Numerical methods for kinetic equations

Lecture 2: Semi-Lagrangian schemes

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Imperial College, October 2-9, 2015

Lecture 2 Outline

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Introduction

- We give a short overview of *semi-Lagrangian* method for kinetic transport equation. The methods are based on a fixed computational grid but take into account the Lagrangian nature of the transport process.
- For their structure semi-Lagrangian methods apply naturally to the linear transport part of kinetic equations, the full equation being often solved by *splitting techniques*.
- These methods can be designed in order to possess many desired properties for a numerical scheme for kinetic equations, namely positivity, physical conservations and robustness when dealing with large velocities.
- These restrictions often prevent a straightforward application of the usual schemes for hyperbolic conservation laws.
- Several approaches can be used to solve efficiently the transport process in kinetic equations, ranging from *particle in cell methods*[1] and *flux-balance methods* [2] to *WENO schemes* [3] and *Discontinuous-Galerkin methods* [4].

[1] C. Birdsall, A. Langdon '91

[2] J. Boris, D. Book '73

[3] J.A. Carrillo, F. Vecil'07

[4] J.-M. Qiu, C.-W. Shu '11; B. Ayuso, J.A. Carrillo, C.-W. Shu '11; R. Heath, I. Gamba, P. Morrison, C. Michler '12

Transport equations

Let us consider the one dimensional linear advection equation

Linear advection

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0, \qquad x \in \mathbb{R}$$

here $f = f(x,t)$, $v \in \mathbb{R}$, with initial datum $f(x,0) = f_0(x)$. The exact solution is

$$f(x,t) = f_0(x - vt).$$

The Semi-Lagrangian methods use the knowledge of the exact solution which is explicitly represented in terms of the initial datum to construct a numerical approximation of the transport equation. In particular, we have

$$f(x_j, t^{n+1}) = f_0(x_j - vt^{n+1}) = f_0(x_j - v\Delta t - vt^n) = f(x_j - v\Delta t, t^n)$$

where we introduced a uniform grid $x_j = j\Delta x$, $j \in \mathbb{Z}$ and discrete time steps $t^n = n\Delta t$. The points in space used to compute the solution are the points that within a single time step are transported by the flow onto the mesh. These points do not lie in the general case on the grid.

Semi-Lagrangian methods

The *backward semi-Lagrangian scheme* can then be obtained as

$$f_j^{n+1} = f^n_{j-v\frac{\Delta t}{\Delta x}} = f^n_{j-k-\alpha}, \qquad k+\alpha = v\frac{\Delta t}{\Delta x}, \quad k = \left[v\frac{\Delta t}{\Delta x}\right],$$

where $[\,\cdot\,]$ denotes the integer part and $\alpha \in (0,1)$ is a non integer index unless the time and space grid satisfy $v\Delta t = k\Delta x$ in which case $\alpha = 0$.

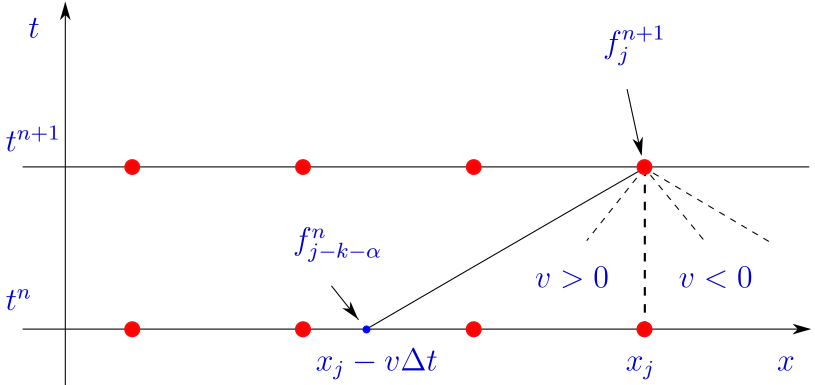

Figure: Sketch of the semi-Lagrangian approach for $v > 0$.

Semi-Lagrangian methods

The type and the degree of interpolation defines then the type of semi-Lagrangian scheme. As an example we consider a simple *linear interpolation*

$$f_j^{n+1} = \alpha f_{j-k-1}^n + (1-\alpha) f_{j-k}^n.$$

If $v\Delta t/\Delta x < 1$ one gets $k=0$, $\alpha = v\Delta t/\Delta x$ and the resulting method is nothing else but the well-known *upwind method*.
In contrast with standard upwind, the scheme holds for any value of $v\Delta t/\Delta x$.
Since the values of the solution at the time level $n+1$ are obtained by linear interpolation of the values at time level n with nonnegative coefficients, a discrete maximum principle holds. No stability conditions are needed and the scheme is well-suited to deal with arbitrary large values of v.
Note also that the exact solution admits the formulation

$$f(x_j + v\Delta t, t^{n+1}) = f(x_j, t^n),$$

which gives the equivalent *forward semi-Lagrangian scheme*

$$f_{j+k+\alpha}^{n+1} = f_j^n, \qquad k+\alpha = v\frac{\Delta t}{\Delta x}, \quad k = \left[v\frac{\Delta t}{\Delta x} \right].$$

Multi-dimensional case

The semi-Lagrangian method can be generalized to the multidimensional case by replacing one dimensional interpolation with multidimensional interpolation techniques. For a space and time dependent velocity field $V(x,t) \in \mathbb{R}^d$ we have

Multidimensional transport equation

$$\frac{\partial f}{\partial t} + V(x,t) \cdot \nabla_x f = 0, \quad x \in \mathbb{R}^d.$$

Under Lipschitz continuity assumptions on the velocity field, the characteristic curves exist. These are defined as the solutions $X(\,\cdot\,; t, x)$ of the ordinary differential equations

$$\frac{d}{ds} X(s;t,x) = V(X(s;t,x), s)$$

with initial data $X(t;t,x) = x$. It is then possible to show that

$$f(x,t) = f(X(s;t,x), s) = f_0(X(0;t,x)).$$

The solution at point x and time t is the initial datum at the foot of the characteristic indicated by $X(0;x,t)$ which passes in x at time t.

Multidimensional semi-Lagrangian methods

Using the formula for the exact solution then a semi-Lagrangian method for the approximation of the multidimensional advection equation can be derive in two steps:

1. At a given time level n compute for each mesh point x an approximate solution of the system of ODEs to determine an estimate of the characteristic $X^*(t^n; t^{n+1}, x)$ which passes at time t^{n+1} at position x.
2. Compute an approximation of the exact solution by interpolating the mesh point values at time level n at the points $X^*(t^n; t^{n+1}, x)$.

This implies that the solution of the PDE is reduced to the solution of a large set ODEs combined with multidimensional interpolation. The most common reconstruction techniques found in literature are *cubic splines*, *Hermite* or *Lagrange polynomials*. More recently *WENO techniques* and *DG methods* have also been used succesfully[5].

[5] X-T.Liu, S.Osher, T.Chan '94; C.-W. Shu '09; B. Cockburn, G. E. Karniadakis, C.-W. Shu (eds.) '00

Semi-Lagrangian scheme for the Vlasov-Poisson system

As an example let us consider the one-dimensional Vlasov-Poisson system

Vlasov-Poisson system

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial v} = 0, \quad x \in \mathbb{R},\, v \in \mathbb{R}$$

$$\frac{\partial^2 \Phi_m}{\partial x^2}(x,t) = 1 - \varrho(x,t) = 1 - \int_{\mathbb{R}} f(x,v,t)dv, \quad E = -\frac{\partial \Phi_m}{\partial x}.$$

Observe that the Vlasov equation can be rewritten in equivalent form as

$$\frac{\partial f}{\partial t} + V \cdot \nabla_{(x,v)} f = 0,\ V(x,v,t) = (v, E)^T$$

which is a linear transport equation in the phase space. Moreover since

$$\nabla_{(x,v)} \cdot V = \frac{\partial v}{\partial x} + \frac{\partial E}{\partial v} = 0,$$

the Vlasov equation can also be written in conservative form as

$$\frac{\partial f}{\partial t} + \nabla_{(x,v)} \cdot (V f) = 0.$$

The method by Cheng and Knorr

The Cheng-Knorr method is one of the first semi-Lagrangian schemes designed for the Vlasov-Poisson system [6]. The method is based on the classical *Strang splitting method*.

1. Starting from f^n compute the electric field E^n solving the Poisson equation.
2. Compute f^* solving
$$\frac{\partial f}{\partial t} + E^n \frac{\partial f}{\partial v} = 0,$$
with initial data f^n, for a half time step $\Delta t/2$.
3. Compute f^{**} solving
$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = 0,$$
with f^* as initial data, for a time step Δt.
4. Compute ϱ^{n+1} from f^{**} and the electric field E^{n+1} solving the Poisson equation.
5. Compute f^{n+1} solving for a half time step $\Delta t/2$
$$\frac{\partial f}{\partial t} + E^{n+1} \frac{\partial f}{\partial v} = 0,$$
with initial data f^{**}.

[6] C. Cheng, G. Knorr '76

Direct multidimensional approach

- The semi-Lagrangian approach with splitting for the resolution of the Vlasov-Poisson system has the big advantage that the characteristic equation can be solved explicitly at each step of the splitting procedure. However, the splitting introduce errors privileging the directions.
- It is then interesting to consider the construction of semi-Lagrangian methods directly without splitting. These methods, however, need a suitable numerical approximation of the characteristic equation.
- The characteristic curve is solution of

$$\frac{dV}{dt} = E(X(t), t), \quad \frac{dX}{dt} = V.$$

The above equations cannot be solved exactly since the electric field E is computed through the Poisson equation which depends on the evolution of the distribution of particles f.

The method by Sonnendrücker et al.

The method by Sonnendrücker et al.[7] permits to pass from time t^n to t^{n+1} in an iterative way. Assume f^n and the electric potential E^n are known, then a second order in time iterative approach is summarized below.

1. Compute an approximation of the electric potential $\tilde{E}^{n+1}$ at time t^{n+1}.
2. Solve for all points in the phase space (x_j, v_k) the characteristics equations with a second order Runge-Kutta method

$$
\begin{aligned}
V^{n+1/2} &= V^{n+1} - \frac{\Delta t}{2}\tilde{E}^{n+1}(X^{n+1}), \\
X^{n} &= X^{n+1} - \Delta t\, V^{n+1/2}, \\
V^{n} &= V^{n+1/2} - \frac{\Delta t}{2}E^{n}(X^{n}).
\end{aligned}
$$

3. Compute the interpolation of f^n at points (X^n, V^n) to obtain an approximation of the distribution function $f^{n+1}(x_j, v_k)$ at time t^{n+1}, which we can use to compute a new value of the electric field $\tilde{E}^{n+1}$.
4. Iterate the scheme up to a prescribed convergence error.

[7] E. Sonnendrücker, J. Roche, P. Bertrand, A. Ghizzo '99

Positive flux-conservative schemes

These schemes are based on a conservative reconstruction strategy along the characteristics curves. For simplicity we restrict to the following one dimensional transport equation

$$\partial_t f + \partial_x (v\, f) = 0,$$

where $v > 0$ is a constant velocity (by symmetry one constructs the method for $v < 0$).

Let us introduce the mesh points $x_{j+1/2} = j\Delta x + \Delta x/2$, $j \in \mathbb{Z}$. Assume the solution is known at time $t^n = n\,\Delta t$, we compute the new values at time t^{n+1} by integration of the exact solution in each cell

$$\int_{x_{j-1/2}}^{x_{j+1/2}} f(t^{n+1}, x)dx = \int_{x_{j-1/2}-v\,\Delta t}^{x_{j+1/2}-v\,\Delta t} f(t^n, x)dx,$$

then, setting

$$G_{j+1/2}(t^n) = \int_{x_{j+1/2}-v\,\Delta t}^{x_{j+1/2}} f(t^n, x)dx,$$

we obtain the conservative form

$$\int_{x_{j-1/2}}^{x_{j+1/2}} f(t^{n+1}, x)dx = \int_{x_{j-1/2}}^{x_{j+1/2}} f(t^n, x)dx + G_{j-1/2}(t^n) - G_{j+1/2}(t^n).$$

Reconstruction via primitive function

The main step is now to choose an efficient method to reconstruct the distribution function from the values on each cell $[x_{j-1/2}, x_{j+1/2}]$. If we denote by

$$f_j^n = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} f(t^n, x)dx,$$

the simplest choice is based on a linear interpolation procedure

$$f_{\Delta x}(x) = f_j + (x - x_j)\frac{f_{j+1} - f_{j-1}}{2\Delta x},$$

which permits an explicit computation of the fluxes. Unfortunately the resulting method does not preserve positivity.

Another approach is based on a reconstruction via primitive function [8]. Let $F(t^n, x)$ be a primitive of the distribution function $f(t^n, x)$, then $F(t^n, x_{j+1/2}) - F(t^n, x_{j-1/2}) = \Delta x\, f_j^n$ and

$$F(t^n, x_{j+1/2}) = \Delta x \sum_{k=0}^{j} f_k^n = w_j^n.$$

[8] F. Filbet, E. Sonnendrücker, P. Bertrand '01

Nonnegative reconstructions

A reconstruction method allowing to preserve positivity and maximum principle can be obtained using a third-order reconstruction with slope correctors

$$
\begin{aligned}
f_{\Delta x}(x) = f_j + & \\
+ \quad & \frac{\theta_j^+}{6\,\Delta x^2}\Big[2\,(x-x_j)(x-x_{j-3/2})+(x-x_{j-1/2})(x-x_{j+1/2})\Big](f_{j+1}-\ f_j) \\
+ \quad & \frac{\theta_j^-}{6\,\Delta x^2}\Big[2\,(x-x_j)(x-x_{j+3/2})+(x-x_{j-1/2})(x-x_{j+1/2})\Big](f_j-\ f_{j-1}),
\end{aligned}
$$

with

$$
\theta_j^{\pm} = \begin{cases} \min\Big\{1;\dfrac{2\,f_j}{f_{j\pm1}-f_j}\Big\}, & \text{if } f_{j\pm1}-f_j>0,\\ \min\Big\{1;-\dfrac{2\,(f_{\max}-f_j)}{f_{j\pm1}-f_j}\Big\}, & \text{if } f_{j\pm1}-f_j<0,\end{cases}
$$

where $f_{\max} = \max_j\{f_j\}$. It can be shown that this reconstruction satisfies

(i) Conservation of the average

$$
\int_{x_{j-1/2}}^{x_{j+1/2}} f_{\Delta x}(x)dx = \Delta x\, f_j, \quad \forall\, j.
$$

(ii) Maximum principle

$$
0 \le f_{\Delta x}(x) \le f_{\max}, \quad \forall\, x.
$$

A numerical example

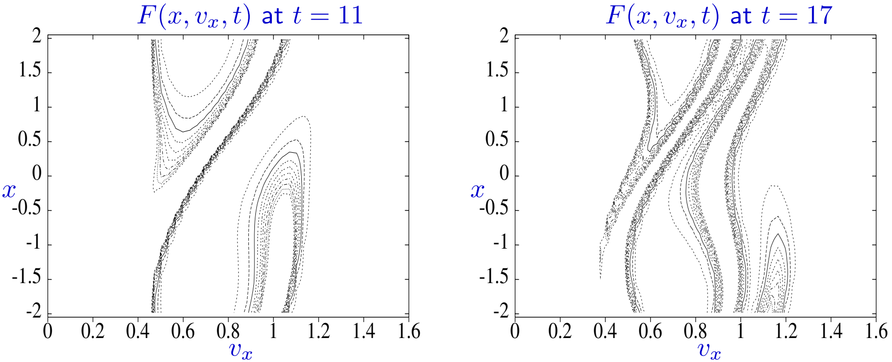

Figure: Evolution of $F(x, v_x, t) = \int_{\mathbb{R}} f(x, v_x, v_y, t)\, dv_y$ with $N_x = 32$, $N_v = 64$.

Initial data

$$f(0, x, v) = \frac{1}{2\pi\,\sigma^2}\, e^{-|v|^2/2\sigma^2}\ (1 + \alpha\cos(2\pi\, x/L))\,, \quad \forall\, x \in (0, L), \quad v \in \mathbb{R}^2,$$

where $\sigma = 0.24$, $\alpha = 0.5$, $L = 4$ and periodic boundary conditions.

Semi-Lagrangian schemes for BGK type equations

Coupling the previous semi-Lagrangian schemes with a collision term can be done in a straightforward way through splitting methods. Here we consider direct semi-Lagrangian approximations.

For simplicity, we restrict to the BGK equation in one space dimension

BGK model

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \nu(M[f] - f),$$

where $\nu > 0$ is a constant. The characteristic formulation of the problem yields

$$\frac{df}{dt} = \nu(M\,[f] - f), \qquad \frac{dx}{dt} = v.$$

Let $f_{j,k}^n$ be the approximate solution at time t^n at the nodes $x_j = j\Delta x$, $v_k = k\Delta v$, $j, k \in \mathbb{Z}$. A simple explicit first order forward semi-Lagrangian scheme reads

$$f(x_j + v_k\Delta t, v_k, t^{n+1}) = f_{j,k}^n(1 - \Delta t\nu) + \Delta t\nu M_{j,k}^n,$$

which do not lie on the grid. Then compute the values of $f_{j,k}^{n+1}$ on the grid by reconstruction from the computed values $f(x_j + v_k\Delta t, v_k, t^{n+1})$.

Computing Maxwellian states

In order to advance in time we must define the approximated Maxwellian distribution $M^n_{j,k}$. The simplest method to do that is given by

$$M^n_{j,k} = \frac{\rho^n_j}{(2\pi R T^n_j)^{1/2}} \exp\left(-\frac{|v_k - u^n_j|^2}{2RT^n_j} \right),$$

where ρ^n_j, T^n_j and u^n_j are approximations of the moments at the grid points. This formula requires the computation of the discrete moments of $f^n_{j,k}$ by some kind of quadrature. For example by simple summations

$$\rho^n_j = \Delta v \sum_h f^n_{j,h}, \quad u^n_j = \frac{\Delta v}{\rho^n_j} \sum_h v_h f^n_{j,h}, \quad T^n_j = \frac{\Delta v}{R\rho^n_j} \sum_h (v_h - u^n_j) f^n_{j,h}.$$

Problems

- $M^n_{j,k}$ is not compactly supported in the velocity space. Problem of the truncation of the velocity domain and the *loss of conservations*.
- There is no CFL-type stability restriction on the time step due to convection. The schemes may suffer from stability restrictions in *stiff regimes* when the collision rate ν is large.

Implicit semi-Lagrangian schemes

By applying simple implicit Euler on the characteristic equation backwards in order to compute $f_{j,k}^{n+1}$ one obtains

$$\begin{aligned} f_{j,k}^{n+1} &= f(t^n, x_j - v_k\Delta t, v_k) + \Delta t\nu(M_{j,k}^{n+1} - f_{j,k}^{n+1}) \\ &= \frac{1}{1+\Delta t\nu} f(t^n, x_j - v_k\Delta t, v_k) + \frac{\Delta t\nu}{1+\Delta t\nu} M_{j,k}^{n+1}, \end{aligned}$$

where $f(t^n, x_j - v_k\Delta t, v_k)$ is computed by suitable reconstruction from $f_{j,k}^n$.

The scheme cannot be directly solved for $f_{j,k}^{n+1}$, because $M_{j,k}^{n+1}$ depends from $f_{j,k}^{n+1}$ itself. However, if the discrete Maxwellian at time t^{n+1} has exactly the same first three moments as $f_{j,k}^{n+1}$

$$\sum_h M_{j,h}^{n+1}\phi_h = \sum_h f_{j,h}^{n+1}\phi_h, \qquad \phi_h = 1, v_h, |v_h|^2,$$

then we have

$$\sum_h f_{j,h}^{n+1}\phi_h = \sum_h f(t^n, x_j - v_h\Delta t, v_h)\phi_h, \qquad \phi_h = 1, v_h, |v_h|^2.$$

Therefore the moments at time t^{n+1} can be computed from the solution at time t^n and this allows and explicit evaluation of $M_{j,k}^{n+1}$.

Remarks

- For consistency, we must construct the approximated Maxwellian values $M_{j,k}^{n+1}$ in such a way that the moments equations are exactly satisfied. This is a transversal problem to most schemes which use a finite grid over a bounded velocity domain.
- Higher order implicit semi-Lagrangian methods for relaxation operators can be constructed using L-stable *diagonally implicit Runge Kutta (DIRK)* schemes[9].
- If the time step is such that $\Delta t = \Delta x / \Delta v$ then the foot of the characteristic is a grid point and no interpolation is required. In such case the semi-Lagrangian schemes becomes particular cases of *Lattice Boltzmann Methods (LBM)*[10].
- The implicit semi-Lagrangian schemes are unconditionally stable. However, large time steps will cause large numerical diffusion in the solution. In particular semi-Lagrangian schemes may suffer of accuracy degradation close to fluid regimes, or equivalently for very large values of ν. The latter aspect can be understood by observing that the characteristic speeds of the system change in such a limit.

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[9] P. Santagati, G. Russo, S.-B. Yun '12

[10] S.Succi '01

Fully conservative methods

Let us consider $f = f(v)$, $v \in \mathbb{R}^d$, $d \geq 1$, and denote by $f_k \approx f(v_k)$, $k = 1, \ldots, N$ the finite grid approximations. We want to define the grid values f_k in such a way that the macroscopic moments of f are preserved at a discrete level. We denote by $U \in \mathbb{R}^{2+d}$ the given set of moments

$$U = \int_{\mathbb{R}^d} f \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv.$$

We use notations $\mathrm{f} = (f_1, \ldots, f_N)^T$ to denote the unknown set of values and $\tilde{\mathrm{f}} = (\tilde{f}_1, \ldots, \tilde{f}_N)^T$ the point values $\tilde{f}_k = f(v_k)$. We also denote by $C \in \mathbb{R}^{(d+2)\times N}$ the matrix containing the parameters of the quadrature formula used to evaluate the discrete moments. Therefore we have $C\tilde{\mathrm{f}} \neq U$, and search for a vector f that it is "close" to $\tilde{\mathrm{f}}$ and such that $C\mathrm{f} = U$.

In order to find a solution to the problem one can consider the *constrained optimization problem* find $\mathrm{f} \in \mathbb{R}^N$ such that

$$\min \left\{ \|\tilde{\mathrm{f}} - \mathrm{f}\|_2^2 \;:\; C\mathrm{f} = U; C \in \mathbb{R}^{(d+2)\times N}, \tilde{\mathrm{f}} \in \mathbb{R}^N, U \in \mathbb{R}^{(d+2)} \right\}.$$

The optimal L_2 Maxwellian

The problem can be solved by a Lagrange multiplier method. Let $\lambda \in \mathbb{R}^{d+2}$ be the Lagrange multiplier vector, the objective function to be minimized is given by

$$L(\mathrm{f}, \lambda) = \sum_{k=1}^{N} |\tilde{f}_k - f_k|^2 + \lambda^T (C\mathrm{f} - U).$$

Next we impose

$$\frac{\partial L(\mathrm{f}, \lambda)}{\partial f_k} = 0, \quad k = 1, \ldots, N \qquad \frac{\partial L(\mathrm{f}, \lambda)}{\partial \lambda_i} = 0, \quad i = 1, \ldots, d+2.$$

The first condition implies $2\mathrm{f} = 2\tilde{\mathrm{f}} + C^T \lambda$ and the second $C\mathrm{f} = U$. Since CC^T is symmetric and positive definite one gets $\lambda = 2(CC^T)^{-1}(U - C\tilde{\mathrm{f}})$ and therefore[11]

$$\mathrm{f} = \tilde{\mathrm{f}} + C^T (CC^T)^{-1} (U - C\tilde{\mathrm{f}}).$$

Reverting now to the full space and time dependent notation, we get

$$\mathrm{M}_j^n = \tilde{\mathrm{M}}_j^n + C^T (CC^T)^{-1} (U_j^n - C\tilde{\mathrm{M}}_j^n),$$

with U_j^n the set of moments, $\mathrm{M}_j^n = (M_{j,1}^n, \ldots, M_{j,N}^n)^T$ and $\tilde{\mathrm{M}}_j^n$ defined similarly.

[11] I. Gamba, S. Tharkabhushanam '09

Remarks

- The method only involves a matrix-vector multiplication. Moreover, since the matrix C depends only on the parameter of the discretization, the matrix $C^T(CC^T)^{-1}$ can be precomputed and stored in memory. This makes the technique extremely efficient for multi-dimensional computations.
- Positivity of the solution is lost in general, as well as the monotonicity property induced by the entropy inequality.
- For Maxwellian densities, these properties can be recovered considering a constrained minimization problem with respect to the entropy of the solution. However, solving such a minimization problem implies the solution of a system of $d+2$ nonlinear equations at each time step.

The discrete entropic Maxwellian

Let $\mathcal{V} = \left\{ v_k \in \mathbb{R}^3, k = 1, \ldots, N_v \right\}$ be a discrete-velocity grid of N_v points. A classical way to recover the exact moments and the minimum entropy property of the Maxwellian in a finite computational domain is based on the theory of *discrete velocity models* [12].

The discrete Maxwellian state $M_k[\mathrm{f}]$, where $\mathrm{f} = (f_1, \ldots, f_{N_v})^T$, should be such that $\log(M_k[\mathrm{f}]) \in \mathrm{span}\{1, v_k, |v_k|^2\}$ which implies

$$M_k[\mathrm{f}] = \exp(a + b \cdot v_k + c|v_k|^2), \quad c < 0,$$

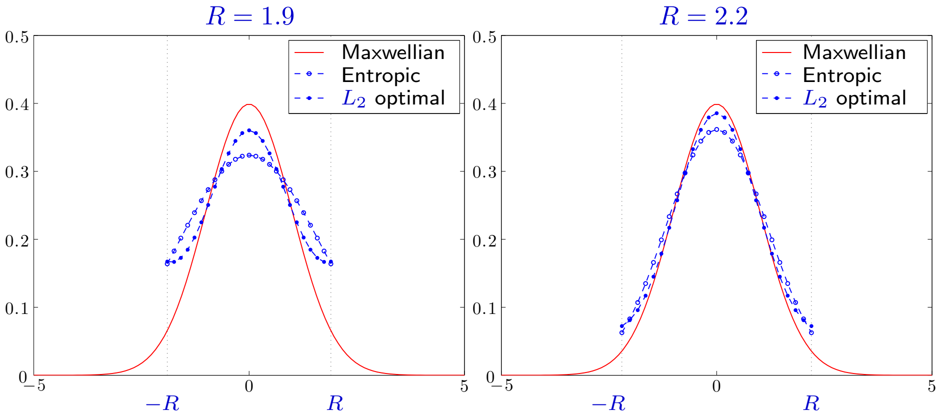
where $a, c \in \mathbb{R}$, $b \in \mathbb{R}^3$ are obtained from the solution of the nonlinear system

$$\sum_{h=1}^{N_v} f_h (v_h)^s \quad = \quad \sum_{h=1}^{N_v} M_h[\mathrm{f}] (v_h)^s, \qquad s = 0, 1, 2.$$

Note that, due to the particular choice of the grid, not all set of moments may be realizable by the discrete velocity model.

[12] H.Cabannes '81, L. Mieussens '00

Discrete Maxwellian states



Further reading

- E. Sonnendrücker (2013), Numerical methods for Vlasov equations, Technical report, MPI TU Munich. (http://www-m16.ma.tum.de/foswiki/pub/M16/Allgemeines/NumMethVlasov/Num-Meth-Vlasov-Notes.pdf).