ENTROPY AND H THEOREM

THE MATHEMATICAL LEGACY OF LUDWIG BOLTZMANN

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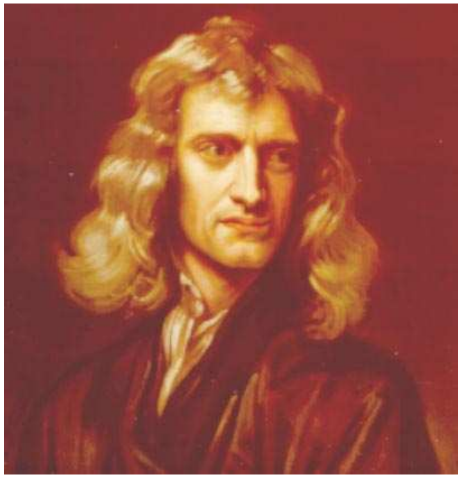
Cutting-edge physics at the end of nineteenth century

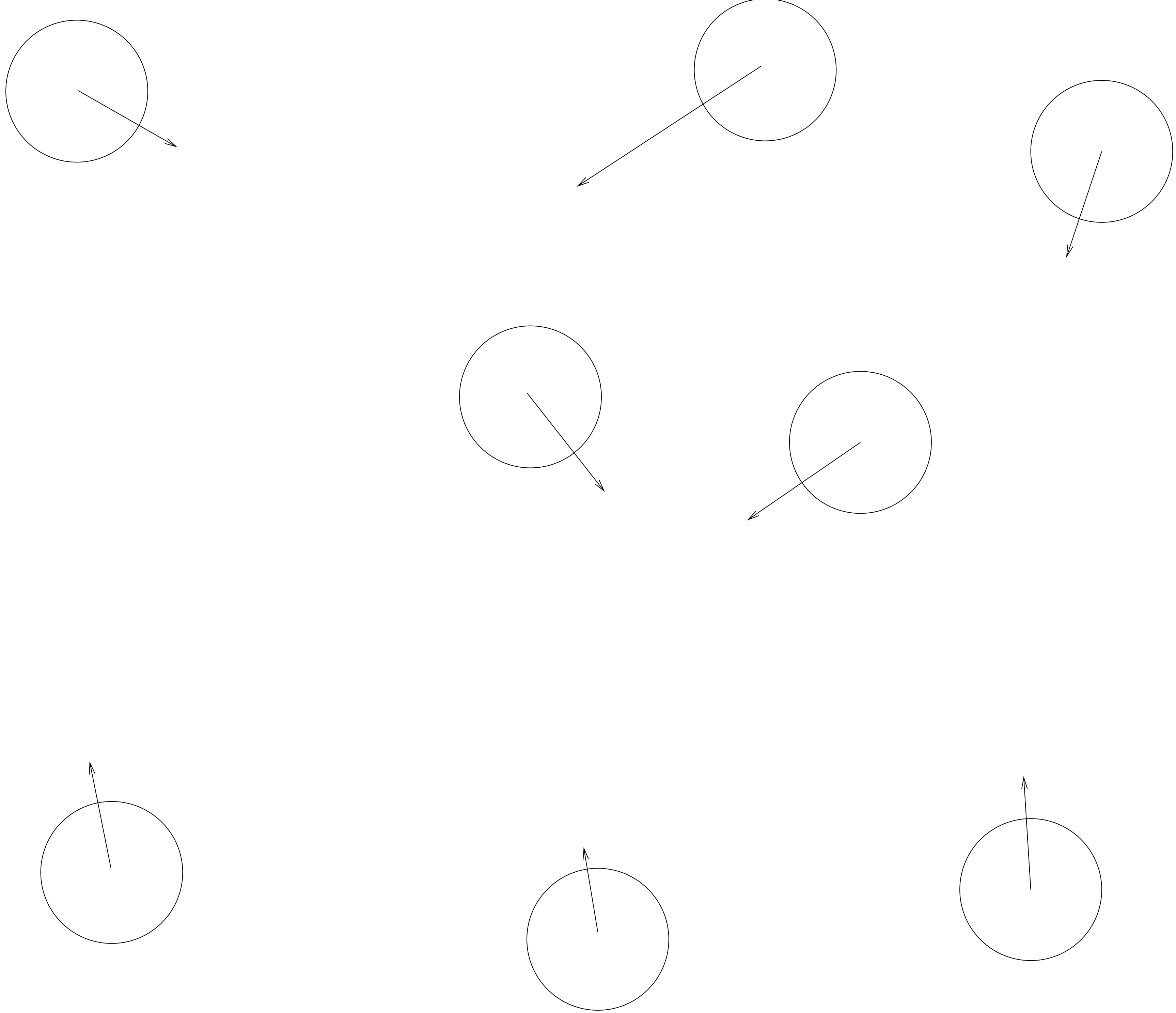
Long-time behavior of a (dilute) classical gas

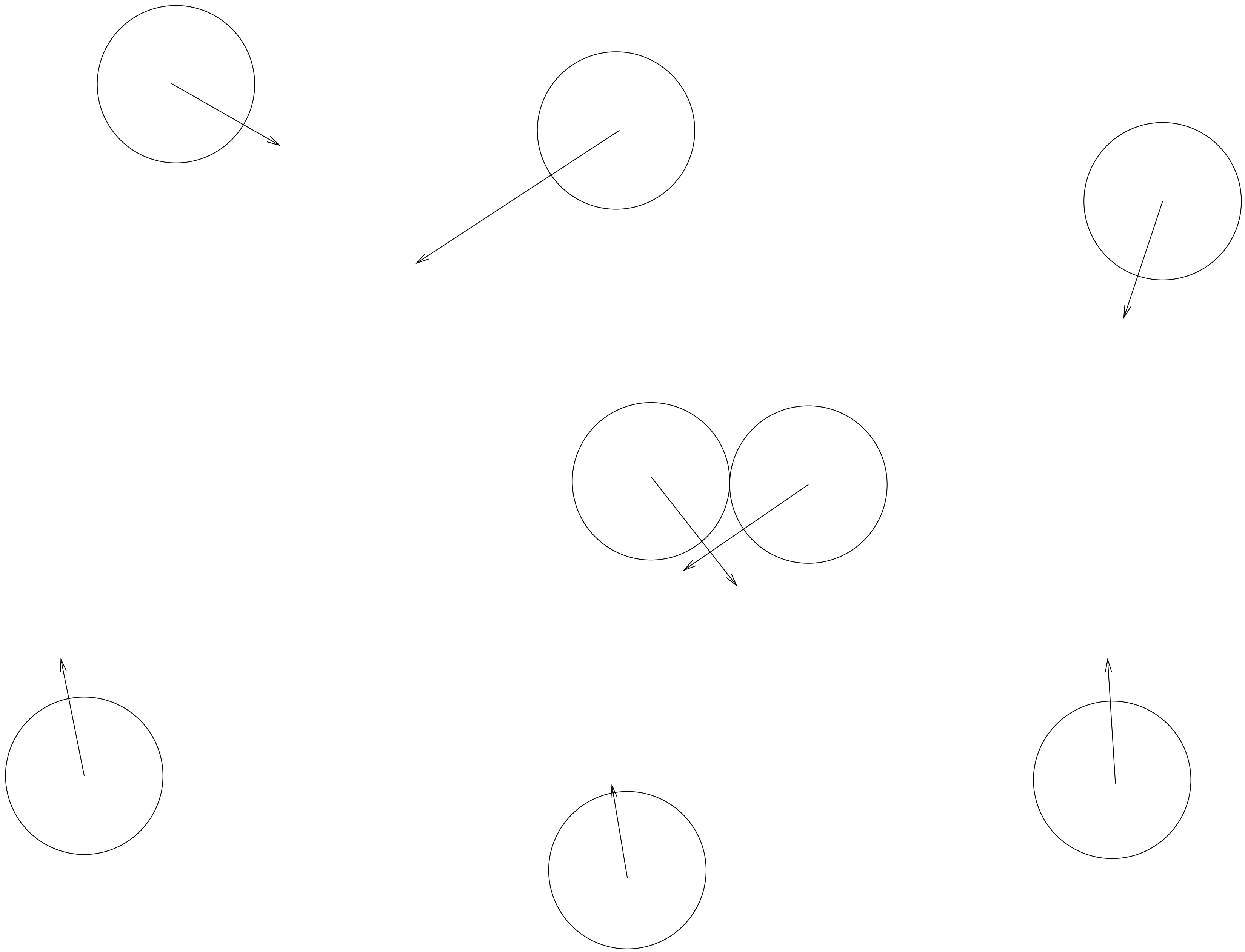
Take many (say 10^{20}) small hard balls,

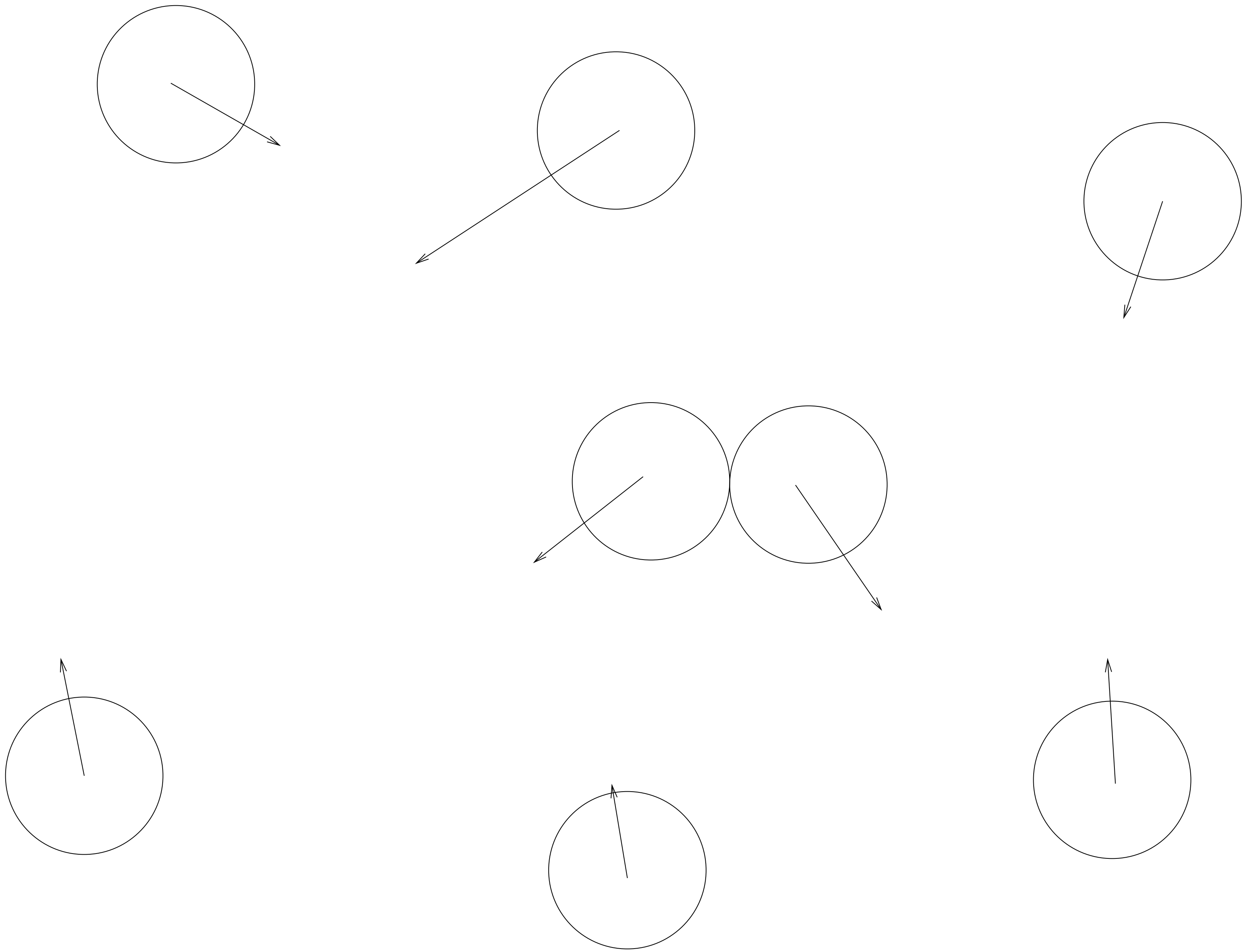
bouncing against each other, in a box

Let the gas evolve according to Newton's equations









Prediction by Maxwell and Boltzmann

The distribution function is asymptotically Gaussian

$$f(t,x,v) \simeq a\, \exp\left(-\frac{|v|^2}{2T}\right) \qquad \text{as } t \to \infty$$

Based on four major conceptual advances 1865-1875

- Major modelling advance: Boltzmann equation
- Major mathematical advance: the statistical entropy
- Major physical advance: macroscopic irreversibility
- Major PDE advance: qualitative functional study of the large-time limit

Let us review these advances

$\Longrightarrow$ journey around centennial scientific problems

Probabilistic point of view

$y_1 = (x_1, v_1)$, y_2, ..., y_N ...

Microscopic state: e.g. $N \gtrsim 10^{10} \gg 1$

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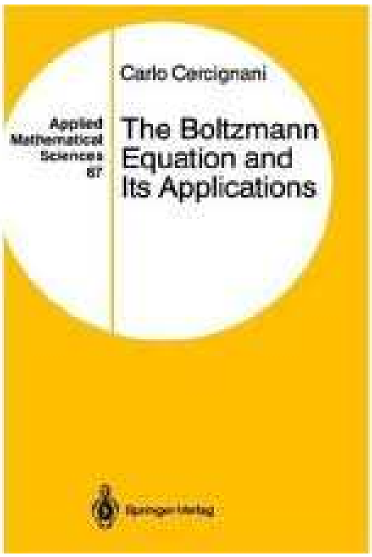
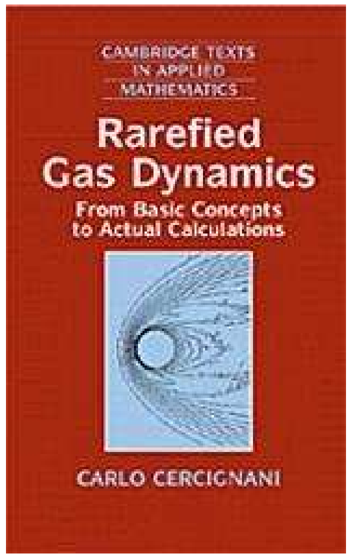
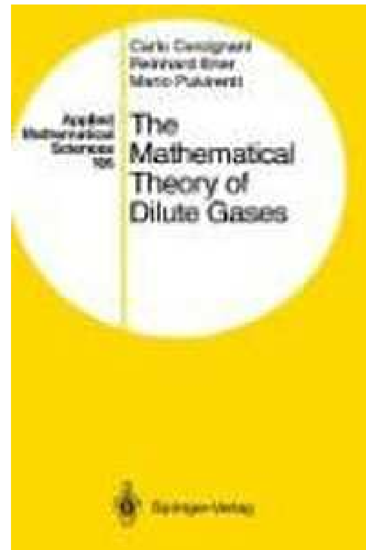
Closed equation on f?

The Boltzmann equation

Models rarefied gases (Maxwell 1865, Boltzmann 1872)







$f(t,x,v)$: density of particles in (x,v) space at time t

$f(t,x,v)\,dx\,dv =$ fraction of mass in $dx\,dv$

The Boltzmann equation (without boundaries)

Unknown = time-dependent distribution $f(t,x,v)$:

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} v_i \, \frac{\partial f}{\partial x_i} = Q(f,f) =$$

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

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$$\begin{cases} v' = v - (v-v_*)\cdot\omega\,\omega \\ \\ v'_* = v_* + (v-v_*)\cdot\omega\,\omega \end{cases}$$

$$(x,v) + (x+r\omega, v_*) \longleftrightarrow (x,v') + (x+r\omega, v'_*)$$

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Conceptually tricky!

Molecular chaos: No correlations between particles

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However correlations form due to collisions!

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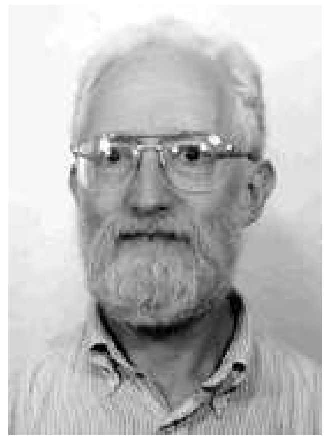
One-sided chaos: No correlations on pre-collisional configurations, but correlations on post-collisional configurations [which topology??]

...and this should be preserved in time,

although correlations continuously form!

... Valid approximation? 100 years of controversy

Lanford's Theorem (1973)



- Rigorously derives the Boltzmann equation from Newtonian mechanics of N hard spheres of radius r, as $Nr^2 \to 1$, for microscopic distributions with Gaussian velocity decay, under an assumption of strong molecular chaos at initial time, on a short time interval.
- Improved (Illner & Pulvirenti): rare cloud in $\mathbb{R}^3$
- Quantum: Erdös–Yau, Lukkarinen–Spohn...

Leaves many open issues

- Large data? Box? Long-range interactions?
- Nontrajectorial proof??
- Propagation of one-sided chaos???

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Qualitative properties?

- Fundamental properties of Newtonian mechanics: preservation of volume in configuration space
- What can be said about the volume in this infinite-dimensional limit??

Boltzmann's H functional

$$S(f) = -H(f) := -\int_{\Omega_x \times \mathbb{R}^3_v} f(x,v) \log f(x,v)\, dv\, dx$$

Boltzmann identifies S with the entropy of the gas

and proves that S can only increase in time

(strictly unless the gas is in a hydrodynamical state)

— an instance of the Second Law of Thermodynamics

The content of the H functional

Mysterious and famous, also appears in Shannon's theory of information

In Shannon's own words:

I thought of calling it 'information'. But the word was overly used, so I decided to call it 'uncertainty'. When I discussed it with John von Neumann, he had a better idea: (...) "You should call it entropy, for two reasons. In first place your uncertainty has been used in statistical mechanics under that name, so it already has a name.

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Information theory

The Shannon–Boltzmann entropy $S = -\int f \log f$ quantifies how much information there is in a "random" signal Y, or a language.

$$H_\mu(\nu) = \int \rho \log \rho \, d\mu; \qquad \nu = \rho \, \mu.$$

... Entropy = mean value of $\log \dfrac{1}{\rho(Y)}$ ...

Microscopic meaning of the entropy functional

Measures the volume of microstates associated,

to some degree of accuracy in macroscopic observables,

to a given macroscopic configuration (observable distribution function)

$\Longrightarrow$ How exceptional is the observed configuration?

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Boltzmann's formula

$$S = k \log W$$


S = k. log W
LVDWIG
BOLTZMANN
1844 - 1906
GEB. CHIARI

$\longrightarrow$ How to go from $S = k \log W$ to $S = -\int f \log f$?

Famous computation by Boltzmann

N particles in k boxes

$f_1, \ldots, f_k$ some (rational) frequencies; $\sum f_j = 1$

N_j = number of particles in box $\#j$

$\Omega_N(f)$ = number of configurations such that $N_j/N = f_j$

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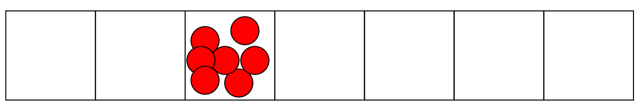

$f = (0, 0, 1, 0, 0, 0, 0)$

$$\boxed{\Omega_N(f) = 1}$$

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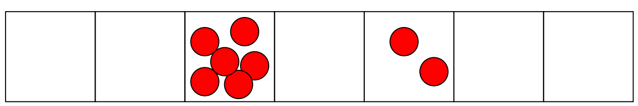

$f = (0, 0, 3/4, 0, 1/4, 0, 0)$

$$\boxed{\Omega_8(f) = \frac{8!}{6!\, 2!}}$$

$\longrightarrow$ How to go from $S = k \log W$ to $S = -\int f \log f$?

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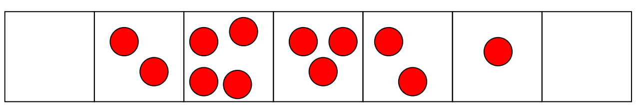

$f = (0, 1/6, 1/3, 1/4, 1/6, 1/12, 0)$

$$\boxed{\Omega_N(f) = \frac{N!}{N_1! \ldots N_k!}}$$

$\longrightarrow$ How to go from $S = k \log W$ to $S = -\int f \log f$?

Famous computation by Boltzmann

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$\Omega_N(f)$ = number of configurations such that $N_j/N = f_j$

Then as $N \to \infty$

$$\#\Omega_N(f_1, \ldots, f_k) \sim e^{-N \sum f_j \log f_j}$$

$$\frac{1}{N} \log \#\Omega_N(f_1, \ldots, f_k) \simeq -\sum f_j \log f_j$$

Sanov's theorem

A mathematical translation of Boltzmann's intuition

$x_1, x_2, \ldots$ ("microscopic variables") independent, law μ;

$$\widehat{\mu}^N := \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i} \text{ (random measure, "empirical")}$$

What measure will we observe??

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Rigorous writing: $H_\mu(\nu) = \lim_{k\to\infty} \limsup_{\varepsilon\to 0} \limsup_{N\to\infty}$

$$-\frac{1}{N} \log \mathbb{P}_{\mu^{\otimes N}} \left[\left\{ \forall j \leq k, \quad \left| \frac{\varphi_j(x_1) + \ldots + \varphi_j(x_N)}{N} - \int \varphi_j \, d\nu \right| < \varepsilon \right\} \right]$$

Universality of entropy

Lax entropy condition

Entropy is used to select physically relevant shocks in compressible fluid dynamics

(Entropy should increase,

i.e. information be lost, not created!!)

Universality of entropy

Voiculescu's classification of II_1 factors

Think of $(A_1, \ldots, A_n)$ in $(\mathcal{A}, \tau)$ as the observable limit of a family of "microscopic systems" = large matrices

$$\Omega(N, \varepsilon, k) :=$$

$$\Big\{(X_1, \ldots, X_n),\ N \times N \text{ Hermitian; } \forall P \text{ polynomial of degree} \leq k,$$

$$\left| \frac{1}{N} \operatorname{tr} P(X_1, \ldots, X_n) - \tau(P(A_1, \ldots, A_n)) \right| < \varepsilon \Big\}$$

$$\chi(\tau) := \lim_{k \to \infty} \limsup_{\varepsilon \to 0} \limsup_{N \to \infty} \left[\frac{1}{N^2} \log \operatorname{vol}(\Omega(N, \varepsilon, k)) - \frac{n}{2} \log N \right]$$

Universality of entropy

Ball–Barthe–Naor's quantitative central limit theorem

$X_1, X_2, \ldots, X_n, \ldots$ identically distributed, independent real random variables;

$\mathbb{E}X_j^2 < \infty, \quad \mathbb{E}X_j = 0$

Then $\dfrac{X_1 + \ldots + X_N}{\sqrt{N}} \xrightarrow[N\to\infty]{}$ Gaussian random variable

Ball–Barthe–Naor (2004): Irreversible loss of information

$$\text{Entropy}\left(\frac{X_1 + \ldots + X_N}{\sqrt{N}}\right) \quad \text{increases with } N$$

(some earlier results: Linnik, Barron, Carlen–Soffer)

Back to Boltzmann: The H Theorem

Boltzmann computes the rate of variation of entropy along the Boltzmann equation:

$$\frac{1}{4}\int \Big(f(v)f(v_*) - f(v')f(v'_*) \Big) \log \frac{f(v)f(v_*)}{f(v')f(v'_*)} \, B \, d\omega \, dv \, dv_* \, dx$$

Obviously ≥ 0

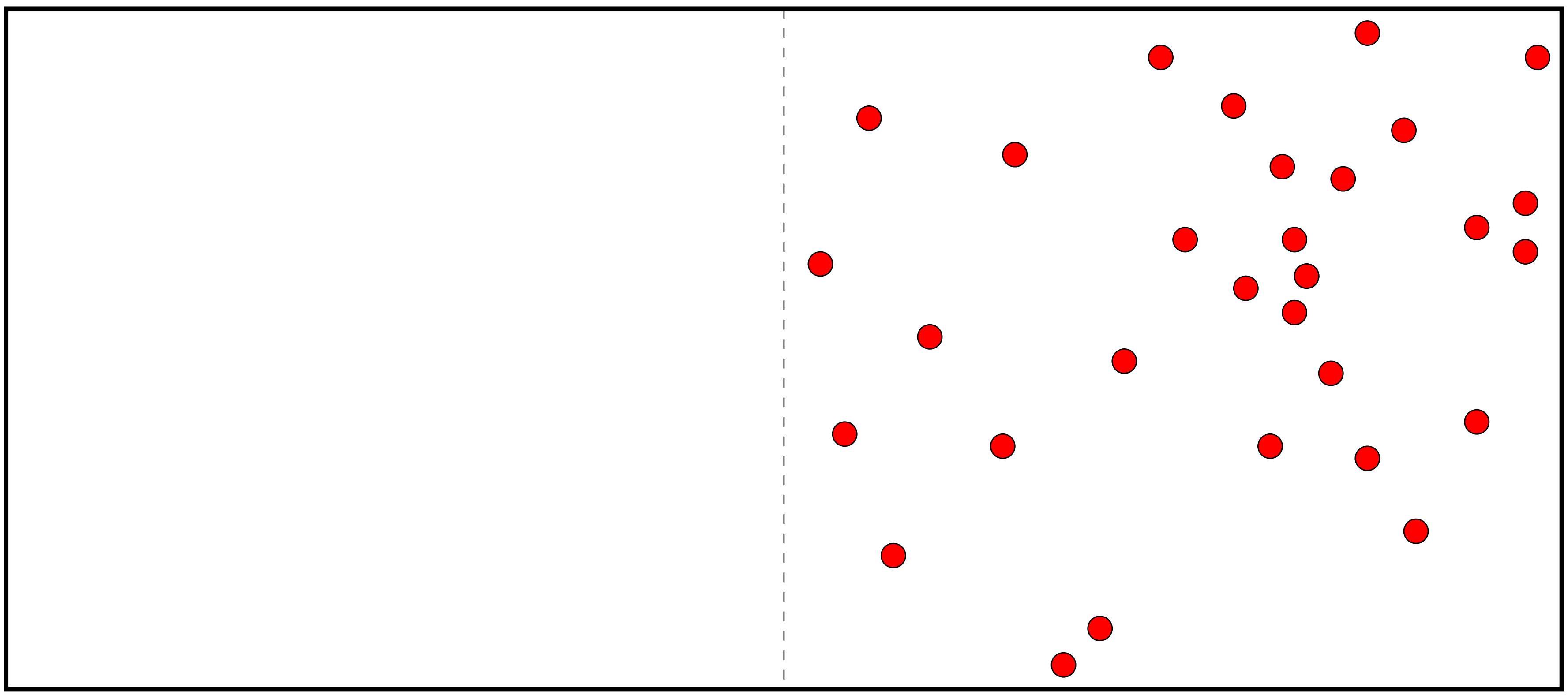
Moreover, $\quad = 0$ if and only if $f(x,v) = \rho(x) \dfrac{e^{-\frac{|v-u(x)|^2}{2T(x)}}}{(2\pi\, T(x))^{3/2}}$

$=$ Hydrodynamic state

Reversibility and irreversibility

Entropy increase, but Newtonian mechanics is reversible!?

Ostwald, Loschmidt, Zermelo, Poincaré... questioned Boltzmann's arguments



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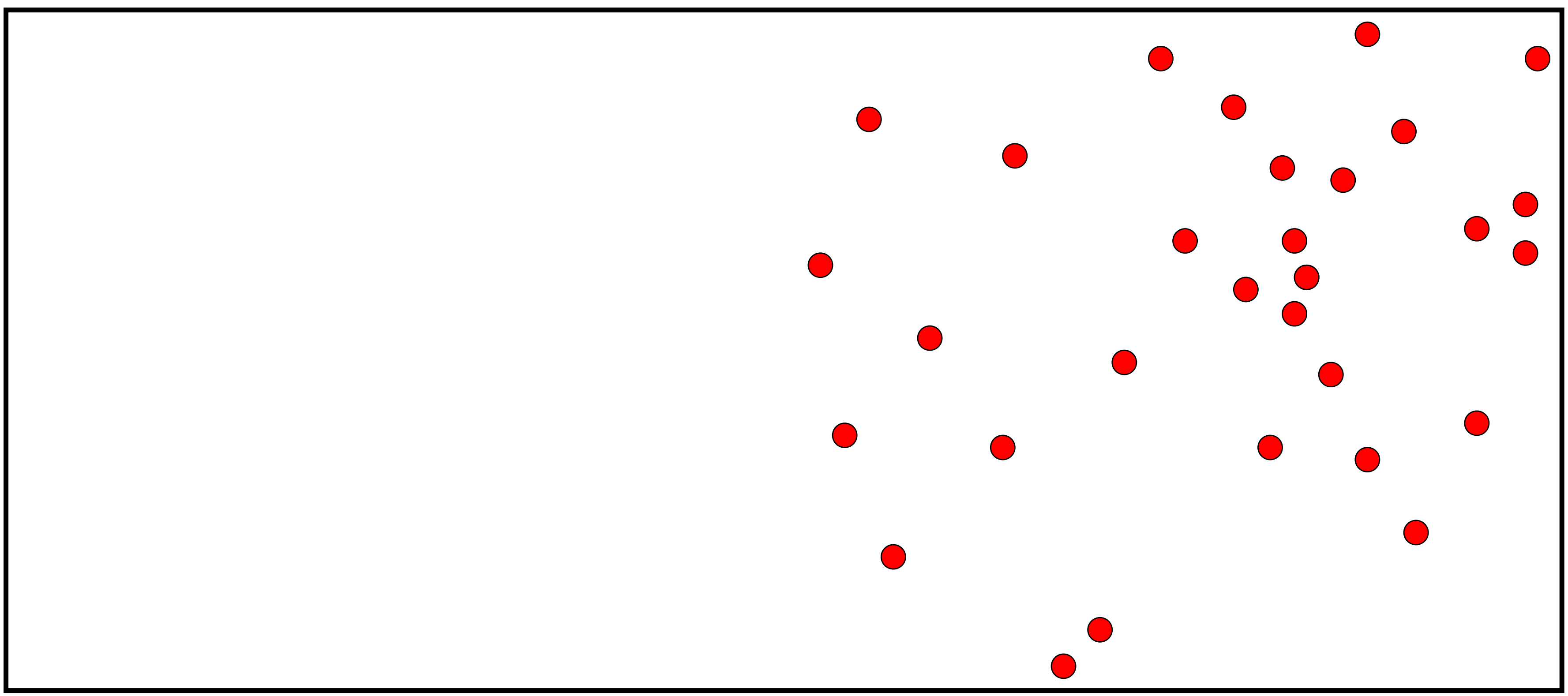

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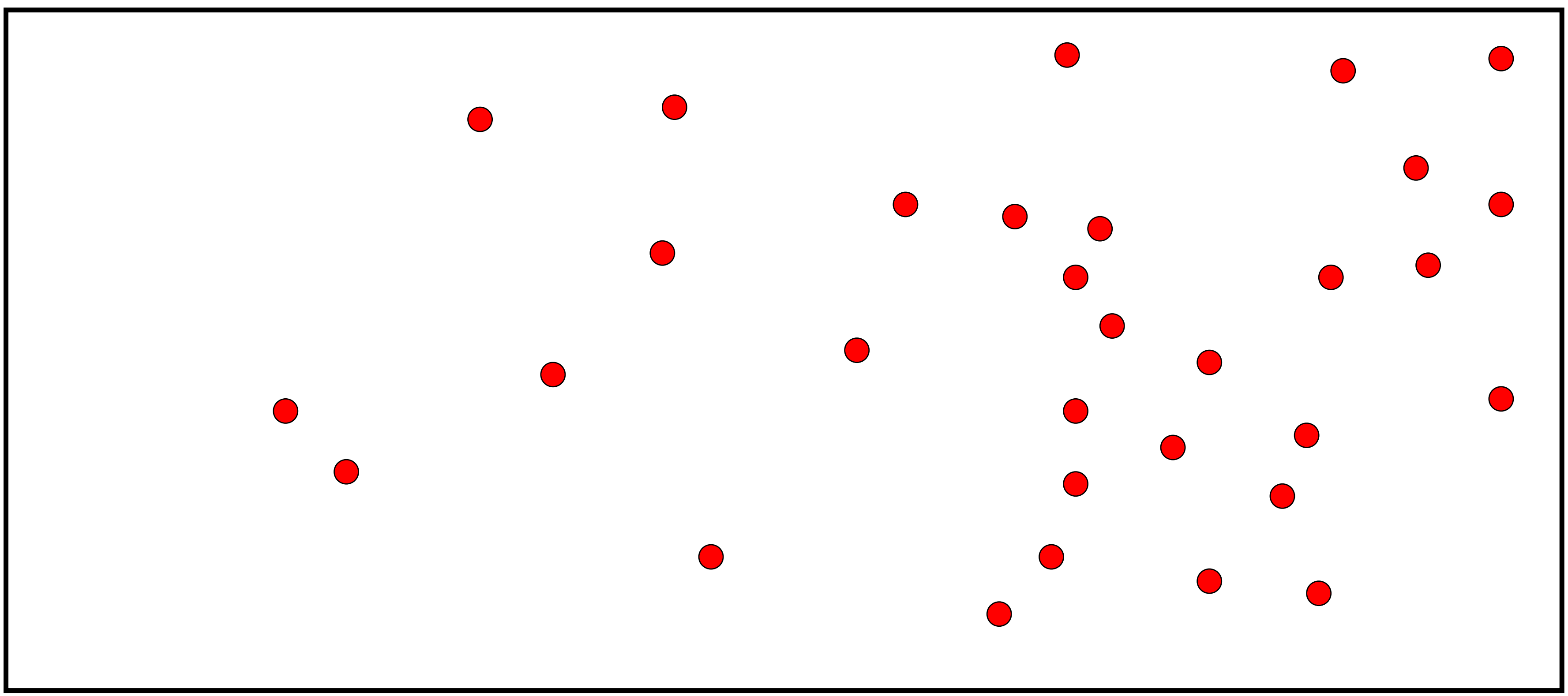

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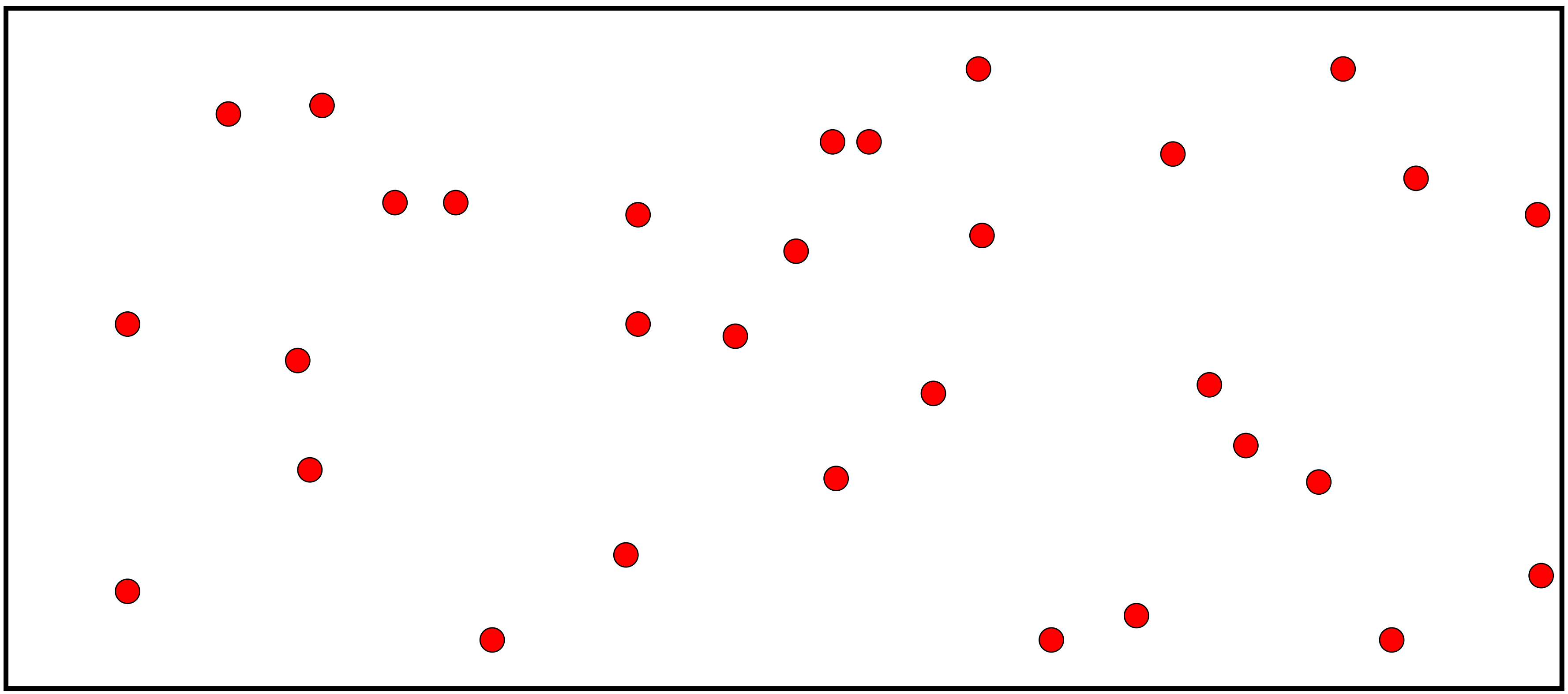

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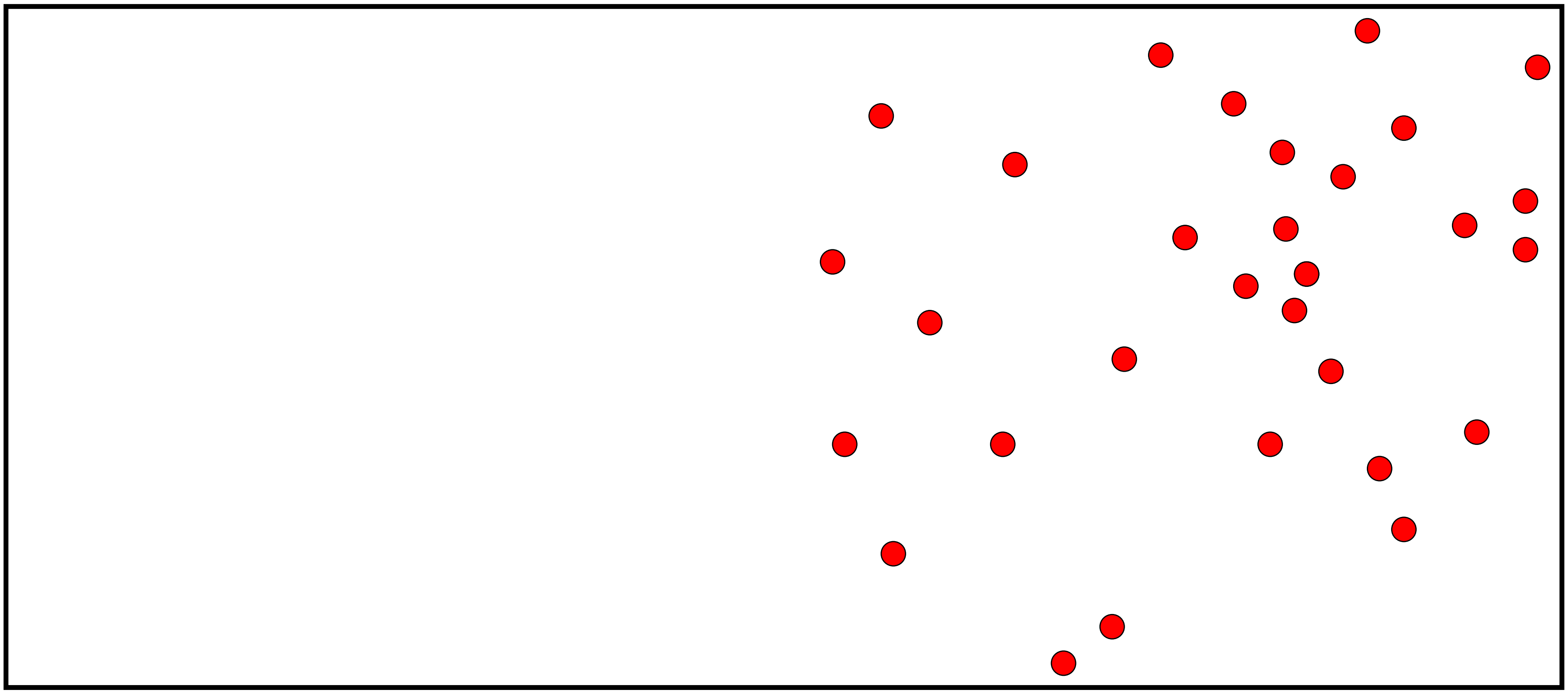

Power of combinatorics

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Gas in half-box $\Longrightarrow$ gas in whole box

Entropy goes up by $\log 2$, say $N = 10^{17}$

$\Longrightarrow$ Volume of microstates is $2^{10^{17}}$ times larger

$$\frac{\text{Vol of microstates in whole box}}{\text{Vol of microstates in half box}} \geq \left(\frac{\text{Vol of galaxy}}{\text{Vol of electron}}\right)^{200000000000000}$$

Loschmidt's paradox

At time t, reverse all velocities (entropy is preserved), start again (entropy increases) but go back to initial configuration (and initial entropy!)

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... Importance of the prepared starting state:

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... Subtleties of one-sided chaos

... Importance of the prepared starting state:

- low macroscopic entropy (unlikely observed state),
- high microscopic entropy (no initial correlations)

Loschmidt's paradox

At time t, reverse all velocities (entropy is preserved), start again (entropy increases) but go back to initial configuration (and initial entropy!)

Boltzmann: "Go on, reverse them!"

Later allowed by the spin echo experiment

... Subtleties of one-sided chaos

... Importance of the prepared starting state:

- low macroscopic entropy (unlikely observed state),
- high microscopic entropy (no initial correlations)

Knowing $\widehat{\mu}_0^N \simeq \mu_0, \quad \mu_0^{\otimes N}$ is the microscopic probability with maximum entropy (Cf. max likelihood)

Micro/macro (ir)reversibility

If there is macroscopic determinism:

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remain typical microstates at time t (profile μ_t)

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$$\boxed{\text{Microscopic reversibility} \Longrightarrow \text{macroscopic increase of entropy}}$$

... Microscopic irreversibility usually leads to nothing!!

Back to Boltzmann – Mathematicians chose their side

All of us younger mathematicians stood by Boltzmann's side.

Arnold Sommerfeld (about a 1895 debate)

Boltzmann's work on the principles of mechanics suggest the problem of developing mathematically the limiting processes (...) which lead from the atomistic view to the laws of motion of continua.

David Hilbert (1900)

Boltzmann summarized most (but not all) of his work in a two volume treatise *Vorlesungen über Gastheorie*. This is one of the greatest books in the history of exact sciences and the reader is strongly advised to consult it.

Mark Kac (1959)

Back to Boltzmann equation: Major PDE advance

Recall: The most important nonlinear models of classical mechanics have not been solved

(compressible and incompressible Euler, compressible and incompressible Navier–Stokes, Boltzmann, even Vlasov–Poisson to some extent)

But Boltzmann's H Theorem was the first qualitative estimate!

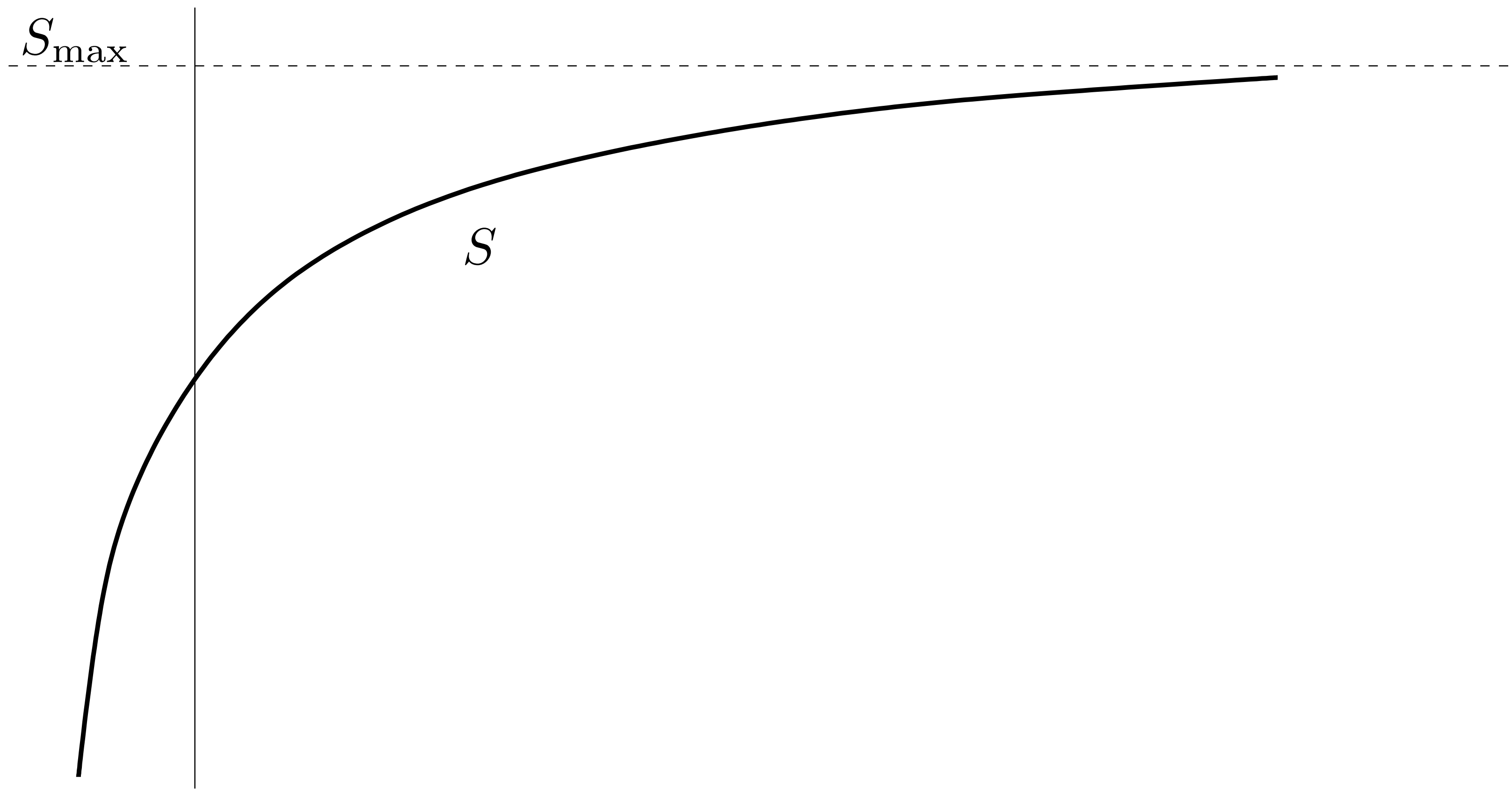
- Finiteness of the entropy production prevents clustering, providing compactness, crucial in the Arkeryd and DiPerna–Lions stability theories
- The H Theorem is the main "explanation" for the hydrodynamic approximation of the Boltzmann equation

Large-time behavior

The state of maximum entropy given the conservation of total mass and energy is a Gaussian distribution

... and this Gaussian distribution is the only one which prevents entropy from growing further

Plausible time-behavior of the entropy



If this is true, then f becomes Gaussian as $t \to \infty$!

What do we want to prove?

Prove that a “nice” solution of the Boltzmann equation approaches Gaussian equilibrium: short and easy (basically Boltzmann’s argument)

Get quantitative estimates like “After a time ....., the distribution is close to Gaussian, up to an error of 1 %”: tricky and long (1989–2004 starting with Cercignani, Desvillettes, Carlen–Carvalho)

One big problem: degeneracy: If the distribution becomes hydrodynamical but not homogeneous then entropy production vanishes although not at equilibrium!

Conditional convergence theorem (Desvillettes – V)

Let $f(t,x,v)$ be a solution of the Boltzmann equation, with appropriate boundary conditions. **Assume** that

(i) f is very regular (uniformly in time): all moments ($\int f|v|^k\,dv\,dx$) are finite and all derivatives (of any order) are bounded;

(ii) f is strictly positive: $f(t,x,v) \geq K e^{-A|v|^q}$.

Then $f(t) \longrightarrow f_\infty$ at least like $O(t^{-\infty})$ as $t \to \infty$

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- Regularity assumptions can be weakened
- Gualdani–Mischler–Mouhot complemented this with a rate $O(e^{-\lambda t})$ for hard spheres

The proof uses differential inequalities of first and second order, coupled via many inequalities including:

- precised entropy production inequalities (information theoretical input)

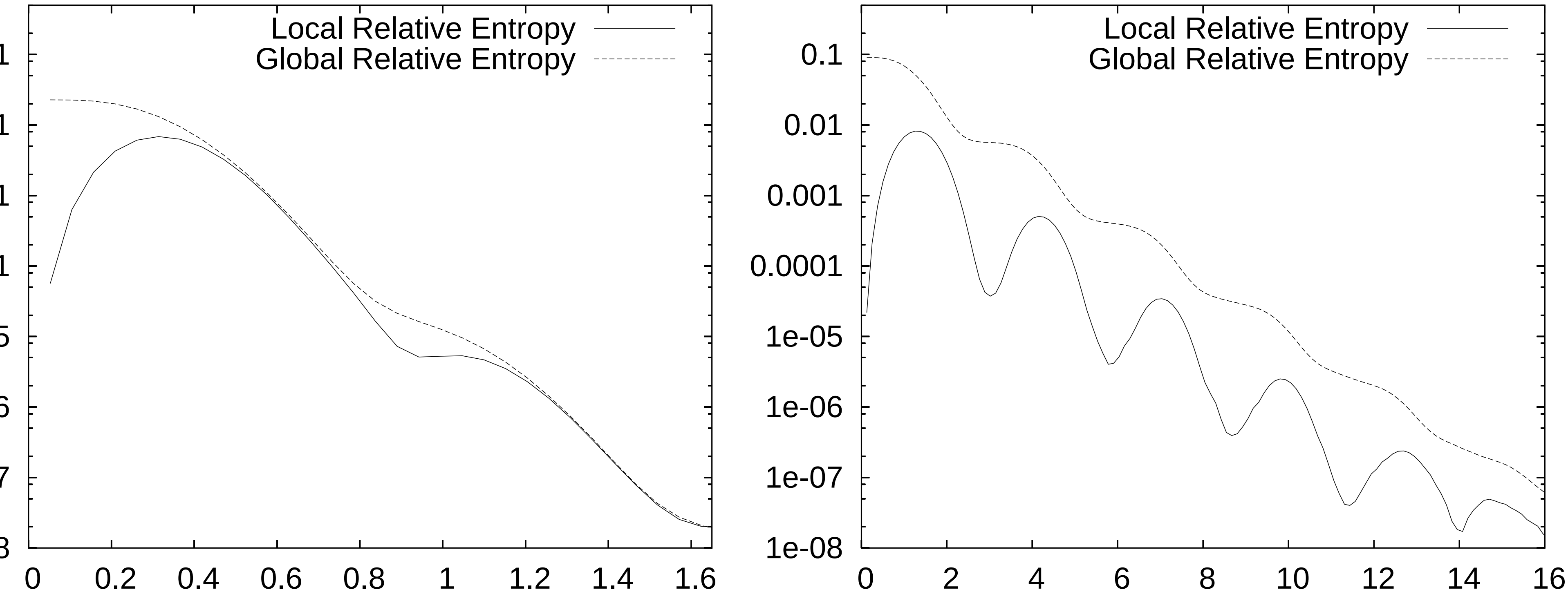
- Instability of hydrodynamical description (fluid mechanics input).

- decomposition of entropy in kinetic and hydrodynamic parts

- functional inequalities coming from various fields (information theory, quantum field theory, elasticity theory, etc.)

It led to the discovery of oscillations in the entropy production

Numerical simulations by Filbet



These oscillations of the entropy production slow down the convergence to equilibrium (fluid mechanics effect)

and are related to current research on the convergence for nonsymmetric degenerate operators ("**hypocoercivity**")

Other quantitative use of entropy a priori estimates

- Instrumental in Nash's proof of continuity of solutions of linear diffusion equations with nonsmooth coefficients

- Allowed Perelman to prove the Poincaré conjecture

- Used by Varadhan and coworkers/students for (infinite-dimensional) hydrodynamic problems

- Basis for the construction of the heat equation in metric-measure spaces (... Otto ... V ... Savaré, Gigli ...)

- ...

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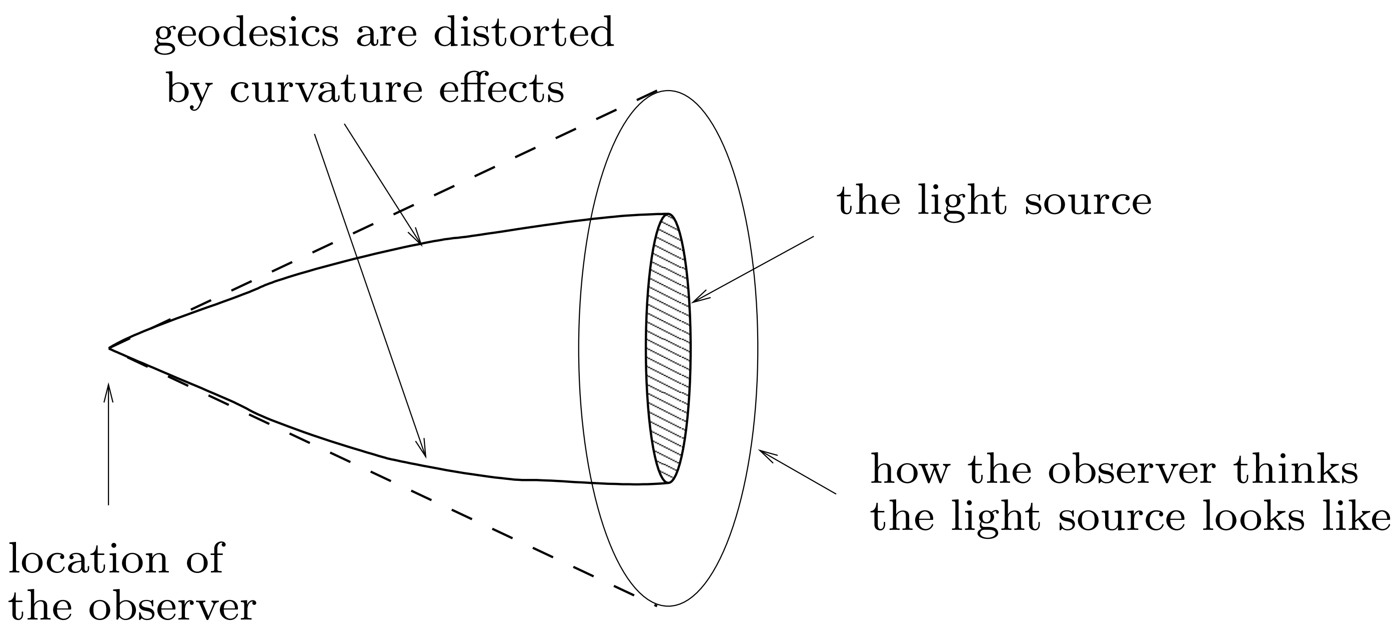
A final example of universality of entropy: Ricci curvature

Distortion interpretation of Ricci



Because of positive curvature effects, the observer overestimates the surface of the light source; in a negatively curved world this would be the contrary.

$$[\,\text{Distortion coefficients always} \geq 1\,] \quad \Longleftrightarrow \quad [\,\mathrm{Ric} \geq 0\,]$$

The lazy gas experiment (Otto.... Lott–Sturm–Villani)

Describes the link between Ricci, optimal transport and entropy