Statistical mechanics as a paradigm for complex systems
Motivation, foundations and limitations

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Onthology droplet
São Paulo, January 2014

A little history

Target: matter = system with huge number of components
Order: Avogadro number

$$6.02 \cdot 10^{23} \quad \sim \quad \text{\# molecules in 1 cubic inch of water}$$
$$\sim \quad 10 \cdot \text{\# grains of sand in the Sahara}$$

(c.f. brain = 10^{10} neurons)

Two observational levels:

▶ Microscopic: laws followed by the different components

▶ Macroscopic: laws followed by "bulk" matter

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Complex microscopic laws:

- ▶ Complex interaction processes, in fact not totally known
- ▶ Processes involving a huge number of degrees of freedom

Simple equilibrium macroscopic description:

- ▶ Few variables suffice: P, V, T, composition, ...
- ▶ Variables related by a simple equation of state: e.g.

$$PV = nRT$$

Macroscopic state: Specification of P, V, T, composition, ...

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Macroscopic transformations

Simple and efficient description:

- ▶ Two state functions:
  - ▶ internal energy
  - ▶ entropy
  - ▶ By Legendre transform enthalpy, free energy
- ▶ Two laws (*thermodynamic laws*)
  - ▶ Conservation of energy (heat = energy)
  - ▶ Non decrease of entropy (closed system)

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Dramatic changes at *very precise* values of P, V, T, ...

Different types:

- ▶ *First order:* Coexistence of more than one state (=phases)
- ▶ *Second order:* Large fluctuations

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Explain

- ▶ Transition complex micro → simple macro
- ▶ Thermodynamic laws
    - ▶ What is entropy?
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The tenets

Detailed micro description: unfeasible (too much, too long)

Solution? **Stochastic description**

- ▶ Microscopic state = **probability distribution** (measure)
- ▶ Macroscopic simplicity: $0 - 1$ laws, ergodic theory
- ▶ Entropy?
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Which measure?

Boltzmann!

- ▶ Closed system:
  - ▶ equiprobable configurations (respecting conservation laws)
  - ▶ Explains entropy: Boltzmann formula
- ▶ Small box inside a large closed system (reservoir)
  - ▶ probability $\sim e^{-E/T}$
  - ▶ T = temperature (fixed by reservoir)
  - ▶ E = energy = Hamiltonian
  - ▶ E must be sum of terms involving few components each

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To explain phase transitions:

► Must consider exterior conditions to the box

► At zero degrees:

  ► Exterior ice → interior ice

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► Boltmann prescription + limits with boundary conditions:

Gibbs measures

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Advantages of Gibbsianness

Gibbs measures explain thermodynamics

Furthermore, they have several mathematical advantages:

- ▶ Parametrized by a few constants (couplings)
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Limitations of Gibbsianness

- ▶ Gibbs measures are *designed to describe equilibrium*
- ▶ No guarantee of applicability in evolutions
- ▶ A limit state of an evolution need not be Gibbs
- ▶ Gibsianness can be destroyed by
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  - ▶ Change of observational scale
  - ▶ Projections
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