Numerical methods for kinetic equations

Lecture 1: Preliminaries on kinetic equations

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

http://www.lorenzopareschi.com

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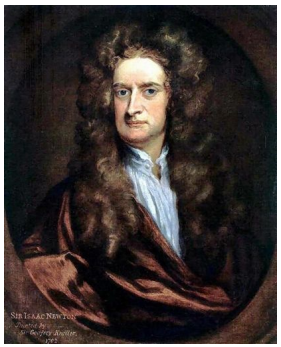
Plan of the lectures

1. Lecture 1: Preliminaries on kinetic equations
2. Lecture 2: Semi-Lagrangian schemes
3. Lecture 3: Discrete velocity and spectral methods
4. Lecture 4: Breaking complexity: fast algorithms
5. Lecture 5: Asymptotic-preserving schemes
6. Lecture 6: Fluid-kinetic coupling and hybrid methods

Lecture 1 Outline

Levels of description

- 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.



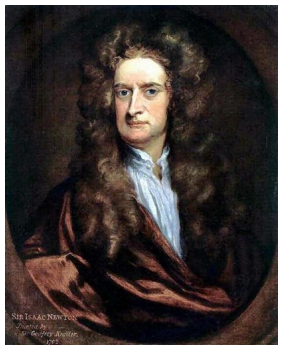
I.Newton

L.Euler

- Particle systems can be described at the microscopic level by particle dynamics (*Newton's equations*) describing the individual motions of the particles. Particle dynamic may be impossible to use, due to the large number of equations that must be solved simultaneously.
- At the macroscopic level models (such as the *Euler or Navier-Stokes equations*) describe averaged quantities, local density, momentum, energy... These models are based on equilibrium assumptions which may not be valid everywhere (or may even not be known in analytical form in some cases).

Levels of description

- There is a need to bridge the gap between particle dynamics and macroscopic models. The problem is slightly simplified by introducing an intermediate step between particle systems and macroscopic models: the so-called kinetic level.


I.Newton


L.Boltzmann


L.Euler

- These kind of models, characterized by *mean field* and *Boltzmann equations*, represent a way of describing the time evolution of a system consisting of a large number of particles by means of a quantity, the distribution function, which is the density of particles in phase-space (say position and velocity).
- Due to the high number of dimensions and their intrinsic physical properties, the construction of numerical methods represents a challenge and requires a careful balance between *accuracy* and *computational complexity*.

Microscopic particle dynamics

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

Newton's equations

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

where $F_i(x_1, \dots, x_N)$ 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

$$F_i = -\nabla_{x_i} \Phi(x_1, \dots, x_N)$$

where $\Phi(x_1, \dots, x_N)$ is a scalar potential function.
For forces originated from binary interactions the potential Φ is given by

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

with $\Phi_{int}(x)$ the interaction potential and $\Phi_{ext}(x)$ the external potential.

Microscopic particle dynamics

The force is then given by

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

with $F_{int} = -\nabla \Phi_{int}$ the interaction force and $F_{ext} = -\nabla \Phi_{ext}$ 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

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

The description of particle systems by Newton's equation of motion is the most fundamental one. However, for systems composed by large number of particles, Newton's equations are intractable from a numerical point of view, and bring little intuition on how a large particle system behaves.

Kinetic level

Kinetic models intend to describe large particle systems by means of a nonnegative *distribution function*

$$f(x, v, t) \geq 0.$$

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 $dxdv$ about the point (x, v). Macroscopic quantities (mass, momentum, energy) can be recovered taking moments of f

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

A thorough treatment of the derivation of kinetic models is beyond the scope of our discussion. We recall some of the basic ideas that lead to the two models that can be considered as prototypes for the development of the numerical methods, the *Vlasov mean-field* equation and the *Boltzmann equation*.

Non-interacting particles

To obtain the equation satisfied by f, it is easier to consider first the case of non-interacting particles $F_{int} = 0$. In such a situation, all particles issued from the same point (x, v) of phase-space follow the same trajectory

$$\dot{X} = V \qquad \dot{V} = F_{ext}(X, t)$$

Furthermore, since the vector field $(v, F_{ext}(x, t))$ is divergence-free (in phase space), the volume element $dxdv$ does not change along the solutions.
It follows that f satisfies

$$\frac{d}{dt} f(X(t), V(t), t) = 0.$$

Applying the chain rule, we get

Free transport Vlasov equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F_{ext}(x, t) \cdot \nabla_v f = 0.$$

Mean-field interacting particles

In the case of particles interacting through a smooth potential in absence of external forces $F_{ext} = 0$, we obtain

Vlasov mean-field equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F_m \cdot \nabla_v f = 0,$$

where F_m is the mean-field force given by

$$F_m(t) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} F_{int}(x-y) f(y,v,t)\, dv\, dy = \int_{\mathbb{R}^3} F_{int}(x-y)\rho(y,t)\, dy.$$

Typically we shall restrict to internal forces which derive from an interaction potential Φ_{int} so that $F_{int} = -\nabla_x \Phi_{int}$, and therefore F_m can also be written as

$$F_m = -\nabla_x \Phi_m, \quad \Phi_m = \int_{\mathbb{R}^3} \Phi_{int}(x-y)\rho(y)\, dy.$$

Vlasov-Poisson systems

One of the most important examples for applications is the *Coulomb potential*

$$\Phi_i(x) = \frac{q}{4\pi r}, \quad r = |x|,$$

where $q = 1$ corresponds to the repulsive case (like e.g. the electrostatic interaction) and $q = -1$ to the attractive case (like e.g. gravitation).
Then $\Delta\Phi_i(x) = -q\delta(x)$, where $\delta(x)$ is the delta distribution at 0 and

$$\Delta\Phi_m(x,t) = \int_{\mathbb{R}^3} \Delta\Phi_i(x-y)\rho(y,t)\,dy = -q\rho(x,t).$$

We obtain

Vlasov-Poisson system

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f - \nabla_x \Phi_m \cdot \nabla_v f = 0,$$
$$\Delta\Phi_m(x,t) = -q\rho(x,t).$$

In the case of negative charged particles in a uniform neutralizing background the Poisson equation reads

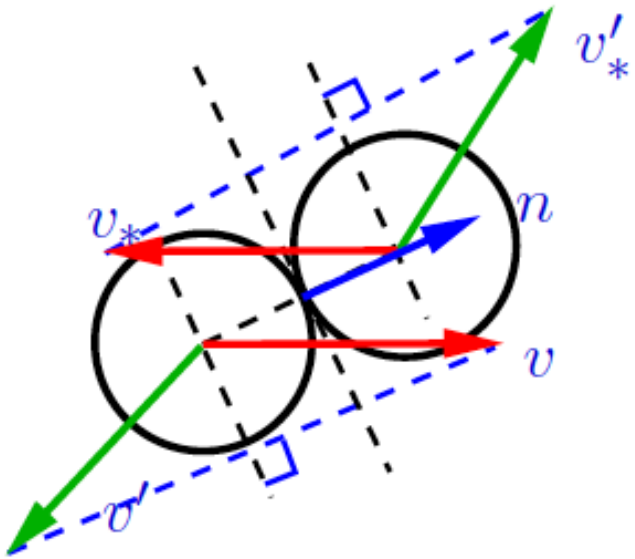
$$\Delta\Phi_m(x,t) = 1 - \rho(x,t).$$

Hard-sphere dynamic

The *Boltzmann equation* is the fundamental model for the kinetic description of a dilute gas. The classical *hard sphere case* considers particles as solid spheres of diameter d which do not interact as long as they do not enter in contact.
In contrast with the Vlasov description, the interaction potential is non smooth

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

where (x, v) and (x_*, v_*) are the centers and velocities of the two spheres. When $|x - x_*| = d$, the spheres undergo a collision and the collision instantaneously changes the velocities to v' and v'_*.



Hard sphere collision. Here $n = (x_* - x)/d$.

Colliding 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

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

Another common way to parametrize this solution is

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

where now ω is the unit vector

$$\omega = g - 2(g \cdot n)n, \quad g = \frac{v - v_*}{|v - v_*|}.$$

The collision operator

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 $Q(f)$ modeling the rate of change of f due to collisions.
This leads to

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

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

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

The collision operator

In this case the interaction operator has a bilinear structure, $Q = Q(f, f)$ and is obtained in the *Boltzmann-Grad limit* where the number of particles $N \to \infty$, $d \to 0$ in such a way that Nd^2 is kept constant. In this limit, the collision operator converges to[1]

Hard spheres collision operator

$$Q(f,f)(x,v,t) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} |v - v_*| [f(v')f(v'_*) - f(v)f(v_*)] \, d\omega \, dv_* .$$

The operator may be decomposed in two terms

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

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

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

More general interactions

Although a mathematical theory is still lacking, the Boltzmann equation is often used in connection with smooth potentials. Formally, for interactions forces described by an inverse power law we have the Boltzmann collision operator

General collision operator

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

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 $B(v,v_*,\omega) = b_0(\cos\theta)$.

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 equivalently

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

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

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

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

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

The H-function is monotonically decreasing until f reaches the Maxwellian state.

Hydrodynamic approximations

Integrating the Boltzmann equation against the collision invariants $\phi(v)$ yields a system of macroscopic conservation laws

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

The system is not closed since it involves higher order moments of f.
The simplest way to find an approximate closure is to assume $f \approx M$. Higher order moments of f can be computed as function of ρ, u, and T and we obtain

Compressible Euler equations

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

Other closure strategies, like the *Navier-Stokes* approach, lead to more accurate macroscopic approximations of the moment system.

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*[2] 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*[3]

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

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

[2] M.Kac, 1959
[3] D.Benedetto, E.Caglioti, M.Pulvirenti, 1997, Toscani 2000

BGK

A simplified model Boltzmann equation is given by the *BGK model*[4]. 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[5].

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

[5] 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

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

  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 (Maxwellian, Fermi-Dirac) and $\sigma(v,v_*)$ describes the interaction of carriers with phonons.
- *Boltzmann-like models*: vehicular traffic flows, social sciences, swarming models, finance, ...[6]

[6] L.Pareschi, G.Toscani '13

Numerical challenges

From the above picture it is clear that the numerical solution of a kinetic equation involves several problems of different nature. Aside from the high dimensionality of the problem, in general $(x, v, t) \in \mathbb{R}^7$, let us shortly summarize some of the additional numerical difficulties and requirements specific to kinetic equations:

(i) *Conservation properties*. Physical conservation properties are very important since they characterize the steady states. Methods that do not maintain such properties at the discrete level need special care in practical applications.

(ii) *Computational cost*. The collision operator may be described by a high dimensional integral in velocity space at each point x in physical space. In such cases fast solvers are essential to avoid excessive computational cost.

(iii) *Velocity range*. The significant velocity range may vary strongly with space position (steady states are not compactly supported in velocity space and in some applications may present power law tails). Methods that use a finite velocity range may be inadequate in some circumstances.

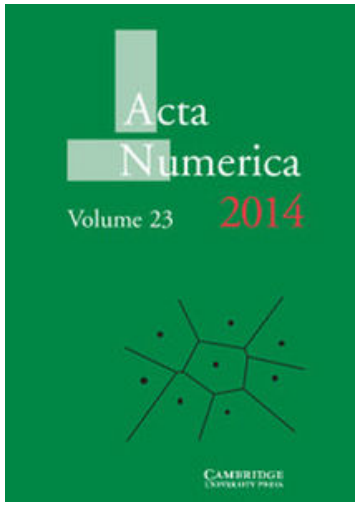
(iv) *Presence of multiple scales*. In presence of multiple space-time scales and/or large velocities the kinetic equation becomes stiff. Classical stiff solvers may be hard to use when we have to invert a very large nonlinear system.

Some final considerations

In these lectures we review some of the main results in this field for deterministic numerical methods.

- The material is mostly based on the recent survey

  G. Dimarco, L. Pareschi, Acta Numerica, 2014.



Another class of methods, that we will not cover in the present lectures, is based on *stochastic Monte-Carlo techniques*. The most famous example is the Direct Simulation Monte-Carlo (DSMC) methods [7]. Some related topics based on the use of hybrid stochastic-deterministic methods will be discussed in the last lecture.

[7] G.Bird '4, K.Nanbu '80