Monte Carlo methods for kinetic equations

Lecture 1: Kinetic models and computational challenges

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Tutorial Outline

1. Lecture #1: Kinetic models and numerical challenges
2. Lecture #2: Monte Carlo simulation methods
3. Lecture #3: Methods for the fluid-limit
4. Lecture #4: Hybrid methods and variance reduction

Lecture #1 Outline

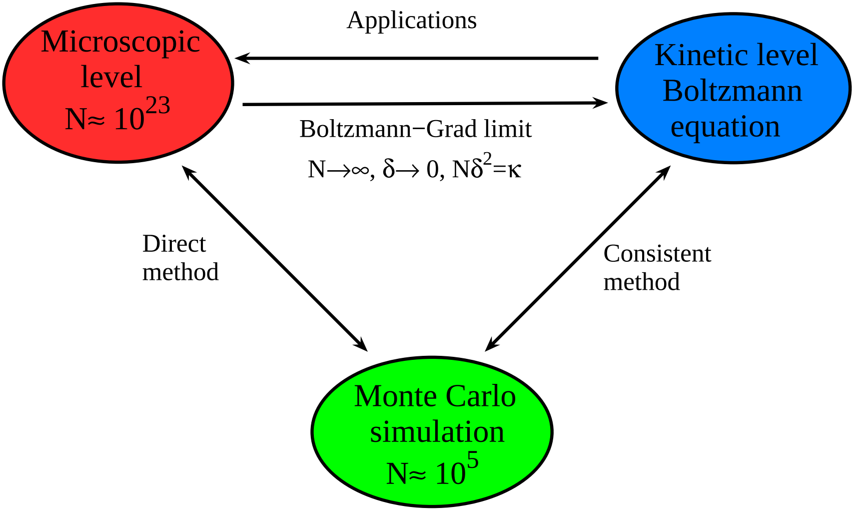
Levels of representation

- Interacting particle systems are ubiquitous in nature: gases, fluids, plasmas, solids (metals, semiconductors or insulators), vehicles on a road, economic agents can be considered as interacting particle systems.
- Particle systems can be described at the microscopic level by particle dynamics (*Newton's equations*) describing the individual motions of the particles. However, particle dynamic is impossible to use in most practical cases, due to the extraordinary large number of equations that must be solved simultaneously.
- At the macroscopic level fluid models (such as the *Euler or Navier-Stokes equations*) describe averaged quantities, local density, momentum, energy... However, fluid models involve constants (viscosity, heat conductivity, diffusion) which depend on the microscopic properties of the elementary particles interactions.

Levels of representation

- There is a need to bridge the gap between particle dynamics and fluid models. This question of how to pass from microscopic properties of matters to macroscopic properties of systems is one of the most fundamental ones in physics. It is also one of the most difficult.
- The problem is slightly simplified by introducing an intermediate step between particle systems and fluid models: the so-called kinetic level. These models, characterized by *Boltzmann equations*, deal with a quantity, the distribution function, which is the density of particles in phase-space (say position and velocity).
- The essential idea of *Monte Carlo* or *particle* simulations for the Boltzmann equation is to return to the particle description with a number of particles small enough to make the situation computationally treatable but "sufficiently close" to the physical situation. As we will see this will involve evaluations of high dimensional integrals for which Monte Carlo methods arise quite naturally.

Microscopic, kinetic and computational levels



Microscopic level

Let us consider N interacting particles and denote their positions and velocities by $x_i(t)$ and $v_i(t)$ with $i = 1, \ldots, N$. Newton's equations reads

$$\dot{x}_i = v_i, \qquad \dot{v}_i = F_i(x_1, \ldots, x_N),$$

where the dots denote time derivatives and $F_i(x_1, \ldots, x_N)$ is the force exerted on the i-th particle by the other particles and by external forces.
We shall consider forces which derive from an interacting potential

$$F_i = -\nabla_{x_i}\phi(x_1, \ldots, x_N)$$

where $\phi(x_1, \ldots, x_N)$ is a scalar potential function.
In most cases, the force originates from a binary interaction. The potential ϕ is given by

$$\phi(x_1, \ldots, x_N) = \frac{1}{2}\sum_{j \neq k} \phi_{int}(x_j - x_k) + \sum_j \phi_{ext}(x_j)$$

where $\phi_{int}(x)$ is the binary interaction potential and $\phi_{ext}(x)$ is the potential of external forces.

Microscopic level

The force is then given by

$$F_i(x_1,\ldots,x_N) = \frac{1}{2}\sum_{k\neq i} F_{int}(x_i - x_k) + \sum_k F_{ext}(x_k)$$

and $F_{int} = -\nabla\phi_{int}$ is the binary interaction force while $F_{ext} = -\nabla\phi_{ext}$ is the external force.

Often, one considers that the binary interaction is well described by a central force with inverse power law $F_{int}(x) = F_{int}(|x|)$ with

$$F_{int}(r) = C\frac{1}{r^s}\frac{x}{r}, \quad r = |x|.$$

This is a model for the interaction force between molecules in a gas.

The description of particle systems by Newton's equation of motion is the most fundamental one. One important feature of Newton's equations of motion for N-particle dynamics is their time reversibility. However, it is untractable from a numerical point of view, and brings little intuition on how a large particle system behaves.

Kinetic level

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. $f(x, v, t)dxdv$ is the number of particles at time t in a small volume $dx\ dv$ in position-velocity space about the point (x, v).
Macroscopic quantities (mass, momentum, energy) can be recovered taking moments of f

$$\rho = \int_{\mathbb{R}^3} f\, dv, \quad \rho u = \int_{\mathbb{R}^3} f\, v\, dv, \quad E = \frac{1}{2}\int_{\mathbb{R}^3} f\, v^2\, dv.$$

A thorough treatment of the derivation of kinetic models is beyond the scope of our discussion. But we may sketch the basic ideas that lead to the celebrated *Boltzmann equation*.

Hard-sphere dynamic

We restrict to the case of N-particle systems interacting via *hard-sphere dynamics*. Particles consist of indeformable solid spheres of diameter δ which do not interact as long as they do not enter in contact. Consider a sphere with center x and velocity v and a sphere centered at x_* with velocity v_*

$$F_{int}(x - x_*) = 0\,, \quad \forall\, x,\, x_* \text{ s.t.} |x - x_*| > \delta.$$

When $|x - x_*| = \delta$, the spheres undergo a collision. Define $n = (x_* - x)/\delta$ the unit vector joining the centers of the two spheres. The collision instantaneously changes the velocities to v' and v'_*.

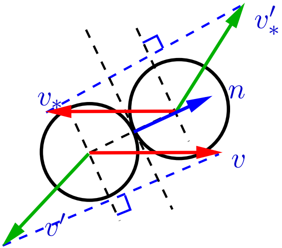


Figure 1: Hard sphere collision

Interacting particles

The collision mechanism must satisfy:

(i) Conservation of momentum:

$$v + v_* = v' + v'_* \,.$$

(ii) Conservation of energy:

$$v^2 + v_*^2 = {v'}^2 + {v'_*}^2 \,.$$

(iii) From conservation of momentum and energy, we have a system of 4 scalar equations for 6 scalar unknowns. Then it is natural to expect that its solutions can be defined in terms of 2 parameters.
Using the unit vector n, by conservation of angular momentum (spheres are not rotating), we can represent this solution in the form

$$v' = v - ((v - v_*) \cdot n)n \,, \quad v'_* = v_* + ((v - v_*) \cdot n)n \,.$$

The collision operator

We now outline what a kinetic equation for hard-sphere dynamics could be. Such a kinetic equation is obtained when one formally lets $N \to \infty$, and simultaneously, $\delta \to 0$.

Note that in the absence of collisions all particles issued form the same point (x, v) follows the same trajectory

$$\dot{X} = V\,, \quad \dot{V} = 0\,,$$

and consequently, the distribution function f is invariant along the particle paths.

To take into account collisions, one introduces a quantity denoted by $Q(f, f)$ modeling the rate of change of f due to collisions.

This leads to

$$\frac{d}{dt} f(X(t), V(t), t) = \left(\frac{\partial f}{\partial t} + v \cdot \nabla_x f \right) |_{(X(t),V(t),t)} = Q(f, f)|_{(X(t),V(t),t)}\,.$$

$Q(f, f)$ is called the *collision operator*. A kinetic equation for colliding hard spheres should therefore be written as

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

The collision operator

The collision operator is supposed local in time, because the collision dynamics is instantaneous.
The operator may be decomposed in two terms

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

The loss term $Q^-(f,f)$ models the decay of the distribution function $f(x,v)$ due to particles of velocity v changing to velocity v' during a collision, while the gain term $Q^+(f,f)$ describes the increase of $f(x,v)$ due to particles changing from any other velocity to v during a collision.

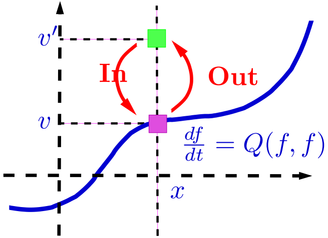


Figure 2: Gain and loss in $Q(f,f)$

Boltzmann-Grad limit

The Boltzmann equation is obtained in the limit $\delta \to 0$, $N \to \infty$, with $N\delta^2 = \kappa$ kept constant. This is the so-called *Boltzmann-Grad limit*. In this limit, the collision operator converges to[1]

Boltzmann collision operator I

$$Q(f,f) = \kappa \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_+} |(v - v_*) \cdot n| \, [f(x,v')f(x,v'_*) - f(x,v)f(x,v_*)] \, dn \, dv_*,$$

where

$$v' = v - ((v - v_*) \cdot n)n \,, \quad v'_* = v_* + ((v - v_*) \cdot n)n \,.$$

The sign restriction on n is due to the fact that in the loss term v and v_* refer to pre-collisional velocities and particles are moving towards each other before the collision. Similarly in the gain term v and v_* are post-collisional velocities and particles are moving in opposite directions after a collision.

[1] L.Boltzmann, 1872 - J.C. Maxwell, 1867 - C.Cercignani, 1988 - C.Cercignani, R.Illner, M.Pulvirenti, 1995

An alternative representation

The collision integral $Q(f, f)$ can be written in different equivalent forms, accordingly to the parametrization used for the collisional velocities. Using the identity

$$\int_{\mathbb{S}^2_+} |u \cdot n| \phi(n(u \cdot n))\, dn = \frac{|u|}{4} \int_{\mathbb{S}^2} \phi\left(\frac{u - |u|\omega}{2}\right) d\omega$$

obtained by the transformation $\omega = u/|u| - 2(u \cdot n/|u|)n$, we get the form

Boltzmann collision operator II

$$Q(f, f)(v) = \frac{\kappa}{4} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} |v - v_*| [f(x, v') f(x, v'_*) - f(x, v) f(x, v_*)]\, d\omega\, dv_*,$$

where now

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

The collision sphere

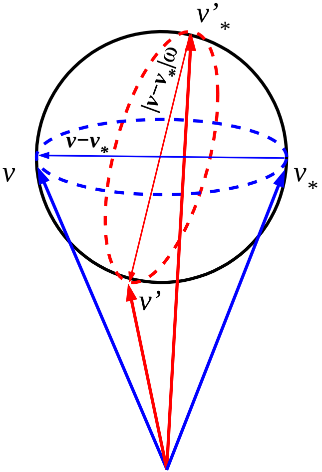


Figure 3: Collision sphere in the alternative representation

The general case

In non-dimensional form the general case has the form

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* proportional to the mean free path.
The collision operator is given by

Collision operator

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

with $B(v, v_*, \omega)$ is a nonnegative collision kernel.

The collision kernel

The collision kernel $B(v, v_*, \omega)$ for inverse s-th power forces reads

$$B(v, v_*, \omega) = b_\alpha(\cos\theta)|v - v_*|^\alpha, \quad \alpha = (s-5)/(s-1), \quad \cos\theta = \frac{(v - v_*)}{|v - v_*|} \cdot \omega.$$

For $s > 5$ we have *hard potentials*, for $2 < s < 5$ we have *soft potentials*. The special situation $s = 5$ gives the *Maxell model* with $B(v, v_*, \omega) = b_0(\cos\theta)$. For the Maxwell case the collision kernel is independent of the relative velocity. This case has been widely studied theoretically, in particular exact analytic solutions can be found in the space homogeneous case[2].

For numerical purposes a generalization of the hard sphere kernel is given by the so-called *variable hard sphere*[3] (VHS) kernel

$$B(v, v_*, \omega) = C_\alpha|v - v_*|^\alpha, \quad 0 \le \alpha \le 1,$$

where $C_\alpha > 0$ is a constant.

[2] A.V.Bobylev, 1977 - M.Krook, T.T.Wu, 1976

[3] G.Bird, 1976

Conservations

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

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

The above properties are a consequence of the following identity that can be easily proved for any test function $\phi(v)$

$$\int_{\mathbb{R}^3} Q(f,f)\phi(v)\,dv = -\frac{1}{4}\int_{\mathbb{R}^6}\int_{\mathbb{S}^2} B(v,v_*,\omega)[f'f'_* - ff_*][\phi' + \phi'_* - \phi - \phi_*]\,d\omega\,dv_*\,dv.$$

where we have omitted the explicit dependence from x and v, v_*, v', v'_*.
In order to prove this identity we used the micro-reversibility $B(v,v_*,\omega) = B(v_*,v,\omega)$ and the fact that the Jacobian of the transformation $(v,v_*) \leftrightarrow (v',v'_*)$ is equal to 1.

Collision invariants

A function ϕ such that

$$\phi(v') + \phi(v'_*) - \phi(v) - \phi(v_*) = 0$$

is called a *collision invariant*. It can be shown that a continuous function ϕ is a collision invariant if and only if $\phi \in \mathrm{span}\{1, v, |v|^2\}$ or equivalentely

$$\phi(v) = a + b \cdot v + c|v|^2, \quad a, c \in \mathbb{R}, \quad b \in \mathbb{R}^3.$$

Assuming f strictly positive, for $\phi(v) = \ln(f(v))$ we obtain

$$\begin{aligned}
&\int_{\mathbb{R}^3} Q(f,f) \ln(f) dv \\
&= -\frac{1}{4} \int_{\mathbb{R}^6} \int_{\mathbb{S}^2} B(v, v_*, \omega)[f' f'_* - f f_*][\ln(f') + \ln(f'_*) - \ln(f) - \ln(f_*)]\, d\omega\, dv_*\, dv \\
&= -\frac{1}{4} \int_{\mathbb{R}^6} \int_{\mathbb{S}^2} B(v, v_*, \omega)[f' f'_* - f f_*] \ln\left(\frac{f' f'_*}{f f_*}\right) d\omega\, dv_*\, dv \leq 0,
\end{aligned}$$

since the function $z(x,y) = (x-y)\ln(x/y) \geq 0$ and $z(x,y) = 0$ only if $x = y$. In particular the equality holds only if $\ln(f)$ is a collision invariant that is

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

Maxwellian states

If we define the density, mean velocity and temperature of the gas by

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

we obtain

Maxwellian state

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

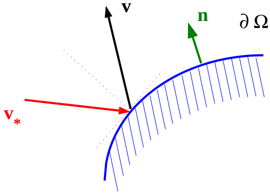
where $R = K_B/m$, K_B is the Boltzmann constant and m the mass of a particle. Boltzmann's H-theorem implies that any function f s.t. $Q(f,f)=0$ is a Maxwellian. If we define the *H-function* we have

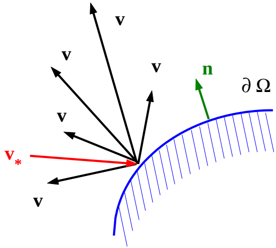
$$H(f) = \int_{\mathbb{R}^3} f\ln(f)\,dv \quad \Rightarrow \quad \frac{\partial}{\partial t}\int_{\mathbb{R}^3} H(f)\,dx = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} Q(f,f)\ln(f)\,dv\,dx \leq 0.$$

The H-function is monotonically decreasing until f reaches the Maxwellian state. This shows that one cannot come back to the original state by a simple reversal of the particle velocities. The Boltzmann dynamic is irreversible.

Boundary conditions

The Boltzmann equation is complemented with the boundary conditions for $v \cdot n \geq 0$ and $x \in \partial\Omega$, where n denotes the unit normal, pointing inside the domain Ω. Usually the boundary represents the surface of a solid object (an obstacle or a container). The particles of the gas that hit the surface interact with the atoms of the object and are reflected back into the domain Ω.





Commonly used reflecting boundary conditions are the so-called *Maxwell's conditions*. From a physical point of view, one assumes that a fraction α of molecules is absorbed by the wall and then re-emitted with the velocities corresponding to those in a still gas at the temperature of the wall, while the remaining fraction $(1 - \alpha)$ is specularly reflected.

Boundary conditions

This is equivalent to impose for the ingoing velocities

Maxwell's boundary condition

$$f(x,v,t) = (1-\alpha)Rf(x,v,t) + \alpha Mf(x,v,t), \quad x \in \partial\Omega, \quad v \cdot n(x) \geq 0.$$

The coefficient α, with $0 \leq \alpha \leq 1$, is called the *accommodation coefficient* and

$$Rf(x,v,t) = f(x, v - 2n(n \cdot v), t), \quad Mf(x,v,t) = \mu(x,t)M_w(v).$$

If we denote by T_w the temperature of the solid boundary, M_w is given by

$$M_w(v) = \exp(-\frac{v^2}{2T_w}),$$

and μ is determined by mass conservation at the surface of the wall

$$\mu(x,t)\int_{v \cdot n \geq 0} M_w(v)|v \cdot n| dv = \int_{v \cdot n < 0} f(x,v,t)|v \cdot n| dv.$$

Fluid limit

The most natural method to derive fluid equations is the *moment method*. Let us multiply the Boltzmann equation by its collision invariants and integrate

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} f\phi(v)\,dv + \nabla_x\left(\int_{\mathbb{R}^3} vf\phi(v)\,dv\right) = 0, \quad \phi(v) = 1, v_1, v_2, v_3, |v|^2.$$

These equations descrive the balance of mass, momentum and energy. The system is not closed since it involves higher order moments of f.

As $\varepsilon \to 0$ we have formally $Q(f,f) \to 0$ and thus $f \to M$. Higher order moments of f can be computed as function of ρ, u, and T and we obtain

Compressible Euler equations

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho u) = 0$$
$$\frac{\partial \rho u}{\partial t} + \nabla_x \cdot (\rho u \otimes u + p) = 0$$
$$\frac{\partial E}{\partial t} + \nabla_x \cdot (Eu + pu) = 0, \quad p = \rho T = \frac{2}{3}E - \frac{1}{3}\rho u^2.$$

Hydrodynamic limits

Different strategies can be used to go beyond the Euler equations.

- The distribution function can be expanded in terms of the small parameter ε. There are two ways to deal with this, the *Hilbert* and the *Chapman-Enskog expansions*[4]. Roughly speaking the idea is to write

$$f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \dots$$

  To the leading order we have $f_0 = M$ and we get the Euler system, to the next order we obtain the *compressible Navier-Stokes* system.
- One can also consider higher order moment closures, which originates models such as the *Extended Thermodynamic*.[5]
- The other important type of asymptotic limit that give rise to fluid equations are *diffusion limits*. These limits were studied first in the context of neutron transport. Many other applications were investigated, such as semiconductors, plasmas, mathematical biology and others.[6]

[4] D.Hilbert, 1916 - S. Chapman, 1916 - D.Enskog, 1917

[5] H. Grad, 1949 - I.Mueller, T.Ruggeri, 1998

[6] E.W.Larsen, 1975 - F.Poupaud, 1991 - P.Degond, 2000 - H.G.Othmer, T.Hillen, 2002.

One-dimensional models

In one-dimension in velocity the collision operator vanishes since imposing conservation of momentum and energy we have a system of two equations in two unknowns v' and v'_* which has the trivial unique solution $v' = v$ and $v'_* = v_*$.
A model that considers only energy conservation is *Kac's model*[7] of a Maxwell gas

$$Q(f,f) = \int_{\mathbb{R}} \int_0^{2\pi} \beta(\theta)[f(v')f(v'_*) - f(v)f(v_*)]d\theta\, dv_*,$$

with $v' = v\cos(\theta) - v_* \sin(\theta)$, $v'* = v\sin(\theta) + v_* \cos(\theta)$.
If we assume energy dissipation we have a *granular gas model*[8]

$$Q(f,f) = \int_{\mathbb{R}} |v - v_*|[\frac{1}{e} f(v')f(v'_*) - f(v)f(v_*)]\, dv_*,$$

with $v' = \frac{1}{2}(v + v_*) + \frac{1}{2}(v - v_*)e$, $v'_* = \frac{1}{2}(v + v_*) - \frac{1}{2}(v - v_*)e$, $0 < e < 1$.

[7] M.Kac, 1959
[8] D.Benedetto, E.Caglioti, M.Pulvirenti, 1997, Toscani 2000

BGK

A simplified model Boltzmann equation is given by the *BGK model*[9]. In this model the collision operator is replaced by a relaxation operator of the form

BGK operator

$$Q_{BGK}(f,f)(v) = \nu(\rho)(M(f) - f)$$

where $M(f)$ is the Maxwellian and $\nu(\rho)$ is the collisional frequency. Conservation of mass, momentum and energy as well as Boltzmann H-theorem are satisfied. The equilibrium solutions are Maxwellians

$$Q_{BGK}(f,f) = 0 \Leftrightarrow f = M(f).$$

The model has the wrong Prandtl number (the ratio between heat conductivity and viscosity) and therefore incorrect Navier-Stokes limit. Correct Prandtl number $2/3$ can be recovered using $\nu = \nu(\rho, v)$ and *Ellipsoidal Statistical BGK* (ES-BGK) models[10].

[9] P.I.Bhatnagar, E.P.Gross, M.Krook, 1954

[10] F.Bouchut, B.Perthame, 1993 - L.H.Holway, 1966

Further Models

- *Quantum models*: the nonlinear term $f'f'_* - ff_*$ is replaced by

$$f'f'(1 \pm f)(1 \pm f_*) - ff_*(1 \pm f')(1 \pm f'_*).$$

  Sign $-$ Pauli operator, Sign $+$ Bose-Einstein operator.

- *Landau Fokker-Planck models*: Coulomb case ($\alpha = -3$) in plasma physics

$$Q_L(f,f)(v) = \nabla_v \cdot \int_{I\!R^d} A(v - v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*} f(v_*)]\, dv_*$$

  where $A(z) = \Psi(|z|)\Pi(z)$ is a $d \times d$ nonnegative symmetric matrix, $\Pi(z) = (\pi_{ij}(z))$ is the orthogonal projection upon the space orthogonal to z, $\pi_{ij}(z) = \left(\delta_{ij} - z_i z_j/|z|^2\right)$ and $\Psi(|z|) = \Lambda|z|$, $\Lambda > 0$.

- *Semiconductor models*: linear equation for semiconductor devices

$$Q_S(f,M) = \int \sigma(v,v_*)\{M(v)f(v_*) - M(v_*)f(v)\}\, dv_*,$$

  where M is the normalized equilibrium distribution (Maxwellian, Fermi-Dirac) at the temperature of the lattice. The function $\sigma(v,v_*)$ describes the interaction of carriers with phonons.

- *Boltzmann-like models*: vehicular traffic flows, biomathematics, finance, internet ...

Numerical challenges

We can summarize the main different numerical difficulties and requirements specific to the approximation of kinetic equations as follows.

- Physical *conservation properties*, positivity and entropy inequality are very important since they characterize the steady states. Methods that do not maintain such properties need special attention in practical applications.
- The operator $Q(f, f)$ may contain an highly dimensional integral in velocity space. In such cases *fast solvers* are essential to avoid excessive computational cost. Otherwise fully realistic simulations would be impossible even with today faster computers.
- The significant *velocity range* may vary strongly with space position (steady states may not be compactly supported in velocity space). Thus methods that use a finite velocity range require a great care and may be inadequate in some circumstances.

Numerical challenges

- *Stiffness* of the problem for small mean free paths and/or large velocities. Stiff solvers for small mean free path problems may be hard to use when we have to invert a large nonlinear system. As we will see operator splitting may loose accuracy in such cases.
- Schemes must be capable to deal with *boundary conditions* in complicated geometries and with shocks without introducing excessive numerical dissipation.
- For such reasons realistic numerical simulations are based on *Monte-Carlo techniques*. The most famous examples are the Direct Simulation Monte-Carlo (DSMC) methods by Bird and by Nanbu. These methods guarantee efficiency and preservation of the main physical properties. However, avoiding statistical fluctuations in the results becomes extremely expensive in presence of non-stationary flows or close to continuum regimes.