Kinetic equations: computation

Synonyms

Collisional equations, Transport equations, Boltzmann equations

Mathematics Subject Classification

65D32, 65M70, 65L04, 68Q25, 82C40

Short Definition

Kinetic equations bridge the gap between a microscopic description and a macroscopic description of the physical reality. Due to the high dimensionality the construction of numerical methods represents a challenge and requires a careful balance between accuracy and computational complexity.

Description

Kinetic equations

Particle systems can be described at the microscopic level by particle dynamics, i.e. systems of differential equations describing the individual motions of the particles.
However, they are extremely costly from a numerical point of view, and bring little intuition on how a large particle system behaves. Therefore, one is led to seek reduced descriptions of particle systems which still preserve an accurate description of the physical phenomena. Kinetic models intend to describe particle systems by means of a distribution function $f(x, v, t)$. This object represents a number density in phase space, i.e. $f \, dx \, dv$ is the number of particles in a small volume $dx \, dv$ in position-velocity space about the point $(x, v)$ of this space.

In this short entry we will focus on computational methods for the interacting particle case described by the Boltzmann equation. This is motivated by its relevance for applications and by the fact that it contains all major difficulties present in other kinetic equations. From a numerical perspective, most of the difficulties are due to the multidimensional structure of the distribution function. In particular the approximation of the collisional integral is a real challenge for numerical methods, since the integration runs on a highly-dimensional unflat manifold and is at the basis of the macroscopic properties of the equation. Further difficulties are represented by the presence of fluid-kinetic interfaces and multiple scales where most numerical methods lose their efficiency because they are forced to operate on a very short time scale.

Although here we review briefly only deterministic numerical methods let us mention that several realistic numerical simulations are based on Monte-Carlo techniques [1; 10; 15]. In the next paragraphs we summarize the main ideas at the basis of two of the most popular way to approximate the distribution function in the velocity space, namely the discrete-velocity method [16; 2; 3; 11] and the spectral method [12; 13; 9; 7; 14]. Finally we shortly introduce the basic principles for the construction of schemes which are robust in fluid regions [6; 8; 5].
Boltzmann equation

Taking into account only binary interactions, the behavior of a dilute gas of particles is described by the Boltzmann equation \[ \frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f, f) \] (1)

where \( f(t, x, v), x, v \in \mathbb{R}^d (d \geq 2) \), is the time-dependent particle distribution function in the phase space and the collision operator \( Q \) is defined by

\[ Q(f, f)(v) = \int_{v_* \in \mathbb{R}^d} \int_{\sigma \in S^{d-1}} B(\cos \theta, |v - v_*|) \left[ f'_* f' - f_* f \right] d\sigma dv_* . \] (2)

Time and position act only as parameters in \( Q \) and therefore will be omitted in its description. In (2) we used the shorthands \( f = f(v), f_* = f(v_*), f' = f(v'), f'_* = f(v'_*) \).

The velocities of the colliding pairs \((v, v_*)\) and \((v', v'_*)\) are related by

\[ v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma. \]

The collision kernel \( B \) is a non-negative function which only depends on \(|v - v_*|\) and \( \cos \theta = ((v - v_*)/|v - v_*|) \cdot \sigma \). Boltzmann’s collision operator has the fundamental properties of conserving mass, momentum and energy

\[ \int_{v \in \mathbb{R}^d} Q(f, f) \phi(v) dv = 0, \quad \phi(v) = 1, v, |v|^2 \] (3)

Moreover, any equilibrium distribution function \( M \) such that \( Q(M, M) = 0 \) has the form of a locally Maxwellian distribution

\[ M(\rho, u, T)(v) = \frac{\rho}{(2\pi T)^{d/2}} \exp \left( -\frac{|u - v|^2}{2T} \right), \] (4)

where \( \rho, u, T \) are the density, mean velocity and temperature of the gas

\[ \rho = \int_{v \in \mathbb{R}^d} f(v) dv, \quad u = \frac{1}{\rho} \int_{v \in \mathbb{R}^d} vf(v) dv, \quad T = \frac{1}{d\rho} \int_{v \in \mathbb{R}^d} |u - v|^2 f(v) dv. \] (5)
**Discrete velocity methods**

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

\[ V_N = \{ v_1, v_2, v_3, \ldots, v_N \}, \quad v_i \in \mathbb{R}^d, \]

and denote by \( f_j(x, t) = f(v_j, x, t), \quad j = 1, \ldots, N \). The collision pair \((v_i, v_j) \leftrightarrow (v_k, v_l)\) is admissible if \( v_i, v_j, v_k, v_l \in V_N \) and preserves momentum and energy

\[ v_i + v_j = v_k + v_l, \quad |v_i|^2 + |v_j|^2 = |v_k|^2 + |v_l|^2. \]

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

The discrete collision operator is obtained as a quadrature formula based on the weights \( a_{kl}^{ij} \) related to the collision \((v_i, v_j) \leftrightarrow (v_k, v_l)\) which must satisfy the relations

\[ a_{ij}^{kl} \geq 0, \quad \sum_{k,l=1}^{N} a_{ij}^{kl} = 1, \forall i, j = 1, \ldots, N. \]

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

\[ \frac{\partial f_i}{\partial t} + v_i \cdot \nabla_x f_i = Q_i(f, f), \]

with

\[ Q_i(f, f) = \sum_{j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j). \]

The discretized Boltzmann equation has the nice property of preserving the essential physical features (conservations, H-theorem, equilibrium states). However, from a computational point of view the discrete Boltzmann equation presents two main drawbacks. First the computational cost is larger than \( O(N^2) \) and second the accuracy is rather poor, less then first order accurate (see [11] for example).
Spectral methods

Spectral methods have been constructed recently with the goal to compensate the drawbacks of discrete velocity approximation. For the sake of simplicity we summarize their derivation in the case of the space homogeneous Boltzmann equations, although the schemes can be effectively used to compute the collision integral in a general setting.

The approximate function $f_N$ is represented as the truncated Fourier series

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

The spectral equation is the projection of the collision integral $Q_R(f, f)$, truncated over the ball of radius $R$ centered in the origin, in $P^N$, the $(2N+1)^d$-dimensional vector space of trigonometric polynomials of degree at most $N$ i.e.

$$\frac{\partial f_N}{\partial t} = \mathcal{P}_N Q^R(f_N, f_N)$$

where $\mathcal{P}_N$ denotes the orthogonal projection on $P^N$ in $L^2(D^d)$. A straightforward computation leads to the following set of ordinary differential equations

$$\frac{d\hat{f}_k(t)}{dt} = \sum_{l,m=-N}^{N} \hat{\beta}(l, m) \hat{f}_l \hat{f}_m, \quad k = -N, ..., N$$  

where $\hat{\beta}(l, m)$ are the kernel modes, given by $\hat{\beta}(l, m) = \beta(l, m) - \beta(m, m)$ with

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

and

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

As shown in [9] when $B$ satisfies the decoupling assumption $\tilde{B}(x, y) = a(|x|) b(|y|)$, it is possible to approximate each $\hat{\beta}(l, m)$ by a sum

$$\beta(l, m) \simeq \sum_{p=1}^{A} \alpha_p(l) \alpha'_p(m).$$  

(7)
This gives a sum of $A$ discrete convolutions, with $A \ll N$, and by standard FFT techniques a computational cost of $O(A N^d \log_2 N)$. Denoting by $N = (2N + 1)^d$ the total number of grid points this is equivalent to $O(A N \log_2 N)$ instead of $O(N^2)$.

Moreover, one gets the following consistency result of spectral accuracy [9]

**Theorem 1.** For all $k > d - 1$ such that $f \in H^k_p$

$$
\|Q^R(f, f) - P_NQ^{R,M}(f_N, f_N)\|_{L^2} \leq C_1 \frac{R^k \|f_N\|_{H^k_p}^2}{M^k} + C_2 \frac{R^k}{N^k} \left( \|f\|_{H^k_p} + \|Q^R(f_N, f_N)\|_{H^k_p} \right).
$$

**Asymptotic-preserving methods**

Let us now consider the time discretization of the scaled Boltzmann equation

$$
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f),
$$

where $\varepsilon > 0$ is the Knudsen number. For small value of $\varepsilon$ we have a stiff problem and standard time discretization methods are forced to operate on a very small time scale. On the other hand in such regime formally $Q(f, f) \approx 0$ and the distribution function is close to a local Maxwellian. Thus the moments of the Boltzmann equation are well-approximated by the solution to the Euler equations of fluid-dynamics

$$
\partial_t u + \nabla_x \cdot F(u) = 0,
$$

with

$$
u = (\rho, w, E)^T, \quad F(u) = (\rho w, \rho w \otimes (w + pI), Ew + pw)^T, \quad p = \rho T,
$$

where $I$ is the identity matrix and $\otimes$ denotes the tensor product.

We say that a time discretization method for (8) of stepsize $\Delta t$ is asymptotic preserving (AP) if, independently of the stepsize $\Delta t$, in the limit $\varepsilon \to 0$ becomes a consistent time discretization method for the reduced system (9).

When $\varepsilon \ll 1$ the problem is stiff and we must resort on implicit integrator to avoid small time step restriction. This however requires the inversion of the collision integral $Q(f, f)$ which is prohibitively expensive from the computational viewpoint.
On the other hand when \( f \approx M[f] \) we know that the collision operator \( Q(f, f) \) is well approximated by its linear counterpart \( Q(M, f) \) or by a simple relaxation operator \((M - f)\). If we denote by \( L(f) \) the selected approximate linear operator we can rewrite the equation introducing a penalization term as

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon}(Q(f, f) - L(f)) + \frac{1}{\varepsilon}L(f).
\]  

(10)

The idea now is to be implicit (or exact) in the linear part \( L(f) \) and explicit in the deviations from equilibrium \( Q(f, f) - L(f) \). This approach has been successfully presented in [6] using implicit-explicit integrators and in [8, 5] by means of exponential techniques.

**Conclusions**

Computational methods for kinetic equations represent an emerging field in scientific computing. This is testified by the large amount of scientific papers which has been produced on the subject in recent years. We do not seek to review all of them here and focused our attention to the challenging case of the Boltzmann equation of rarefied gas dynamic. The major difficulties in this case are represented by the discretization of the multi-dimensional integral describing the collision process and by the presence of multiple time scales. Fast algorithms and robust stiff solvers are then essential ingredients of computational methods for kinetic equations.

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