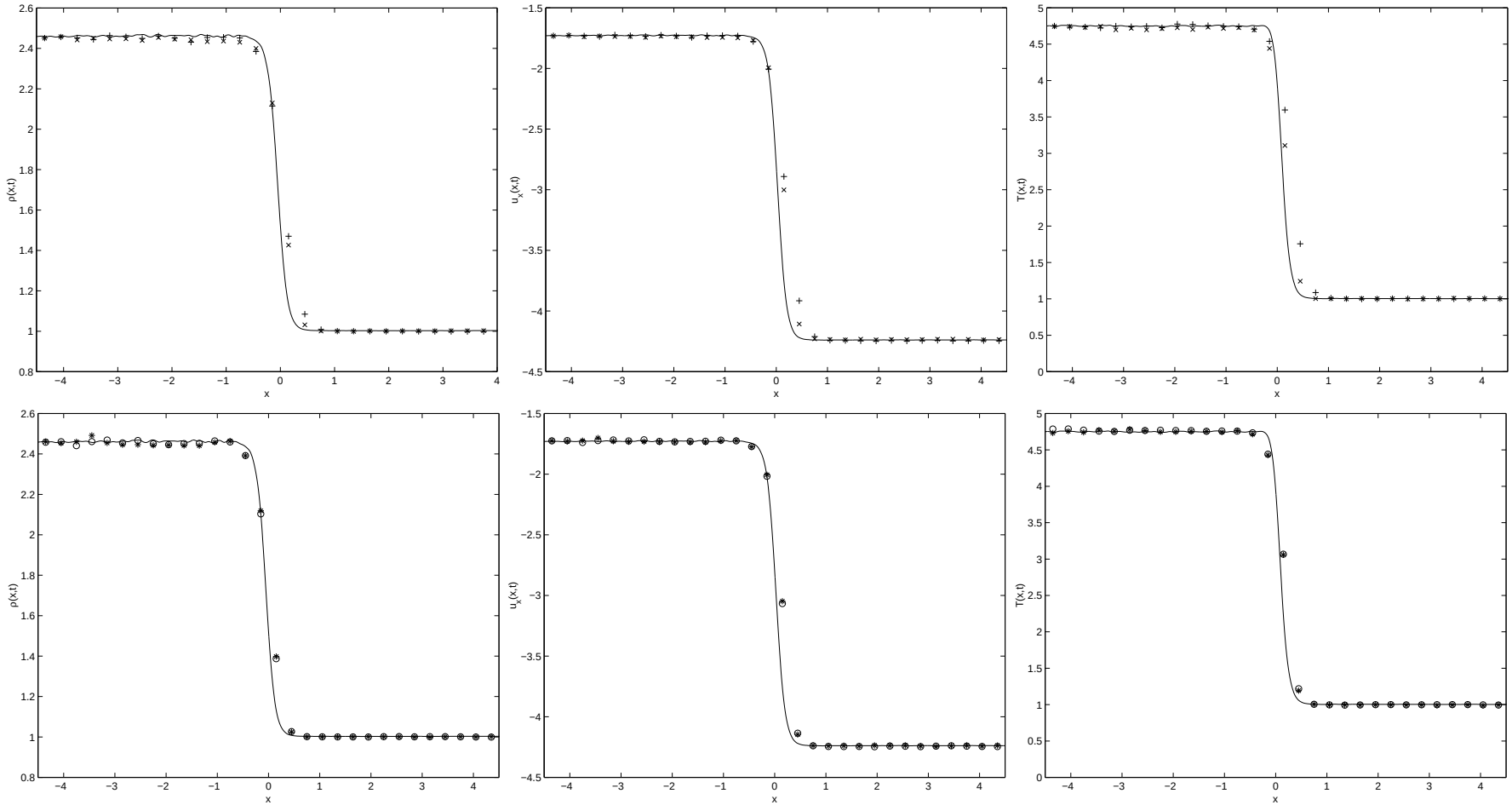
Shock profile rarefied regime

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



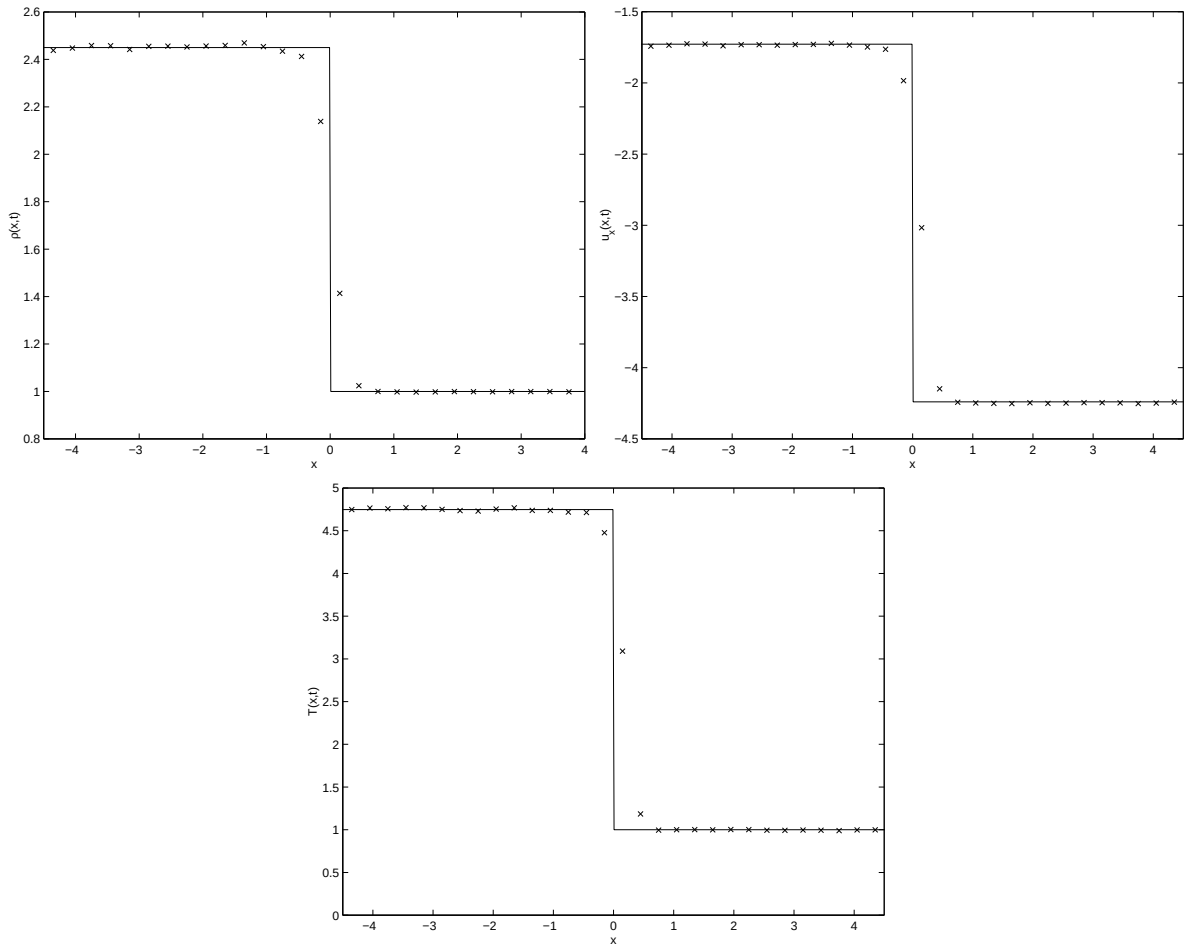
Shock profile intermediate regime

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

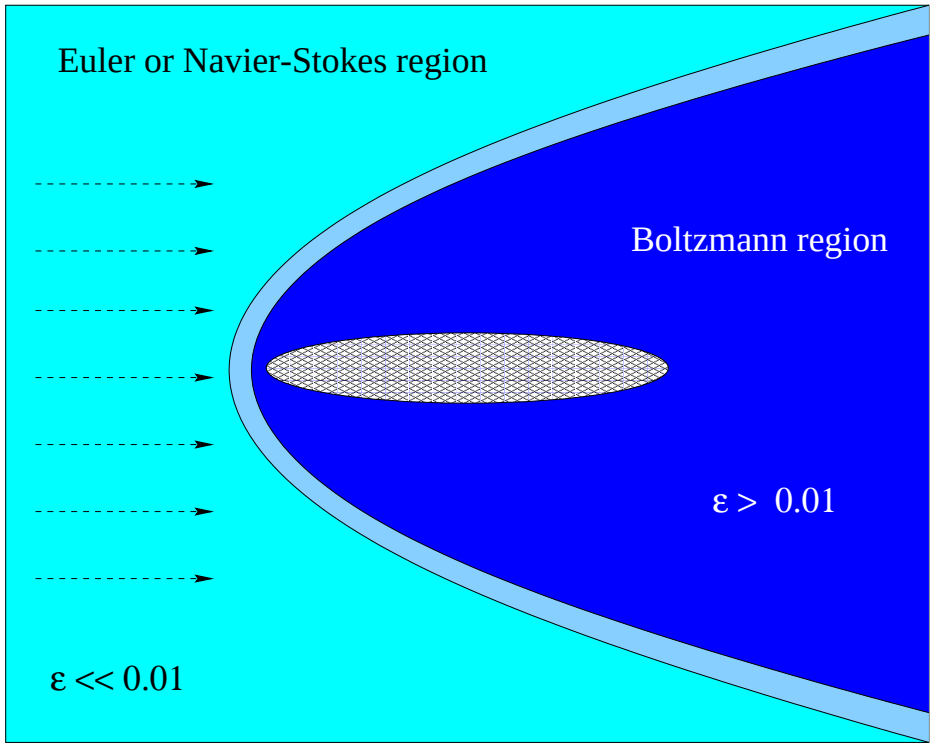


Shock profile fluid regime

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



2D Flow past an ellipse



NB, TRMC1 and TRMC2 schemes

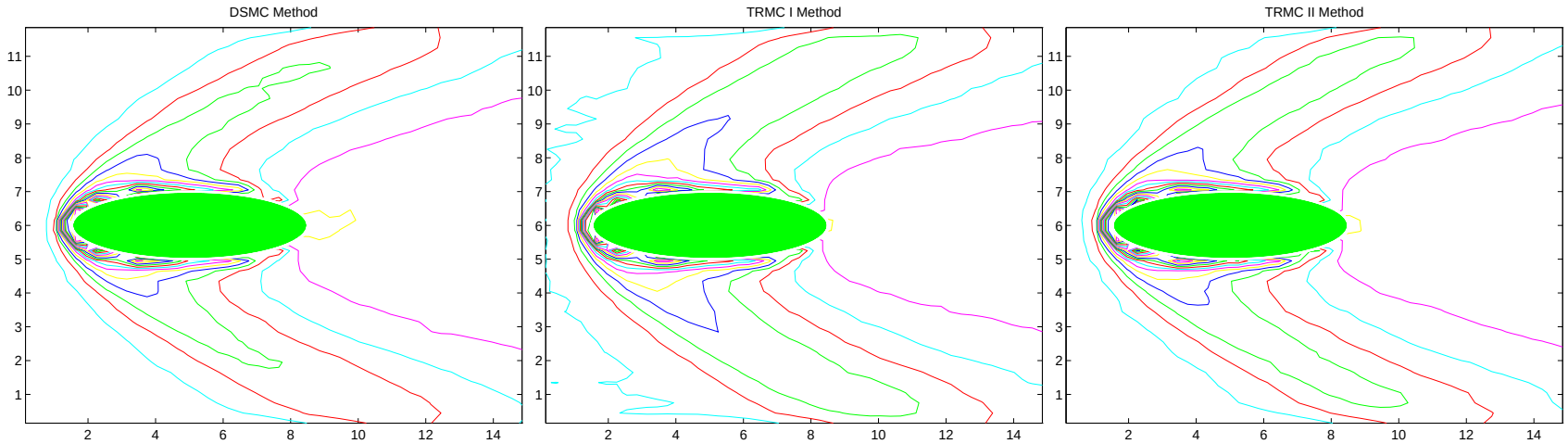
$Ma = 20$, $\rho_{inf} = 0.01$, $T_{inf} = 200$, $T_{obj} = 1000$, $\epsilon = 0.1, 0.01, 10^{-6}$

Test problem :

• *Hard spheres*: 75×60 space cells and 100 particles in each cell at 'infinity'. Full accomodation boundary condition.

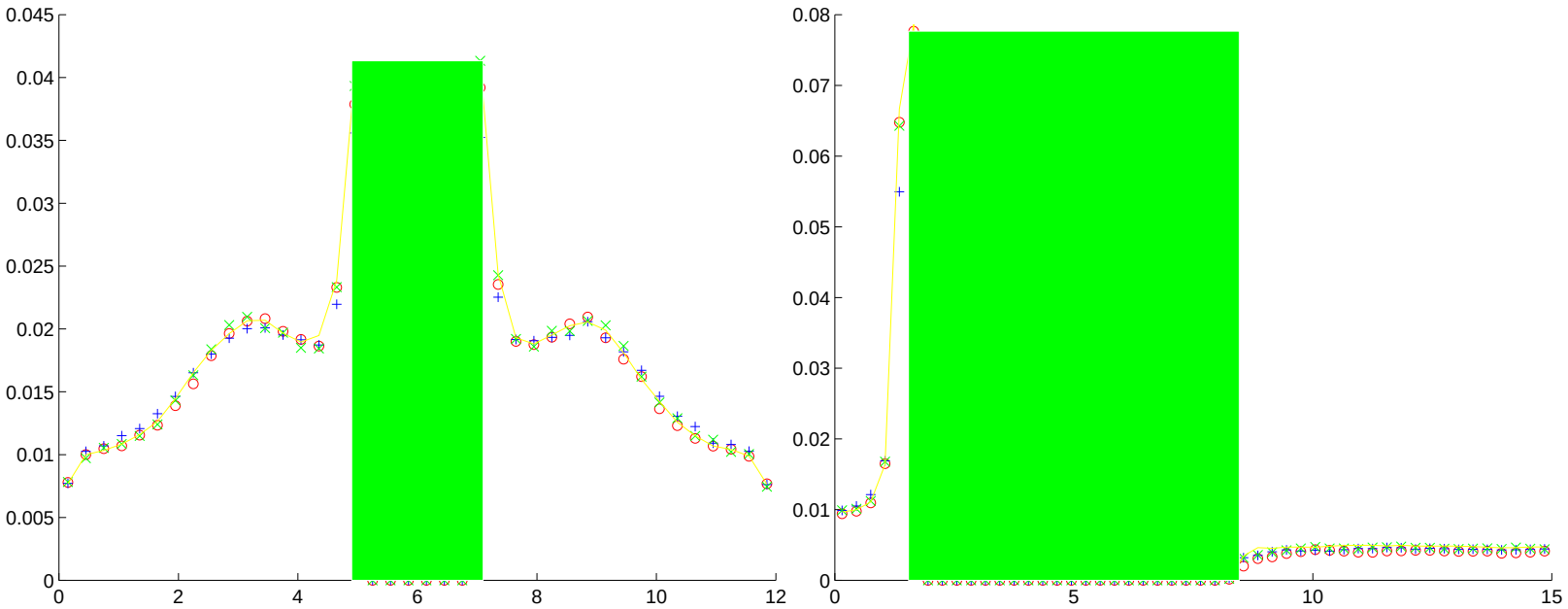
2D flow: $\varepsilon = 0.1$

NB, TRMC1 and TRMC2 solution for the mass ρ.



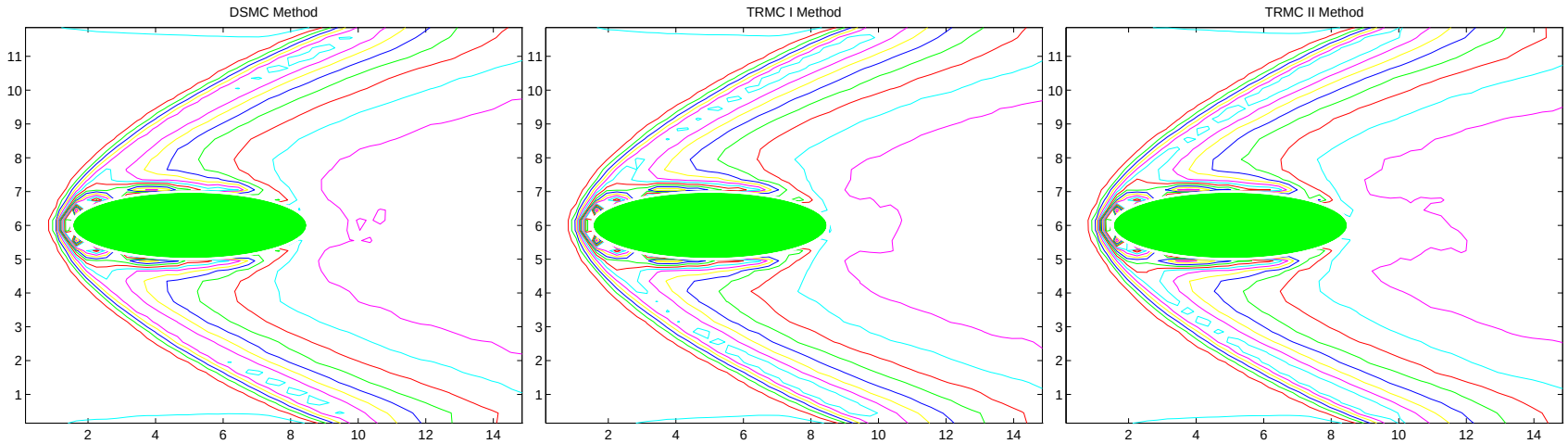
2D flow: $\varepsilon = 0.1$

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



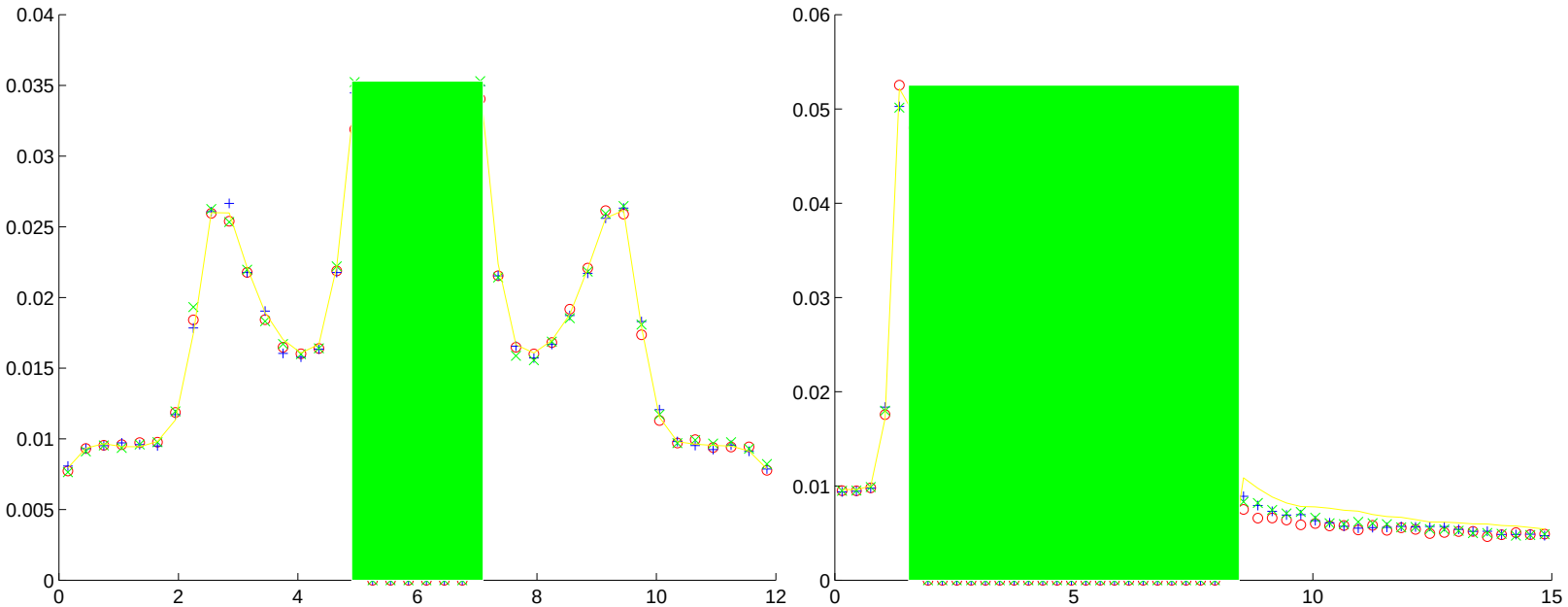
2D flow: $\varepsilon = 0.01$

NB, TRMC1 and TRMC2 solution for the mass ρ.



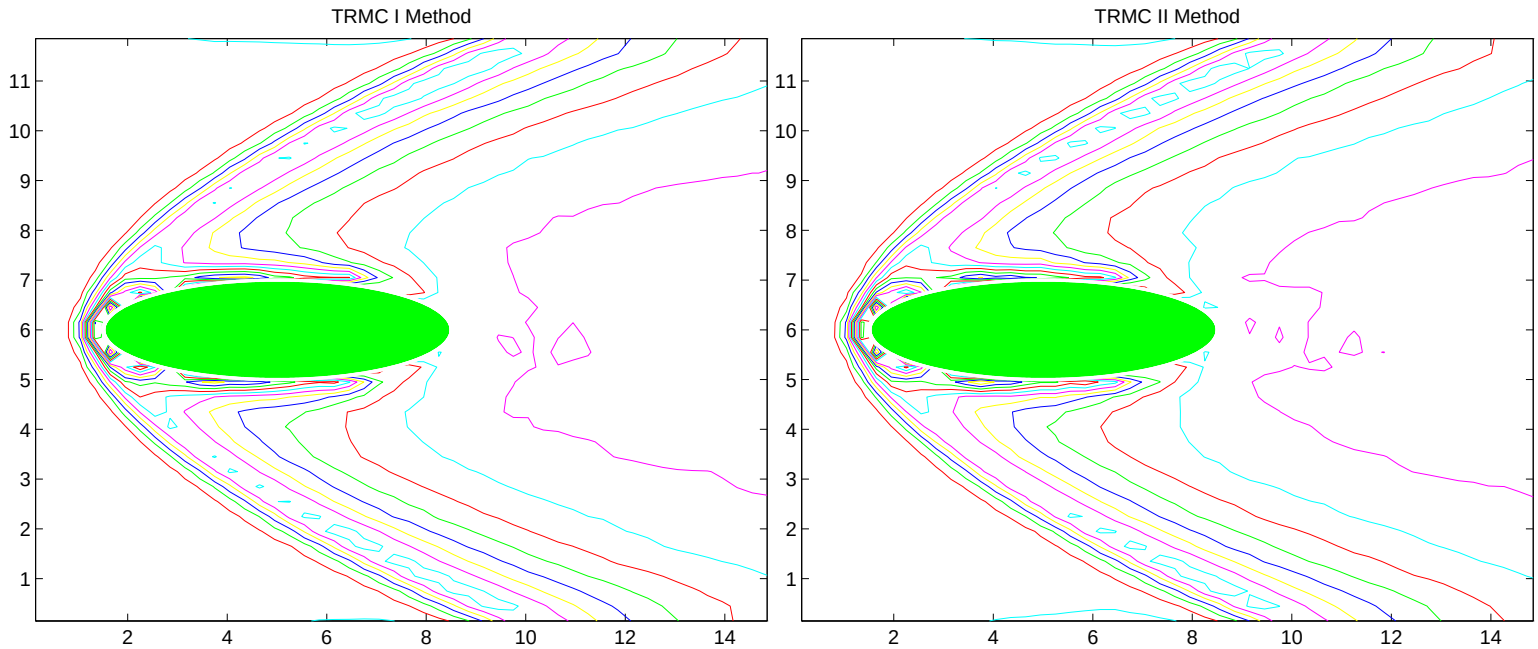
2D flow: $\varepsilon = 0.01$

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



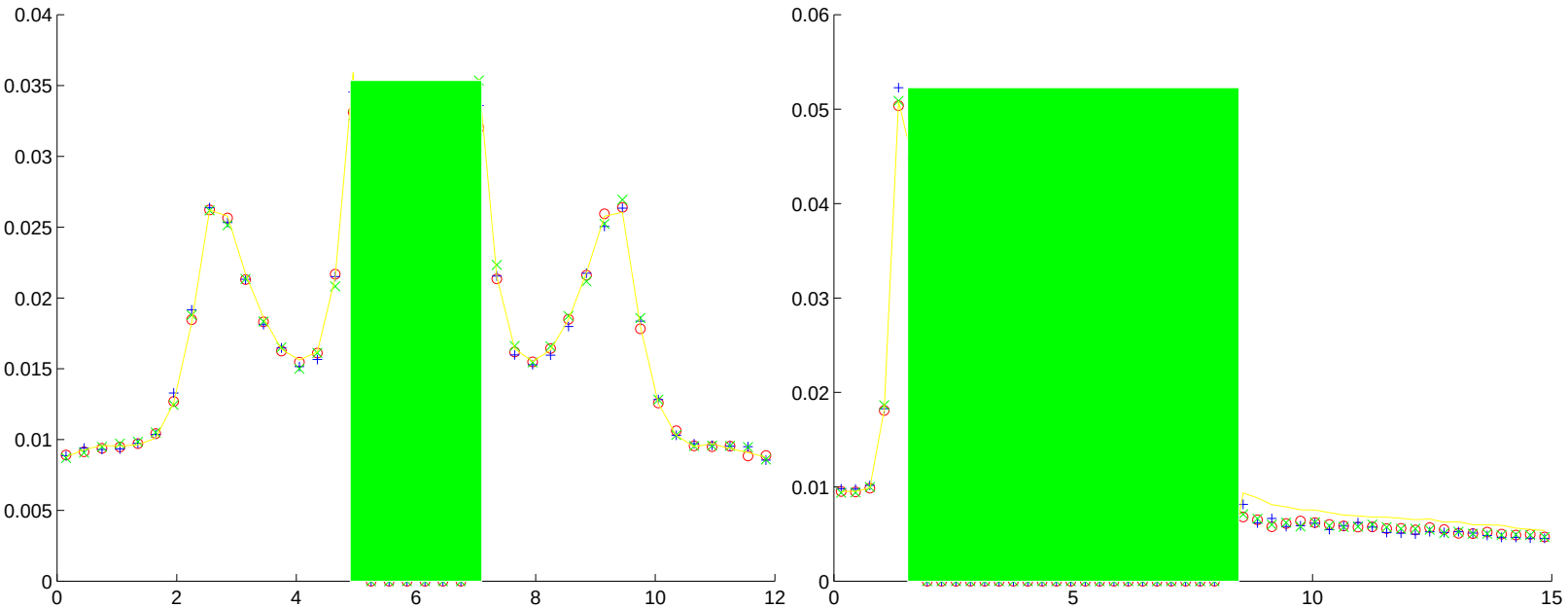
2D flow: $\varepsilon = 10^{-6}$

NB, TRMC1 and TRMC2 solution for the mass ρ.



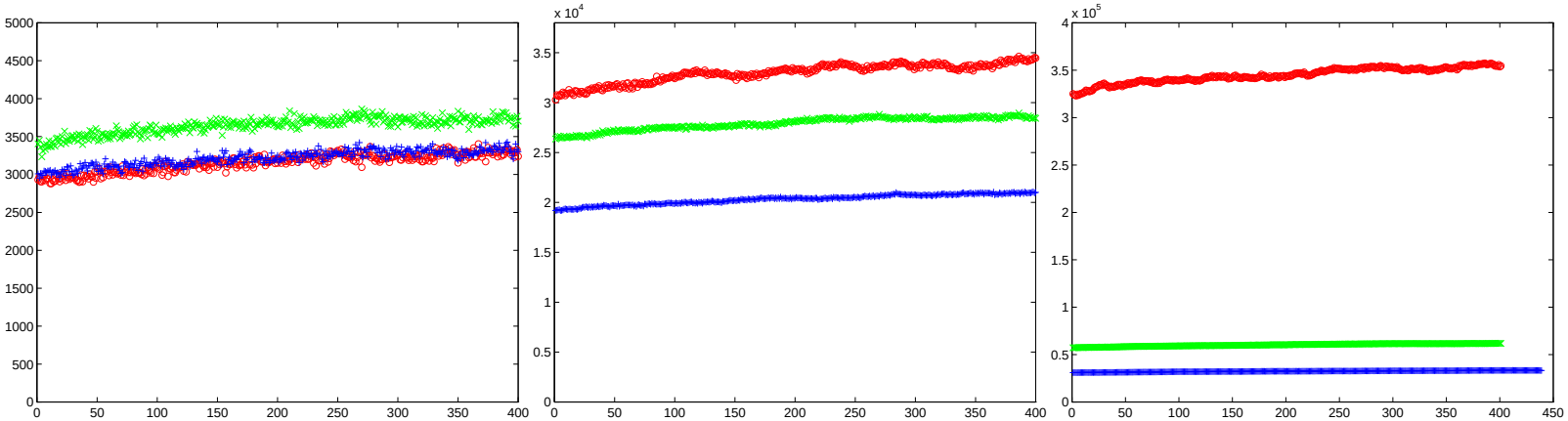
2D flow: $\varepsilon = 10^{-6}$

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



2D flow: Number of "Collisions"

From left to right $\epsilon = 0.1, 0.01, 0.001$; NB ($\circ$), TRMC1 ($+$), TRMC2 ($\times$).



Recursive sampling

Let us first consider the simpler case of a *Maxwellian kernel* and show how we can sample from the whole exponential expansion

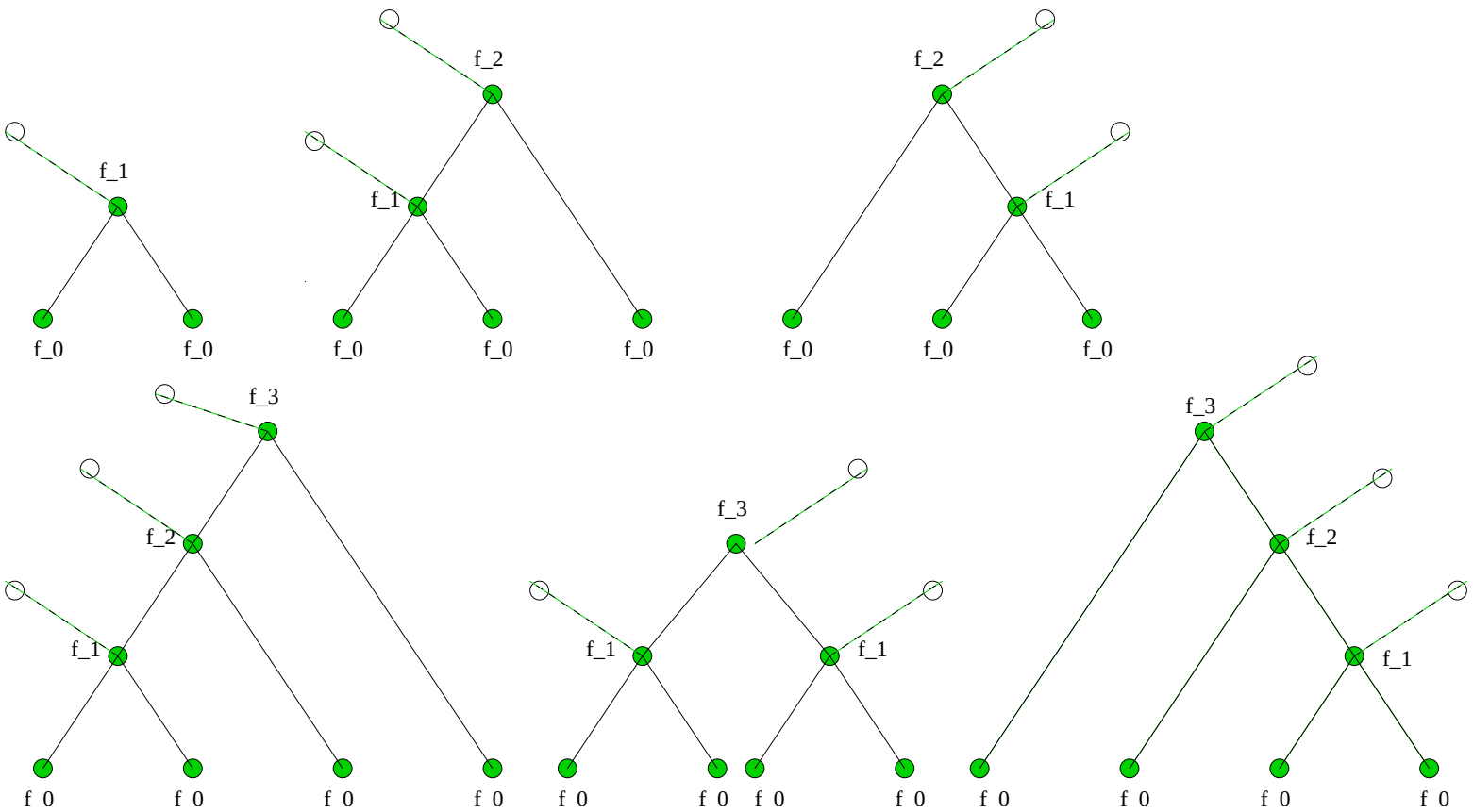
$$f^{n+1}(v) = e^{-\mu\Delta t/\varepsilon} \sum_{k=0}^{\infty} (1 - e^{-\mu\Delta t/\varepsilon})^k f_k^n(v).$$

This sum has a clear probabilistic interpretation.

- The distribution of particles that do not collide is just f_0 and the probability of this event is $e^{-\mu\Delta t/\varepsilon}$.
- In the same way f_1 is the velocity distribution for particles which have been involved in exactly one collision, and the probability of that is $e^{-\mu\Delta t/\varepsilon}(1 - e^{-\mu\Delta t/\varepsilon})$.
- At least f_m is the velocity distribution given that exactly $m+1$ particles have been involved in their collision history back to the initial time. To be able to find a sample of f_m, we must assume that the densities $f_k, 0 \leq m-1$ are all already known. Off course the only one of these that is really known is f_0, the initial distribution.

Collision trees

It is useful to use a representation of the collision process through the *collision trees*, sometimes called *Mc Kean graphs*. Note that "re-collisions" are not allowed.



Mc Kean graphs for f_1, f_2 and f_3

Structure of the recursive sampling algorithm

- The velocity distribution f_k can be drawn from the starting distribution f_0, choosing the different collisional trees with the same probability in mean. In general we need $k+1$ particles from f_0 to get two particles from f_k.
- Two particles are produced in every collisional event (as in standard DSMC), and only one of these is used to complete the collisional process.
- The particle not used is stored in a list, for its direct utilization in a future collisional process. In this way we can increase the efficiency of the method (if a particle sampled from a velocity density f_k already exist it will not be necessary to obtain it by the complete collisional process).
- If we start from a finite set of N particles initially then the above strategy yields a natural truncation of the sum, since the maximum possible length of a collision process is $m_{max} = N - 1$, and guarantees the exact conservation of moments.

Recursive Time relaxed Monte Carlo

The methods can be generalized to time relaxed approximations of order m

$$f^{n+1}(v) = (1 - A(\Delta t)) \sum_{k=0}^{m} A(\Delta t)^k f_k^n(v) + A(\Delta t)^{m+1} M(v),$$

with $A(\Delta t) = 1 - \exp(-\mu \Delta t/\varepsilon)$.
Let us start from a set of N particles initially[8].

- We split the N particles into m collision sets N_i, $i = 0, \ldots, m$ where each set N_i characterizes the particles that undergo i collisions in a time step Δt.
- Sampling starts recursively from f_m and then in decreasing order $f_{m-1}, f_{m-2}, \ldots, f_1, f_0$.
- All particles having more then m collisions in the time step are thermalized (i.e. replaced with an equilibrium particle taken from the local Maxwellian).

Note that if m is too large compared to the initial number of particles then thermalization never occurs.

[8] L.Pareschi, B.Wennberg '01

A numerical example

Maxwell molecules in 2D, $N = 10^5$ particles, $\Delta t = t$. Relative L_2 error norm in time for the *Ernst-Bobylev solution*.

m_{max}	1000	100	25	
$t = 0$	0.013312	0.013312	0.013312	
$t = 1$	0.012055	0.012055	0.012055	$m = 22$
$t = 2$	0.012209	0.012209	0.012114	$m = 64$
$t = 3$	0.012389	0.013130	0.013446	$m = 156$
$t = 5$	0.012737	0.013762	0.016806	$m = 881$
$t = 7$	0.011303	0.012881	0.014775	$m > 1000$
$t = 10$	0.011896	0.012847	0.012998	$m > 1000$
$t = 15$	0.012479	0.012479	0.012479	$m > 1000$

VHS collision kernels

- The simple recursive algorithm described for Maxwellian molecules can be extended to more general collision kernels by using "dummy" collisions and *acceptance-rejection technique*.
- This is equivalent to sample the post collisional velocity according to $P(f,f)/\mu$, where $\mu = 4\pi\Sigma$ and Σ is an *upper bound of the scattering cross section* for the given set of particles.
- The upper bound Σ should be chosen as small as possible, to avoid inefficient rejection, and it should be computed fast. Typically the upper bound used is $\Sigma = \sigma(2\Delta v)$,

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

- As a result of the acceptance-rejection technique we obtain longer (virtual) collision trees compared to the Maxwellian case.

Adaptive techniques

- In practical simulations the number m can be very large, depending on the Knudsen number, on the upper bound Σ and on the number of test particles.
- Small values of m make the algorithm faster, because the collision process is replaced by the projection to the local Maxwellian equilibrium, but far from the fluid regime keeping m too small can produce less accurate results.
- The main problem is to choose the right maximum depth of the trees, in order to have the best combination between *efficiency and accuracy*.
- One possibility is to use an *adaptive technique* based on evaluating the distance of the solution from the equilibrium through a suitable indicator. This can be performed measuring the *variation of some macroscopic variables* (such as the fourth order moment or the components of the shear stress tensor).

An example algorithm

Let S be the macroscopic variable selected. Then define the quantity

$$E_1 = \frac{|S^{n+1,m_{\max}} - S^n|}{|S^n|}.$$

that represents the relative variation at time step $n+1$ of the macroscopic variable S computed with the solution obtained using $m_{\max}$ as *maximum depth* of the collision trees.
If we fix an interval $[\delta_1, \delta_2]$, $0 < \delta_1 < \delta_2$ then we can apply the following criteria

- if $E_1 < \delta_1$ the solution is accepted and $m_{\max} = m_{\max}/2$ in the next time step $n+2$;
- if $\delta_1 \leq E_1 \leq \delta_2$ the solution is accepted and $m_{\max}$ is unchanged in the next time step $n+2$;
- if $E_1 > \delta_2$ the solution is discarded and the calculation is performed again using $m_{\max} = 2m_{\max}$.

Efficiency considerations

The algorithm has optimal efficiency if the collisions computed with the "wrong" $m_{\max}$ are kept and reused with $2m_{\max}$. This can be done observing that if

$$f^{n+1,m} = (1 - A(\Delta t)) \sum_{k=0}^{m} A(\Delta t)^k f_k + A(\Delta t)^{m+1} M$$

then

$$f^{n+1,2m} = f^{n+1,m} + (1 - A(\Delta t)) \sum_{k=m+1}^{2m} A(\Delta t)^k f_k + [A(\Delta t)^{2m+1} - A(\Delta t)^{m+1}] M$$

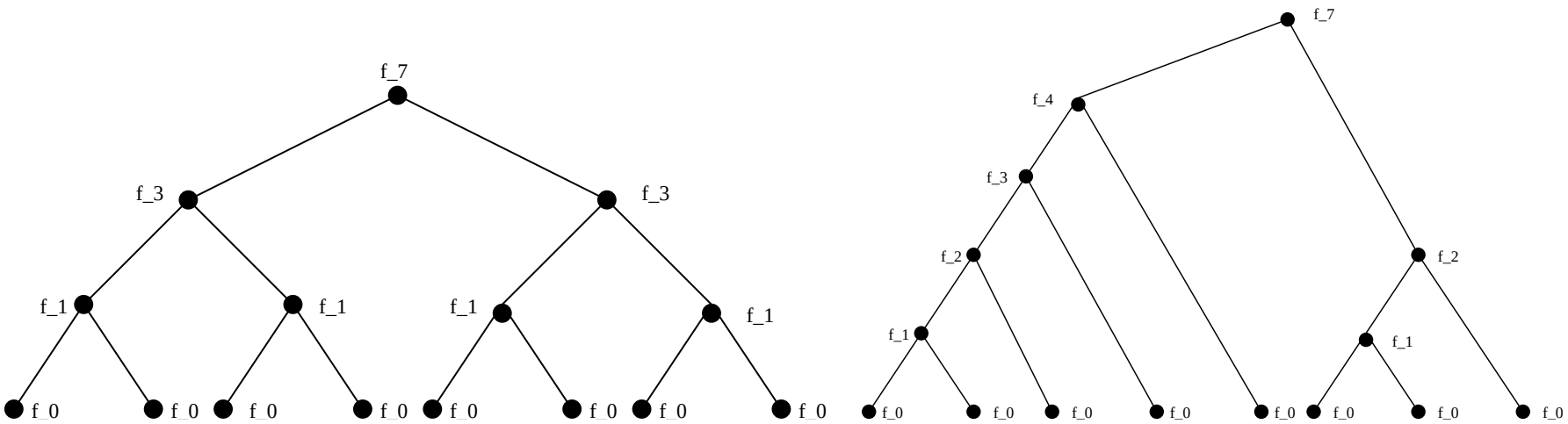
So when increasing the length of the trees we proceed as follows

- the collisions computed with m are kept;
- the fraction $A(\Delta t)^{m+1} M$ is discarded;
- the fraction $\sum_{k=m+1}^{2m} A(\Delta t)^k f_k$ is computed by the recursive collision process;
- the fraction $[A(\Delta t)^{2m+1} - A(\Delta t)^{m+1}]$ is sampled by a Maxwellian.

Note that for estimation purposes the sampling from the Maxwellian can be avoided using a *direct analytical computation*.

Well balanced trees

In TRMC we sample directly from the local Maxwellian if $k > m_{\max}$, otherwise the whole collision tree is evaluated. This simple choice however does not take into account the *shape of the collision trees* and then the effective collision history of the sampled particle.



Well balanced (left) and not well balanced tree (right)

The idea is to consider other indicators $L(k)$, capable to distinguish between *well balanced* and not well balanced trees, and the *thermalization criteria* $L(k) > m_{\max}$. The simplest definition corresponds to $L(k) = k$.

Thermalization indicators

Different length indicators L can be constructed using recursivity. For example

$$\begin{aligned} L(k = h + j + 1) &= 1 + \min\{L(h), L(j)\}, \\ L(k = h + j + 1) &= 1 + \text{mean}\{L(h), L(j)\}. \end{aligned}$$

In table we show the values of the length indicators for the two collision trees of the previous Figure.

Indicator	left tree	right tree
simple	7	7
min	3	2
mean	3	43/16

The implementation of such strategy inside the recursive algorithm needs the evaluation of collision trees and their *storage* without performing collisions. Only non thermalized trees are then computed effectively.

Space homogeneous case

We consider a simple space homogeneous test for a VHS kernel.

- The initial data is the *sum of two Maxwellians*. The solutions is computed in one single run using $N = 5 \times 10^4$ particles. The reference solution has been obtained by a large number of averages on *Bird's DSMC* method.
- We compare the results for the *fourth order moment*

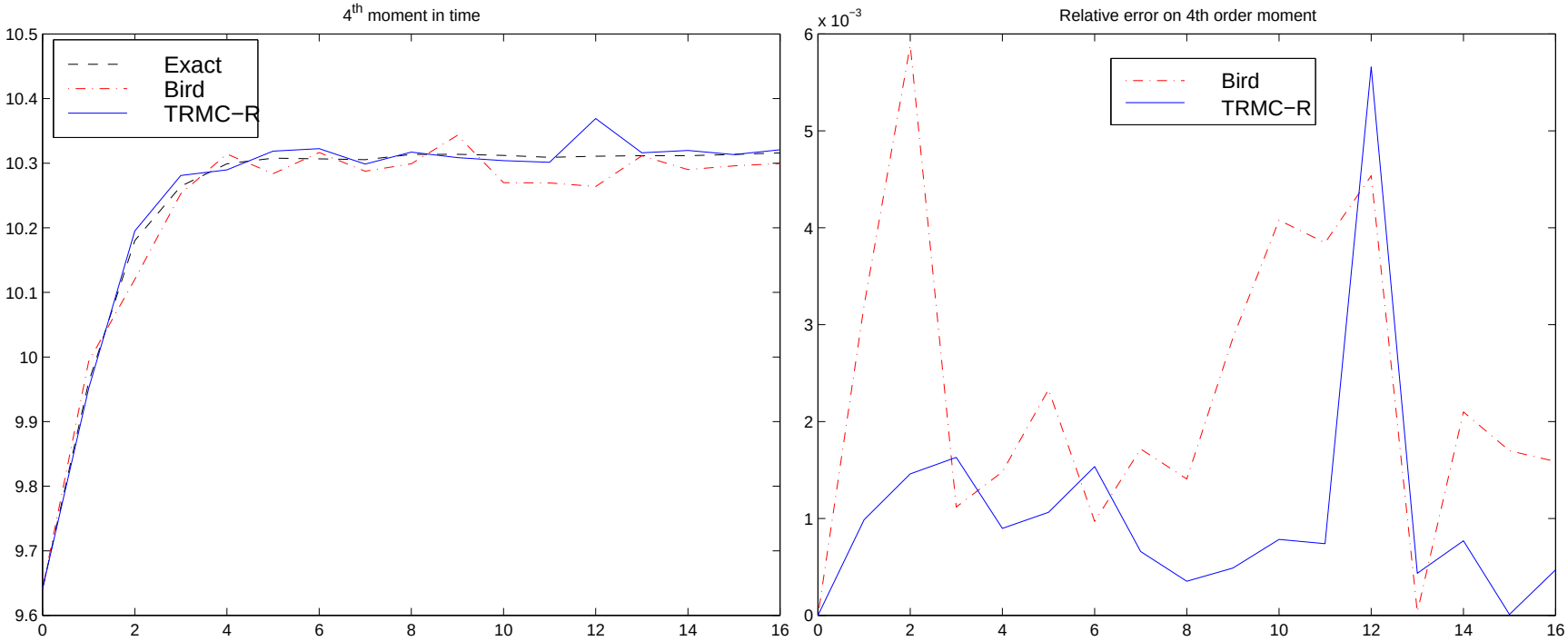
$$M_4 = \int_{\mathbb{R}^3} f v^4 \, dv.$$

- We use the notations *TRMC-R* for the basic recursive method, *TRMC-RAD* for same scheme improved by the adaptive truncation of the collision trees, based on the shear stress tensor

$$P_{xx} = \int_{\mathbb{R}^3} f (v_1 - u_1)^2 \, dv,$$

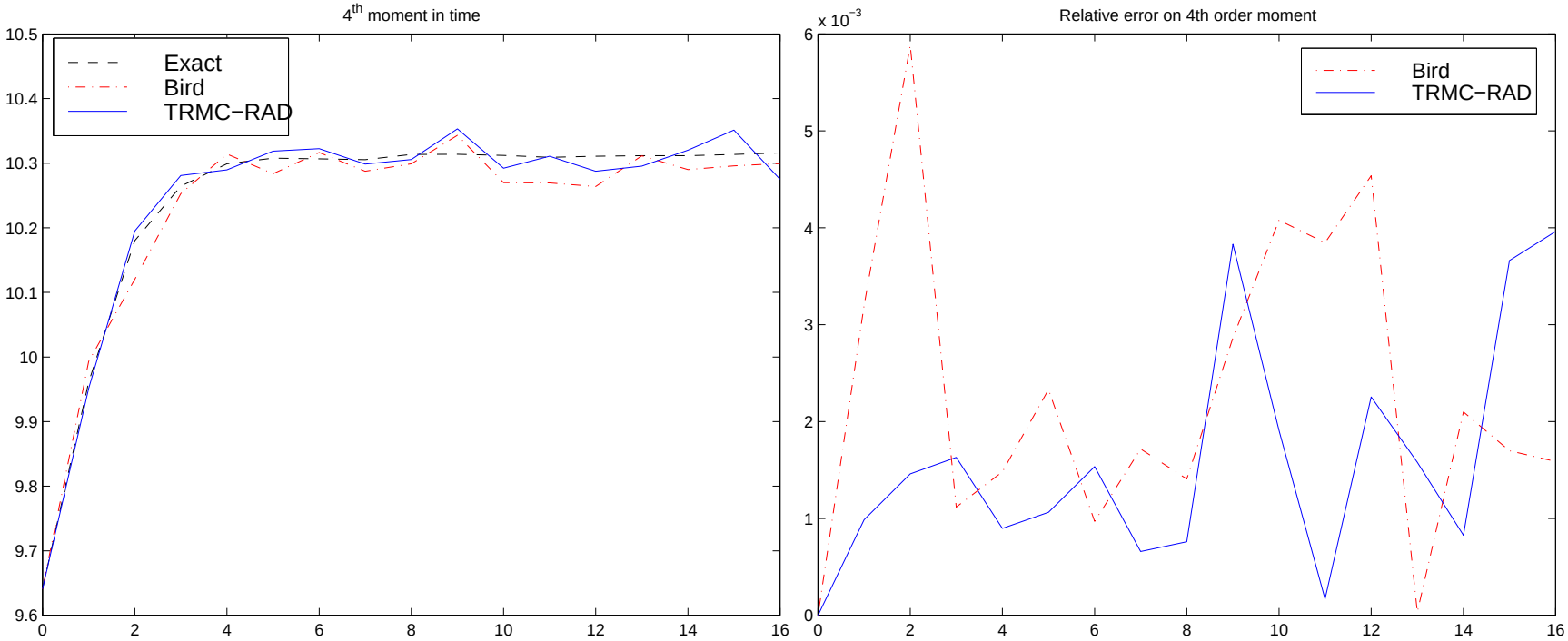
as equilibrium indicator, and *TRMC-WB* for the method based on the well balanced truncation of the collision trees.

Evolution of the fourth order moment (TRMC-R)



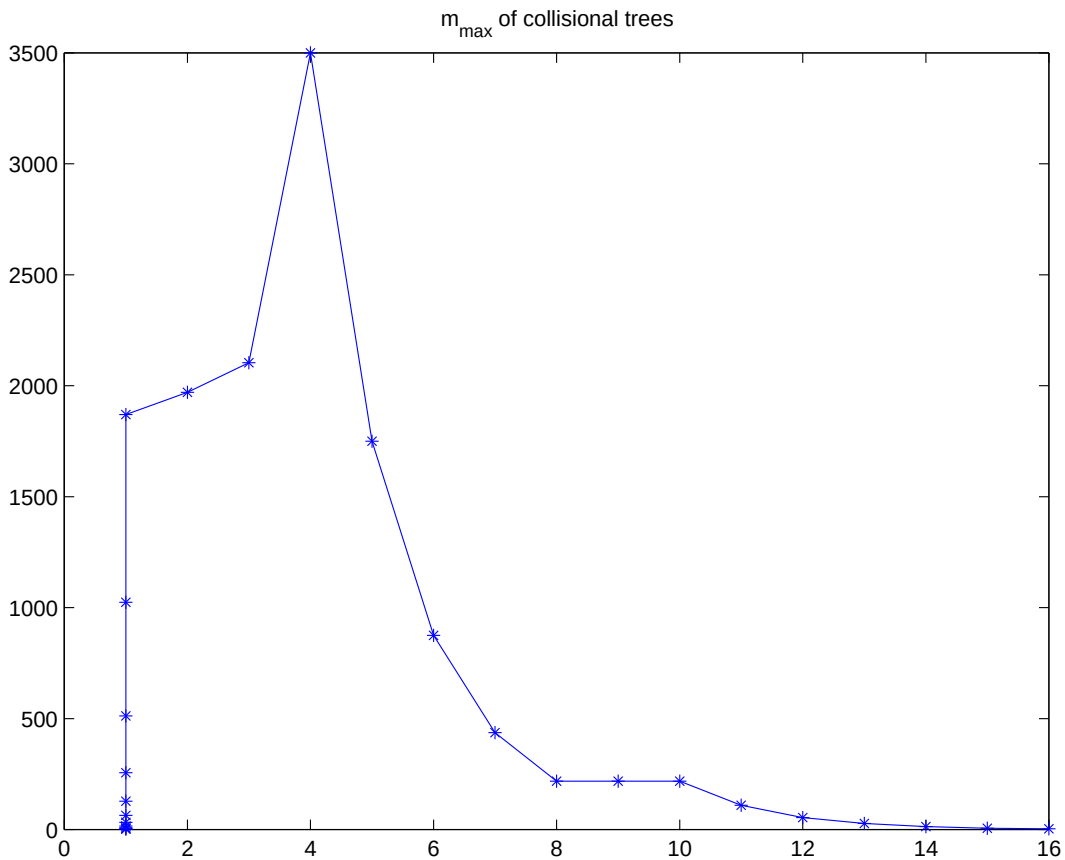
Evolution in Time of 4^{th} order moment (left) and relative error (right) for TRMC-R and Bird's method.

Evolution of the fourth order moment (TRMC-RAD)



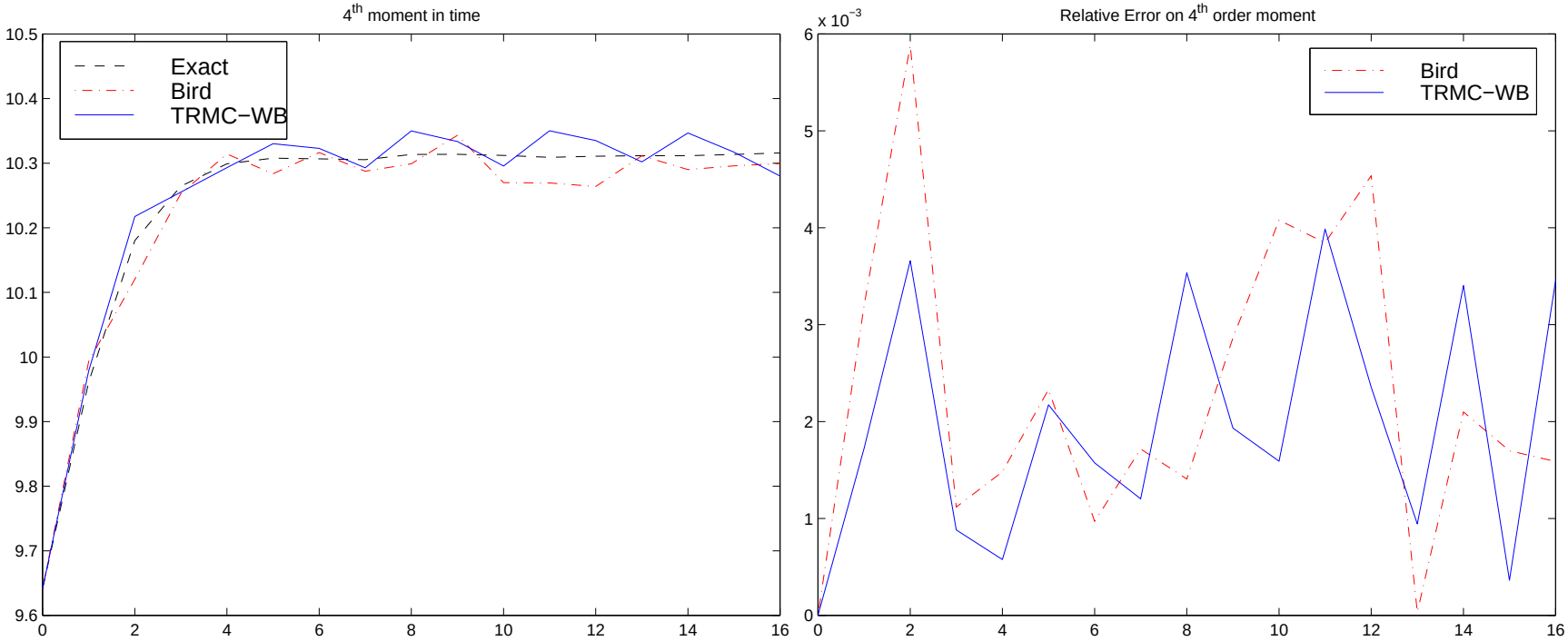
Evolution in Time of 4^{th} order moment (left) and relative error (right) for TRMC-RAD and Bird's method.

Length of the collision trees (TRMC-RAD)



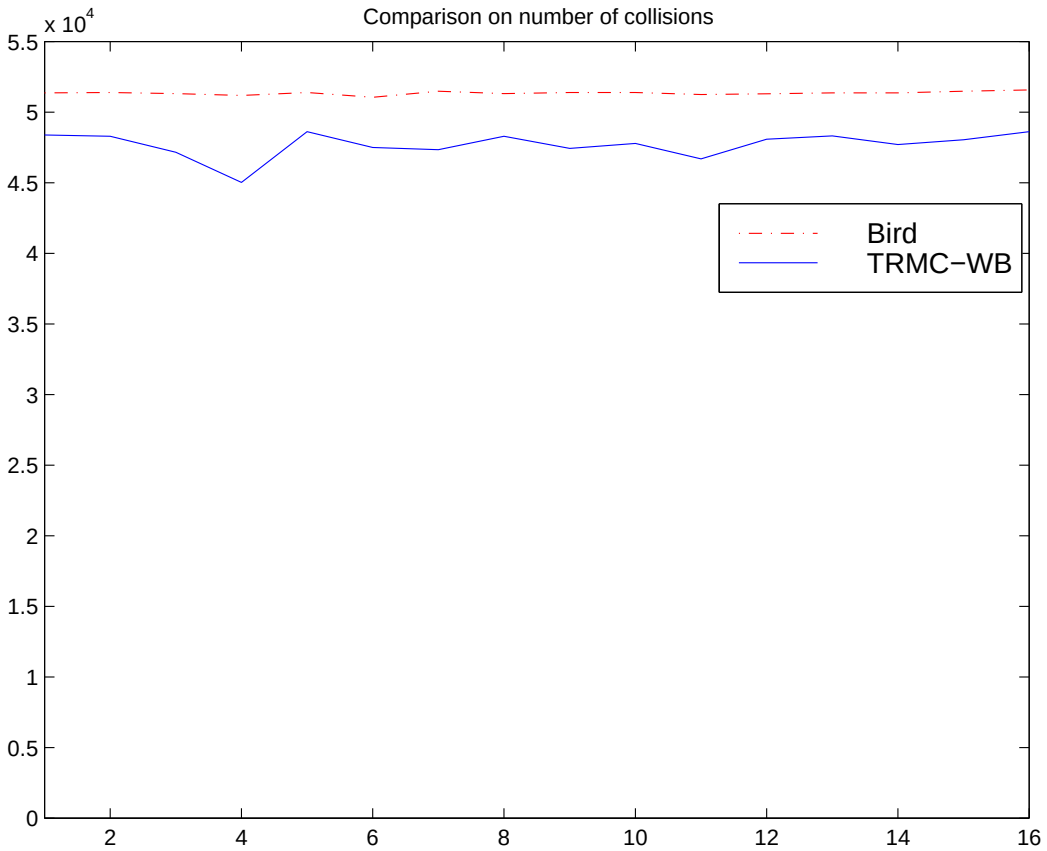
Maximum depth m_{max} of a collision tree in time for TRMC-RAD

Evolution of the fourth order moment (TRMC-WB)



Evolution in Time of 4^{th} order moment (left) and relative error (right) for TRMC-WB and Bird's method.

Total number of collisions (TRMC-WB)



Total number of collisions for TRMC-WB and Bird's method.

Stationary shock in 1D

Next we consider a stationary shock problem characterized by the *Rankine-Hugoniot* relations

$$\rho_L u_L = \rho_R u_R,$$

$$\rho_L u_L^2 + p_L = \rho_R u_R^2 + p_R,$$

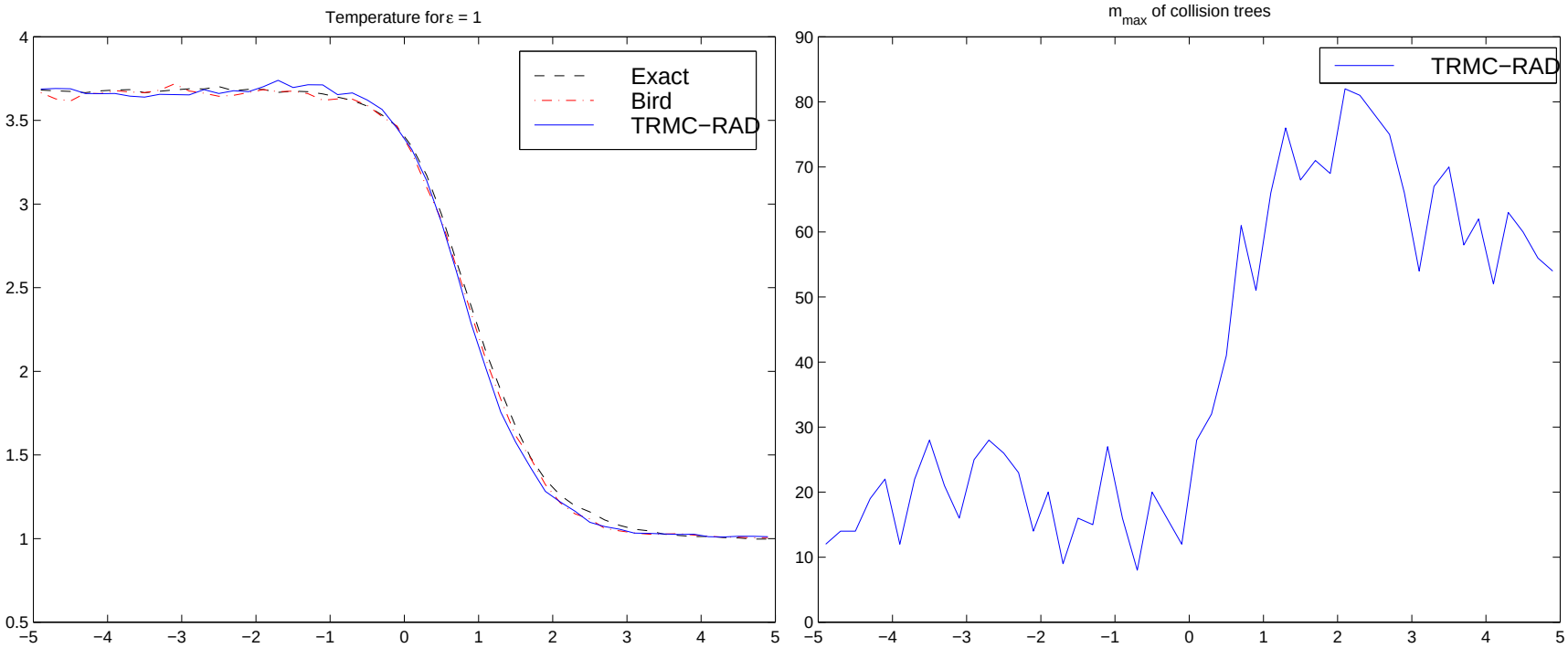
$$u_L(E_L + p_L) = u_R(E_R + p_R).$$

The values used in the simulation are

- $M_{a_L} = 3$ (*Mach Number*)
- $T_L = 1$
- $u_{x_L} = -M\sqrt{\gamma T_L}$, $u_{y_L} = 0$, $u_{z_L} = 0$ $\gamma = 5/3$
- $\rho_L = 1$

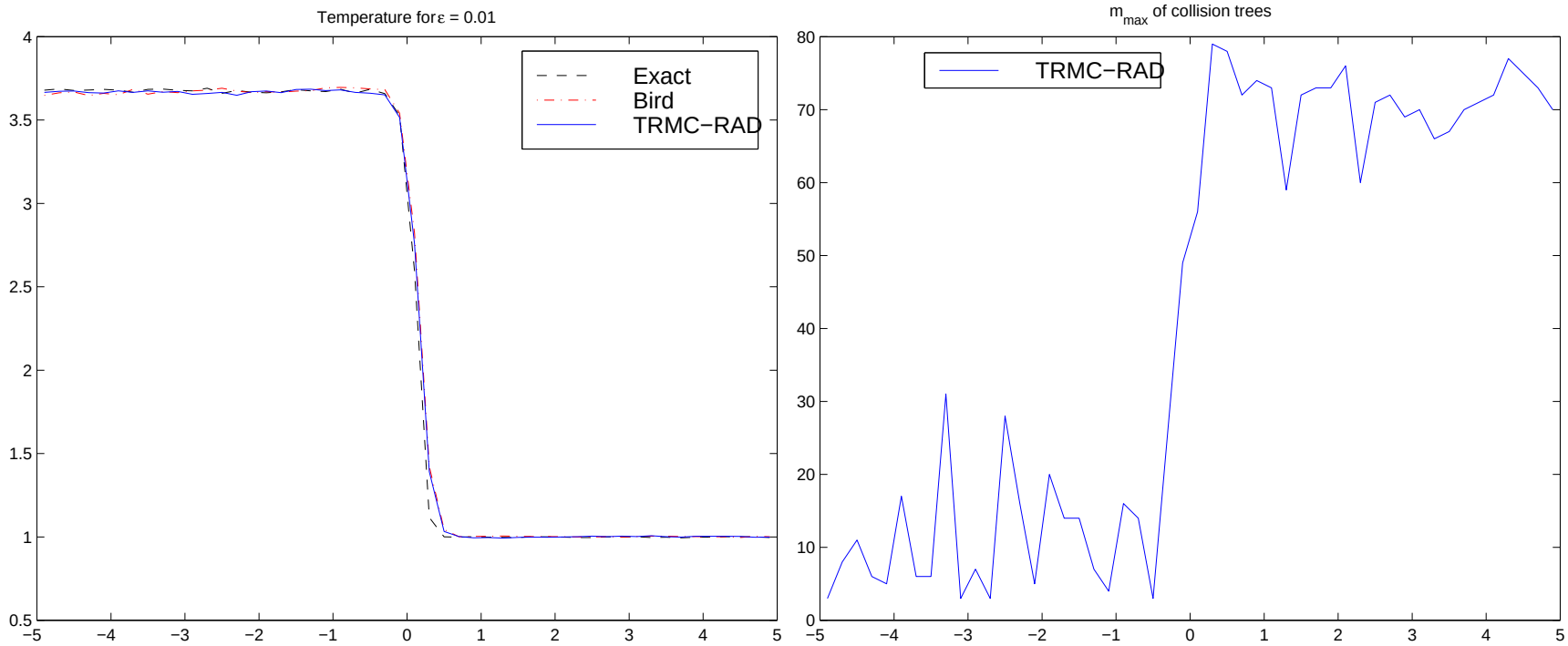
The numerical solution has been obtained using TRMC-RAD and Bird's method with 50 spatial cells and 1000 particles in each cell. Reference 'Exact' solution has been performed by Bird's standard DSMC method using 50 spatial cells and 3000 particles in each cell.

Rarefied regime (TRMC-RAD)



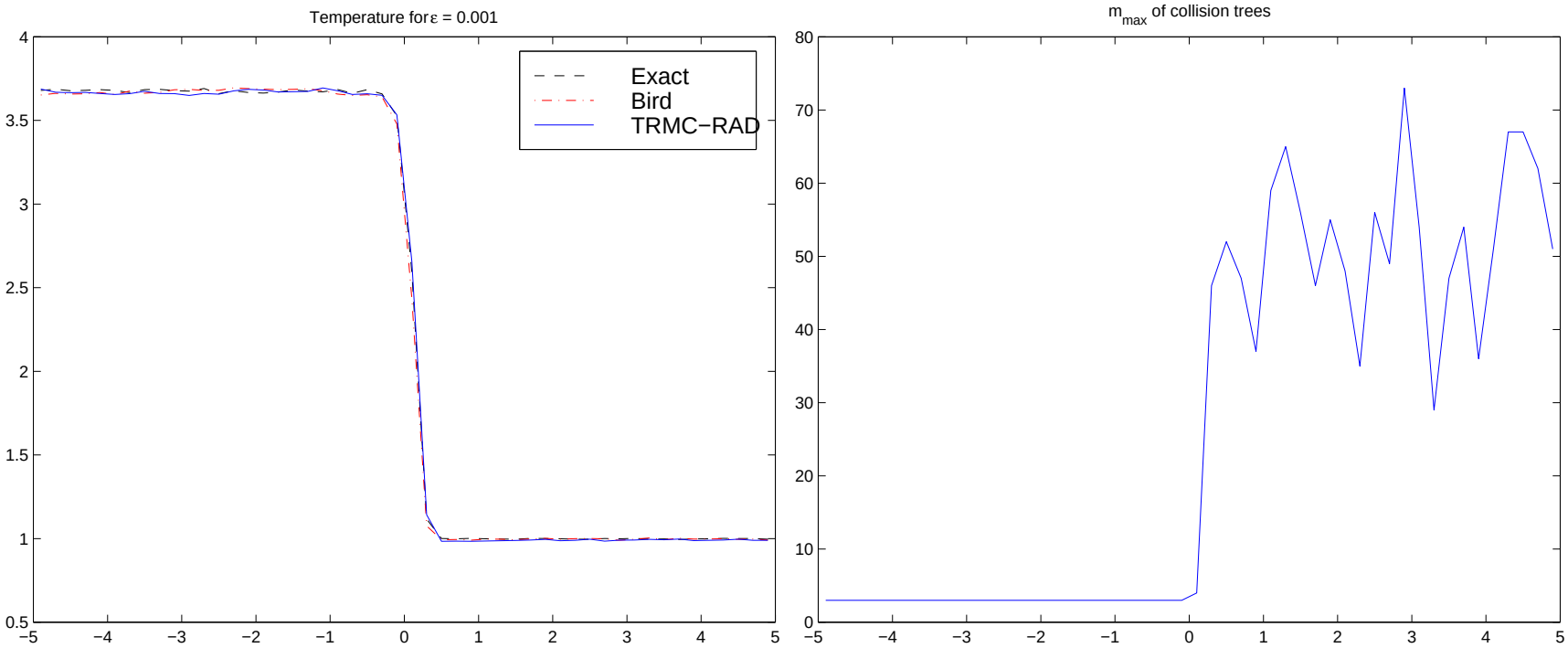
Rarefied regime ($\varepsilon = 1$). Temperature (left) and maximum length of the collisional trees in each cell for TRMC-RAD.

Intermediate regime (TRMC-RAD)



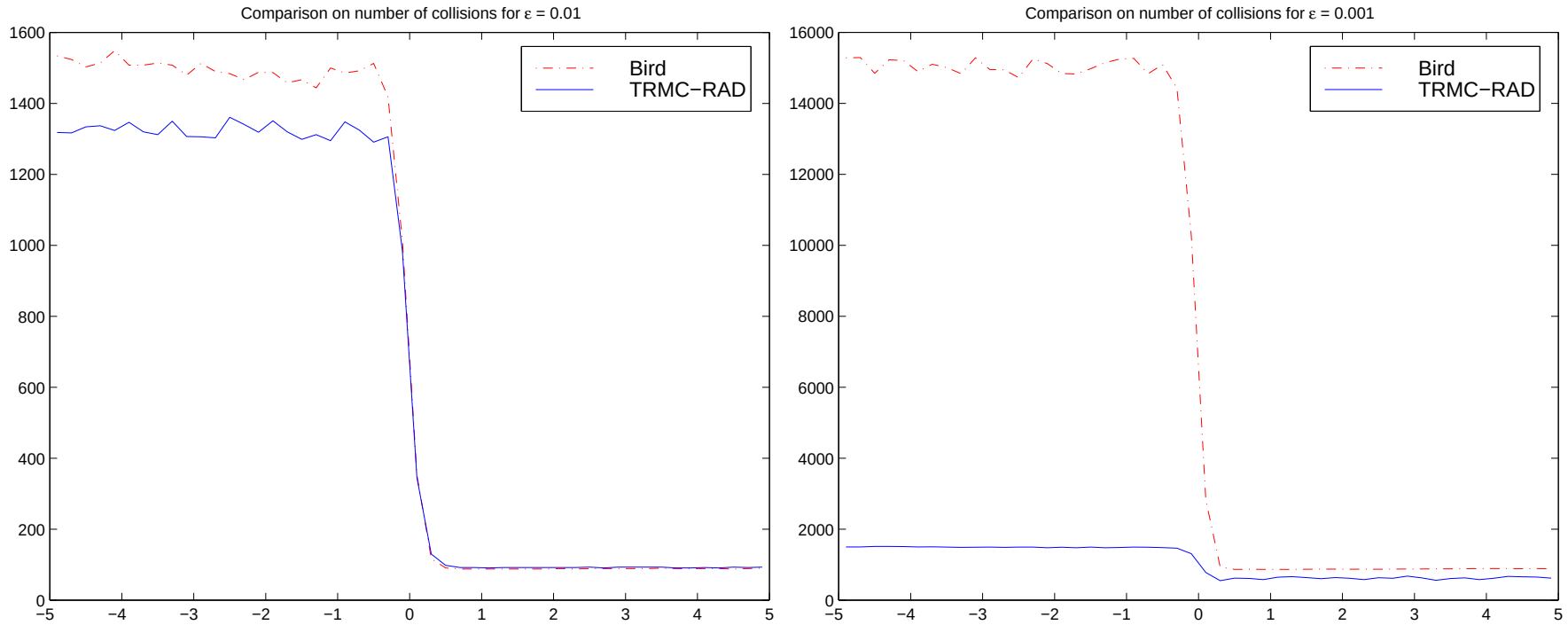
Intermediate regime ($\varepsilon = 0.1$). Temperature (left) and maximum length of the collisional trees in each cell for TRMC-RAD.

Fluid regime (TRMC-RAD)



Fluid regime ($\varepsilon = 0.001$). Temperature (left) and maximum length of the collisional trees in each cell for TRMC-RAD.

Number of collisions (TRMC-RAD)



Number of collisions for TRMC-RAD and Bird's method for $\varepsilon = 0.1$ (left) and $\varepsilon = 0.001$ (right).