Metastability for Interacting Particle Systems

– Introduction –

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§ WHAT IS METASTABILITY?

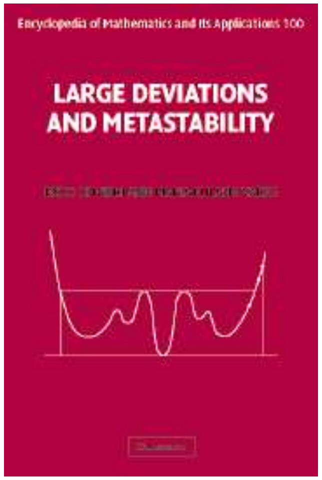
Metastability is the phenomenon where a system, under the influence of a stochastic dynamics, undergoes slow transitions between different phases. It is observed in a variety of physical, chemical and biological settings.

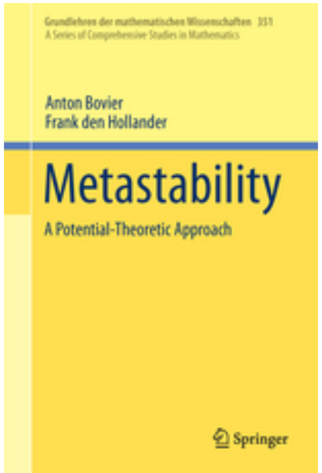
The challenge is to propose mathematical models and to explain the experimentally observed universality.

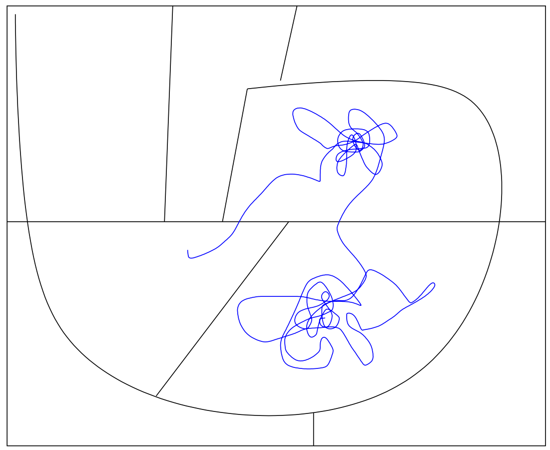
MONOGRAPHS:

Olivieri, Vares 2005

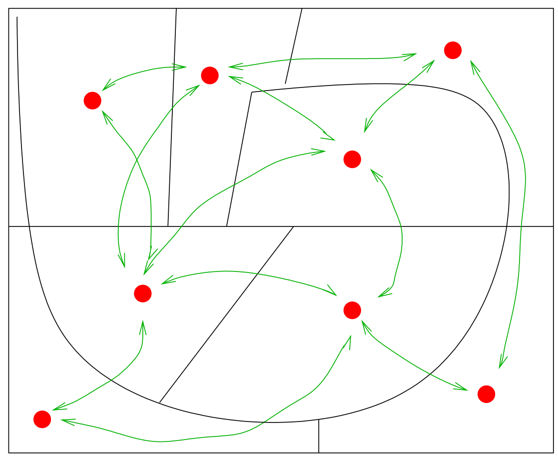
Bovier, den Hollander 2015







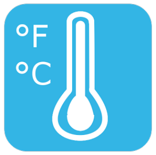
Fast transitions within phases.



Slow transitions between phases.

§ METASTABILITY IN STATISTICAL PHYSICS

Within the narrower perspective of statistical physics, the phenomenon of metastability is a dynamical manifestation of a first-order phase transition. A well-known example is condensation:

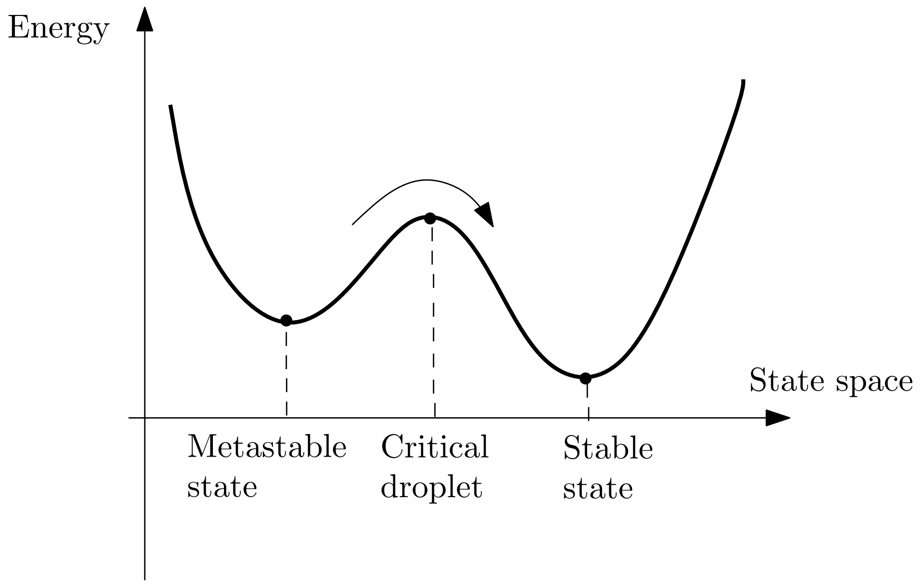


When a vapour is cooled down slowly, it persists for a long time in a metastable vapour state, before transiting to a stable liquid state under the influence of random fluctuations.

The crossover occurs after the system manages to create a critical droplet of liquid inside the vapour, which once present grows and invades the whole system.

While in the metastable vapour state, the system makes many unsuccessful attempts to form a critical droplet.

PARADIGM PICTURE:



metastable crossover: super-saturated vapour

metastable crossover: super-cooled water

metastable crossover: snow avalanche

Statistical physics has been very successful in describing discrete particle systems. Over the years a broad and deep understanding of critical phenomena has emerged:

spin-flip systems
particle-hop systems
cellular automata
...

Much less is known for continuous particle systems, which are very hard to analyse. In fact, a rigorous proof of the presence of a phase transition has so far been achieved for very few models only.

§ HISTORICAL PERSPECTIVE

Early work on metastability was done by van 't Hoff and Arrhenius in the 1880s, to develop a theory for chemical reaction rates. Mathematically, metastability took off with the work of Kramers in the 1940s.

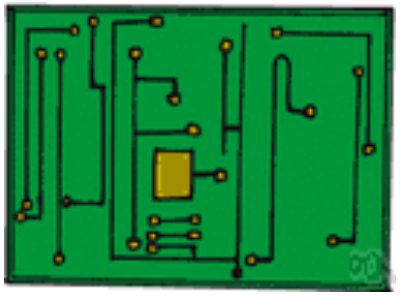
Since then, various approaches to metastability have been developed, with different pros and cons.

Lebowitz, Penrose	1960–1970	van der Waals
Freidlin, Wentzell	1960–1970	SDE
Cassandro, Galves, Olivieri, Vares	1980–1985	path LDP
Davies	1980–1985	spectra

§ POTENTIAL-THEORETIC APPROACH TO METASTABILITY

Bovier, Eckhoff, Gayrard, Klein 2000

Bovier, den Hollander 2015



With the help of potential theory, the problem of how to understand metastability of Markov processes translates into the study of capacities in electric networks.

Dictionary:

state	$\longrightarrow$	node
transition	$\longrightarrow$	edge
rate	$\longrightarrow$	conductance
hitting time	$\longrightarrow$	effective resistance

INTERACTING PARTICLE SYSTEMS:

We think of an interacting particle system whose state space consists of a finite set of configurations Ω and whose evolution is given by a Markov generator L acting on a class of test functions $\phi\colon\ \Omega \to \mathbb{R}$.

The dynamics is assumed to have a reversible equilibrium given by a Gibbs measure

$$\mu(\eta) = \frac{1}{\Xi}\, \mathrm{e}^{-\beta H(\eta)} \mathcal{Q}(\eta), \qquad \eta \in \Omega,$$

where Ξ, β, H and $\mathcal{Q}$ have the following interpretation:

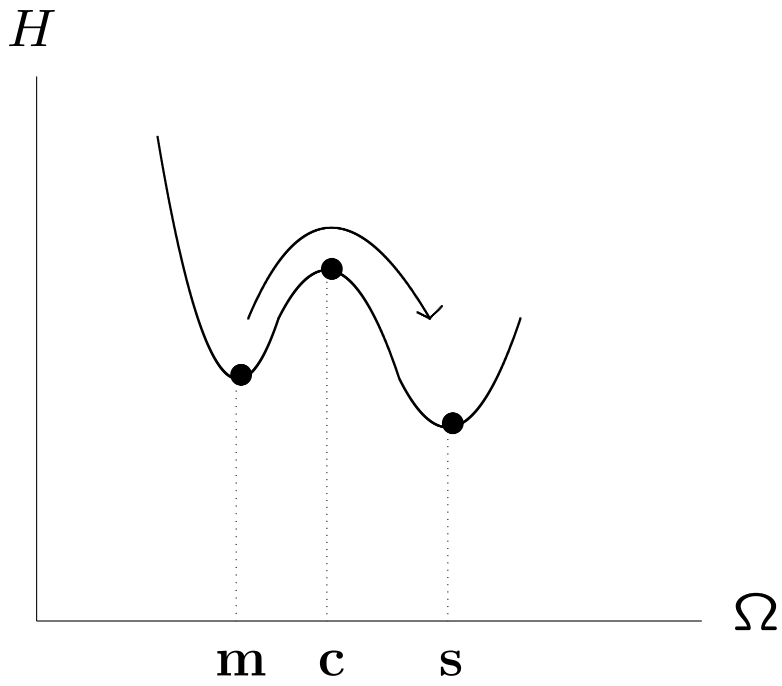
- $H \colon \Omega \to \mathbb{R}$ is the Hamiltonian that associates with each configuration η an energy $H(\eta)$.
- $\beta \in (0, \infty)$ is the inverse temperature (= interaction strength).
- $\mathcal{Q}$ is the reference measure on Ω.
- Ξ is the normalising partition function.

The proper choice of Ω, H, β and $\mathcal{Q}$ depends on the model at hand. For $\beta \to \infty$ we may expect to see metastability under certain conditions.

metastable regime

Typically, the Hamiltonian H has three important sets of configurations:

- Global minimum $\mathbf{s}$: stable state.
- Local minimum $\mathbf{m}$: metastable state.
  (= bottom of the deepest valley not containing $\mathbf{s}$).
- Saddle point $\mathbf{c}$: critical droplet.
  (= ridge between the valleys containing $\mathbf{m}$ and $\mathbf{s}$).



Caricature of the energy lanscape.

Examples of dynamics:

spin-flip systems
particle-hop systems
cellular automata
. . .

If $\mathbf{m}$ is a single configuration, then the average metastable crossover time from $\mathbf{m}$ to $\mathbf{s}$ is given by

$$\boxed{E_{\mathbf{m}}(\tau_{\mathbf{s}}) = \frac{\sum_{\eta \in \Omega} \mu(\eta)\, h_{\mathbf{m},\mathbf{s}}(\eta)}{\mathrm{cap}(\mathbf{m},\mathbf{s})}}$$

EXERCISE!

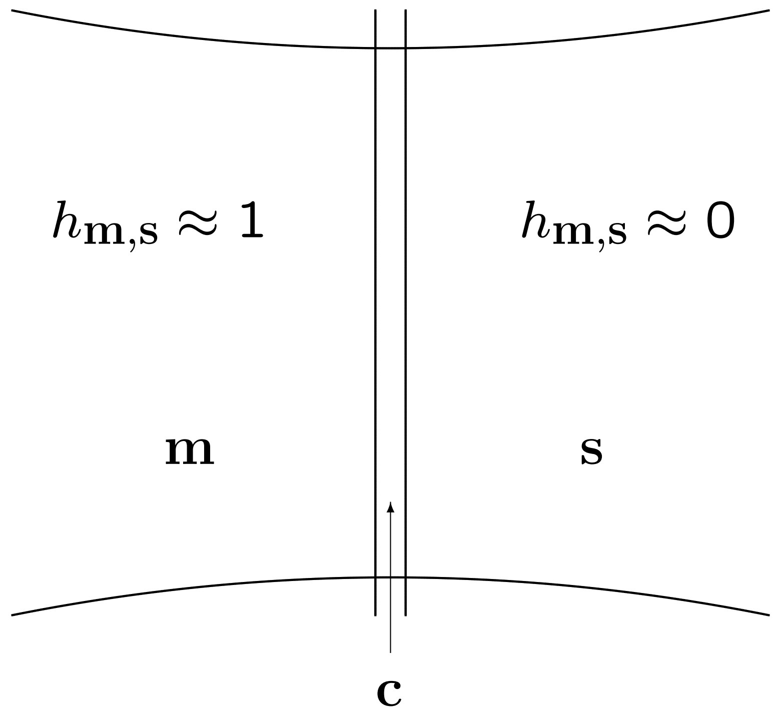
where

$$h_{\mathbf{m},\mathbf{s}}(\eta) = P_\eta(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}), \qquad \eta \in \Omega,$$

is the harmonic function and

$$\mathrm{cap}(\mathbf{m},\mathbf{s}) = \sum_{\eta \in \mathbf{m}} \mu(\eta)(-L h_{\mathbf{m},\mathbf{s}})(\eta)$$

is the capacity, with L the generator of the underlying Markov dynamics.



Schematic picture of the harmonic function $h_{\mathbf{m},\mathbf{s}}$:

trivial inside the valleys around $\mathbf{m}$ and $\mathbf{s}$, nontrivial around $\mathbf{c}$.

In metastable regimes it often turns out that

$$\sum_{\eta \in \Omega} \mu(\eta)\, h_{\mathbf{m},\mathbf{s}}(\eta) = [1 + o(1)]\, \mu(\mathbf{m})$$

in which case

$$E_{\mathbf{m}}(\tau_{\mathbf{s}}) = [1 + o(1)]\, \frac{\mathrm{e}^{-\beta H(\mathbf{m})}}{\Xi\, \mathrm{cap}(\mathbf{m}, \mathbf{s})}.$$

This formula shows that the average metastable crossover time is essentially controlled by the capacity, which in turn is essentially controlled by the harmonic function near the critical set.

§ DIRICHLET PRINCIPLE

The capacity of $\mathbf{m}, \mathbf{s}$ is given by the Dirichlet Principle

$$\boxed{\text{cap}(\mathbf{m}, \mathbf{s}) = \inf_{\phi \in \Phi_{\mathbf{m},\mathbf{s}}} \mathcal{E}(\phi, \phi)}$$

where

$$\Phi_{\mathbf{m},\mathbf{s}} = \{\phi\colon\ \Omega \to [0, 1]\colon\ \phi(\mathbf{m}) = 1,\ \phi(\mathbf{s}) = 0\}$$

and

$$\mathcal{E}(\phi, \phi) = \sum_{\eta, \eta' \in \Omega} \mu(\eta) c(\eta, \eta') [\phi(\eta') - \phi(\eta)]^2$$

is the Dirichlet form associated with the dynamics. Here, $c(\eta, \eta')$ represents the rate at which the dynamics moves from η to η'.

§ THOMSON PRINCIPLE

A unit flow from $\mathbf{m}$ to $\mathbf{s}$ is a map $u\colon \Omega \times \Omega \to \mathbb{R}$ such that the flows into and out of nodes in $\Omega \setminus \{\mathbf{m}, \mathbf{s}\}$ equal 0, while the flows out of node $\mathbf{m}$ and into node $\mathbf{s}$ equal 1.

The Thomson Principle reads

$$\boxed{\text{cap}(\mathbf{m}, \mathbf{s}) = \sup_{u \in \mathcal{U}_{\mathbf{m},\mathbf{s}}} \frac{1}{\mathcal{D}(u,u)}}$$

where $\mathcal{U}_{\mathbf{m},\mathbf{s}}$ is the set of unit flows from $\mathbf{m}$ to $\mathbf{s}$, and

$$\mathcal{D}(u,u) = \sum_{\eta,\eta' \in \Omega} \frac{1}{\mu(\eta) c(\eta,\eta')} u(\eta,\eta')^2$$

is a dual of the Dirichlet form.

§ CAPACITY ESTIMATES

The estimation of capacity proceeds via

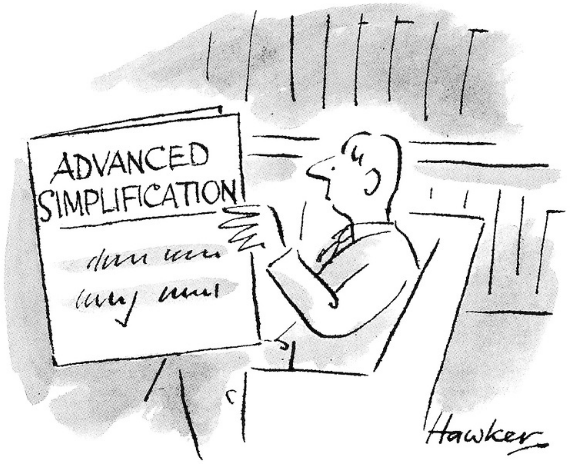
- Dirichlet principle:
  cap$(\mathbf{m},\mathbf{s}) \leq \mathcal{E}(\phi,\phi)$,

- Thomson principle:
  cap$(\mathbf{m},\mathbf{s}) \geq 1/\mathcal{D}(u,u)$,

where ϕ, u are properly chosen test functions and test flows that live in the vicinity of the critical droplet.

The choice of ϕ, u requires physical insight into what drives the metastable crossover.

The key idea is that in metastable regimes the high-dimensional Dirichlet form and dual Dirichlet form are largely controlled by the low-dimensional set of critical droplets.



GUIDING PRINCIPLE:

The formula relating metastable crossover time to capacity effectively links non-equilibrium to equilibrium. The inverse of the capacity plays the role of effective resistance.

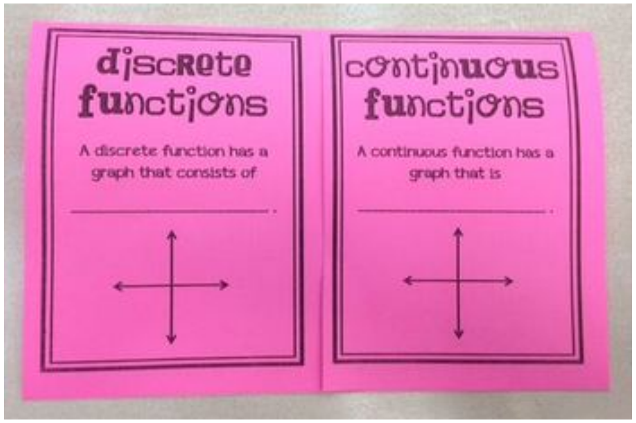
ASYMPTOTICS:

The Dirichlet Principle and Thomson Principle allow for the derivation of upper and lower bounds on capacity. With care, these can be made to match asymptotically.

§ DICRETE VERSUS CONTINUOUS

Definitions and computations become more involved when the state space Ω is infinite discrete or continuous.

Often $\mathbf{m}$, $\mathbf{c}$ and $\mathbf{s}$ are not single configurations but are sets of configurations with an interesting geometric structure.



OUTLINE

- Lecture1:
  Kawasaki dynamics on lattices.

- Lecture 2:
  Glauber dynamics on random graphs.

- Lecture 3:
  Widom-Rowlinson dynamics on the continuum.

firework ahead