From molecular dynamics to kinetic theory and fluid mechanics.

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Microscopic description

System of $N$ particles of size $\varepsilon$
Newton’s equations

Macroscopic description

Continuous fluid equations of hydrodynamics
(Euler, Navier-Stokes...)

$N\varepsilon^{d-1} >> 1$, $N\varepsilon^d << 1$
**Microscopic description**

System of $N$ particles of size $\varepsilon$

Newton’s equations

$N \gg 1$, $N \varepsilon^{d-1} = \alpha$

Low density limit

$N \varepsilon^{d-1} \gg 1$, $N \varepsilon^{d} << 1$

**Mesoscopic description**

Large system of particles with negligible size

Boltzmann’s kinetic equation

$\alpha \gg 1$

Fast relaxation limit

**Macroscopic description**

Continuous fluid equations of hydrodynamics

(Euler, Navier-Stokes...)

$N \gg 1$, $N \varepsilon^{d} = \alpha$
The Boltzmann equation:
A statistical description
A probability as unknown

- The state of a monatomic gas (constituted of indistinguishable particles) is characterized by its **distribution function**

\[ f(t, x, v) = \frac{\text{number of particles of position } x \text{ and velocity } v \text{ at time } t}{\text{total number of particles}} \]

- This function cannot be measured, but allows to compute observables (such as the temperature or the bulk velocity) by taking **averages**.
A billiard dynamics

• In vacuum, particles are just transported

\[ \frac{dX(t)}{dt} = V(t). \]

• Here velocities are modified by collisions
Transport and collisions

• Under the effect of **transport and collisions**, the distribution $f$ of particles evolves according to the integro-differential equation

$$
\partial_t f(t, x, v) + v \cdot \nabla_x f(t, x, v) = \alpha \int \int (f(t, x, v')f(t, x, v') - f(t, x, v)f(t, x, v_2)) |(v - v_2) \cdot v_2| dv_2 dv_2
$$

• By integration in $v$, we recover the **local conservations** of mass, momentum and energy.
Conservation laws

- The symmetries $v \leftrightarrow v_2$ and $(v, v_2) \leftrightarrow (v', v'_2)$ imply

$$\int Q(f, f)\varphi(v)dv = \frac{1}{4} \int\int (\varphi(v) + \varphi(v_2) - \varphi(v') - \varphi(v'_2))$$

$$(f(v')f(v'_2) - f(v)f(v_2))|(v - v_2) \cdot v_2|dvdv_2dv_2$$

- In particular, mass, momentum and kinetic energy are collision invariants:

$$\left\{ \begin{array}{l}
\partial_t \int fdv + \nabla_x \cdot \int fvdv = 0, \\
\partial_t \int fvdv + \nabla_x \cdot \int f v \otimes vdv = 0, \\
\partial_t \int f|v|^2dv + \nabla_x \cdot \int f|v|^2vdv = 0.
\end{array} \right.$$
Boltzmann’s H-theorem

• The symmetries of the collision integral also imply

\[ \int Q(f, f) \log f(t, x, v) dv \leq 0. \]

• This means that the Boltzmann equation describes an **irreversible evolution**: the entropy

\[ S(t) = -\int\int f \log f(t, x, v) dx dv \]

is an increasing function of time!
Return to equilibrium

• The maxima of the entropy under the constraints of mass, momentum and energy are given by Lagrange’s theorem

\[ \log f(v) = \gamma + u \cdot v + \beta |v|^2 \]

The equilibrium distribution (the attractor as time \( t \to \infty \)) is a Gaussian, as predicted by Maxwell.
Formal derivation from system of particles
A statistical point of view

The Boltzmann equation is non deterministic. It governs an average with respect to initial (symmetric) configurations.

- The starting point is the Liouville equation

\[ \partial_t f_N + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} f_N = 0 \text{ on } D_\varepsilon^N := \{(X_N, V_N) / \forall i \neq j, \quad |x_i - x_j| > \varepsilon\} \]

\[ f_N(Z_N) = f_N(Z'_N) \text{ on } \partial D_\varepsilon^N. \]

- We are then interested in the first marginal

\[ f_N^{(1)}(z_1) = \int f_N(Z_N) dz_2 \ldots dz_N. \]
The Boltzmann-Grad scaling

• The transport and collision process have the same time scale if

\[ N \varepsilon^{d-1} = \alpha \sim 1 \]

which only holds for perfect gases.

N spheres of size \( \varepsilon \) on a lattice

Volume covered by one particle of velocity \( v \) during a time \( t : |v|t \varepsilon^{d-1} \)
The low density limit

The first marginal of the N-particles distribution then satisfies a **collisional transport equation** similar to the Boltzmann equation

- By Green’s formula and the symmetry,

\[(\partial_t + v_1 \cdot \nabla_{x_1})f_{N}^{(1)}(t, z_1) = (N - 1)\varepsilon^{d-1}(C_{1,2}f_{N}^{(2)})(t, z_1)\]

\[(C_{1,2}f_{N}^{(2)})(z_1) = \int_{S^1 \times \mathbb{R}^2} f_{N}^{(2)}(x_1, v_1, x_1 + \varepsilon v_2, v_2) \left((v_2 - v_1) \cdot \nu\right) dv_2 dv_2\]

- The collision integral can be split according to 
\[\text{sign}((v_2 - v_1) \cdot \nu)\] (using the scattering if positive)
The chaos assumption

The joint probability can be expressed in terms of the one particle distribution under some independence or chaos assumption:

\[ f_N^{(2)}(t, z_1, z_2) = f_N^{(1)}(t, z_1)f_N^{(1)}(t, z_2). \]

This identity cannot be true for all times!
- At time 0, small error due to the exclusion.
- For further times, we expect propagation of chaos with small error in the low density limit.
Lanford’s convergence result
Lanford’s theorem

Theorem (Lanford)

Consider $N$ hard spheres on $T^d \times \mathbb{R}^d$, initially “independent” and identically distributed according to $f_0$

$$f_0(x, v) \leq \exp \left( -\mu - \frac{\beta}{2} |v|^2 \right).$$

Then, in the Boltzmann-Grad limit $N \to \infty$ with $N\varepsilon^{d-1} = \alpha$, the distribution $f^{(1)}_N(t, x, v)$ of a typical particle converges almost everywhere to the solution $f$ of the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \alpha Q(f, f)$$

on a short time interval $[0, T^*(\beta, \mu)/\alpha]$. 
Paradoxes of Loschmidt and Zermelo

How can the entropy increase even though the equations of mechanics are reversible? (1876)

How can the gas relax to equilibrium while Poincaré’s theorem predicts a recurrence? (1896)
A weak notion of convergence

Some trajectories are far from the Boltzmann dynamics, but their contribution to the average vanishes in the limit.

Irreversibility comes from a loss of information at each collision.
A short-time convergence

Poincaré’s recurrence time diverges with N, it is much bigger than the **expected validity** of the Boltzmann approximation.

Actually Lanford’s theorem gives only a very short time convergence. In particular, it does not say anything about the relaxation \( \alpha \to \infty \), and the hydrodynamic limits.
Strategy of the proof
Collision trees

Solutions of the molecular dynamics can be represented by **collision trees**, with transport and scattering operators.
Recollisions

Solutions of the Boltzmann equation provide a good approximation as long as there is no recollision (i.e. no collision between two particles which are not independent)
Geometric control of recollisions

- Solutions of the Boltzmann equation provide a good approximation as long as there is no recollision (i.e. no collision between two particles which are not independent)

- By a geometric study of the free transport, we can prove that recollisions are of vanishing probability as $\varepsilon \to 0$. 

$$S(0, \varepsilon)$$

$$X_1 - X_2$$
About the size of the trees

• The previous truncation is admissible only for relatively small trees (with a number of branching points at most of the order of log N).

• In general, the size of the trees can be controlled only for very short times, by some Cauchy-Kowalewski estimate for the BBGKY hierarchy.