Exponential methods for kinetic equations

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Outline

Motivations

- One of the major computational challenges for Boltzmann-like kinetic equations is the difficulty to compute *near-continuum regimes* where the collisional time is small enough that the collision rate is large, but not small enough that the flow is well described by fluid mechanics.
- A classical example is given by *rarefied gas dynamic* (RGD) simulations. Since accuracy of DSMC depends on resolution of the collisional length and time scales, it becomes slower and less accurate in this regime.
- 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 methods*[1] as well as in *Monte Carlo methods*[2].

[1] C.Buet '96, L.P.,G.Russo '00, A.Bobylev, S.Rijasanow '97, F.Filbet '03,...
[2] G.Bird '94, K.Nanbu '80, H.Babovsky, R.Illner '89, W.Wagner '92, ...

Main goal

The goal is to construct simple and efficient time discretizations for the solution of kinetic equations in regions with a large variation in the mean free path.

Requirements

- For large Knudsen numbers, the methods behave as standard explicit methods.
- For intermediate Knudsen numbers, the methods are capable to speed up the computation, allowing larger time steps, without degradation of accuracy.
- In the limit of very small Knudsen numbers, the collision step replaces the distribution function by the local Maxwellian. This property is usually referred to as *asymptotic preserving (AP)* since it implies consistency with the underlying system of *Euler equations* of gas dynamics.
- The main physical properties are preserved by the schemes. Namely mass, momentum, energy, nonnegativity of the solution and entropy inequality.

In the sequel we will present some recent advances in this direction based on the use of *exponential methods*[3]

[3] L.P. '96, E.Gabetta, L.P., G.Toscani '97, G.Dimarco, L.P. '10

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 $p = \rho T$.

History of exponential expansions

Let us consider a kinetic equation of the type

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

where $\mu > 0$ and P a bilinear operator.
The solution admits the following *exponential expansion (Wild sum)*[4]

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

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 time* variables

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

[4] E. Wild '51

Application to the Boltzmann equation

The starting point of most numerical methods for the Boltzmann equation is a *splitting method* in time, which consists of solving in two separate steps the free transport equation (i.e., $Q \equiv 0$) and the space homogeneous equation.
After this splitting, most of the computational difficulties concern the solution of the space homogeneous equation

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

Assuming that the collision kernel B is bounded by σ taking

$$P(f, f) = Q(f, f) + \mu f,$$

with $\mu \geq \mu_* = \sigma \int_{\mathbb{R}^3 \times S^2} f(v_*)\, dv_*\, d\omega = 4\pi\rho\sigma$ the solution can be expanded using the Wild sum.
Note that the coefficients $f_k(v)$ are nonnegative and satisfy

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

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 conservative truncation at the order m of the series is given by

$$f^{n+1}(v) = (1-\tau)\sum_{k=0}^{m} \tau^k f_k^n(v) + \tau^{m+1} f_m^n(v).$$

where $f^n = f(n\Delta t)$ and $\tau = 1 - e^{-\mu \Delta t/\varepsilon}$. The methods can be seen as a particular class of *exponential integrators*[5] and are exact for any linear operator

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

with $G = G(v)$ an arbitrary given function.
The methods have the fundamental property of being a convex combination of the f_k's independently on the value of $\Delta t/\varepsilon$, it is straightforward to verify that they preserve mass, momentum, energy and nonnegativity of the solution. Of course they are not *AP*, since in the limit $\Delta t/\varepsilon \to \infty$ we obtain $f^{n+1}(v) = f_m^n(v)$.

[5] M.Hochbruck, C.Lubich, H.Selhofer '98

Exponential Time Relaxed (ETR) schemes

The coefficients f_k in the exponential expansion are characterized by successive applications of the collision operator, thus one expects that[6]

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

where $M(v) = M[f](v)$ is the local Maxwellian equilibrium.
We can consider a *Maxwellian truncation* for $k > m \geq 1$ to get[7]

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

Since M has the same moments of f^n then f^{n+1} is again a convex combination of density functions. Now the schemes are *AP* since $\lim_{\Delta t/\varepsilon\to\infty} f^{n+1}(v) = M(v)$.
Moreover they are exact for linear problems of the form

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

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

Monotonicity and probabilistic interpretation

- 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[8]

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

  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.

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

Remarks

- Exponential time-relaxed (ETR) schemes have proven to be capable to describe well near-continuum flows allowing larger time steps compared with other time discretizations both in Monte Carlo and deterministic contexts[9]
- They are explicit, and in addition to the physical properties, thanks to their recursive structure, they are suitable for the development of adaptive codes[10].

Drawbacks

- The Maxwellian truncation is based on the physical properties of the equations and it is not derived directly from the equations itself. The truncation is then somewhat not completely justified.
- The schemes have been derived under the assumption $\mu \geq \mu_* = 4\pi\rho\sigma$, so that the choice of the upper bound σ of the collision kernel influences directly the relaxation rate characterized by $\exp(-\mu\Delta t/\varepsilon)$. In principle better estimates for $\mu \geq \int_{\mathbb{R}^3\times S^2} B(|v-v_*|,\omega) f(v_*)\, dv_*\, d\omega$ can be obtained but in general they are computationally very expensive.

[9] L.P., R.Caflisch '99, L.P., G.Russo '01, , F.Filbet, G.Russo '03, ...

[10] L.P., S.Trazzi, B.Wennberg '09

A direct derivation of ETR methods

Let us rewrite the homogeneous equation in the form[11]

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

We can integrate exactly the linear term and rewrite the above system as

$$\frac{\partial (f - M)e^{\mu t/\varepsilon}}{\partial t} = (P(f,f) - \mu M)e^{\mu t/\varepsilon}.$$

We can rescale the time using $\tau = 1 - \exp(\mu t/\varepsilon)$ and consider the Taylor expansion of $F = (f - M)\exp(\mu t/\varepsilon)$ around $\tau = 0$ to get

$$\begin{aligned}(f - M)e^{\mu t/\varepsilon} &= (f_0 - M) + (1 - e^{-\mu t/\varepsilon})\left[\frac{P(f_0,f_0)}{\mu} - M\right] \\ &+ \frac{(1 - e^{-\mu t/\varepsilon})^2}{2}\left[\frac{P(P(f_0,f_0),f_0) + P(f_0,P(f_0,f_0))}{\mu^2} - 2M\right] \\ &+ O(\tau^3)\end{aligned}$$

[11] F.Filbet, S.Jin '09, G.Dimarco, L.P. '10

It is easy to show that if we truncate the expansion at the order $m = 1$ in a time interval Δt we obtain exactly the first order ETR scheme

$$f^{n+1} = e^{-\mu \Delta t/\varepsilon} f^n + e^{-\mu \Delta t/\varepsilon}(1 - e^{-\mu \Delta t/\varepsilon}) \frac{P(f^n, f^n)}{\mu} + (1 - e^{-\mu \Delta t/\varepsilon})^2 M,$$

similarly at the order $m = 2$ we obtain the second order ETR scheme

$$\begin{aligned} f^{n+1} &= e^{-\mu \Delta t/\varepsilon} f^n + e^{-\mu \Delta t/\varepsilon}(1 - e^{-\mu \Delta t/\varepsilon}) \frac{P(f^n, f^n)}{\mu} \\ &+ e^{-\mu \Delta t/\varepsilon}(1 - e^{-\mu \Delta t/\varepsilon})^2 \frac{P(P(f^n, f^n), f^n) + P(f^n, P(f^n, f^n))}{2\mu^2} \\ &+ (1 - e^{-\mu \Delta t/\varepsilon})^3 M \end{aligned}$$

In this way we recover directly all ETR schemes at the different orders.
Note that if we consider all the terms in the exponential expansion then, due to cancelations, we recover again the original Wild sum derived before.

Exponential Runge-Kutta

More in general if we consider a system of ODEs with the general structure

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

we can apply an explicit exponential Runge-Kutta method in the form [12]

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

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*.

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

IF-RK methods

Various schemes come from the different choices of the underlying method. The two most popular approaches are the integrating factor (IF) and the exponential time differencing (ETD) methods[13].
For the so-called *Integrating Factor* methods we have

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

When applied to the Boltzmann equation the first order IF-RK scheme gives[14]

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

Note that again the scheme is a convex combination of particle densities independently of $\Delta t/\varepsilon$ and satisfies conservations, nonnegativity and asymptotic preservation.

[13] J. Lawson, '67, A. Friedli, '78
[14] G.Dimarco, L.P. '10

Higher order schemes can be constructed in the same way. Note however that in order to be AP the underlying explicit Runge-Kutta method must satisfy $1 > c_i > c_j > 0$, $\forall\, i > j$.
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.
Other semi-implicit discretizations, like *Implicit-Explicit (IMEX)* Runge-Kutta methods[15], can be used. These schemes however do not preserve in general nonnegativity, monotonicity and AP.

[15] U.Asher, S.Ruth, Spiteri, '98, L.P., G.Russo '05

The choice of μ

All first order exponential schemes have the general form

$$f^{n+1} = A_0\left(\frac{\mu\Delta t}{\varepsilon}\right) f^n + A_1\left(\frac{\mu\Delta t}{\varepsilon}\right)\frac{P(f^n, f^n)}{\mu} + A_2\left(\frac{\mu\Delta t}{\varepsilon}\right) M,$$

with $A_0, A_1, A_2 \in [0,1]$ and $A_0 + A_1 + A_2 = 1$ independently of $\mu\Delta t/\epsilon$.
To have nonnegativity we require

$$P(f^n, f^n) = Q(f^n, f^n) + \mu f^n \geq 0.$$

This is guaranteed if $\mu \geq \mu_* = 4\pi\rho\sigma$ which however relates μ to the choice of the upper bound of the cross section.
A different approach is based on searching for the minimal value of μ, as a function of $\Delta t/\varepsilon$, which makes the whole scheme nonnegative not the single $P(f, f)$ term. Note that for $\mu \to 0$ the schemes yield the explicit Euler method.

In order to do that let us rewrite the schemes in the form[16]

$$f^{n+1} = \left(A_0(\lambda) + A_1(\lambda) \left(\frac{\mu - \mu_*}{\mu} \right) \right) f^n + A_1(\lambda) \frac{\mu_*}{\mu} \frac{P_*(f^n, f^n)}{\mu_*} + A_2(\lambda) M,$$

where $P_*(f^n, f^n) = Q(f^n, f^n) + \mu_* f^n \geq 0$ and we have set $\lambda = \mu \Delta t / \varepsilon$.
The condition for nonnegativity is then

$$A_0(\lambda) + A_1(\lambda) \left(\frac{\mu - \mu_*}{\mu} \right) \geq 0.$$

Setting $\lambda_* = \mu_* \Delta t / \varepsilon$ we have the inequality

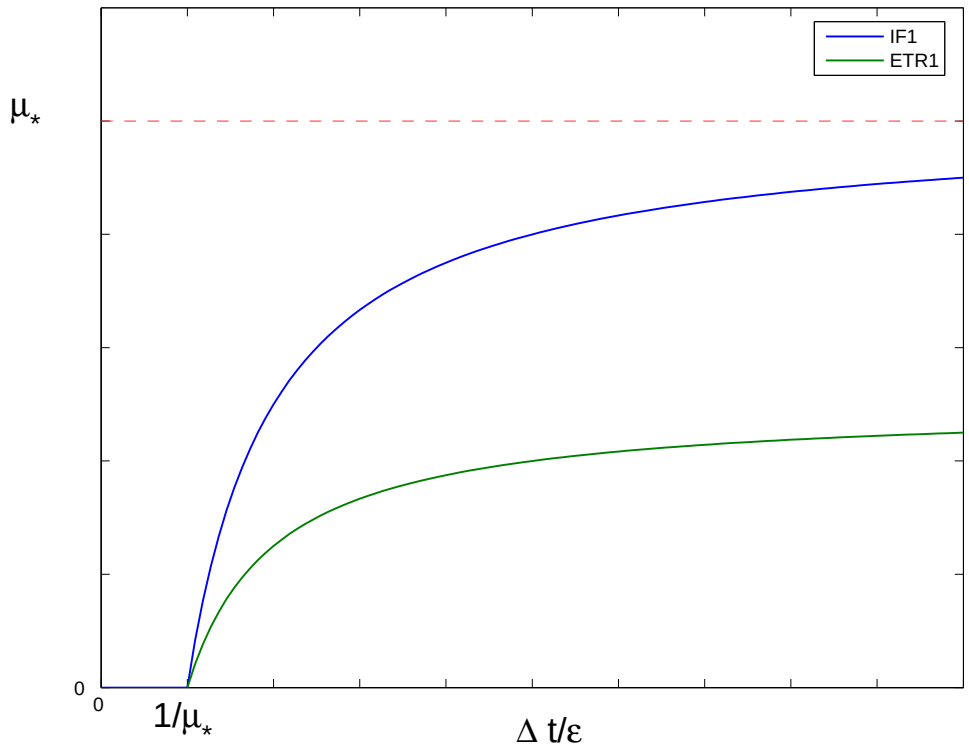
$$\lambda_* \leq s(\lambda) = \frac{A_0(\lambda) + A_1(\lambda)}{A_1(\lambda)} \lambda.$$

Thus we search for the minimum value of λ that satisfies $s(\lambda) \geq \lambda_*$. If $s(\lambda)$ is increasing (as in the case of all schemes considered) the solution is given by

$$\lambda = \begin{cases} 0 & \text{for } \lambda_* \leq 1 \\ s^{(-1)}(\lambda_*) & \text{for } \lambda_* > 1. \end{cases}$$

[16] R.Caflisch, G.Dimarco, L.P.'10

Examples of minimal values for μ

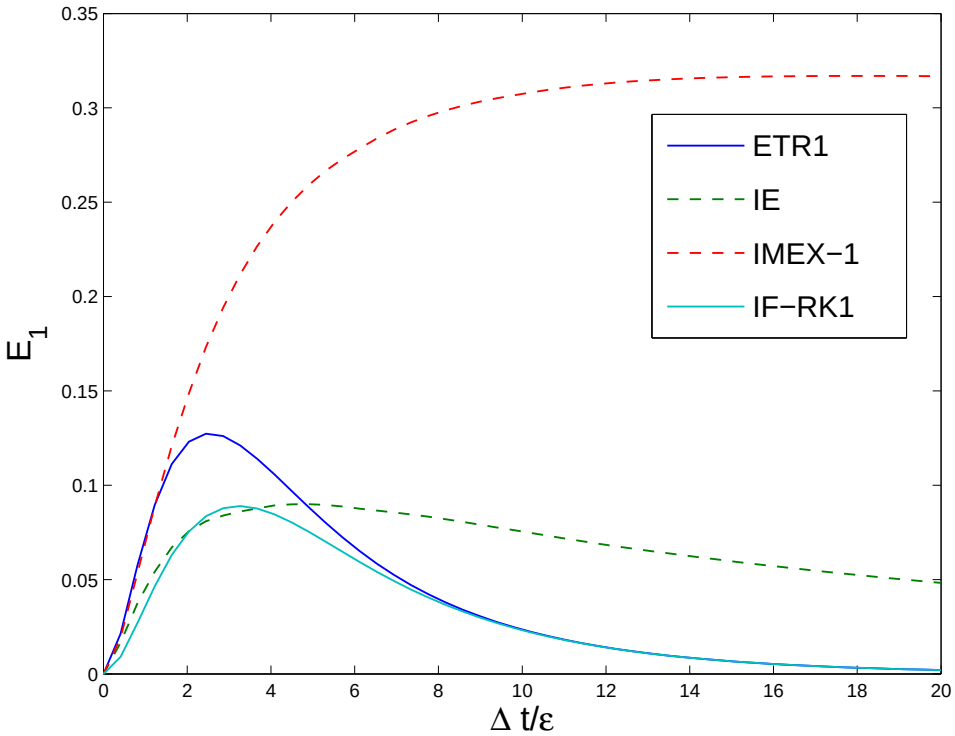


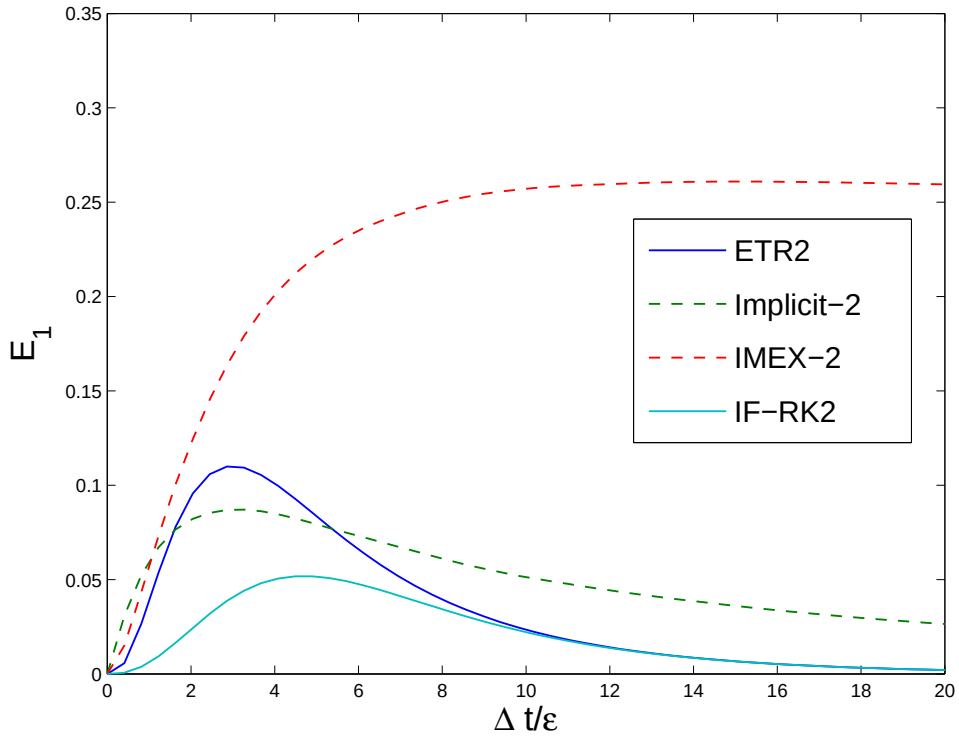
For the IF-RK method we obtain

$$\mu = \begin{cases} 0 & \text{for } \mu_* \Delta t/\varepsilon \leq 1 \\ \mu_* - \varepsilon/\Delta t & \text{for } \mu_* \Delta t/\varepsilon > 1. \end{cases}$$

In the case of the ETR method we don't have an explicit expression, a numerical evaluation is reported in Figure.

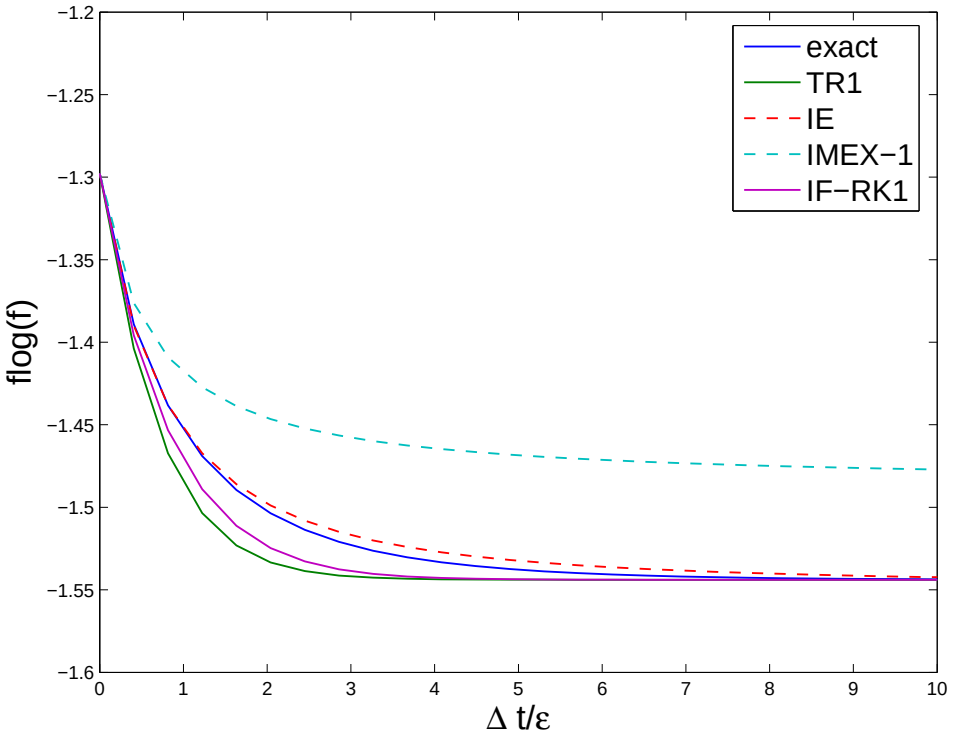
Kac equation: error

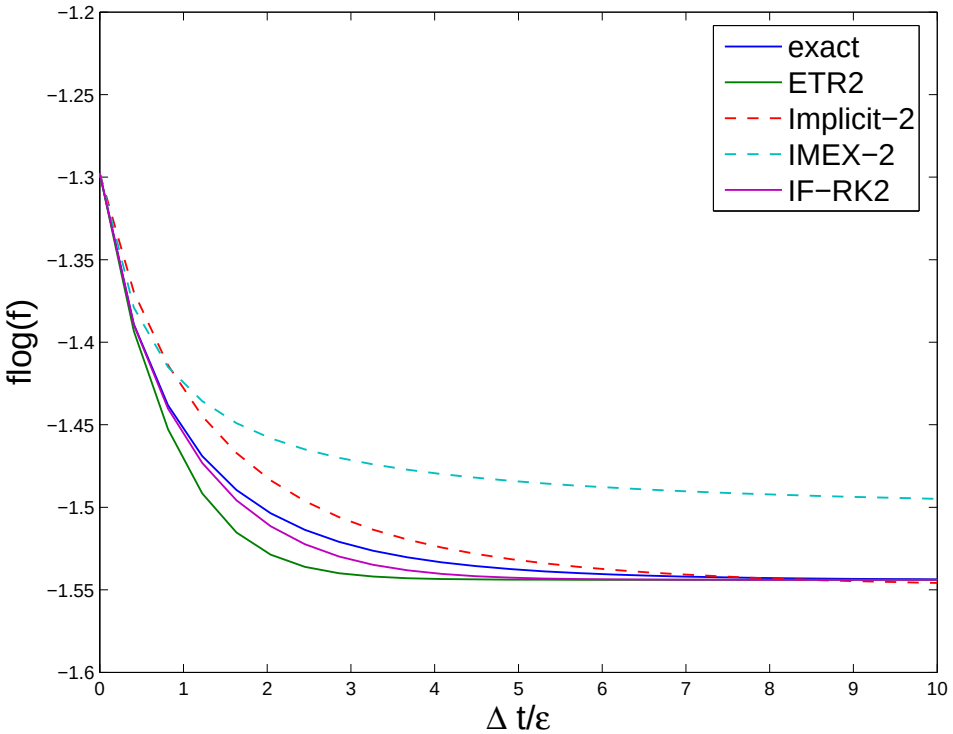




L_1 error for first and second order schemes, stability of Explicit Euler breaks down for $\Delta t/\epsilon > 2/\sqrt{\pi}$.

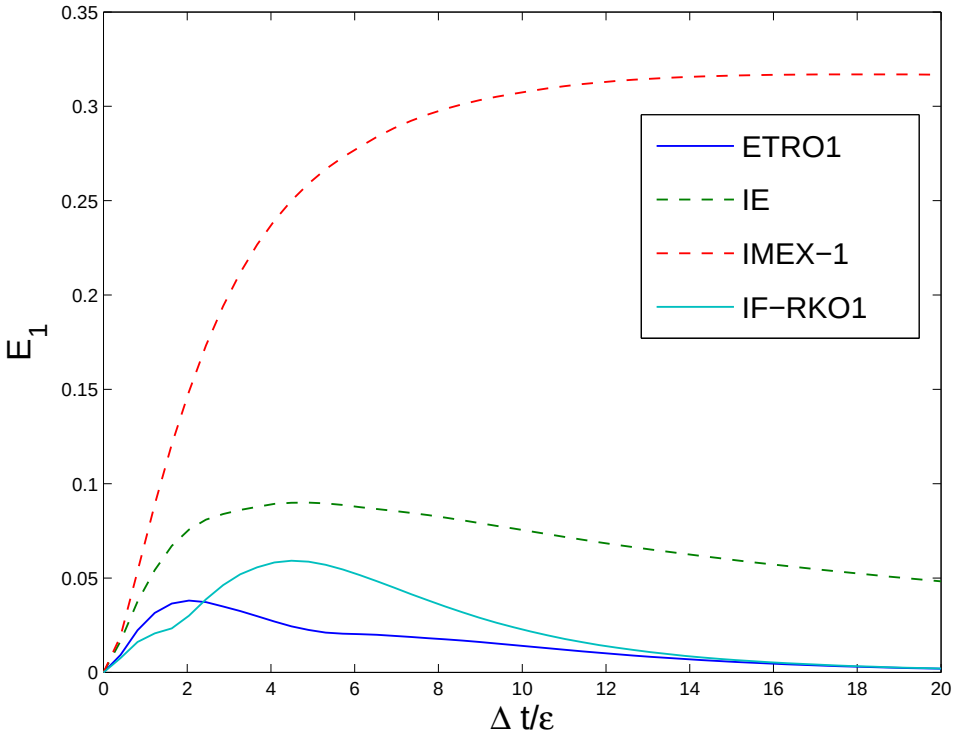
Kac equation: entropy

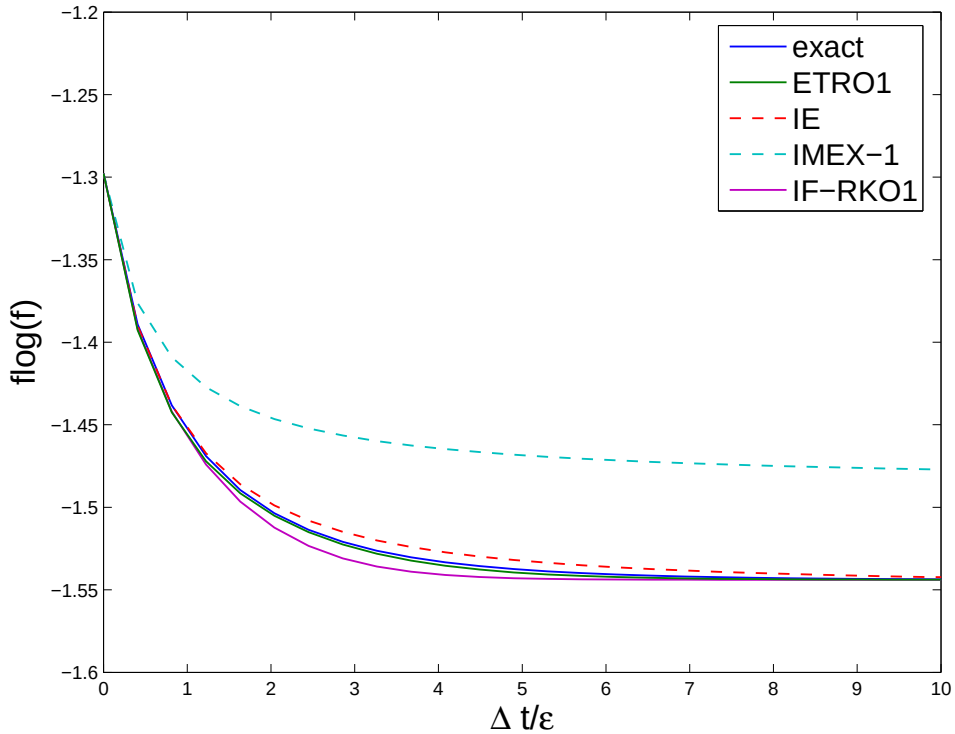




Entropy decay for first and second order schemes.

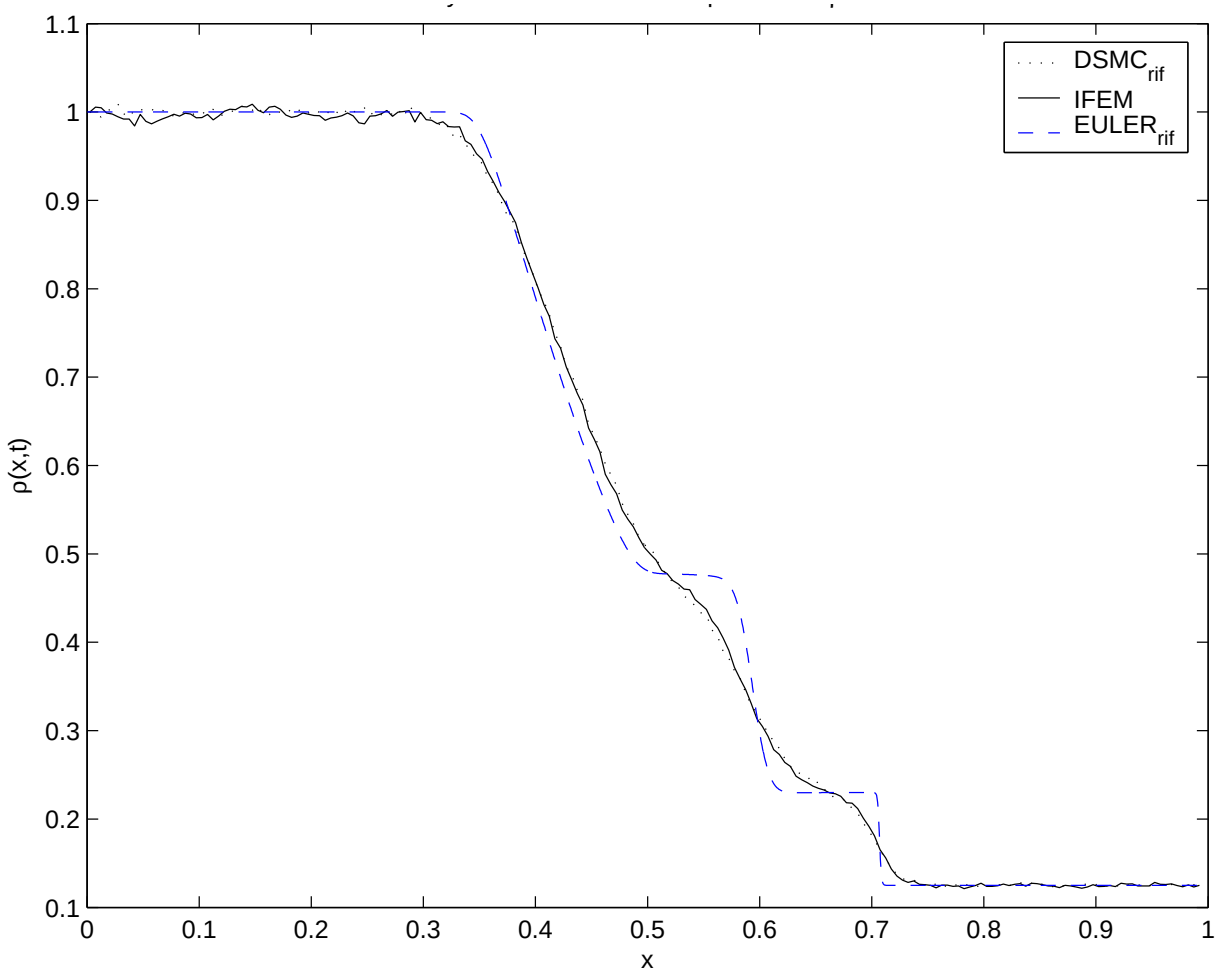
Kac equation: "optimal" μ





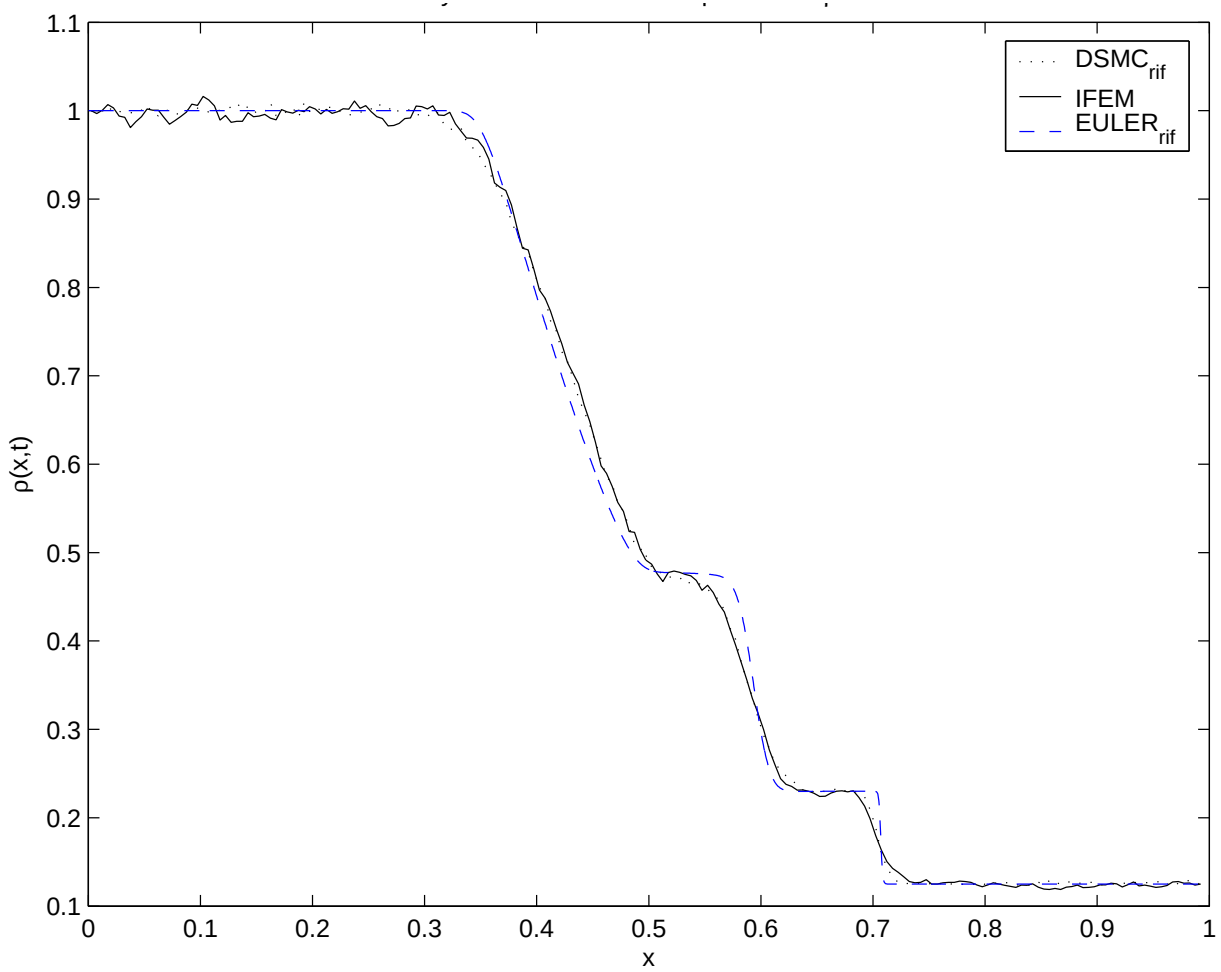
Error and entropy decay for first order "optimal" schemes.

Sod test: rarefied regime



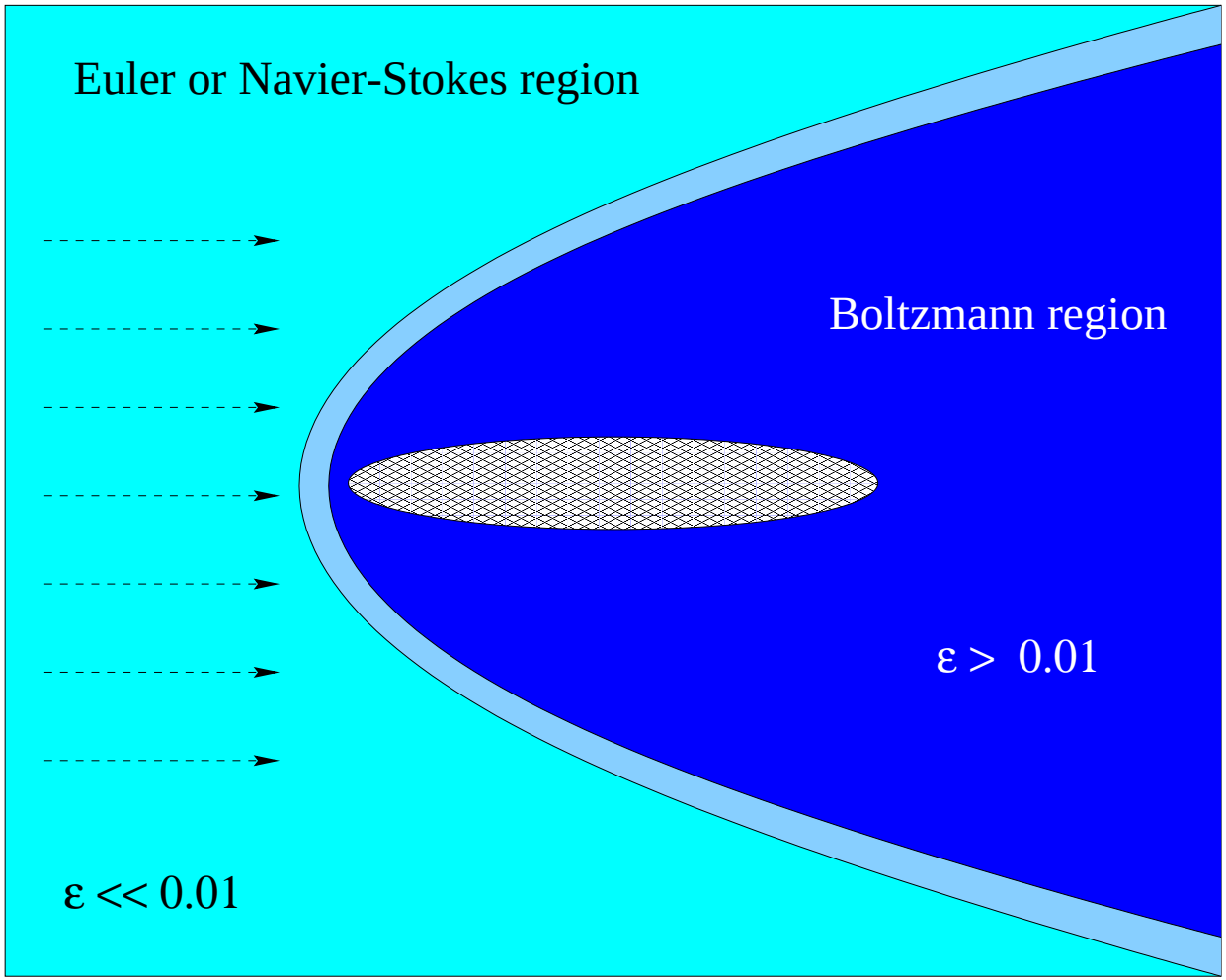
Density for $IF - RK1$ with $\Delta t/\epsilon = 1$ and $\epsilon = 0.01$.

Sod test: near-continuum regime



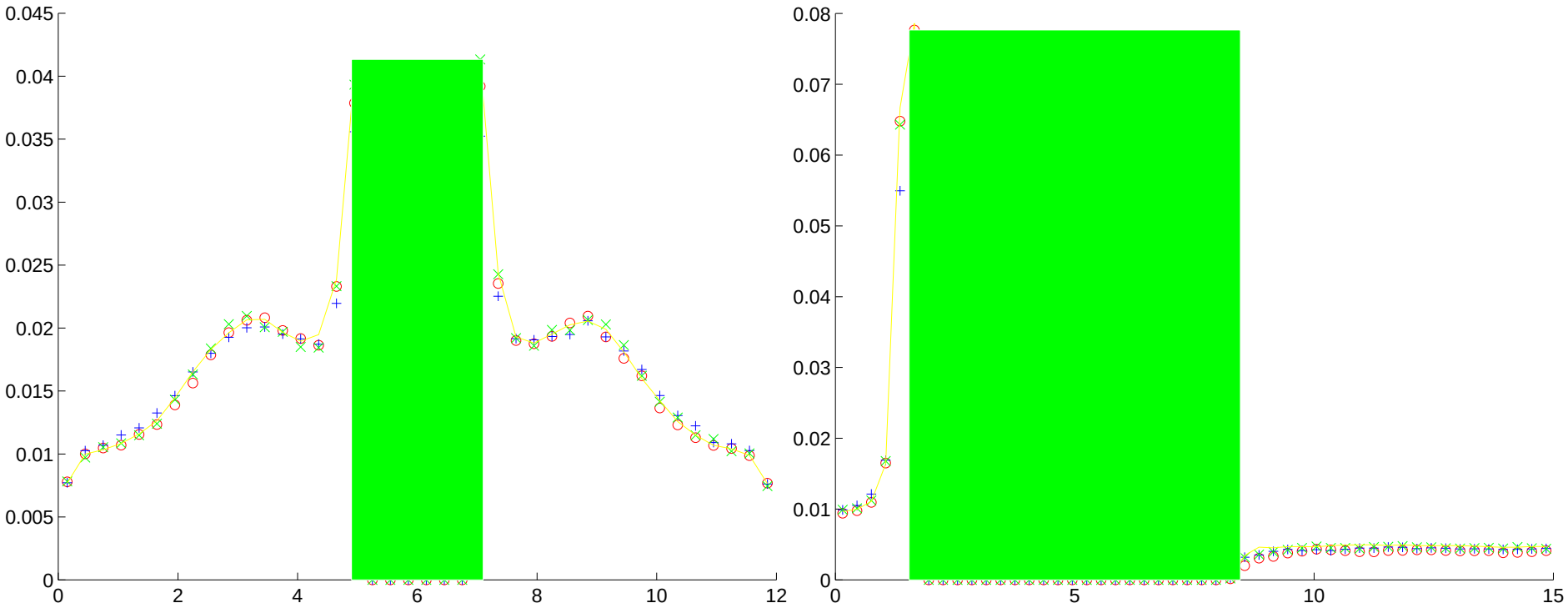
Density for $IF - RK1$ with $\Delta t/\epsilon = 2$ and $\epsilon = 0.001$.

2D flow past an ellipse



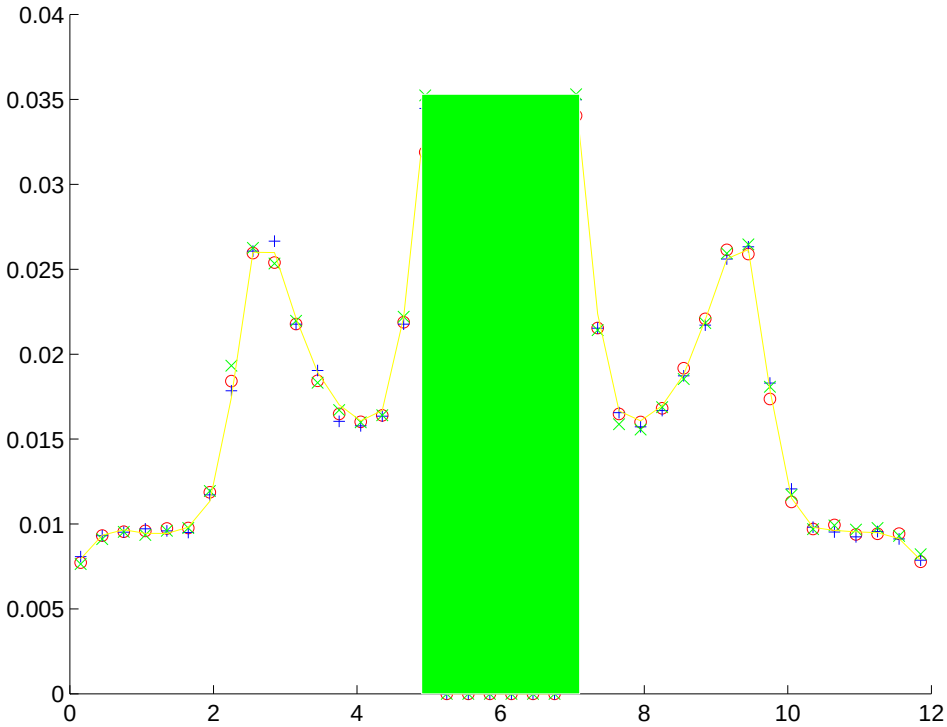
2D flow: rarefied regime

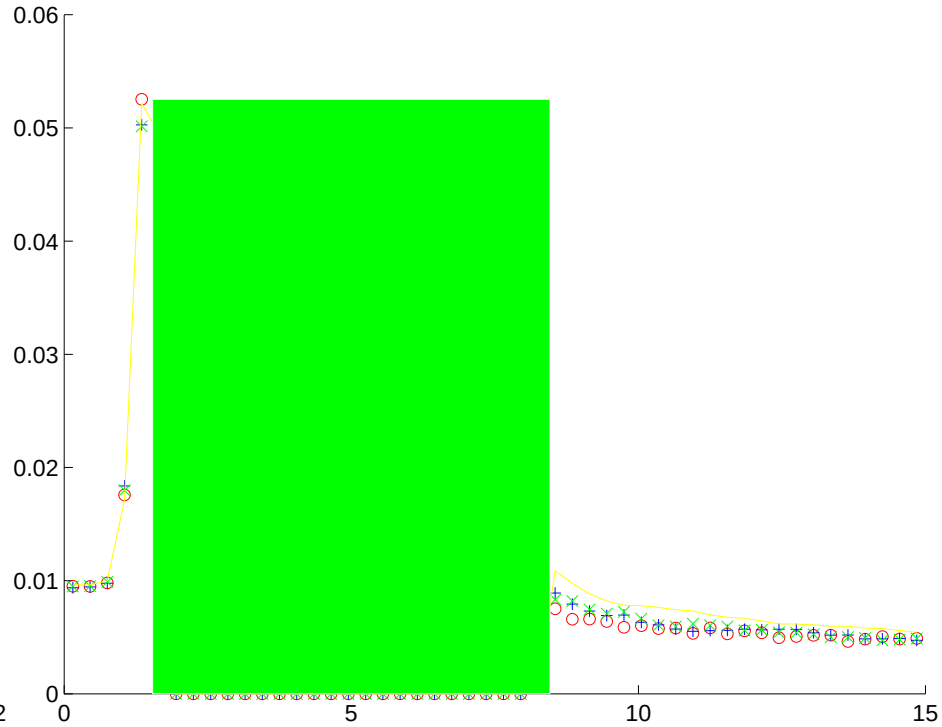
Transversal and longitudinal sections for the mass ρ at $y = 6$ and $x = 5$ respectively for $\Delta t/\epsilon = 1$, $\epsilon = 0.1$ and $M = 20$; EE ($\circ$), ETR1 ($+$), ETR2 ($\times$).



2D flow: near-continuum regime

Transversal and longitudinal sections for the mass ρ at $y = 6$ and $x = 5$ respectively for $\epsilon = 0.01$ and $M = 20$; EE ($\circ$) with $\Delta t/\epsilon = 1$, ETR1 ($+$), ETR2 ($\times$) with $\Delta t/\epsilon = 10$.





Conclusions

- Exponential methods are a powerful tool for the approximation of kinetic equations in regions with strong variations of the mean free path.
- Thanks to the convexity properties they satisfy conservations, nonnegativity and monotonicity. Moreover they can be used both in a deterministic and in a probabilistic setting.
- They can be efficiently blended into domain decomposition and hybrid techniques for multiscale kinetic equations[17].
- Several extensions are possible: Landau-Fokker-Planck equations, quantum kinetic equations, semiconductor models, ... Non splitting based strategies are also under study.

[17] R.Caflisch, L.P '04, G.Dimarco, P.Degond, L.P '10