Numerical methods and uncertainty quantification for kinetic equations

Lecture 2: Semi-Lagrangian, discrete velocity and spectral schemes

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Lecture 2 Outline

1. Semi-Lagrangian schemes
   - Semi-Lagrangian scheme for Vlasov type equations
   - Semi-Lagrangian schemes for BGK type equations
2. Discrete Velocity methods
   - Discrete Boltzmann equation
   - Properties
3. Spectral methods
   - Standard spectral methods
   - Fast spectral methods

Outline

Introduction

- We give a short overview of *semi-Lagrangian*[1] 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*[2] to *WENO schemes*and *Discontinuous-Galerkin methods* [3].

[1] Sonnendrücker, Filbet, Crouseilles, Mehrenberger, Besse, Kormann, Charles, Després, Campos Pinto, Russo, Qiu, Shu, Cottet, Lemou..

[2] C. Birdsall, A. Langdon '91, Sonnendrücker, Campos Pinto, Chacon

[3] Qiu, Shu, Carrillo, Gamba, Navoret, Franck, Helluy, Einkemmer

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

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

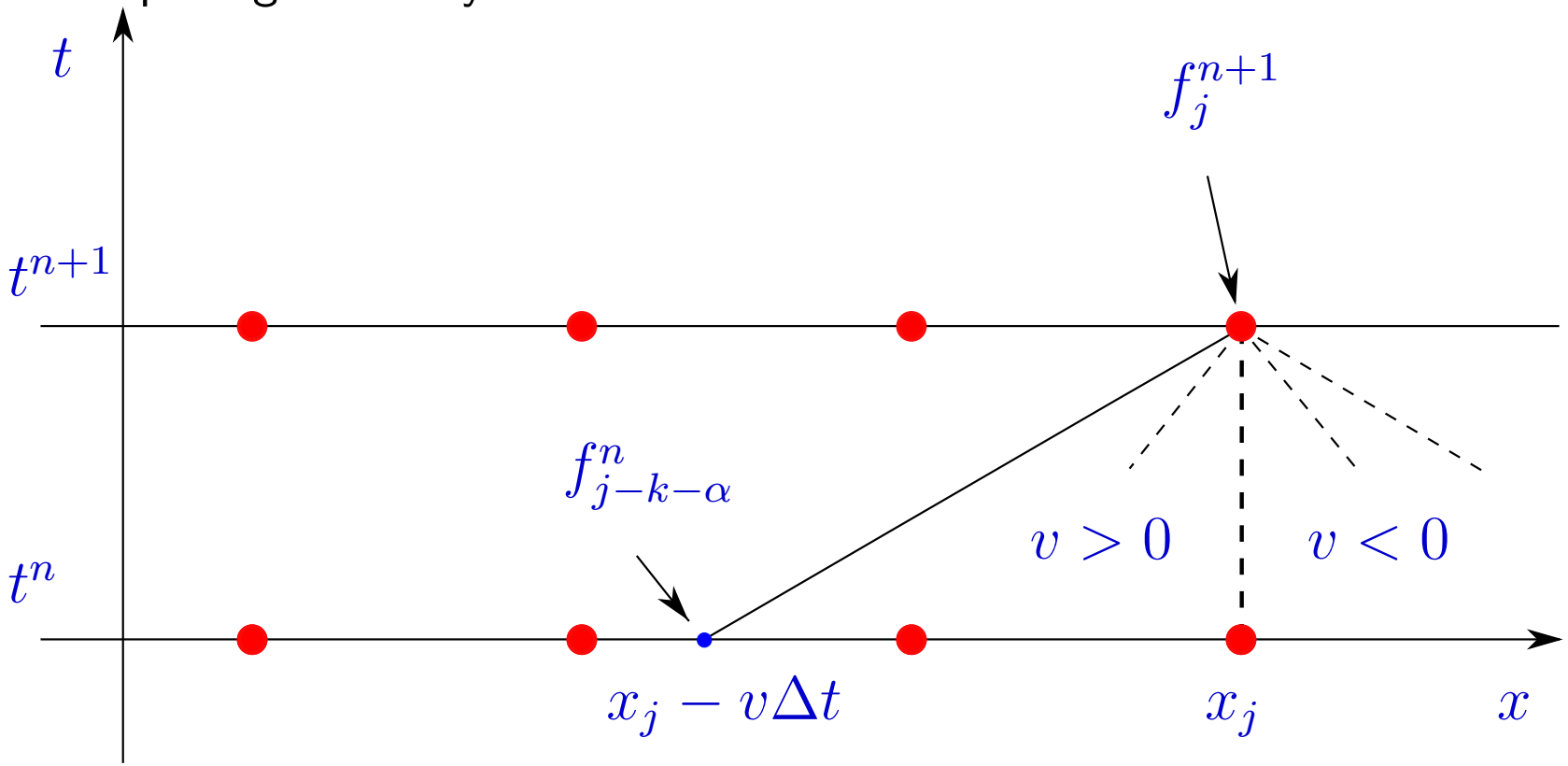
where we introduced a uniform grid $x_j = j\Delta x$, $j \in \mathbb{Z}$ and discrete time steps $t^n = n\Delta t$. The points in space used to compute the solution are the points that within a single time step are transported by the flow onto the mesh. These points do not lie in the general case on 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 $\alpha = 0$.



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[4].

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

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

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

The method by Cheng and Knorr

The Cheng-Knorr method is one of the first semi-Lagrangian schemes designed for the Vlasov-Poisson system [5]. 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^{**}.

[5] 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.[6] 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.

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

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 $M_{j,k}^{n+1}$.

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

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

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[7]

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

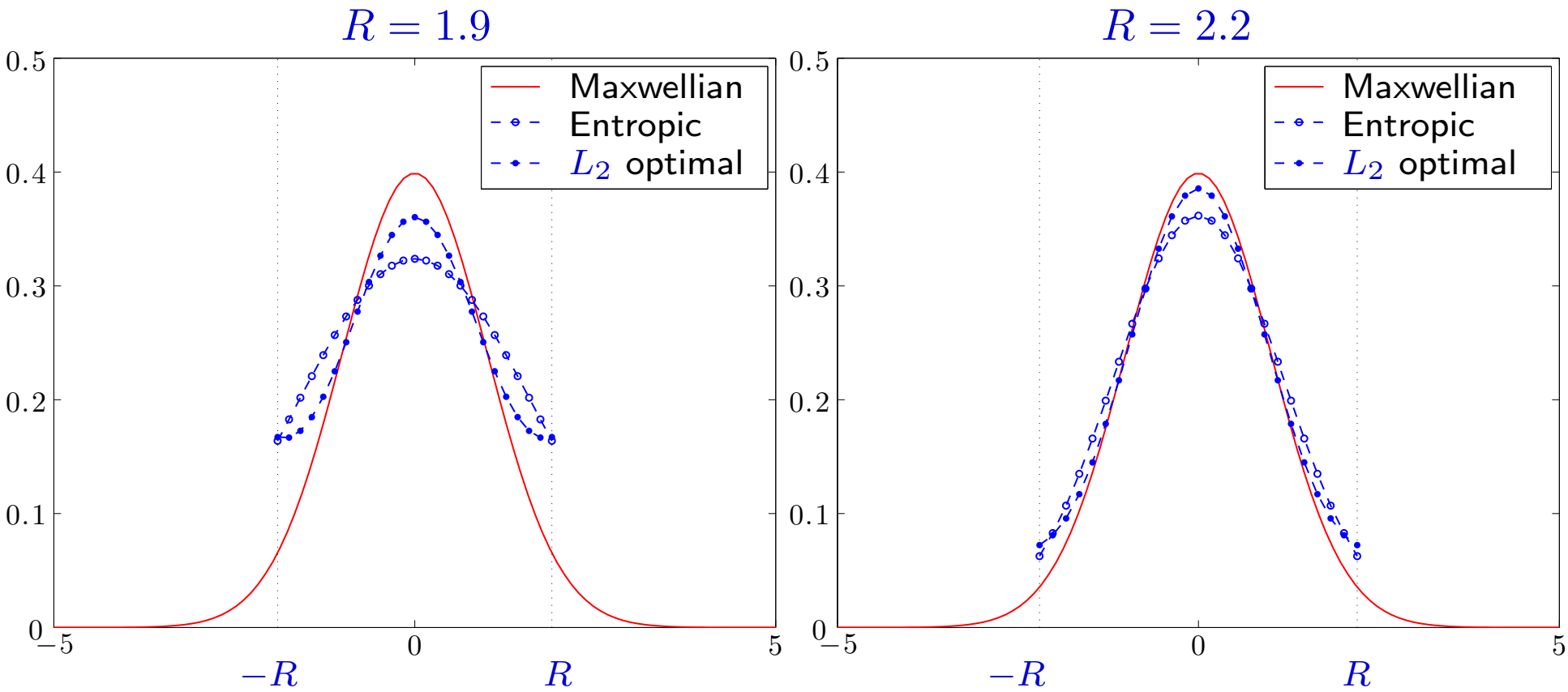
Reverting now to the full space and time dependent notation, we get

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

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

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

Discrete Maxwellian states



Outline

Notations

The Boltzmann equation in non-dimensional form can be written as

Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f, f)$$

where $f = f(x, v, t)$ is the density of particles in (x, v) at time t and

Collision operator

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

with the velocity transformation

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

Physical 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 it satisfies

H-theorem

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

In particular the equality holds in the H-theorem only if

Maxwellian distribution

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

where we defined the density, mean velocity and temperature of the gas by

$$\rho = \int_{\mathbb{R}^3} f\,dv, \qquad u = \frac{1}{\rho}\int_{\mathbb{R}^3} vf\,dv, \qquad T = \frac{1}{3R\rho}\int_{\mathbb{R}^3}[v-u]^2 f\,dv.$$

Discrete velocity methods

Historically this was the first method for discretizing the Boltzmann equation in velocity space[8]. The model is built starting from physical rather then numerical considerations. We assume the gas particles can attain only a finite set of velocities

$$V_N = \{v_1, v_2, v_3, \dots, v_N\}, \quad v_i \in \mathbb{R}^3.$$

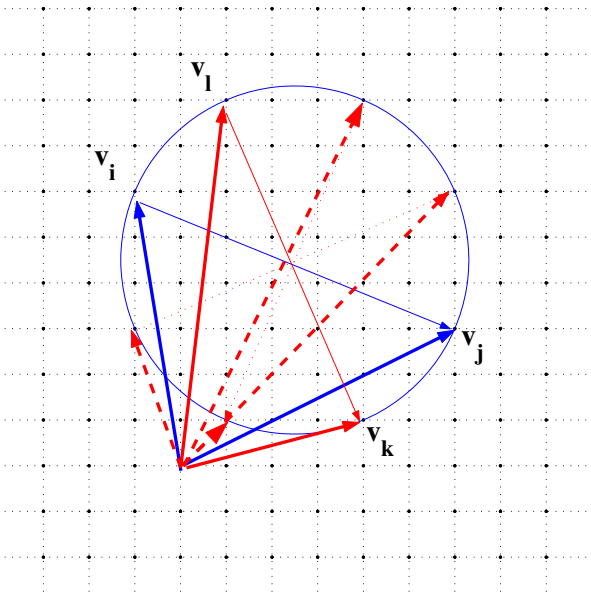
Particles collide by hard spheres dynamic. The collision $(v_i, v_j) \leftrightarrow (v_k, v_l)$ is defined admissible if $v_i, v_j, v_k, v_l \in V_N$ and preserves momentum and energy

$$v_i + v_j = v_k + v_l, \qquad |v_i|^2 + |v_j|^2 = |v_k|^2 + |v_l|^2.$$

The set of admissible output pairs (v_k, v_l) corresponding to a given input pair (v_i, v_j) will be denoted by C_{ij} and its cardinality by q_{ij}.

[8] J.E.Broadwell, 1964 - R.Gatignol, 1975 - H.Cabannes, 1980 - F.Rogier, J.Schneider, 1994 - C.Buet, 1996

Discrete Boltzmann equation



For the collision (v_i, v_j) we have 3 admissible output collision pairs (v_k, v_l) hence $q_{ij} = 3$. In general few grid points will belong to the collision circle.
The discrete collision operator is obtained by computing first the transition probabilities a_{ij}^{kl} of the collision $(v_i, v_j) \leftrightarrow (v_k, v_l)$ which satisfy the relations

$$a_{ij}^{kl} \geq 0, \qquad \sum_{k,l=1}^{N} a_{ij}^{kl} = 1, \; \forall i, j = 1, \dots, N,$$

with $a_{ij}^{kl} = a_{kl}^{ij}$ (simmetry) and $a_{ij}^{kl} = a_{ji}^{kl} = a_{ji}^{lk} = a_{ij}^{lk}$ (microreversibility).

Discrete Boltzmann equation

Example: All output pairs are assumed to be equally probable

$$a_{ij}^{kl} = \begin{cases} \dfrac{1}{q_{ij}} & \text{if } (v_i, v_j) \leftrightarrow (v_k, v_l) \text{ admissible} \\ 0 & \text{if } (v_i, v_j) \leftrightarrow (v_k, v_l) \text{ not admissible.} \end{cases}$$

Next we introduce the transition rates $A_{ij}^{kl} = S|v_i - v_j|a_{ij}^{kl}$, where S is the cross sectional area of particles, and write the discrete Boltzmann equation as

Discrete Boltzmann equation

$$\frac{\partial f_i}{\partial t} + v_i \cdot \nabla_x f_i = Q_i(f,f), \quad Q_i(f,f) = \sum_{j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j)$$

where f_i, f_j, f_k, f_l is the distribution of particles with velocity v_i, v_j, v_k, v_l.

Properties

The discrete Boltzmann equation satisfies for any test function $\phi_i = \phi(v_i)$

$$\sum_{i=1}^{N} Q_i(f,f)\phi_i = -\frac{1}{4}\sum_{i,j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j)(\phi_k + \phi_l - \phi_i - \phi_j),$$

and thus the *discrete collision invariants* satisfy

$$\phi_k + \phi_l - \phi_i - \phi_j = 0.$$

Therefore we have $\phi(v_i) = 1, v_i^x, v_i^y, v_i^z, |v_i|^2$ as collision invariants.
The main macroscopic quantities are defined as

$$\rho = \sum_{i=1}^{N} f_i, \qquad u = \frac{1}{\rho}\sum_{i=1}^{N} f_i v_i, \qquad T = \frac{1}{3R\rho}\sum_{i=1}^{N} f_i (v_i - u)^2.$$

In addition taking $\phi_i = \ln(f_i)$ we obtain

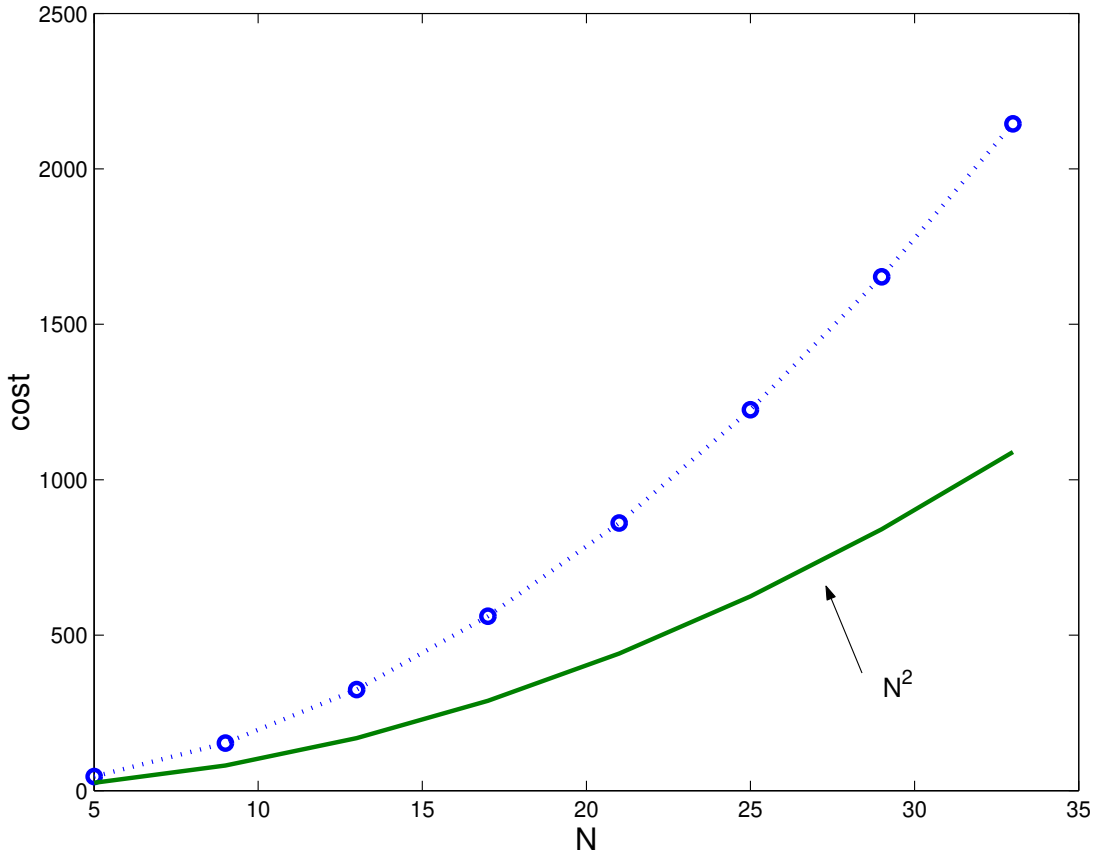
$$\sum_{i=1}^{N} Q_i(f,f)\ln(f_i) = -\frac{1}{4}\sum_{i,j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j)\ln\left(\frac{f_k f_l}{f_i f_j}\right) \leq 0,$$

and hence the discrete analogue of Boltzmann's H-theorem.

Accuracy vs computational cost

The discrete Boltzmann equation has the nice property of preserving the essential physical features (conservations, H-theorem, equilibrium states) however from a computational point of view it presents some drawbacks.

- The computational cost is *high* in general, typically $O(N^\eta)$, with $\eta > 2$.



Computational cost in a 2D model

Accuracy vs computational cost

- The accuracy of the method is *low*, the error behaves as $O(1/n^{\mu})$ with $\mu < 1$ and where n is the number of grid points in each direction.

n	8	10	12	14	16	18	20	22
E_∞	0.044	0.035	0.033	0.028	0.024	0.021	0.019	0.017
T_{sec}	0.38	1.96	7.25	23.01	66.43	135.47	286.94	638.13

Relative L_∞ error and computational cost (in seconds) for $n = 8, 10, 12, 14, 16, 18, 20, 22$.

n	8-10	10-12	12-14	14-16	16-18	18-20	20-22
μ	1.0255	0.3227	1.0659	1.1544	1.1337	0.9499	1.1670
η	2.4506	2.3915	2.4974	2.6466	2.0167	2.3745	2.7953

Convergence rates μ and cost exponents η for $n = 8, 10, 12, 14, 16, 18, 20, 22$.

- The above results have been obtained for the space homogeneous Boltzmann equation using a 3D Maxwell model ($A_{ij}^{kl} = Sa_{ij}^{kl}$) on a regular grid[9].

[9] A.G.Heinz, V.A.Panferov, 2002

Outline

Spectral methods

A different approach is based on the use of spectral methods[10]. After the splitting of the equation we consider the homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = Q(f,f), \quad x, v \in \mathbb{R}^3$$

with $Q(f,f) = Q^+(f,f) - Q^-(f,f)$ and

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

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

The collision transform is

$$v' = \frac{1}{2}(v + v_* + |v - v_*|\omega), \quad v'_1 = \frac{1}{2}(v + v_* - |v - v_*|\omega).$$

Remark: We will restrict to inverse power forces interactions $B = B(|v - v_*|, \theta)$.

[10] L.Pareschi, B.Perthame, '96 - L.Pareschi, G.Russo '00

Spectral-Fourier projection

Let us write the homogeneous Boltzmann equation as

$$\frac{\partial f}{\partial t} + f\, L(f) = Q^+(f,f)$$

The method can be derived in three steps.

1. Change of variables ($v_* \to g = v - v_*$)

Integrating over $g = v - v_*$ gain and loss parts can be rewritten as

$$Q^+(f,f) = \int_{I\!R^3} \int_{\mathbb{S}^2} B(|g|,\theta) f(v') f(v'_*)\, d\omega\, dg,$$

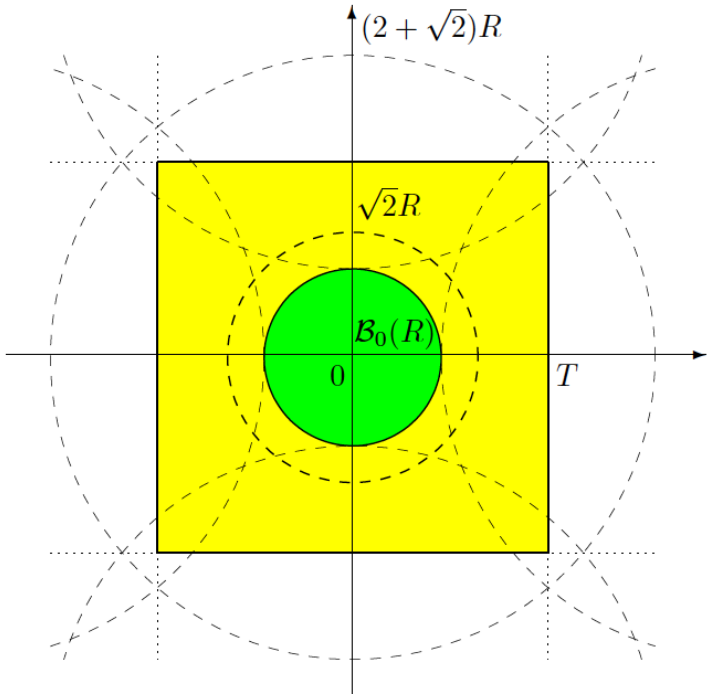
$$L(f) = \int_{I\!R^3} \int_{\mathbb{S}^2} B(|g|,\theta) f(v-g)\, d\omega\, dg,$$

where now

$$v' = v - \frac{1}{2}(g - |g|\omega), \quad v'_* = v - \frac{1}{2}(g + |g|\omega).$$

Spectral-Fourier projection

2. Reduction to a bounded domain



Proposition

Let $\mathrm{Supp}(f(v)) \subset \mathcal{B}(0,R)$ *then* $\mathrm{Supp}(Q(f,f)(v)) \subset \mathcal{B}(0,\sqrt{2}R)$, *and*

$$Q(f,f)(v) = \int_{\mathcal{B}(0,2R)} \int_{S^2} B(|g|,\theta)[f(v')f(v'_*) - f(v)f(v-g)]\, d\omega\, dg,$$

with $v', v'_*, v-g \in \mathcal{B}(0,(2+\sqrt{2})R)$.

Spectral-Fourier projection

3. Fourier-Galerkin projection

Consider the distribution function $f(v)$ restricted on $[-T,T]^3$, using periodicity

$$T \geq R + \frac{(2+\sqrt{2})R - R}{2} = \frac{(3+\sqrt{2})}{2} R = R/\lambda.$$

We set $T = \pi$ and $R = \lambda\pi$.
Assume $f(v) = 0$ on $[-\pi,\pi]^3 \setminus \mathcal{B}(0,\lambda\pi)$, and extend it by periodicity to a periodic function. Then approximate f by the truncated Fourier series

$$f_N(v) = \sum_{k=-N}^{N} \hat{f}_k e^{ik\cdot v}, \quad \hat{f}_k = \frac{1}{(2\pi)^3} \int_{[-\pi,\pi]^3} f(v) e^{-ik\cdot v}\, dv.$$

Fundamental unknowns are the coefficients $\hat{f}_k$, $k = -N,\dots,N$.
To obtain the Fourier-Galerkin method we require that[11]

$$\int_{[-\pi,\pi]^3} \left(\frac{\partial f_N}{\partial t} + f_N\, L(f_N) - Q^+(f_N, f_N) \right) e^{-ik\cdot v}\, dv = 0.$$

[11] C.Canuto, A.Quarteroni,M.Y.Hussaini, T.A.Zang, 1988

Spectral-Fourier projection

By substituting expression for f_N in the Boltzmann equation we get

$$Q^+(f_N, f_N) - f_N\, L(f_N) = \sum_{l,m=-N}^{N} \hat{f}_l\, \hat{f}_m (\hat{B}(l,m) - \hat{B}(m,m)) e^{i(l+m)\cdot v},$$

where the kernel modes $\hat{B}(l,m)$ are given by

$$\hat{B}(l,m) = \int_{\mathcal{B}(0,2\lambda\pi)} \int_{\mathbb{S}^2} B(|g|,\theta) e^{-ig\cdot\frac{(l+m)}{2} - i|g|\omega\cdot\frac{(m-l)}{2}}\, d\omega\, dg.$$

The final scheme is charaterized by a set of ODE's for the Fourier coefficients

Spectral scheme

$$\frac{\partial \hat{f}_k}{\partial t} + \sum_{m=k-N}^{N} \hat{f}_{k-m}\, \hat{f}_m \hat{B}(m,m) = \sum_{m=k-N}^{N} \hat{f}_{k-m}\, \hat{f}_m \hat{B}(k-m,m).$$

Remarks

- Setting $n = N^3$ the evaluation of the spectral scheme requires exactly $O(n^2) \ll O(n^2 M)$ operations where M is the number of angle discretizations.
- The first sum on the left hand side is a convolution sum and can be evaluated in $O(N^3 \log N)$ operations by FFT based transform methods. The most expensive part is thus the right hand side (gain term).
- If we consider the variable hard spheres (VHS) model, the kernel does not depend on the angle θ and $B = C_\alpha |g|^\alpha$.
- In this case $\hat{B}(l, m)$ is a function of $|l - m|$, $|l + m|$ and thus can be efficiently pre-computed and stored in a matrix.
- The scheme preserves the mass (Fourier mode of order zero) but not momentum and energy exactly.
- We will see that however these quantities, except for the error on the initial data, are approximated with spectral accuracy in time.

Properties of the spectral method

If $f \in H_p^r([-\pi,\pi]^3)$, where $r \geq 0$ is an integer and $H_p^r([-\pi,\pi]^3)$ is the subspace of the Sobolev space $H^r([-\pi,\pi]^3)$, which consist of periodic functions, for each $\varphi \in L^2([-\pi,\pi]^3)$ we have

$$| < f, \varphi > - < f, \varphi_N > | \leq ||\varphi||_2 \, ||f - f_N||_2 \leq \frac{C}{N^r} ||\varphi||_2 ||f||_{H_p^r}.$$

Next we state the spectral accuracy of the approximation of the collision operator

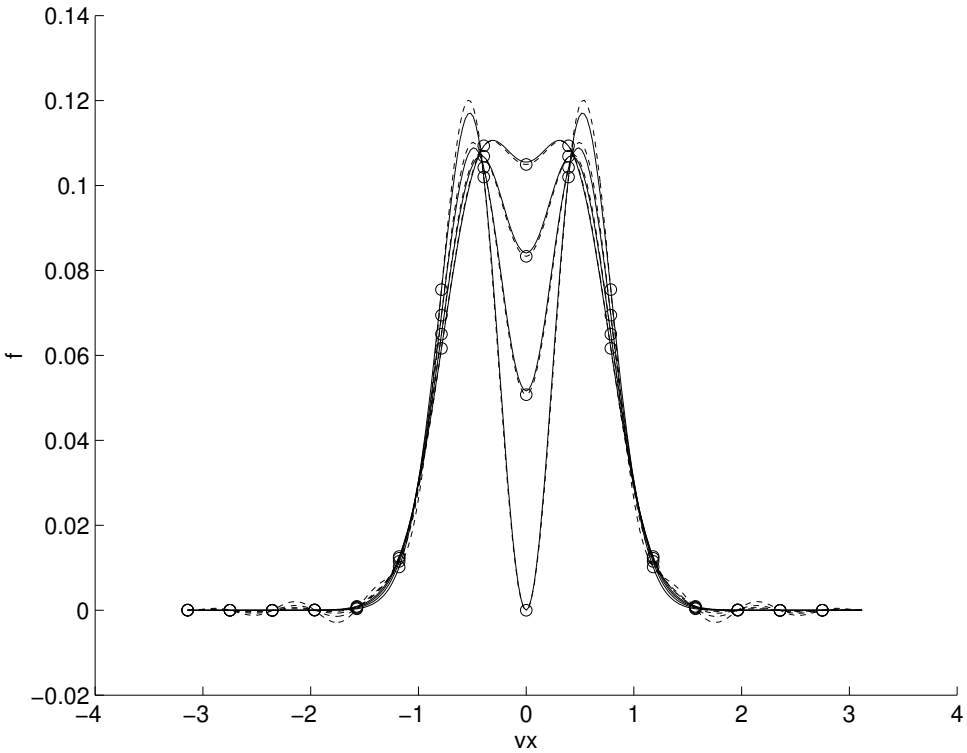
Corollary (Spectral accuracy)

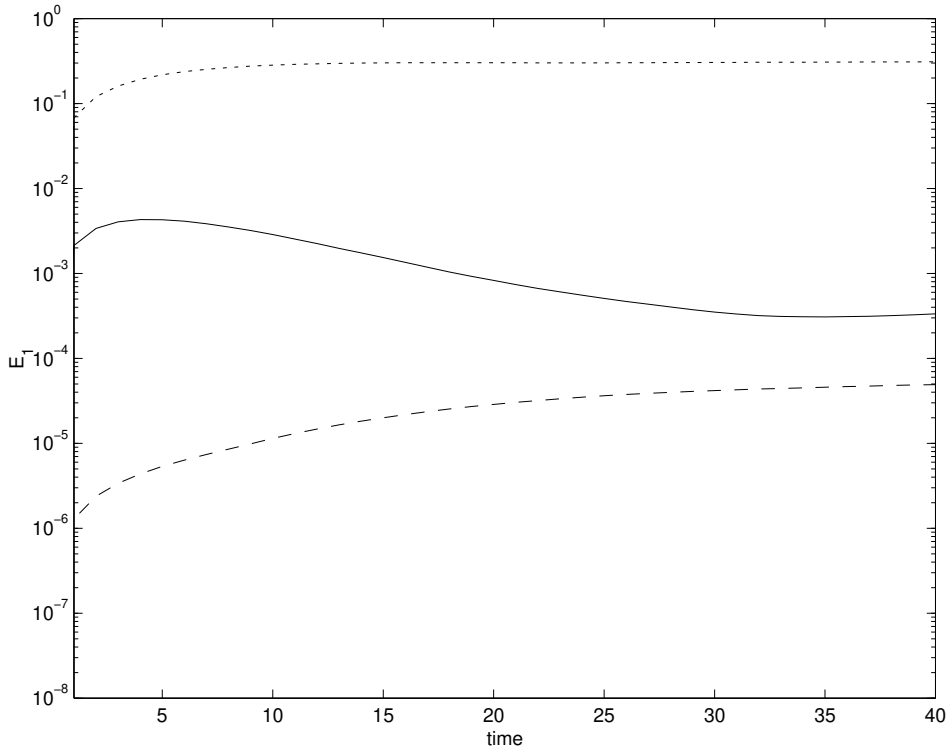
Let $f \in H_p^r([-\pi,\pi]^3)$, $r \geq 0$ then

$$||Q(f) - Q_N(f_N)||_2 \leq \frac{C}{N^r} \left(||f||_{H_p^r} + ||Q(f_N)||_{H_p^r} \right).$$

Test#1 2D Maxwell molecules

Solution at time $t = 0, 3, 6, 9$ (left) and L_1 relative norm of the error vs time (right) for $N = 8, 16$, and 32 modes per direction.





Convergence rates at $t = 5 \Rightarrow 5.6$ $(N = 8 - 16)$ and 9.7 $(N = 16 - 32)$.

Open questions

- We have considered two different deterministic methods for the numerical evaluation of the collision operator.
- Discrete velocity models permit to obtain discretized Boltzmann equation with the correct physical properties.
- Unfortunately the connection with the Boltzmann equation is hard to prove, their accuracy is limited and the computational cost is high. They are rather ad-hoc and not very flexible.
- Spectral methods are obtained directly from the Boltzmann equation. They are very accurate but do not preserve exactly momentum and energy.
- Their computational cost is lower then that of discrete velocity models but still high in general. They are very flexible and can be applied also to Landau-Fokker-Planck equations, granular gases and other kinetic models.
- Is it possible to derive fast algorithms for such methods?
- What about space non homogeneous computations?

Carlemann-like representation

The computational cost of the method can be reduced to $O(n \log_2 n)$ using a different representation of the collision operator[12].
The basic identity we shall need in dimension $d = 2, 3$ is

$$\int_{\mathbb{S}^{d-1}} F(|u|\omega - u)\, d\omega = \frac{2}{|u|^{d-2}} \int_{\mathbb{R}^d} \delta(2\, x \cdot u + |x|^2)\, F(x)\, dx.$$

Using the above identity the collision operator can be written as

Carlemann-like representation

$$Q(f,f)(v) = \int_{x,y \in \mathcal{B}_R} \tilde{B}(x,y)\delta(x \cdot y)\, [f(v+y)f(v+x) - f(v+x+y)f(v)]\, dxdy$$

with $\mathcal{B}_R = \mathcal{B}(0, 2\lambda\pi)$, $v \in [-\pi, \pi]^d$ and

$$\tilde{B}(x,y) = 2^{d-1}\, B\left(-\frac{x \cdot (x+y)}{|x||x+y|}, |x+y|\right) |x+y|^{-(d-2)}.$$

Note that $\tilde{B}(x,y)$ is constant for Maxwell molecules ($B \equiv 1$) in dimension $d = 2$ and for hard spheres ($B \equiv |x+y|$) in dimension $d = 3$.

[12] C.Mouhot, L.Pareschi '05 - F.Filbet, C.Mouhot, L.Pareschi '06

Spectral methods

We can perform the same derivation as in the standard spectral method to obtain

$$\hat{Q}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} (\hat{B}(l,m) - \hat{B}(m,m))\, \hat{f}_l\, \hat{f}_m, \quad k = -N, ..., N$$

where now

New kernel modes

$$\hat{B}(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y)\, e^{il\cdot x}\, e^{im\cdot y}\, dx\, dy.$$

The conventional representation, in the new variables x and y, reads

$$\hat{B}(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y)\, \chi_{\{|x+y|\le R\}}\, e^{il\cdot x}\, e^{im\cdot y}\, dx\, dy.$$

One can notice that here x and y are also restricted to the ball $\mathcal{B}_R$ but the condition $|x+y|^2 = |x|^2 + |y|^2 \le R^2$ couples the two modulus.

Fast algorithms

The search for fast deterministic algorithms consists mainly in identifying some convolution structure in the collision operator.
We make the assumption that

Decoupling assumption

$$\tilde{B}(x,y) = a(|x|)\, b(|y|).$$

This assumption is obviously satisfied if $\tilde{B}$ is constant. This is the case of *Maxwellian molecules* in dimension two, and *hard spheres* in dimension three.
If we now change to spherical coordinates

$$\hat{B}(l,m) = \frac{1}{4}\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \delta(e\cdot e')\left[\int_{-R}^{R} \rho a(\rho) e^{i\rho(l\cdot e)} d\rho\right]\left[\int_{-R}^{R} \rho' b(\rho') e^{i\rho'(m\cdot e')} d\rho'\right] dede'.$$

Fast algorithms

In the case of hard spheres, after integrating e' on $\mathbb{S}^2 \cap e^\perp$ we get

$$\hat{B}(l,m) = \int_{e \in \mathbb{S}^2_+} \phi(l \cdot e)\, \psi\big(\Pi_{e^\perp}(m)\big)\, de$$

where $\mathbb{S}^2_+$ denotes the half-sphere, $\Pi_{e^\perp}$ is the orthogonal projection on $e^\perp$ and

$$\phi(s) = R^2\big(2\,\mathrm{Sinc}(Rs) - \mathrm{Sinc}^2(Rs/2)\big), \quad \psi(s) = \int_0^\pi \phi(s\cos\theta) d\theta.$$

Using spherical coordinates (θ, φ) and taking uniform grids of size M_1 and M_2 we get

Decoupled kernel modes

$$\hat{B}(l,m) \simeq \frac{\pi^2}{M_1 M_2} \sum_{p,q=0}^{M_1,M_2} \alpha_{p,q}(l)\alpha'_{p,q}(m)$$

Computational considerations

- Thanks to periodicity of the integrands the rectangular rule in (θ, φ) is also spectrally accurate.
- Taking $M = M_1 = M_2$ we obtain the computational cost

$$O(M^{d-1} n \log_2 n), \quad n = N^d.$$

The method is therefore faster then the classical if

$$M^{d-1} \log_2 n \ll n.$$

- The angular discretization does not affects the main physical properties of the Boltzmann equation.

Numerical examples

Test problems[13]:

Test#1 2D Maxwellian molecules: Exact solution

This test is used to check spectral accuracy, by comparing the error at a given time, when using $N = 8$, 16, and 32 Fourier modes for each dimension.

Test#2 3D VHS molecules: sum of two Gaussians

This test is used compare the relaxation to equilibrium of the stress tensor for Maxwellian molecules, with the relaxation of other VHS molecules.

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
16	2 $sec.$ 40	1 $sec.$ 15	1 $sec.$ 70	2 $sec.$ 30
32	38 $sec.$ 01	5 $sec.$ 55	8 $sec.$ 47	11 $sec.$ 10
64	616 $sec.$	35 $sec.$ 50	54 $sec.$ 66	71 $sec.$ 27

Comparison of the computational time in $2D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second order Runge-Kutta time discretization.

[13] F.Filbet, C.Mouhot, L.Pareschi, '05

Cost and accuracy

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
16	1 $m.$ 14$s.$	3 $m.$ 31$s.$	7 $m.$ 45 $s.$	13 $m.$ 44 $s.$
32	118 $m.$ 02 $s.$	50 $m.$ 31$s.$	105 $m.$ 19 $s.$	186 $m.$ 18$s.$
64	125h 54 $m.$	8h 45 $m.$ 22$s.$	21h 39 $m.$	35h 01 $m.$ 28$s.$

Comparison of the computational time in $3D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second-order Runge-Kutta time discretization.

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
8	0.02013	0.02778	0.02129	0.02112
16	0.00204	0.00329	0.00238	0.00224
32	1.405E-5	2.228E-5	1.861E-5	1.772E-5

Comparison of the L^1 error in $2D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second-order Runge-Kutta time discretization at time $T_{end} = 1$.

Further reading

- *Semi-Lagrangian* methods are discussed in
  - 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`).
- *Spectral methods* are covered in the general survey used as a reference for the first part of these lectures
  - G. Dimarco, L. Pareschi, *Acta Numerica* 23, 2014.

  DVM are also partially covered in the same reference.
- *Consistency/convergence* results for DVM are found in
  - A. Palczewski, J. Schneider, A. Bobylev, *SINUM* '97;
  - S. Mischler, *ARMA* '97;
  - L. Mieussens, *Comp. Math. App.* '01;
  - V. Panferov, A. Heintz, M^2AS '02