Some results on a simple model of kinetic theory.

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Plan of the talk.

- What is Statistical Mechanics?
- Introduction to the physics of gases.
- Classical heuristic results.
- The Kac model and gas kinetic.
- Classical results on the Kac model.

Gas Kinetic.

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2. the particles are hard spheres of small radius r;
3. the collisions are elastic;
4. the average kinetic energy of the particles is proportional to T.

To get an idea ...

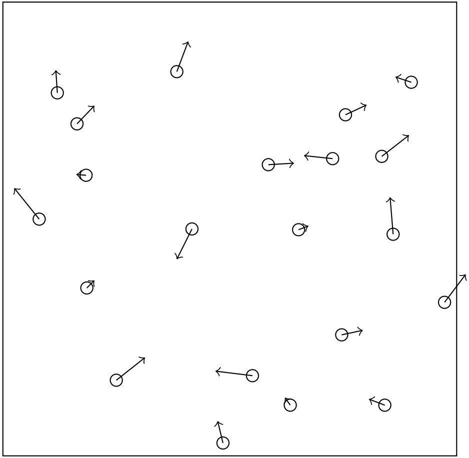
Here are some physical quantities for oxygen at ambient condition

- temperature $T = 273\,\mathrm{K}$
- pressure $P = 1.01 \times 10^5\,\mathrm{N/m^2}$
- number density $\delta = M/V = 2.7 \times 10^{25}\,\mathrm{molecules/m^3}$
- kinetic radius $r = 1.73 \times 10^{-10}\,\mathrm{m}$
- occupied volume fraction $4\pi r^3\delta/3 = 5.85 \times 10^{-4}$
- average speed $v = 1.58 \times 10^2\,\mathrm{m/s}$
- mean free path $\rho = 1.0 \times 10^{-7}\,\mathrm{m}$
- mean free time $\lambda = 0.6 \times 10^{-5}\,\mathrm{s}$

1000 particles initially confined in a quarter of the container and with independent velocity uniformly distributed in $[-1, 1]$.

Left panel: positions. Right panel: histogram of the x-velocity (time smoothed).

Gas Kinetic: schematics



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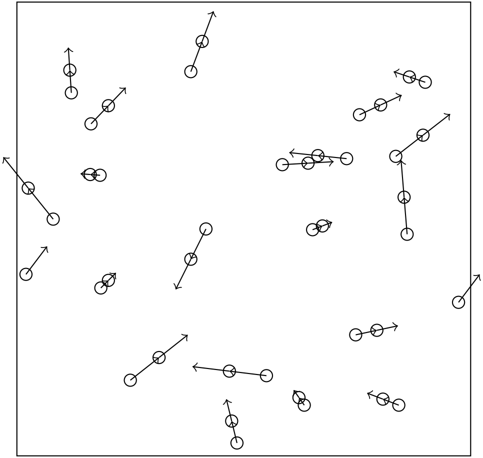

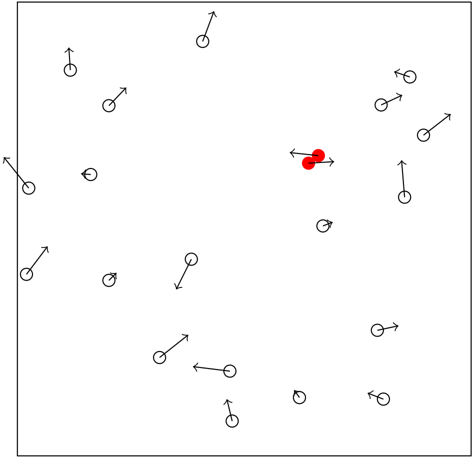

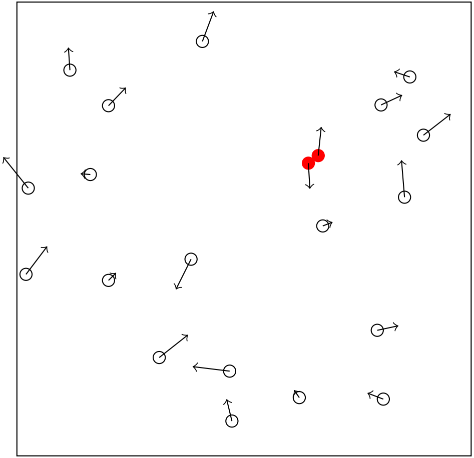

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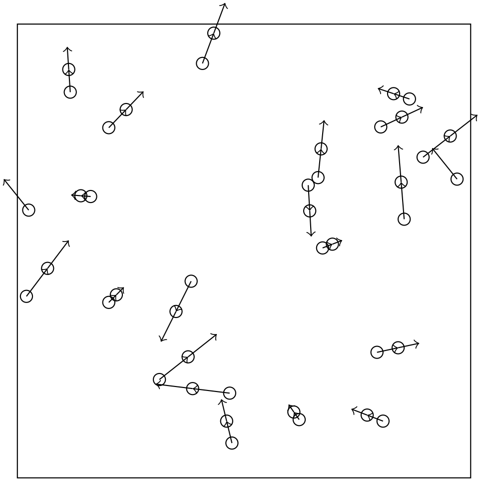

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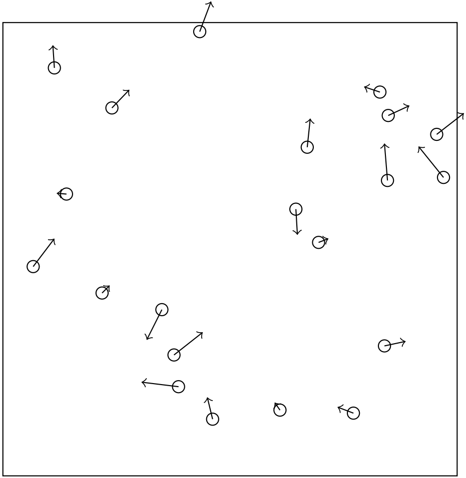

A little history: Fourier.

> *Heat, like gravity, penetrates every substance of the universe, its ray occupy all parts of space. The object of our work is to set forth the mathematical laws which this element obeys. The theory of heat will hereafter form one of the most important branches of general physics.*

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> *But whatever may be the range of mechanical theories, they do not apply to the effects of heat. These make up a special order of phenomena, which cannot be explained by the principles of motion and equilibria.*

— *Ibidem*

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A particle moves on straight line with velocity $\mathbf{p}_i/m$ till it collides with another particle or with the walls of the container.

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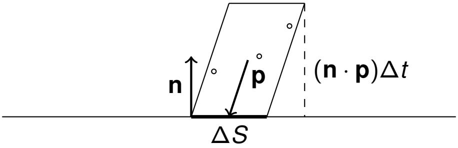

The number of particle with momentum $\mathbf{p}$ that will collide with ΔS in the next Δt is

$$(\mathbf{p} \cdot \mathbf{n}) \Delta S \Delta t \;\; f(\mathbf{p}) \, d\mathbf{p} \;\; \frac{\delta}{m}$$

where $\delta = N/|V|$ is the number density.

Since during a collision a particle momentum changes by $2(\mathbf{p}\cdot\mathbf{n})$, the total momentum exchanged by the gas with ΔS in the time Δt is

$$\Delta\mathbf{P} = 2\int_{(\mathbf{p}\cdot\mathbf{n}<0)} \frac{1}{m}(\mathbf{p}\cdot\mathbf{n})^2 f(\mathbf{p})\, d\mathbf{p}\, \Delta S \Delta t = \frac{2}{3}\int \frac{|\mathbf{p}|^2}{2m} f(\mathbf{p})\, d\mathbf{p}\, \Delta S \Delta t$$

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But we know that the average kinetic energy is proportional to the temperature. More precisely

$$\int \frac{|\mathbf{p}|^2}{2m} f(\mathbf{p})\, d\mathbf{p} = \frac{3}{2} k_B T$$

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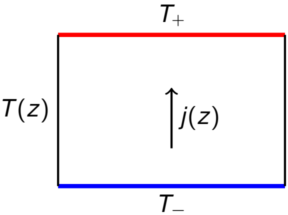

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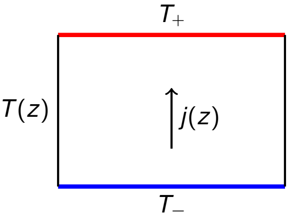

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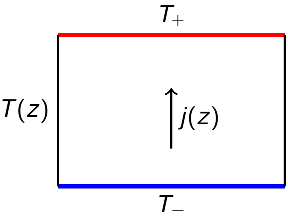

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Fourier's Law states that

$$j(z) = -c(T)\frac{dT(z)}{dz}$$

where $j(z)$ is the heat current in the z direction and $c(T)$ is the thermal conductivity.

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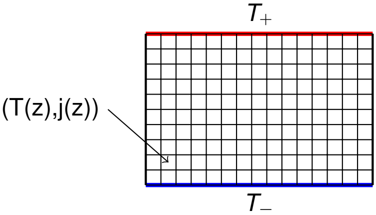

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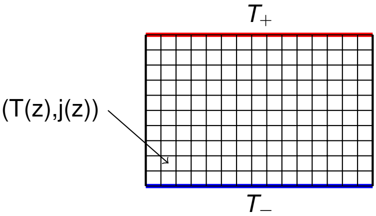

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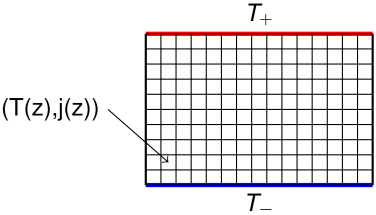

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This is called the *local equilibrium* description of a macroscopic gas (or any other object).

Local equilibrium with 25 volume elements.

de Groot and Mazur

> *It will now be assumed that, although the total system is not in equilibrium, there exists within small mass elements a state of "local" equilibrium for which the local entropy s is the same function of u, v and c_k as in real equilibrium.*

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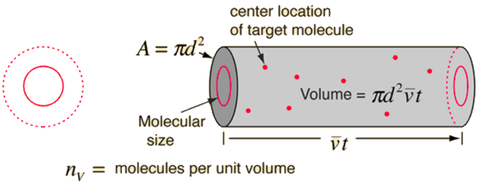
The hypothesis of "local" equilibrium can, from a macroscopic point of view, only be justified by virtue of the validity of the conclusions derived from it.

— *Ibidem*

Mean free time.

The number of collision ν a particle suffers in a time t is:

$$\nu = \pi d^2 \, \bar{v} t \; M/V$$



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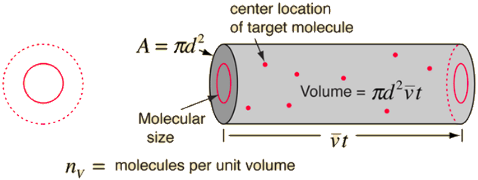

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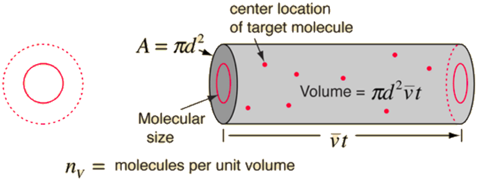

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and the space travelled by the particle between two collisions (*mean free flight*) is:

$$\rho = \lambda \bar{v} \simeq \frac{1}{\delta r^2}.$$

A particle initially at height z with $p_z > 0$ will travel for a distance ρ and will reach, in average, a height $z + \rho/\sqrt{3}$.

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Finally the momentum of the particles at z is, in average, proportional to $\sqrt{T(z)}$.

Putting all together we get

$$j(z) \simeq \delta \sqrt{T(z)} \left(T(z) - T(z + \rho/\sqrt{3}) \right) \simeq -r^{-2} \sqrt{T(z)} \frac{dT(z)}{dz}$$

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The above properties are well verified experimentally at least if T is not too low (quantum effect) or too high (particles are not hard spheres).

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λ_M is fixed in such a way that the average time between two collision of a given particle is independent of M. That is $\lambda_M = 1/(M-1)$. This is called Boltzmann-Grad limit.

Kac vs real gas dynamics

The main simplifications we have introduced are:

1. Collisions times are stochastic and independent from the position and velocity of the particles.
2. Energy and momentum are redistributed randomly.
3. the collision rate between two particles does not depend on their velocities. This are often called “Maxwellian Molecules”.

The evolution.

State of the system

$$f(\underline{v}) : \mathbb{R}^M \to \mathbb{R} \qquad\qquad \underline{v} = (v_1, v_2, \ldots, v_M) \in \mathbb{R}^M,$$

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If f is the state of the system before particle i and j collide, just after the collision the state is

$$R_{i,j} f(\underline{v}) = \int f(r_{i,j}(\theta)\underline{v})d\theta$$

where

$$r_{1,2}(\theta)\underline{v} = (v_1\cos(\theta) - v_2\sin(\theta), v_1\sin(\theta) + v_2\cos(\theta), v_3, \ldots)$$

that is, $r_{i,j}(\theta)$ is a rotation of angle θ in the i, j plane.

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The effect of a collision of a randomly picked pair of particles is

$$Qf = \frac{1}{\binom{M}{2}} \sum_{i<j} R_{i,j} f$$

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$$Qf = \frac{1}{\binom{M}{2}} \sum_{i<j} R_{i,j} f$$

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so that the evolution is given by

$$F_t = e^{-Mt} \sum_{k=0}^{\infty} \frac{t^k}{k!} Q^k f_0 = e^{\mathcal{L}_S t} F_0$$

where

$$\mathcal{L}_S = \frac{2}{M-1} \sum_{i<j} (R_{i,j} - I) = \frac{2}{M-1} \mathcal{K}$$

Thus F_t satisfies the equation:

$$\dot{F}(t) = \mathscr{L}_S f(t)\,.$$

The evolution generated by this equation preserves the total kinetic energy. Thus every rotationally invariant distribution is a steady state.

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Given an initial distribution $f(\underline{v})$, the evolution brings it toward its projection on the rotationally invariant distributions, that is toward

$$F_R(\underline{v}) = \int_{S^{M-1}} F(|\underline{v}|\omega)d\sigma(\omega)$$

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This observation "explain" the movie shown at the beginning.

Convergence to equilibrium.

Carlen-Carvalho-Loss (2000) showed that

$$\left\| e^{t\mathscr{L}_S} f - f_R \right\|_2 \leq Ce^{-L^{(1)}t}$$

where $\|\cdot\|_2$ is the $L^2(\mathbb{R}^M)$ norm and

$$L^{(1)} = \frac{1}{2}\frac{M+1}{M-2}.$$

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The L^2 norm has one major problem. Assume that

$$f(\underline{v}) = \prod_{i=1}^{M} F(v_i) \qquad \text{and} \qquad g(\underline{v}) = \prod_{i=1}^{M} G(v_i)$$

then

$$\|f - g\|_2 \simeq C^M \|F - G\|_2 \qquad \text{with} \qquad C > 1.$$

The entropy with respect to the steady state is defined as

$$\mathscr{S}(f\,|\,f_R) = \int f(\underline{v}) \log\left(\frac{f(\underline{v})}{f_R(\underline{v})}\right) d\underline{v}$$

The entropy with respect to the steady state is defined as

$$\mathscr{S}(f \mid f_R) = \int f(\underline{v}) \log\left(\frac{f(\underline{v})}{f_R(\underline{v})}\right) d\underline{v}$$

In general

$$\mathscr{S}(f \mid f_R) \geq 0 \qquad\qquad \mathscr{S}(f \mid f_R) = 0 \quad \Leftrightarrow \quad f = f_R$$

and

$$\frac{d}{dt}\mathscr{S}(f(t) \mid f_R) \leq 0$$

and

$$f(\underline{v}) = \prod_{i=1}^{M} F(v_i) \qquad \Rightarrow \qquad S(f \mid f_R) = O(M).$$

For the realistic kinetic evolution Cercignani conjectured

$$\mathscr{S}(f(t)\,|\,f_R) \leq e^{-c\,t}\mathscr{S}(f(0)\,|\,f_R).$$

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Cercignani Conjecture

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but for every δ there exists C_δ and f_δ such that

$$-\frac{\dot{\mathscr{S}}(f_\delta\,|\,f_R)}{\mathscr{S}(f_\delta\,|\,f_R)} \leq \frac{C_\delta}{M^{1-\delta}}.$$

Villani (2003), Einav (2011)
Mischler and Muhot obtained polynomial decay unifrom in M.

Suppose that, at least in some approximate form, for every t we have

$$f(\underline{v}, t) = \prod_{i=1}^{M} F(v_i, t) \,.$$

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From the evolution equation, integrating over all variables but one, we get the *Boltzmann-Kac equation*

$$\frac{d}{dt}F(v,t) = 2\int dw \fint d\theta \big(F(v\cos\theta - w\sin\theta, t)F(v\sin\theta + w\cos\theta, t) - F(v,t)F(w,t)\big)$$

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Clearly even if $f(\underline{v}, 0)$ is a product, in general $f(\underline{v}, t)$ is not.

Boltzmann Property

Given a symmetric distribution $f_M(\underline{v}_M)$ we define the k particle marginal as

$$F_M^k(\underline{v}_k) = \int f_M(\underline{v}_M)\, dv_{k+1} \cdots dv_M$$

A sequence of distributions $f_M(\underline{v}_M)$ forms a *chaotic sequence* if

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Theorem (Mc Kean)

If $f_M(\underline{v}, 0)$ forms a chaotic sequence then also $f_M(\underline{v}, t)$ forms a chaotic sequence. It follows that $F^1(v, t)$ satisfies the Boltzmann-Kac equation.

Idea of the proof.

Let $\phi : \mathbb{R}^k \to \mathbb{R}$ be a k variables test function. Then

$$\int_{\mathbb{R}^M} f_M(\underline{v}_M, t)\phi(\underline{v}_k)d\underline{v}_M = \sum_n \frac{t^n}{n!} \int_{\mathbb{R}^M} f_M(\underline{v}_M, 0)(\mathscr{L}_S)^n \phi(\underline{v}_k)d\underline{v}_M$$

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But

$$\mathscr{L}_S\phi = \frac{2}{M-1} \sum_{1\le i<j\le k} (R_{i,j} - I)\phi + \frac{2(M-k)}{M-1} \sum_{i=1}^{k} (R_{i,k+1} - I)\phi \to_{M\to\infty}$$
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Observe that if $\phi : \mathbb{R}^{k_1} \to \mathbb{R}$ and $\psi : \mathbb{R}^{k_2} \to \mathbb{R}$

$$\Lambda\phi\otimes\psi = (\Lambda\phi)\otimes\psi + \phi\otimes(\Lambda\psi)$$

where $\phi\otimes\psi(v_1\ldots, v_{k_1+k_2}) = \phi(v_1\ldots, v_{k_1})\psi(v_{k_1+1}\ldots, v_{k_1+k_2})$.

If now we take $\phi : \mathbb{R} \to \mathbb{R}$, with some straightforward algebra we get

$$\sum_n \frac{t^n}{n!}\Lambda^n \phi^{\otimes k} = \sum_{n_1, n_2, \ldots n_k} \prod_{i=1}^{k} \frac{t^{n_k}}{n_k!}\Lambda^{n_k}\phi$$

so that

$$\lim_{M\to\infty} \int_{\mathbb{R}^M} f_M(\underline{v}_M, t)\phi^{\otimes k}(\underline{v}_k) d\underline{v}_M = \sum_{n_1, n_2, \ldots n_k} \prod_{i=1}^{k} \frac{t^{n_k}}{n_k!} \int_{\mathbb{R}^{n_k+1}} (F^1)^{\otimes n_k+1} \Lambda^{n_k}\phi d\underline{v}_{n_k+1} = \left(\sum_n \int_{\mathbb{R}^{n+1}} (F^1)^{\otimes n+1} \Lambda^n \phi d\underline{v}_{n+1} \right)^k$$

while in the same way we get

$$\lim_{M\to\infty} \int_{\mathbb{R}^M} f_M(\underline{v}_N, t)\phi(v_1) d\underline{v}_M = \sum_n \int_{\mathbb{R}^{n+1}} (F^1)^{\otimes n+1} \Lambda^n \phi d\underline{v}_{n+1}$$

Thank you.