Numerical methods for kinetic equations

Lecture 3: Discrete-velocity and spectral methods

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Lecture 3 Outline

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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

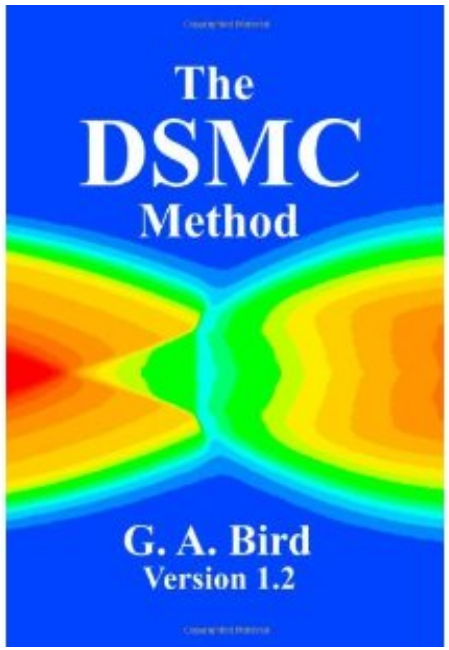
$$\rho = \int_{\mathbb{R}^3} f\,dv, \qquad u = \frac{1}{\rho}\int_{\mathbb{R}^3} vf\,dv, \qquad T = \frac{1}{3R\rho}\int_{\mathbb{R}^3}[v-u]^2 f\,dv.$$

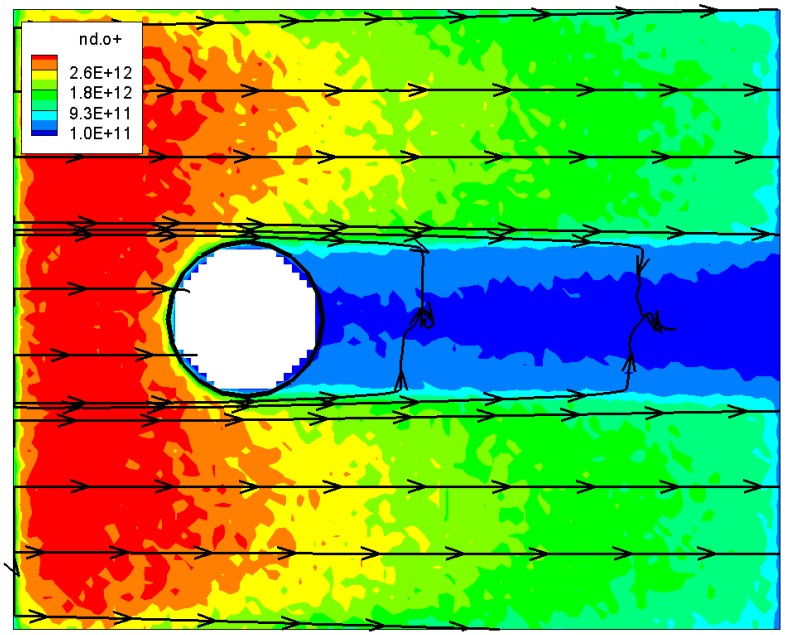
Numerical considerations

- Most difficulties are due to the multidimensional nature of the problem (usually a 7 dimensional problem, 6 space dimensions plus time) and to the structure of the collision integral which leads to the so-called *curse of dimensionality*.
- In the next two lectures we focus on the following major challenges in the numerical solution of the Boltzmann equation.
  - ▷ Computational complexity
  - ▷ Large time behavior
- Both aspects are related to the approximation of the collision integral which involves the velocity space only.
- The same difficulties are shared by most multidimensional kinetic equations.

Monte Carlo methods

- Traditional grid-based methods are often ineffective and the method of choice has been the Monte Carlo method.





- Monte Carlo methods are highly efficient, the computational cost is linear with respect to the particles number, and preserve the main physical properties.
- Monte Carlo method suffers from two difficulties. One is the slow convergence rate. The other is the numerical noise in the solutions.

Discrete velocity methods

Historically this was the first method for discretizing the Boltzmann equation in velocity space[1]. The model is built starting from physical rather then numerical considerations. We assume the gas particles can attain only a finite set of velocities

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

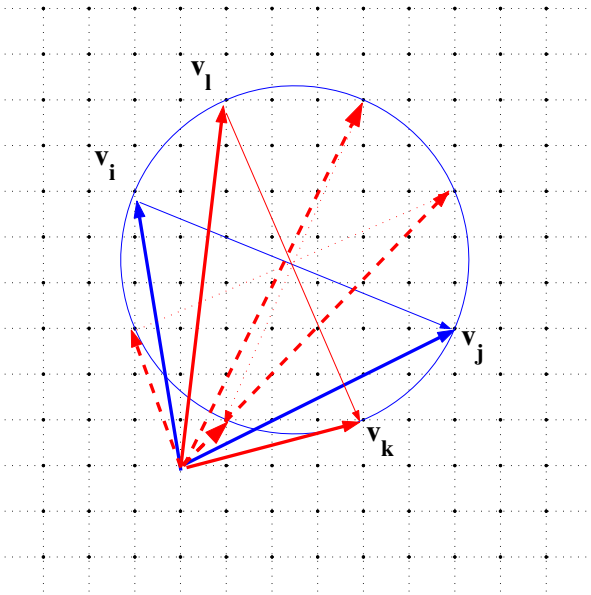
Particles collide by hard spheres dynamic. The collision $(v_i, v_j) \leftrightarrow (v_k, v_l)$ is defined admissible if $v_i, v_j, v_k, v_l \in V_N$ and preserves momentum and energy

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

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}.

[1] 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

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

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.

Equilibrium states

By the same arguments as in the continuous case we obtain that the equilibrium states are characterized by the equation

$$f_i = \exp(a + b \cdot v_i + c|v_i|^2), \quad c < 0.$$

In the discrete case it is not possible to write explicitly a, b, c as functions of the macroscopic quantities ρ, u, T except in some particular cases.
In general one has to solve for a, b, c the system of 5 nonlinear equations

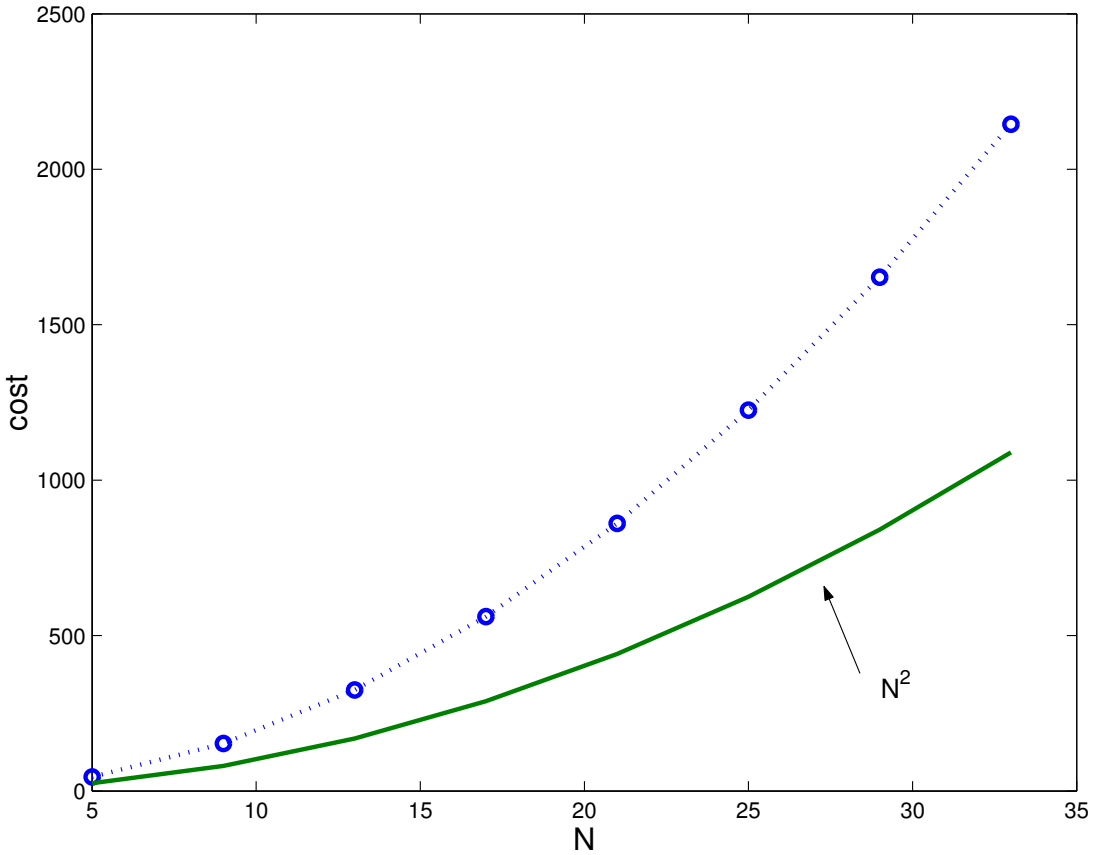
$$\begin{aligned}
\rho &= \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2) \\
u &= \frac{1}{\rho} \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2) v_i, \\
T &= \frac{1}{3R\rho} \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2)(v_i - u)^2.
\end{aligned}$$

Remark: This requires a suitable numerical method if the local Maxwellian equilibrium is needed explicitly. Solvability of the previous system (Moment realization problem).

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[2].

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

Remarks

- The method behaves essentially as a first order scheme $\mu \approx 1$ with a computational cost more then quadratic $\eta \approx 2.5$.
- Numerically the discrete Boltzmann equation corresponds to take a quadrature formula for the Boltzmann equations where

$$V_N = \{v_1, v_2, v_3, \dots, v_N\} \quad \text{quadrature nodes}$$
$$a_{ij}^{kl} \quad \text{quadrature weights.}$$

- Conservations assumptions on the weights typically result in a deterioration of the accuracy of the quadrature formula.
- Recently fast numerical algorithms, based on some of the ideas we will illustrate in lecture 4, have been constructed which reduces the overall cost to $O(N^d \log N)$ [3].

[3] C.Mouhot, L.Pareschi, T.Rey, 2014

Spectral methods

A different approach is based on the use of spectral methods[4]. Let us first write the collision operator as

$$Q(f,f) = Q^+(f,f) - f\,L(f).$$

The method is derived in three subsequent steps.

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

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

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

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

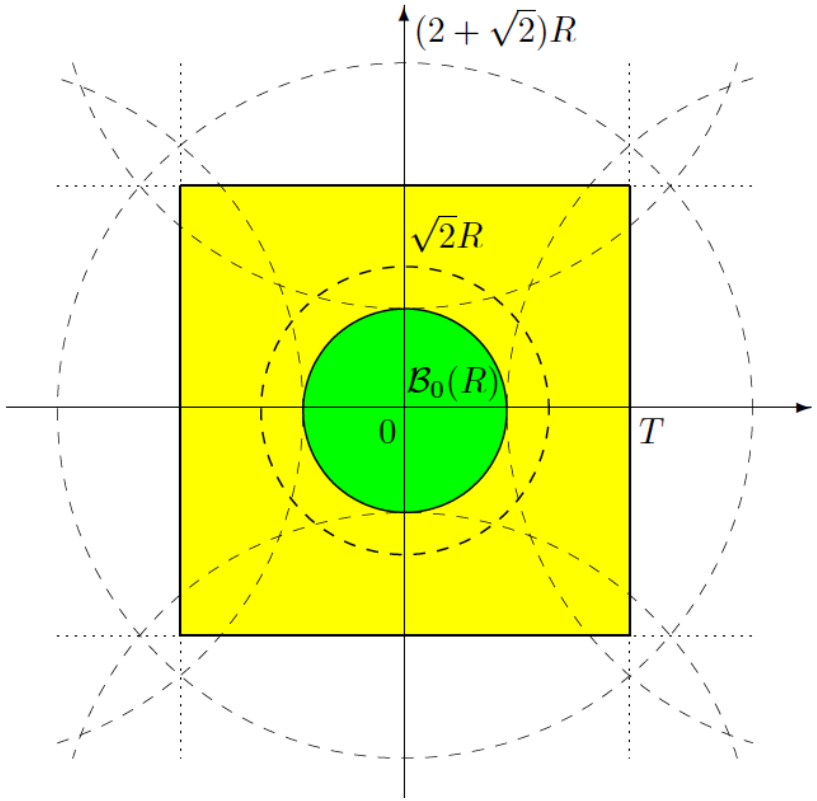
where now

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

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

Spectral methods

2. Periodization and 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 methods

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

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

To obtain the Fourier-Galerkin method we require that

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

Spectral methods

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

Kernel modes

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

The final scheme is charaterized by the computation of the Fourier coefficients of the collision operator

Spectral quadrature

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

Computational considerations

- In dimension d, the direct evaluation of the spectral scheme requires $O(n^2) = O(N^{2d})$ operations, less then $O(N^{2d+1})$ operations of discrete velocity methods.
- The second sum (loss term) is a *convolution sum* and can be evaluated in $O(n \log n)$ operations by *FFT* based transform methods. The most expensive part is thus the first sum (gain term).
- Typically, the kernel modes $\hat{B}(l, m)$ are functions of $|l - m|$, $|l + m|$ and can be efficiently pre-computed and stored. In some cases, like hard spheres for $d = 3$ and Maxwell molecules for $d = 2$, we have explicit analytical expressions [5].
- The scheme preserves the mass (Fourier mode of order zero) but not momentum and energy. However, it can be shown that these quantities are approximated with spectral accuracy in time.

[5] L.Pareschi, G.Russo '00

Notations

For any $t \geq 0$, $f_N(t) \in \mathbb{P}^N$ where

$$\mathbb{P}^N = span\left\{e^{ik\cdot v} \mid -N \leq k_j \leq N,\, j = 1,2,3\right\}.$$

Let $\mathcal{P}_N : L^2([-\pi,\pi]^3) \to \mathbb{P}^N$ be the orthogonal projection upon $\mathbb{P}^N$ in the inner product of $L^2([-\pi,\pi]^3)$.
Hence $\mathcal{P}_N f = f_N$ and we define

$$Q_N(f_N, f_N) = \mathcal{P}_N Q(f_N, f_N)$$

where $Q(f,f)$ denotes the Boltzmann operator with the relative velocity restricted on $\mathcal{B}(0, 2\lambda\pi)$.
Finally, we denote with $H^r_p([-\pi,\pi]^3)$, where $r \geq 0$ is an integer, the subspace of the Sobolev space $H^r([-\pi,\pi]^3)$, which consist of periodic functions.

Consistency and spectral accuracy

Theorem (Pareschi, Russo '00)

Let $f \in L^2([-\pi,\pi]^3)$, *then*

$$||Q(f,f) - Q_N(f_N,f_N)||_2 \leq C\left(||f - f_N||_2 + \frac{||Q(f_N,f_N)||_{H_p^r}}{N^r}\right), \quad \forall\, r \geq 0,$$

where C *depends on* $||f||_2$.

This estimate states that the rate of convergence of $Q_N(f_N,f_N)$ to $Q(f,f)$ depends only on the rate of convergence of f_N to f.
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

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

Numerical validation

Two-dimensional Maxwellian molecules (i.e. $\alpha = 0$, $v \in \mathbb{R}^2$). In the space homogeneous case, this problem has an exact solution given by

$$f(v,t) = \frac{1}{4\pi S^2 \gamma^2}\left(2S - 1 + \frac{1-S}{2S}\frac{v^2}{\gamma^2}\right)\exp\left(-\frac{v^2}{2S\gamma^2}\right), \quad t \geq 0,$$

where $S = 1 - \exp(-\gamma^2 t/8)/2$. The scaling parameter $\gamma = \pi/6$ is chosen in such a way that the numerical support of the initial condition is well approximated by $\mathcal{B}_0(R)$ and and the integration time is $t = 5$.

Table: Convergence test for the homogenous Boltzmann equation.

# modes	Error at time $t = 5$			Convergence rate		
n	$\pi/6$	$\pi/7$	$\pi/8$	$\pi/6$	$\pi/7$	$\pi/8$
8×8	1.51E-01	2.09E-01	2.71E-01	5.64	4.41	3.91
16×16	3.01E-03	9.78E-03	1.78E-03	9.64	10.23	8.19
32×32	3.79E-06	0.81E-05	0.61E-05			

Further reading

- Spectral methods are covered in the *general survey* used as a reference for these lectures
  - G. Dimarco, L. Pareschi, *Acta Numerica* 23, 2014.

  DVM are also partially covered in the same reference.
- An interesting *historical reference* is
  - H. Cabannes, R. Gatignol and L. Luo (2003), *The discrete Boltzmann equation (theory and applications)*, Henri Cabannes, Paris. Revised from the lecture notes given at the University of California, Berkeley, CA, 1980, `http://henri.cabannes.free.fr/Cours_de_Berkeley.pdf`.
- *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