1. Large Deviations and Population Dynamics

Unusual time averages

We ask for the probability that it sustains an unusual time-average for an observable during a long interval:

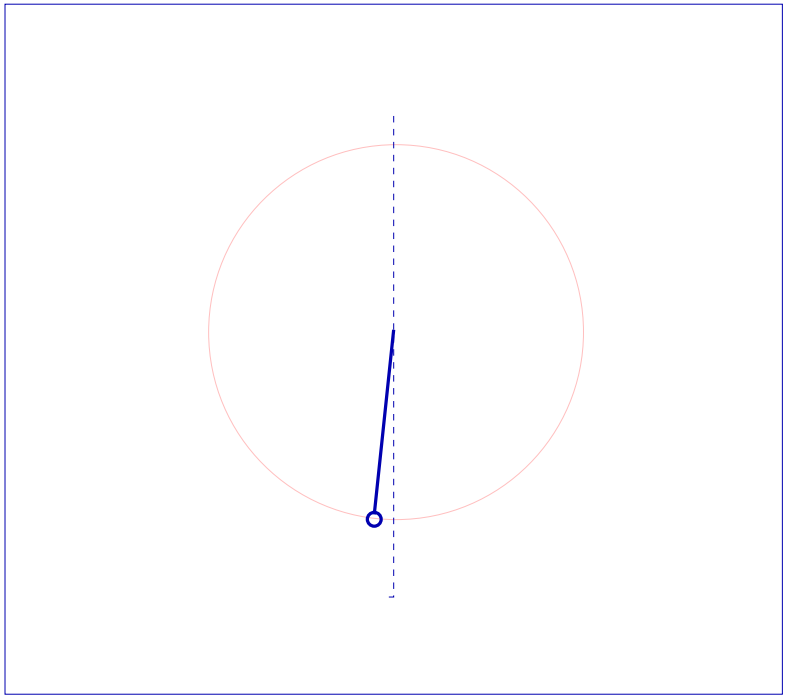
$$\frac{1}{t}\int dt'\ A(t') = \overline{A}$$

The most celebrated example is the average power, which can be interpreted in some cases as entropy production:

$$\sigma_t = -\frac{1}{t}\int_0^t dt'\ \frac{\mathbf{f}\dot{\mathbf{q}}}{T}$$

$$P(A) = \sum_{\text{Trajec.}} (\text{Prob. Trajectory})\,\delta\left(t\overline{A} - \int_o^t dt'\ A(t')\right)$$

a pendulum immersed in a low-temperature bath



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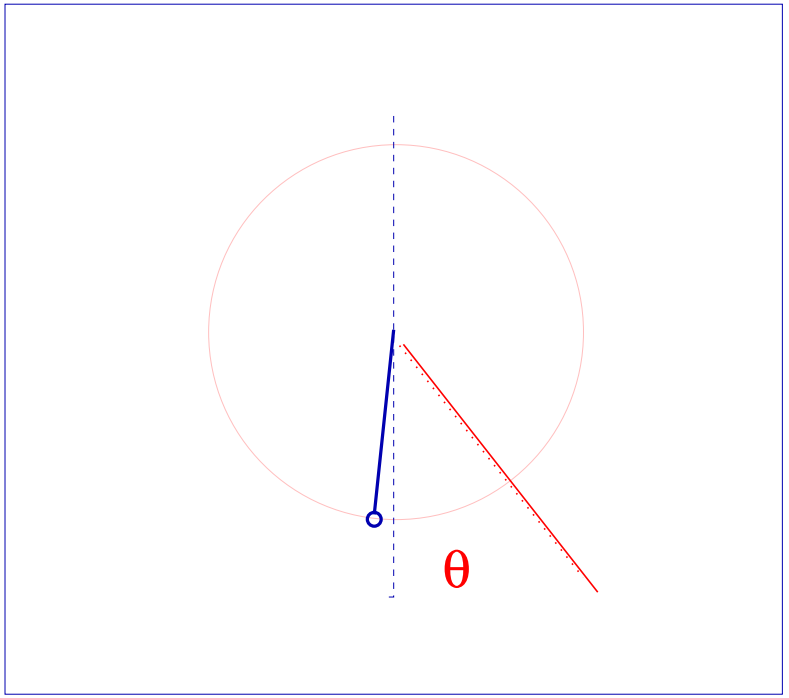
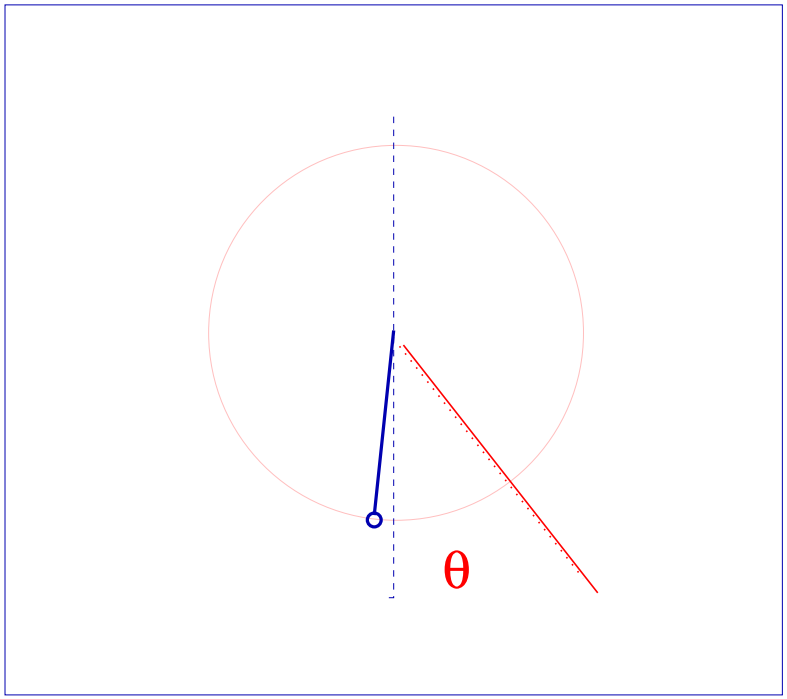
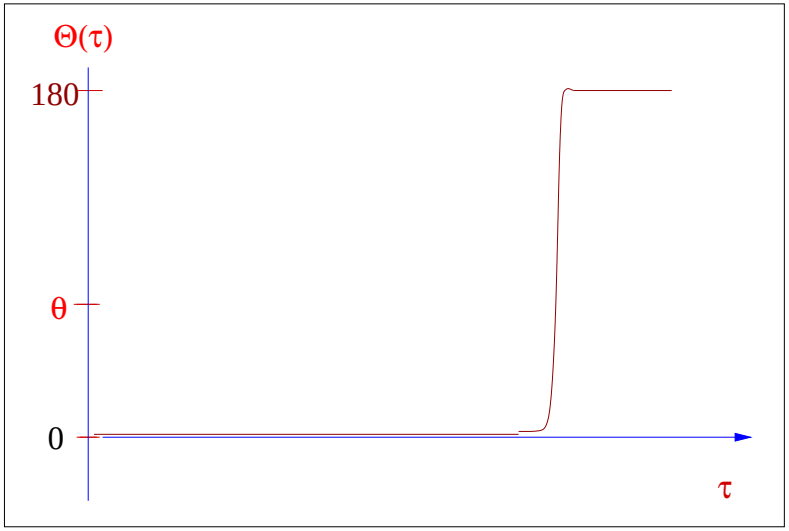


and ask: *given* that during a specific minute the average angle took the value θ

***i)* what is the probability of this?** ***ii)* how does this come about?**



Imposing the average angle, the trajectory shares its time between saddles 0° and 180°



phase-separation, a first order transition!

Consider a process:

$$\frac{dP(q,t)}{dt} = -LP(q,t)$$

$$P(\mathbf{q_o}, t_o \to \mathbf{q}, t) \qquad = e^{-Lt}P(q,0) = \int D[q] \quad \text{(Prob. Trajectory)}$$

$$= \int D[q]\, e^{-\mathcal{L}_t(trajectory)}$$

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Writing the delta function as an exponential

$$\delta\left(t\overline{A} - \int_o^t dt'\ A(t')\right) = \int_{-i\infty}^{+i\infty} d\mu\ e^{\mu\left(t\overline{A} - \int_o^t\ dt'\ A(t')\right)}$$

$$\begin{aligned} P(A) &= \int_{-i\infty}^{+i\infty} d\mu\ e^{\mu t\overline{A}} \underbrace{\int D[\mathbf{q}]\ \text{(Prob. Trajectory)}\, e^{-\mu\int_o^t\ dt'\ A(t')}}_{\downarrow} \\ &= \int_{-i\infty}^{+i\infty} d\mu\ e^{\mu t\overline{A}} \times\ e^{-tG(\mu)} \end{aligned}$$

which defines the large-deviation function $G(\mu)$.

For example, in the Fokker-Planck case, it reads:

$$e^{-tG(\mu)} = \int D[\mathbf{q}] \;\; e^{\int dt' \; \left[\sum_i -\mathcal{L} - \mu \int_o^t \; dt' \; A(t')\right]}$$

What we have done is nothing but the analogue of a passage from a microcanonical calculation of 'entropy' $= \ln \bar{A}$, to a canonical calculation of 'free energy' $G(\mu)/\mu$ at 'inverse temperature' μ. The 'space' in our problem is in fact the time, and 'extensive quantities' are those that are proportional to time: we extracted a time in the definition of $G(\mu)$ in order to make it 'intensive'.

For large t, in analogy with the thermodynamic limit, assuming that $G(\mu)$ has a good limit, we may evaluate the integral over μ by saddle point, to obtain:

$$\ln P(A) \sim t[\mu^* A - G(\mu^*)]$$

$$A(\mu^*) = \left.\frac{dG}{d\mu}\right|_{\mu^*}$$

This is the Legendre transform taking from canonical to microcanonical.
Now, by simple comparison, operator language:

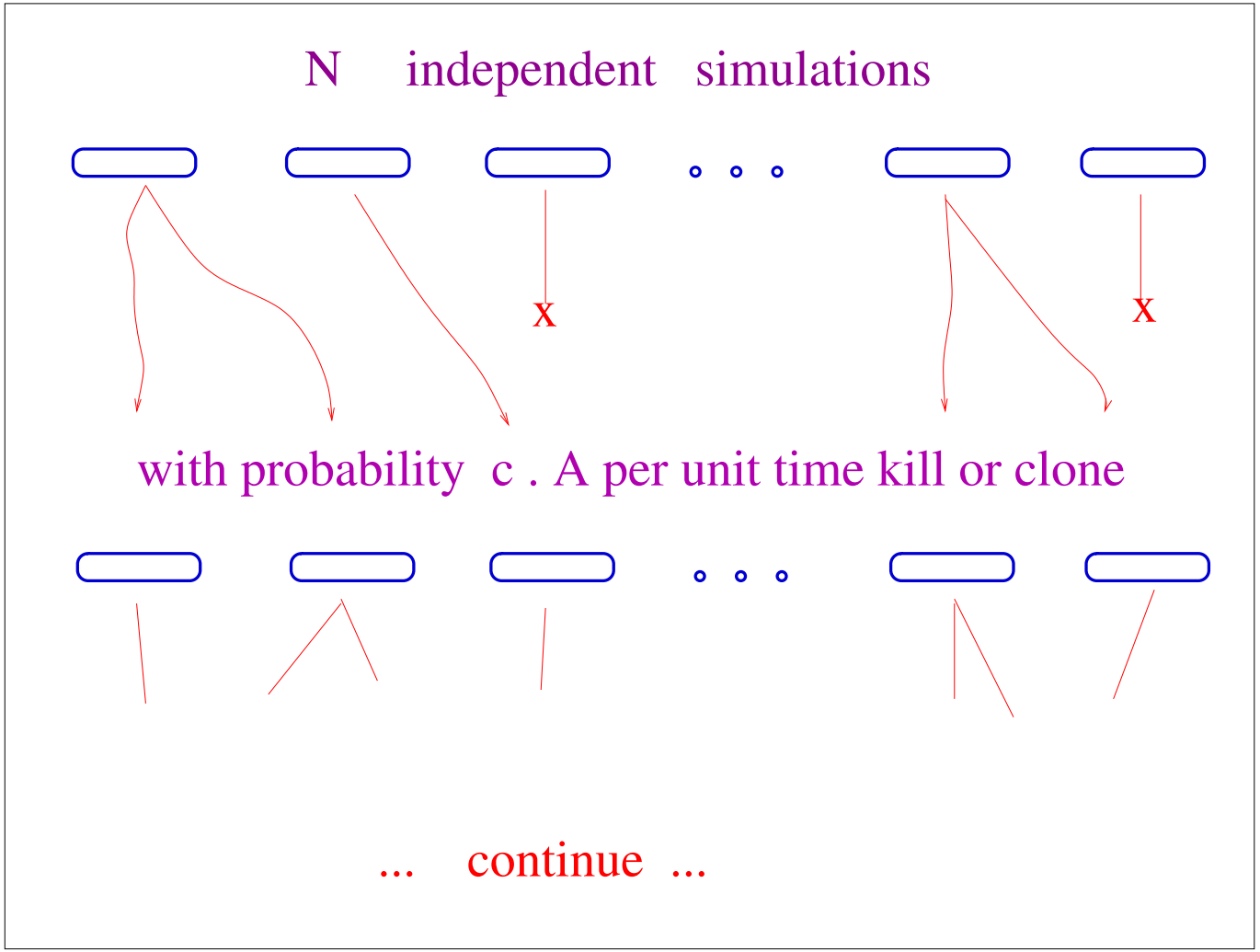
$$e^{-tG(\mu)} = \langle final | e^{-t[L+\mu A(\mathbf{q})]} | init \rangle$$

Note the fundamental difference between this large-deviation functions and those of Friedlin-Wentzell: in that case by 'large' deviations we meant that they are exponentially small in the temperature (or the coarse-graining size) while here we mean that they are sustained for long times, and the only large parameter is precisely the time t.

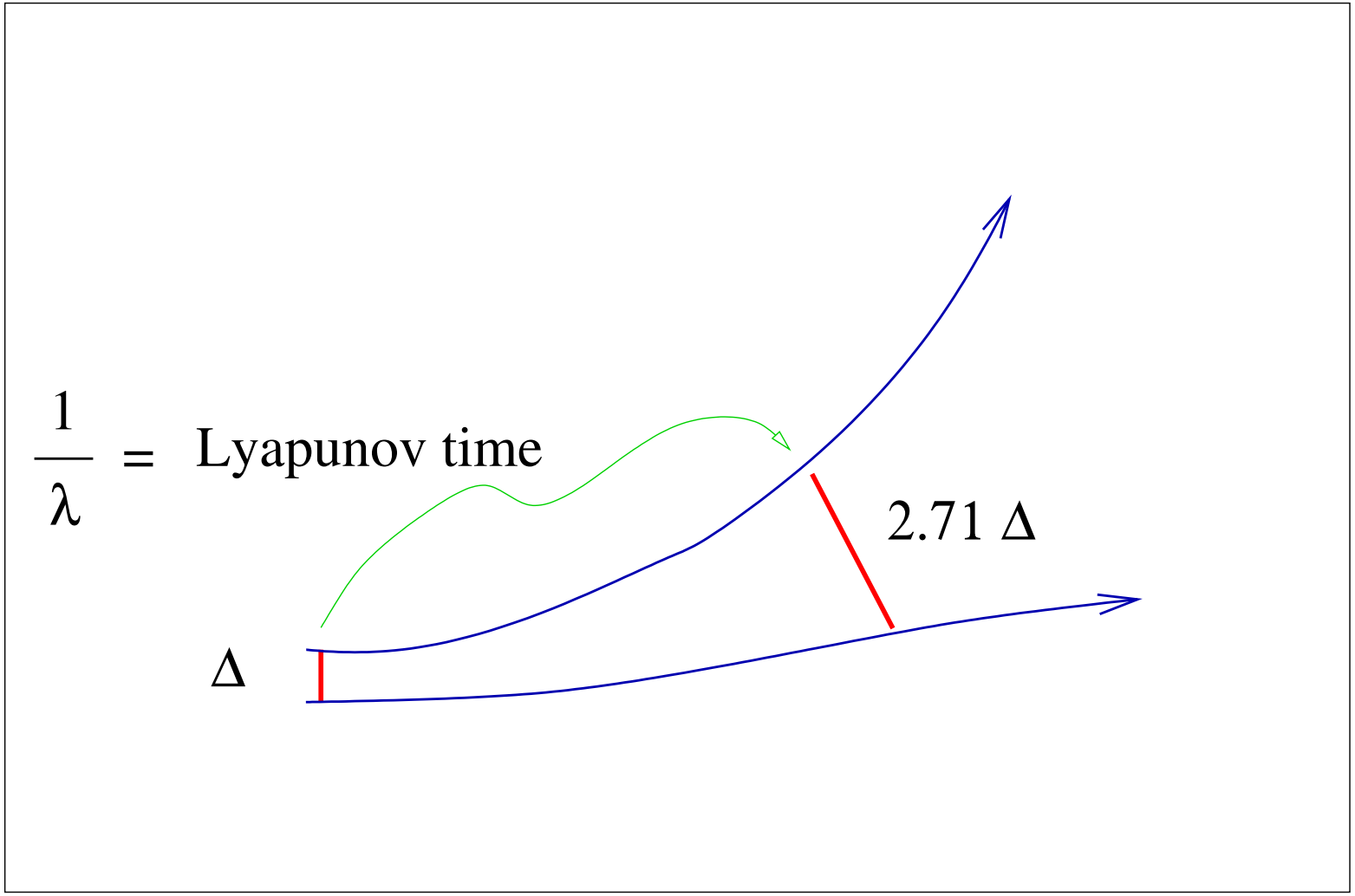
Simulating large deviations – relation with selection

$$\dot{P} = -[L + \mu A]P \quad \rightarrow P(\mathbf{q}, t) = e^{-t[L+\mu A]}$$

We are dealing with a dynamics without probability conservation. In fact, we can reproduce it by using a large number of non-interacting walkers, each performing the original (Langevin) dynamics with independent noises, occasionally giving birth to another walker starting in the same place, or dying. A negative (positive) value of $\mu A(\mathbf{q})$ gives a probability $|\mu A(\mathbf{q})|dt$ of making a clone or of dying, respectively, in a time-interval dt. At each time, the global number of clones $M(t)$ changes, in such a way that for long times $M(t)/M(t=0) \sim e^{-\lambda_{min}(\mu)t}$. In practice, one can normalise the total number periodically by cloning or decimating all walkers with a random factor. The factor needed to keep the population constant is, again, the exponential of the lowest eigenvalue.



a way to count trajectories weighted with e^{cA}

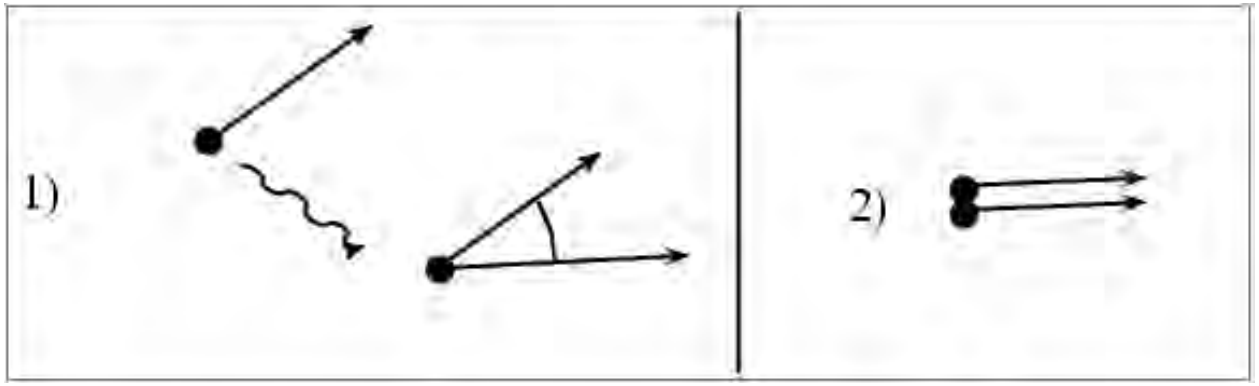


Trajectories with rare values of Lyapunov exponents: vector process

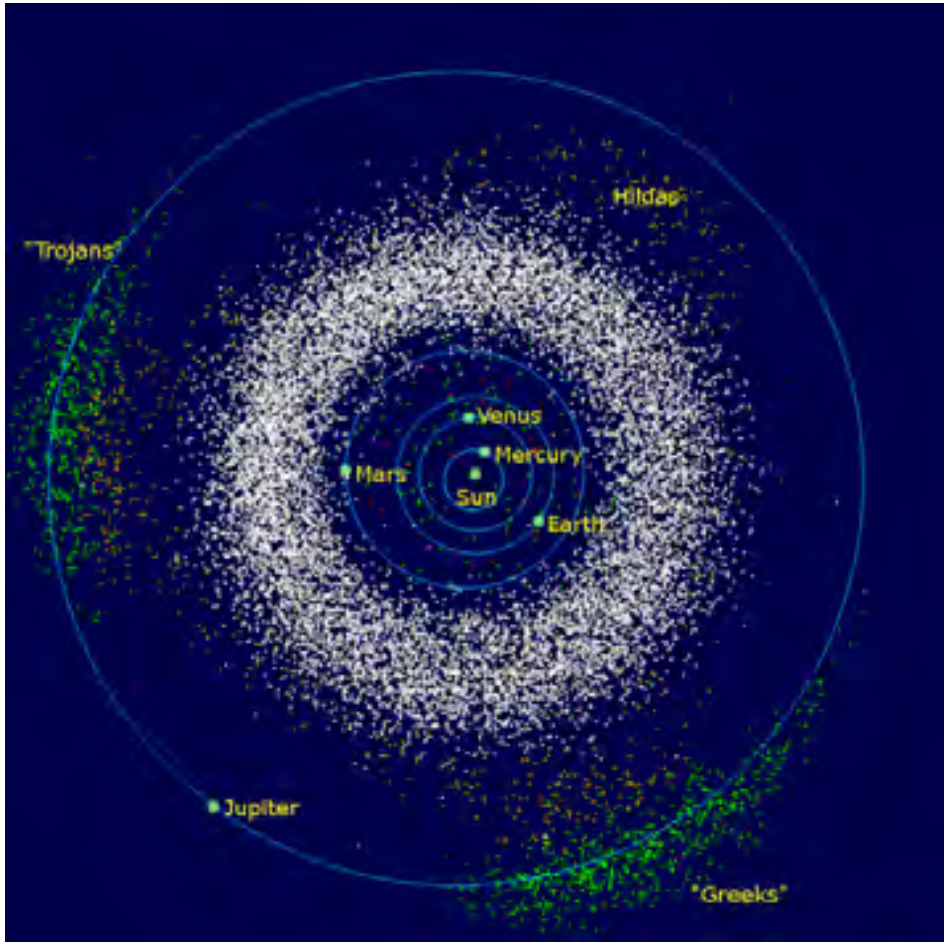
à la Diffusion Monte Carlo: particles have a vector $\vec{u}$ attached, which evolves with

$$\dot{u}_i = -\frac{\partial^2 V}{\partial x_i x_j} u_j$$

Particles perform ordinary diffusion + cloning $\propto \frac{d|u|}{dt}$

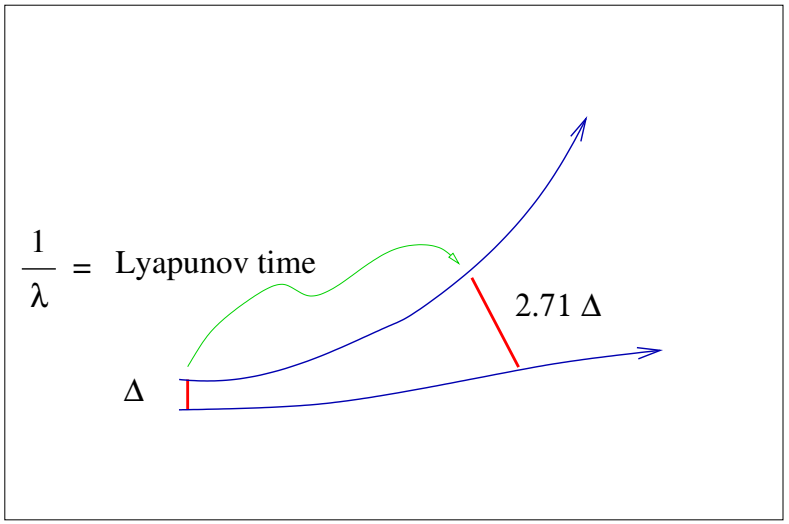


2. Large Deviations: an Advertisement



because planets disturb one another, the dynamics is chaotic

chaotic?

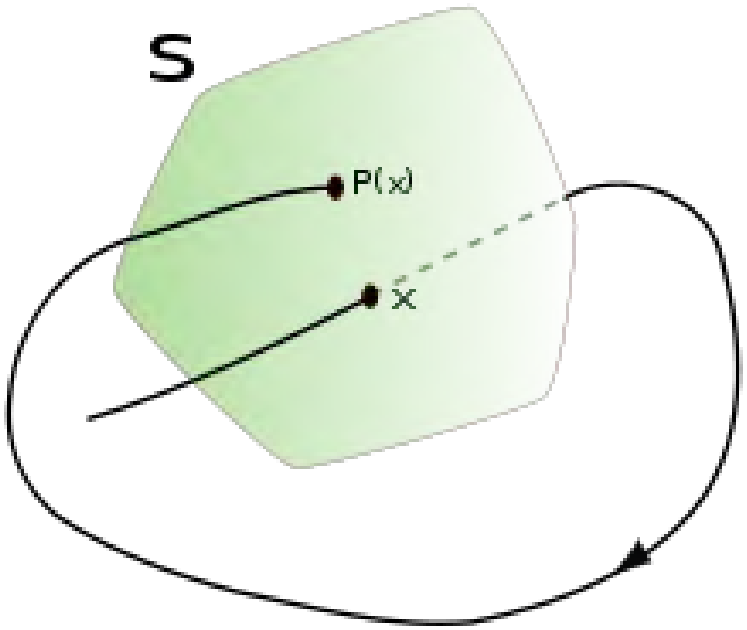


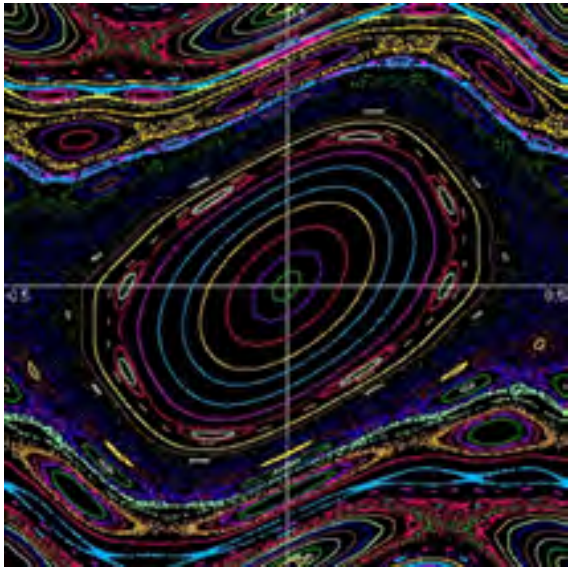
difference between trajectories multiplies by $e = 2.71...$ **every** $\sim 5M$ **years** Laskar

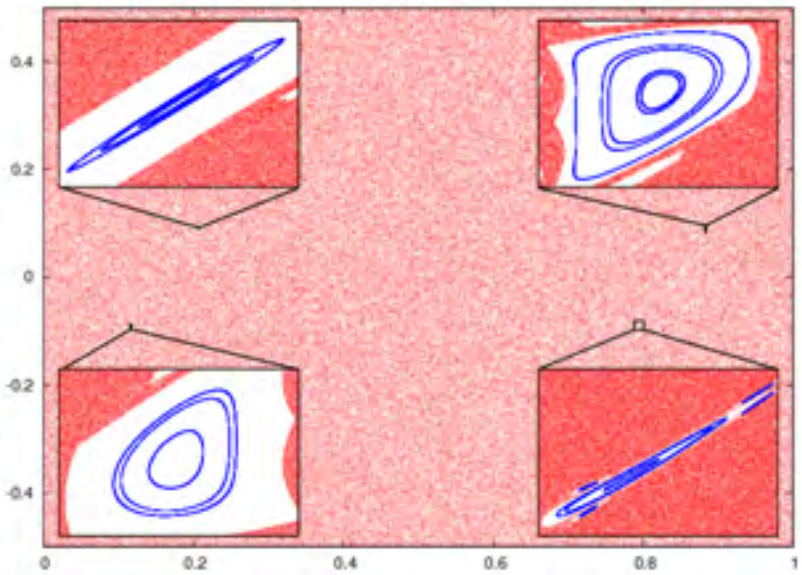
$\lambda \equiv 1/5MYrs$ **is called the *Lyapunov exponent***

$\lambda > 0 \quad \rightarrow$ **chaos**

Poincaré section: a better visualisation:







Consider this:

- The solar system formed $\sim$ 4.5 GYr ago
- starting from the present conditions, *depending on details*, 1% of histories run into trouble in 5 GYr Laskar and Gastineau
- If you start a random planetary system in your computer, almost always it quickly runs into trouble.
- If you observe a planetary system, many conditions within the observational error imply recent formation or immediate destruction

You need to know rare trajectories

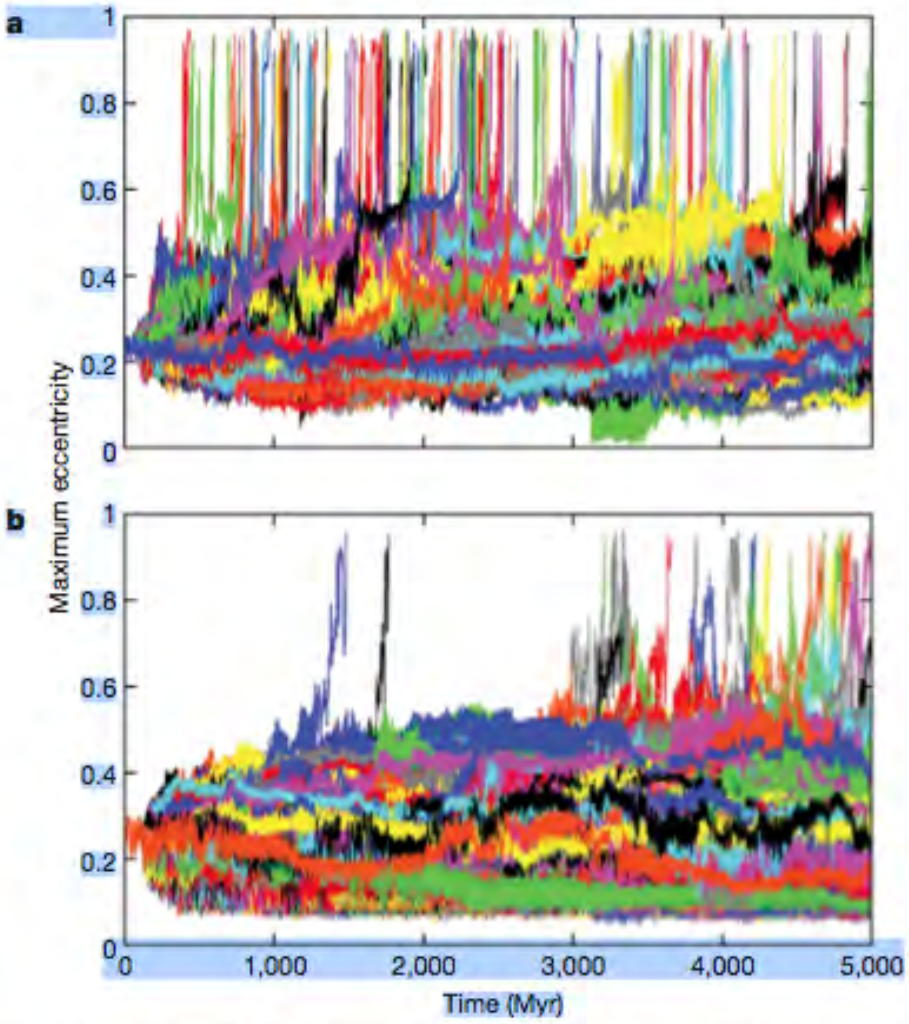
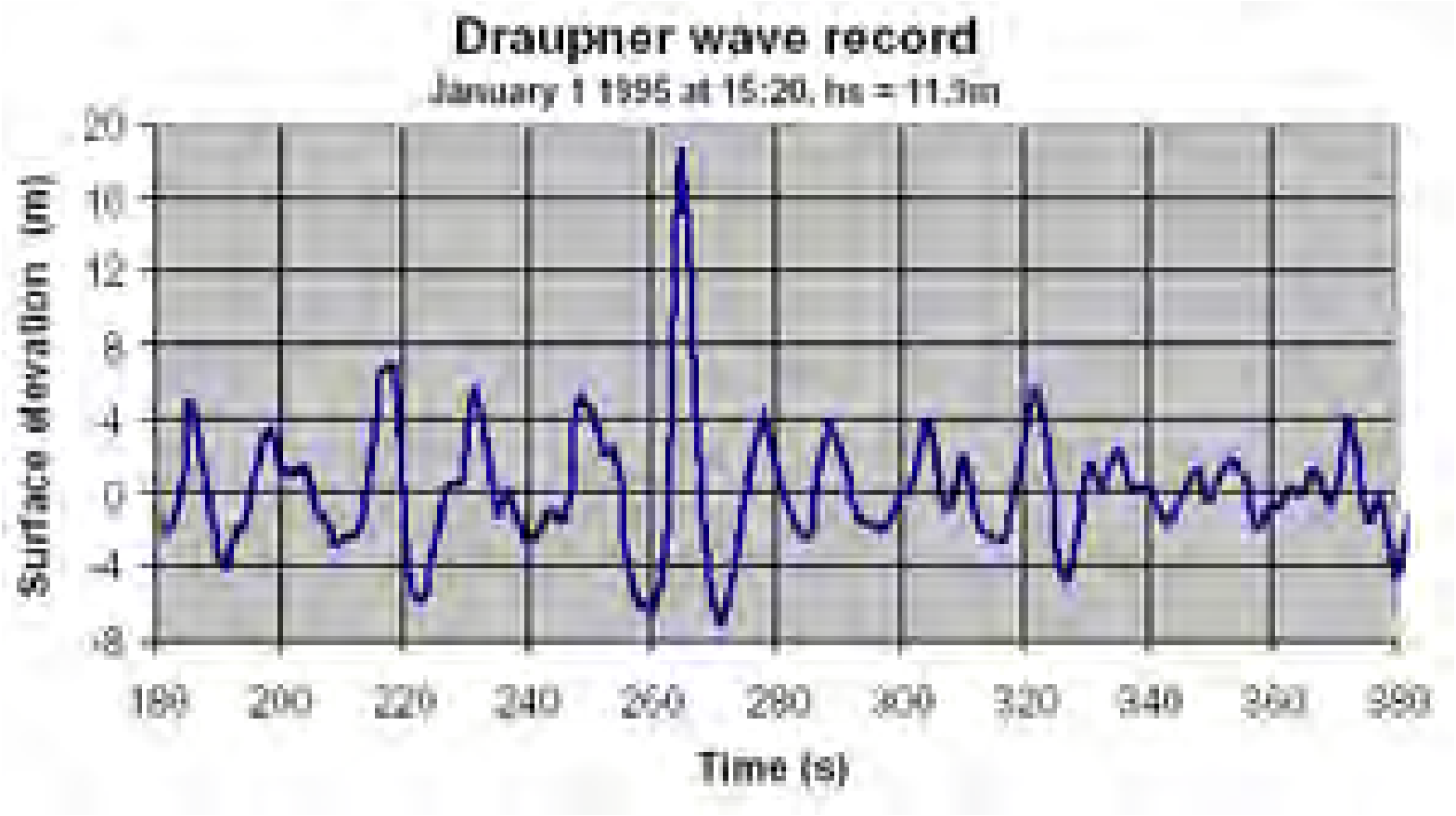


Figure 1 | Mercury's eccentricity over 5 Gyr. Evolution of the maximum

Laskar et al

Another example



The Draupner rogue wave Taylor, Wiki

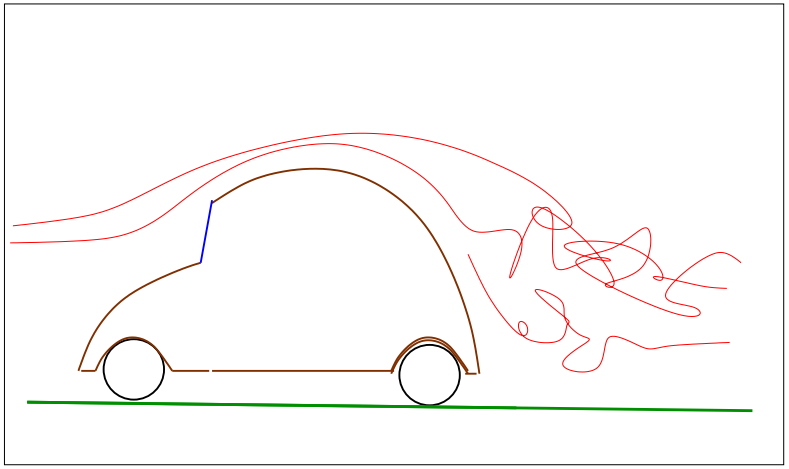
Another example

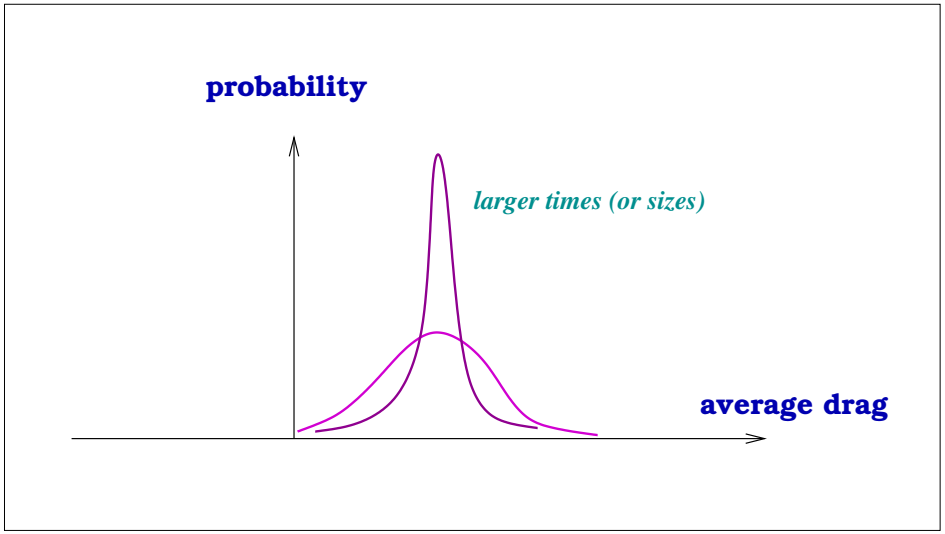
The Draupner rogue wave Taylor, Wiki

Another example

T. Duriez, J..L. Aider, E. Masson, J.E. Wesfreid ; Qualitative investigation of the main flow features over a TGV ; Proceedings of the Euromech Colloquium 509, Vehicle Aerodynamics, Berlin, Allemagne, **2009**, p. 52-57
http://opus.kobv.de/tuberlin/volltexte/2009/2249/

$$\bar{f}_\tau = \frac{1}{\tau} \int_0^\tau f(t)\, dt$$





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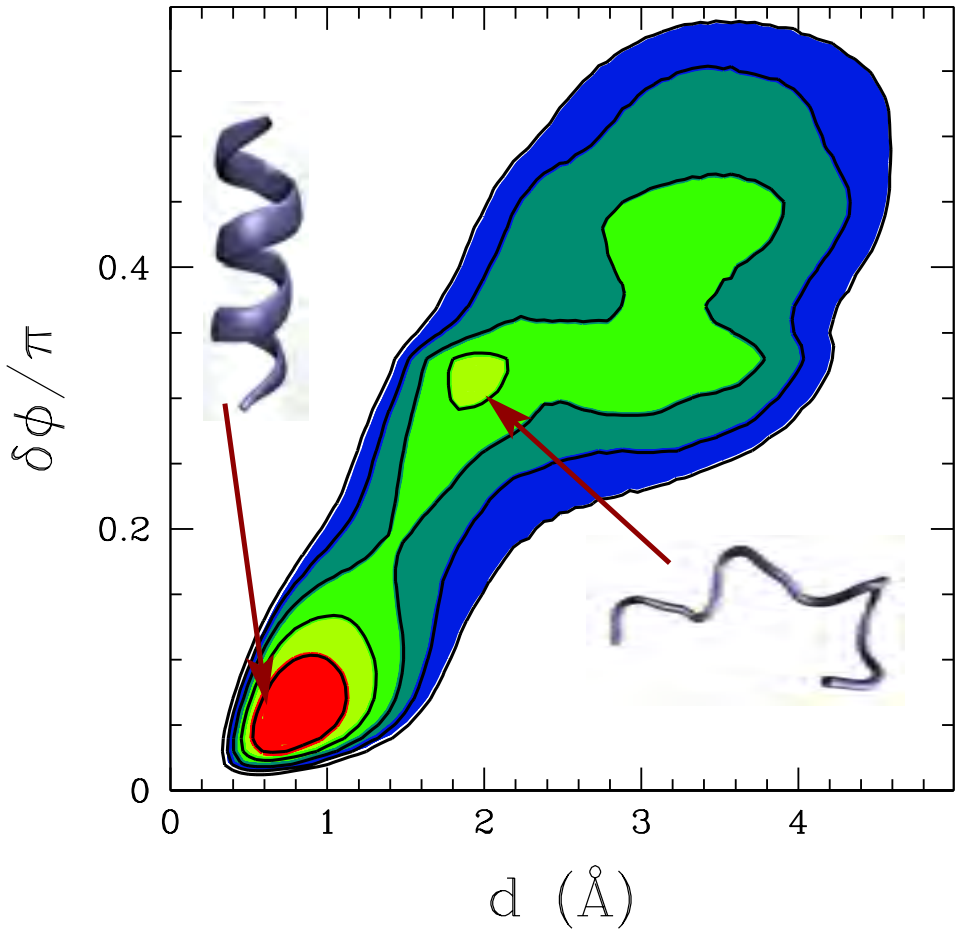
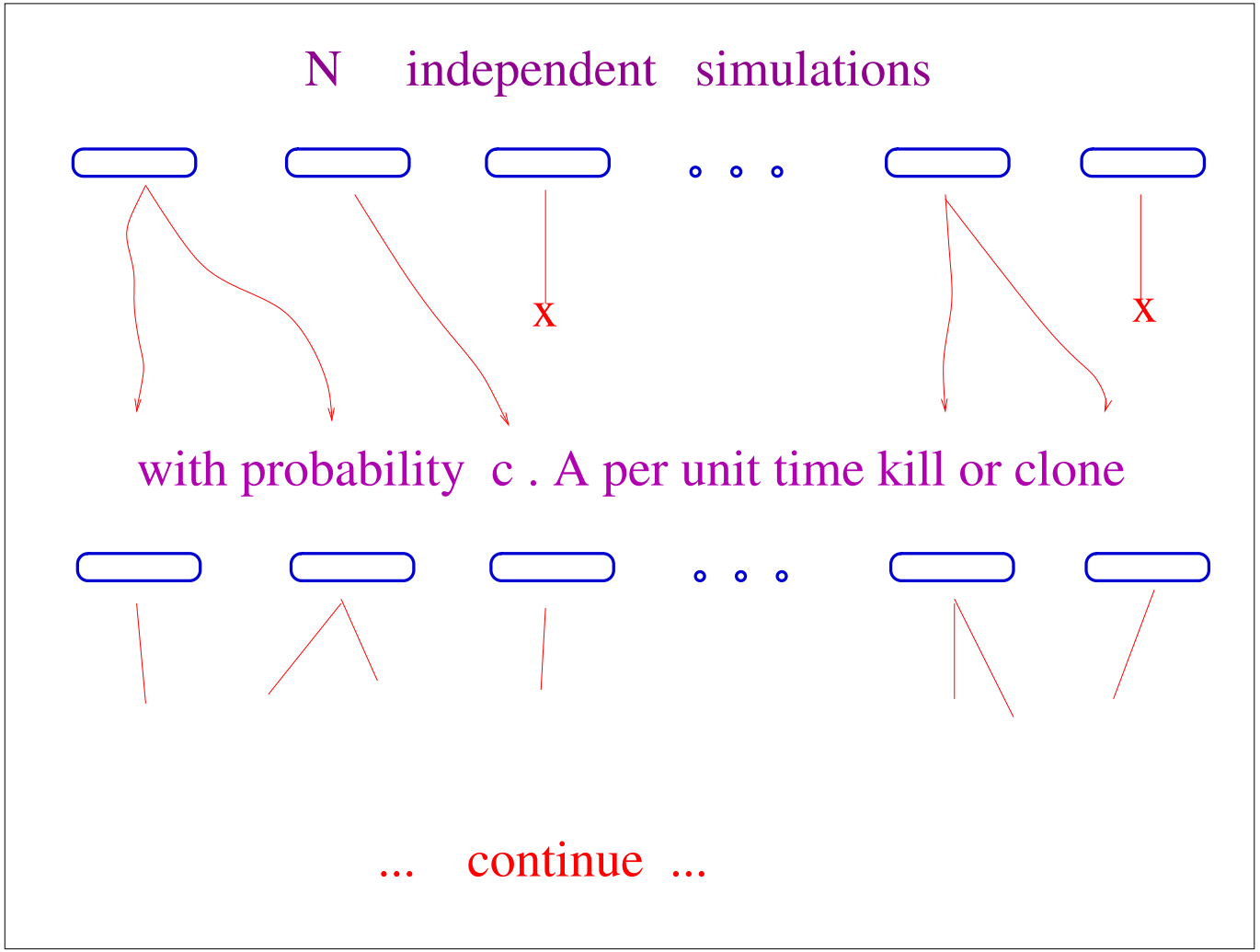


peptide helix-coil transition most trajectories spend their time around one configuration

We wish to simulate an event with an unusually large value of A

without having to wait for this to happen spontaneously

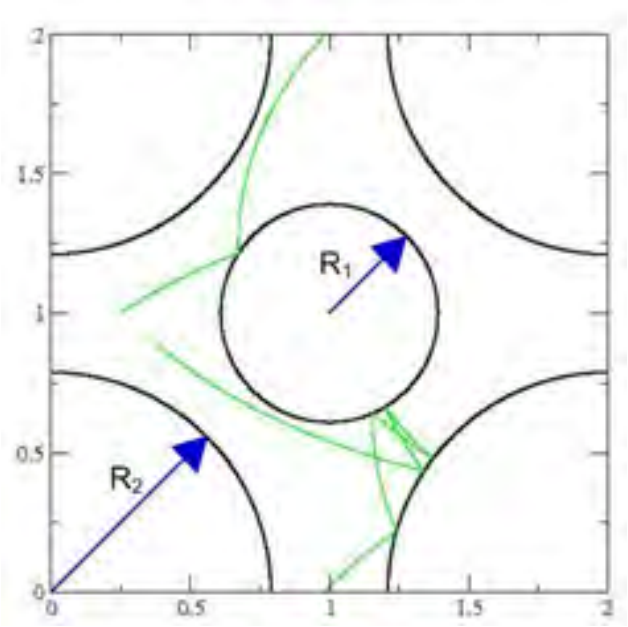
but without forcing the situation artificially

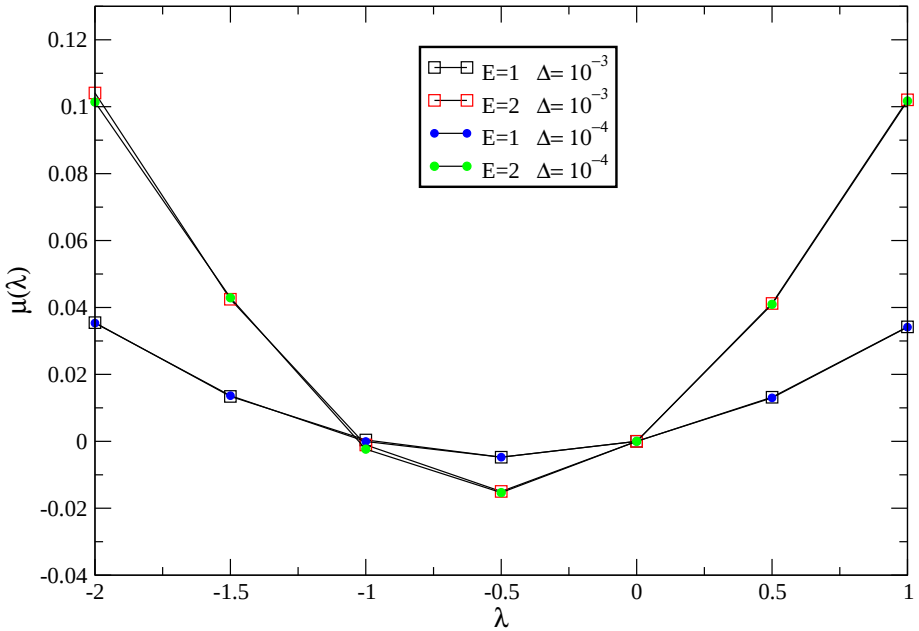


a way to count trajectories weighted with e^{cA}

Some examples

Driven Lorentz Gas



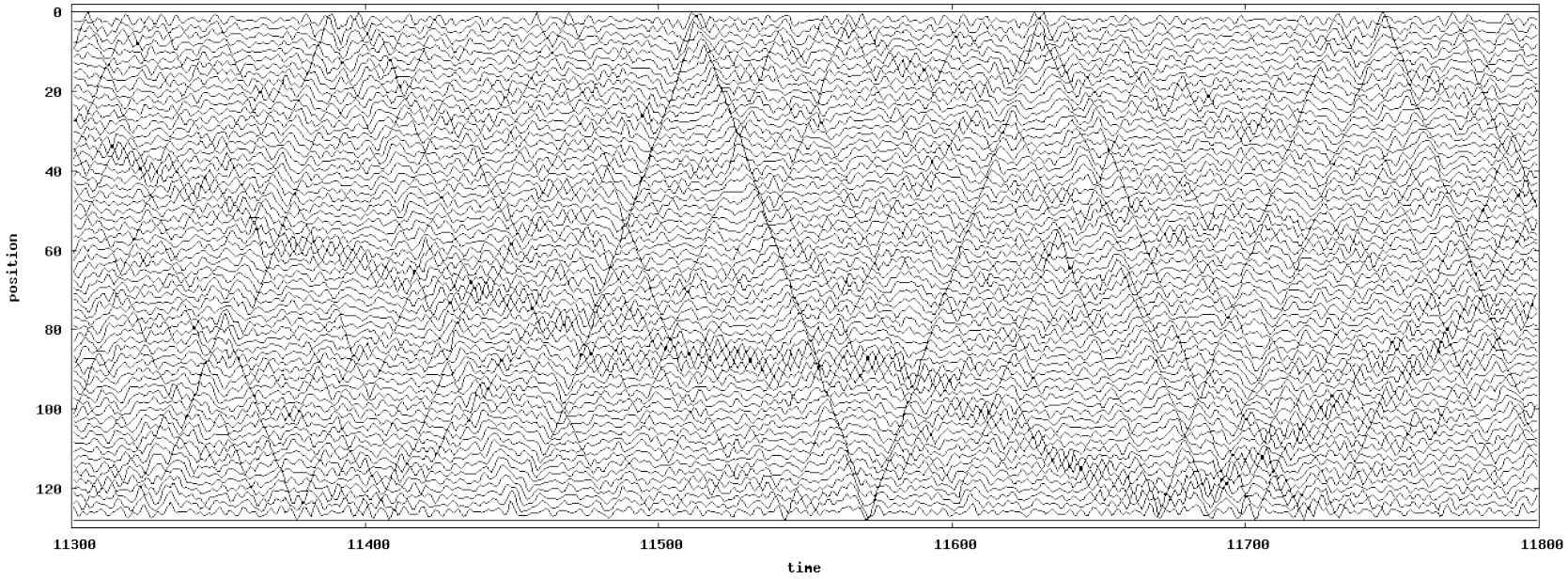


Fermi-Pasta-Ulam chain

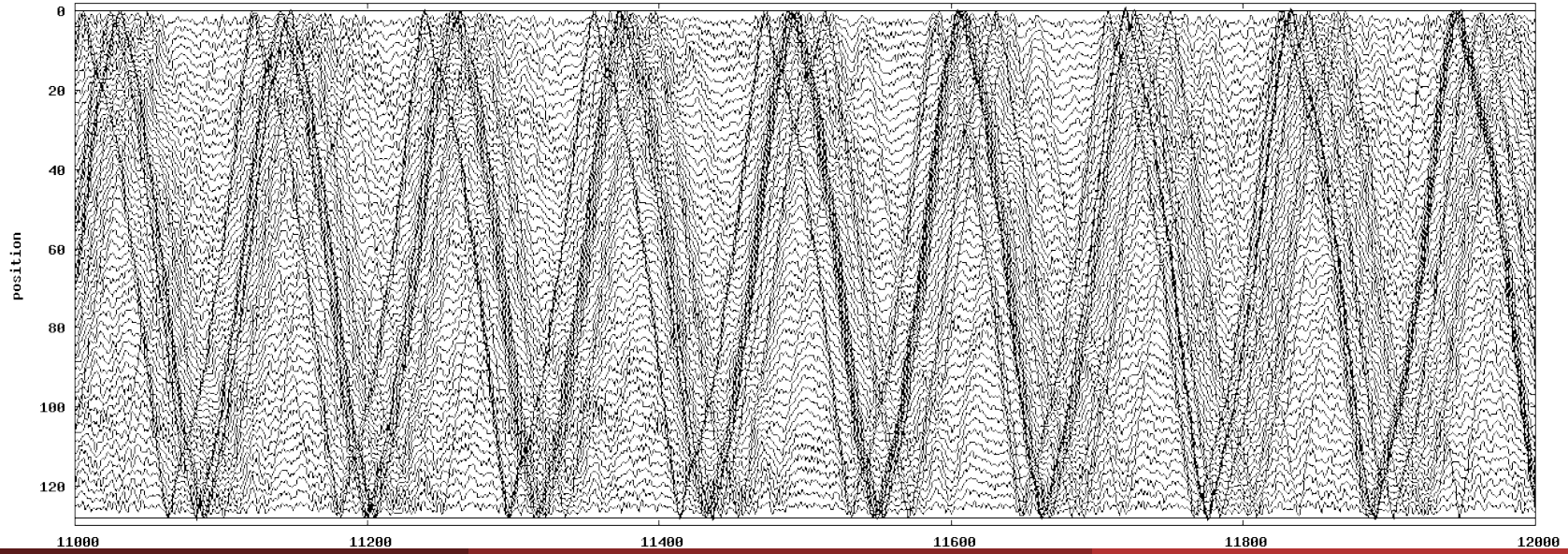
$$H = \sum_{i=1}^{N} \left(\frac{1}{2} p_i^2 + \frac{1}{2} (x_i - x_{i+1})^2 + \frac{\beta}{4} (x_i - x_{i+1})^4 \right)$$

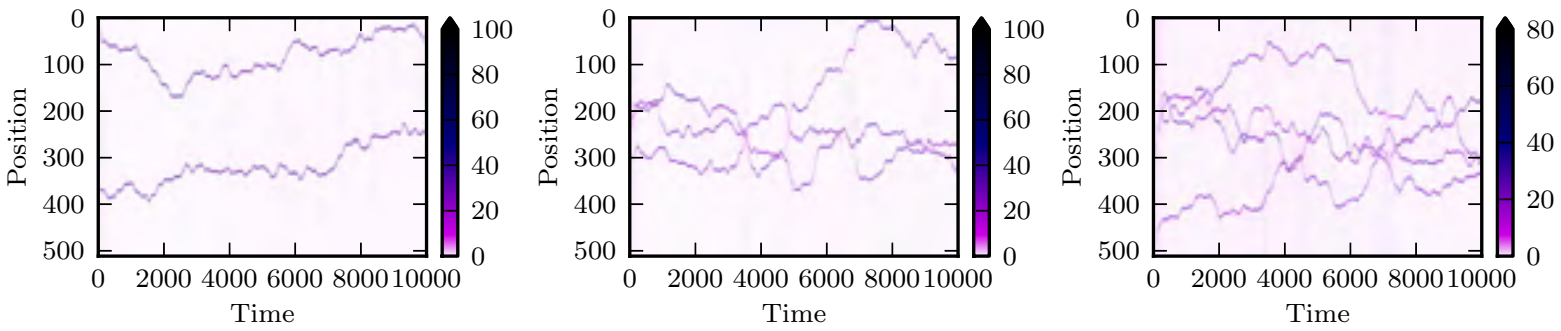
$$A = t * \lambda$$

typical

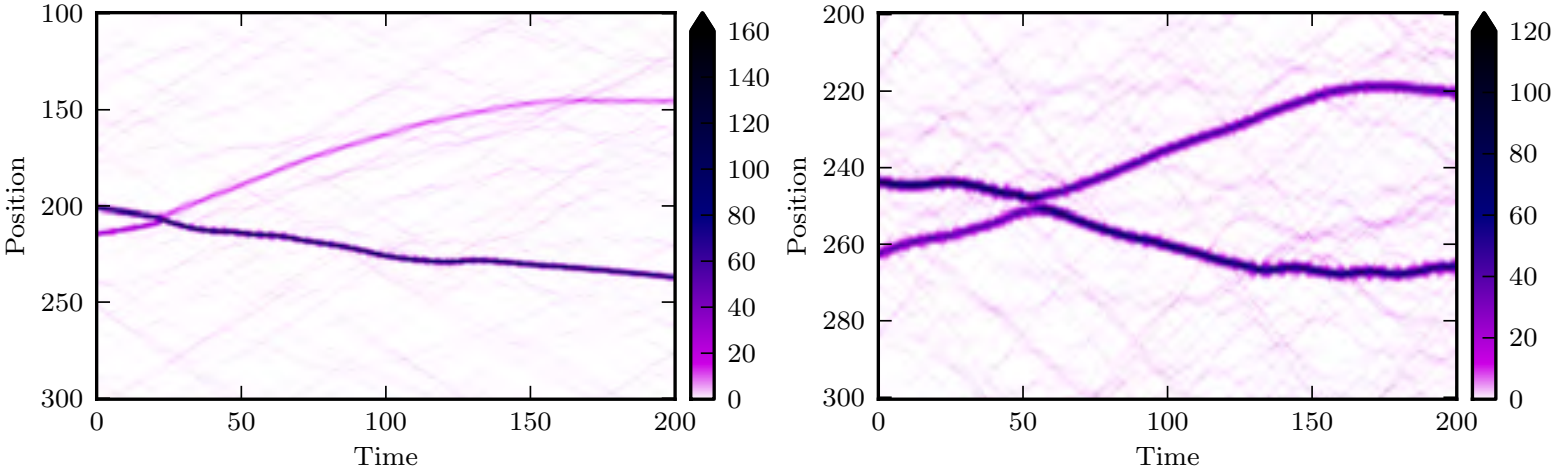


unusually unchaotic

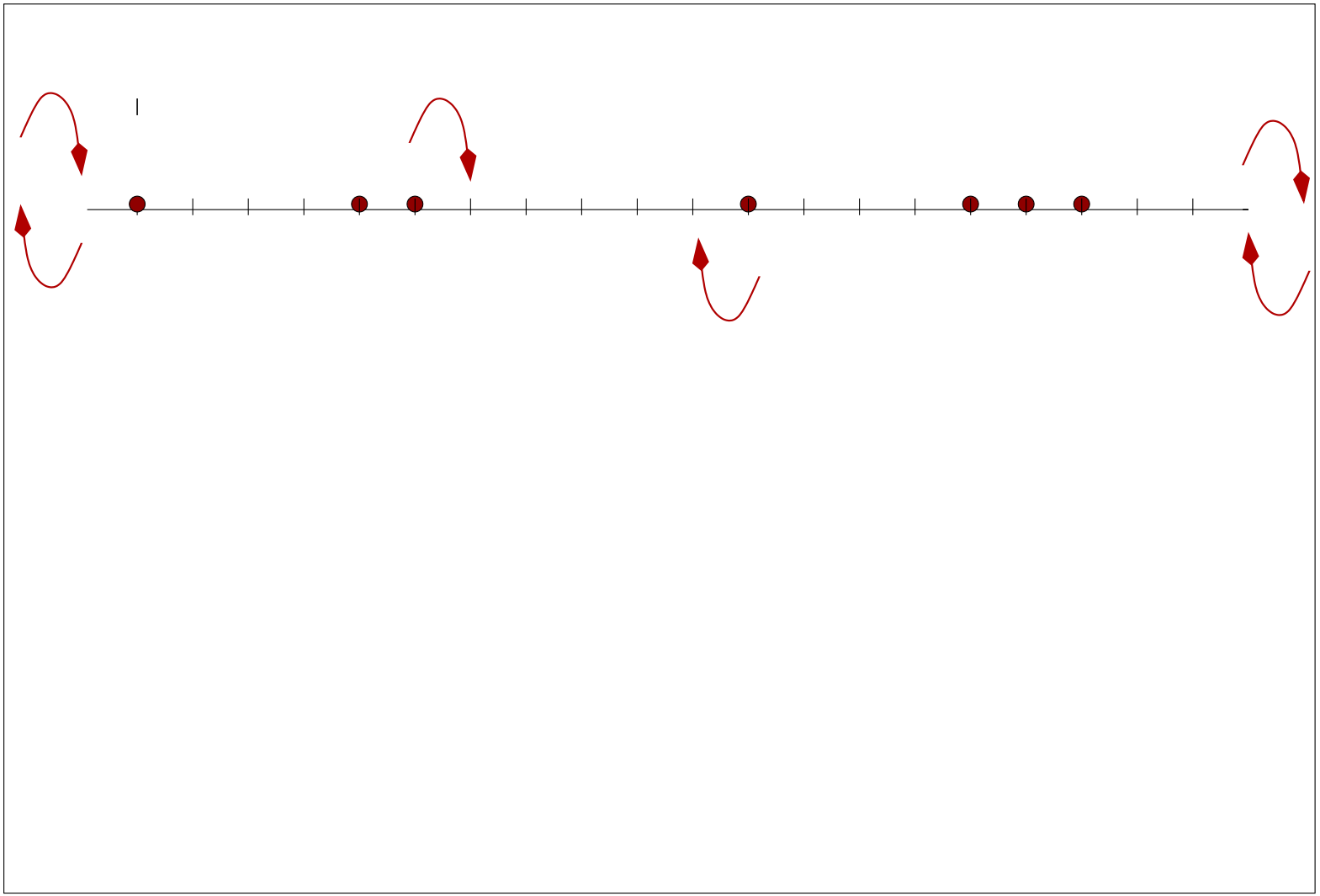




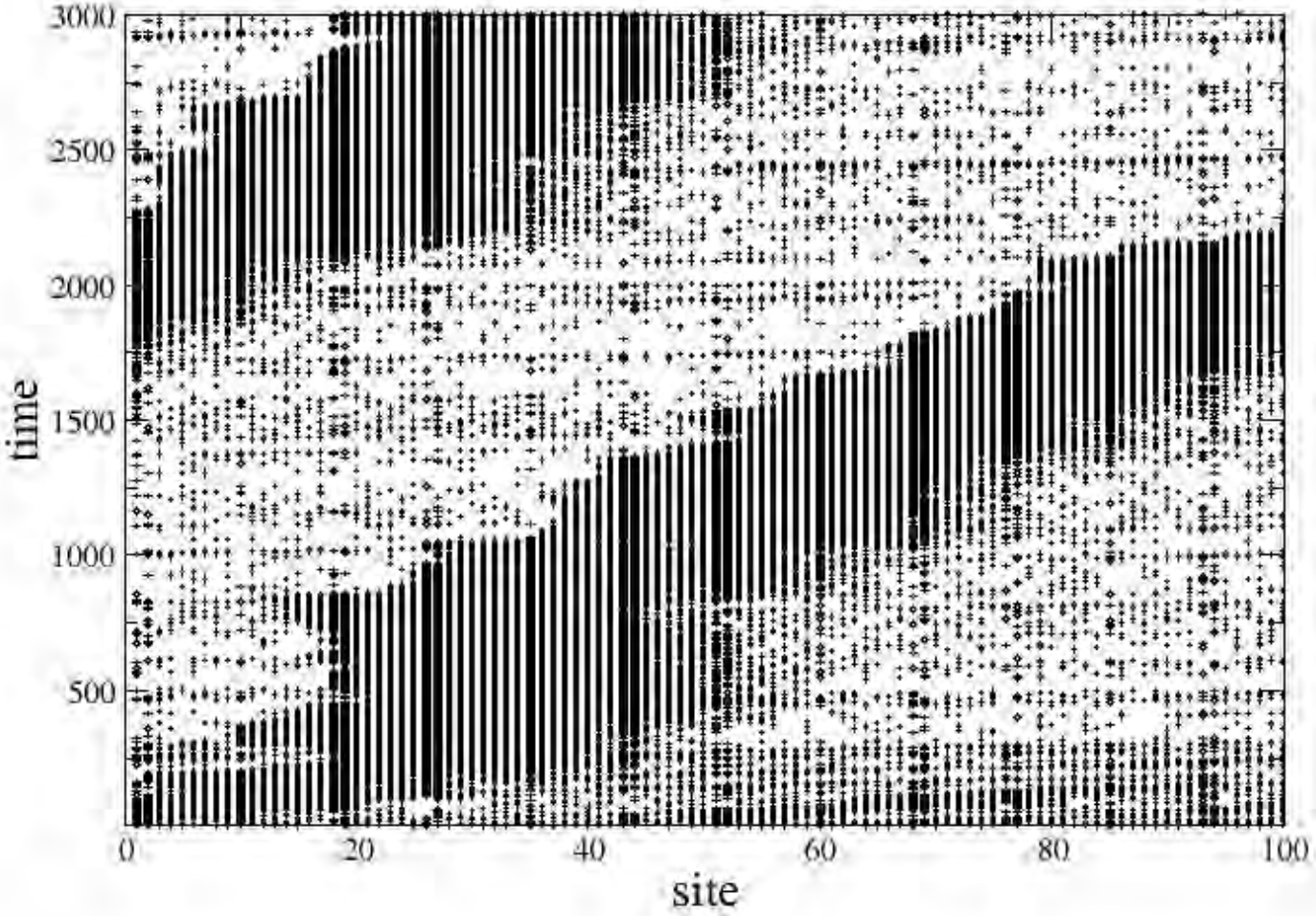
unusually chaotic: breathers (Tailleur et al)



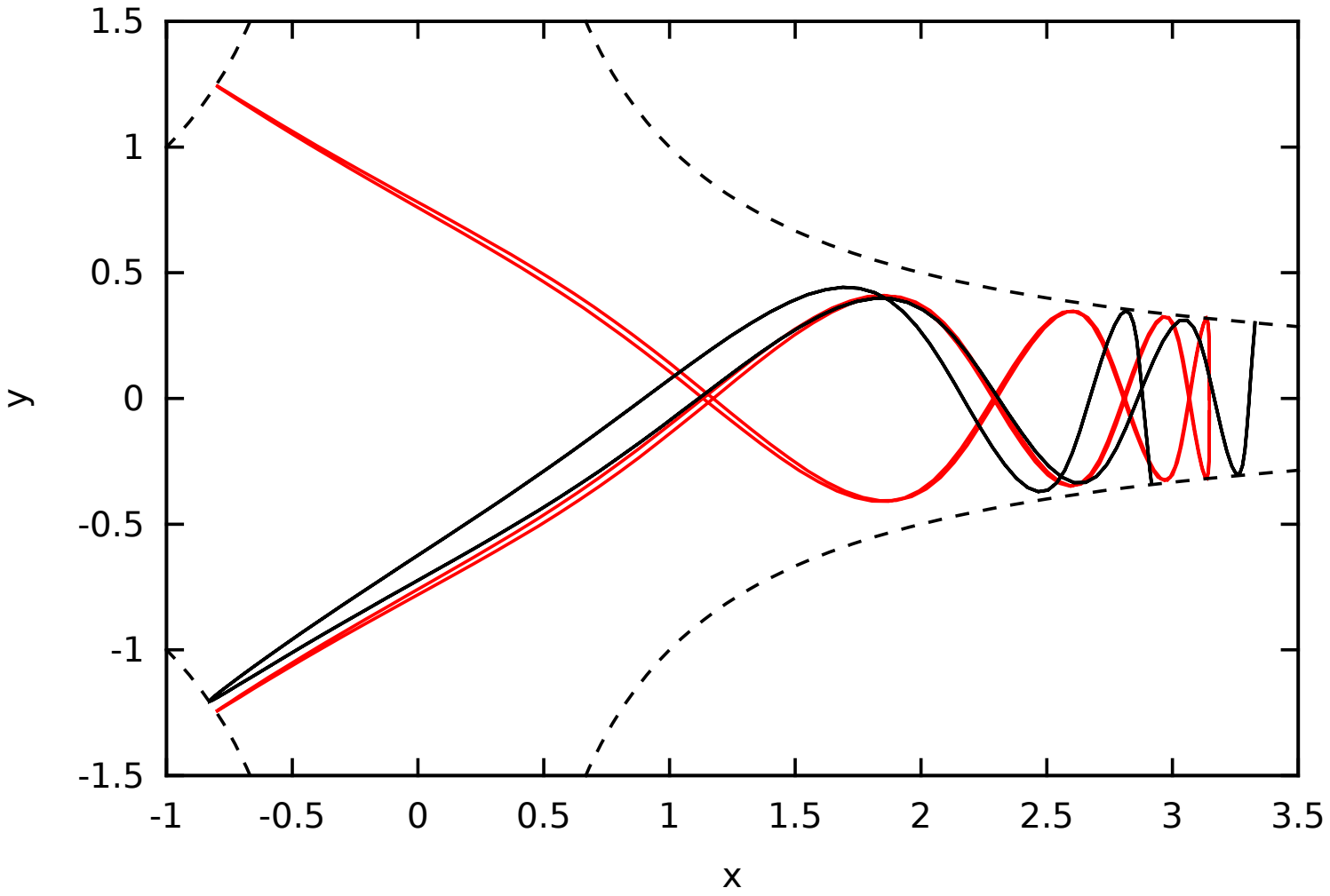
The Symmetric Exclusion Process



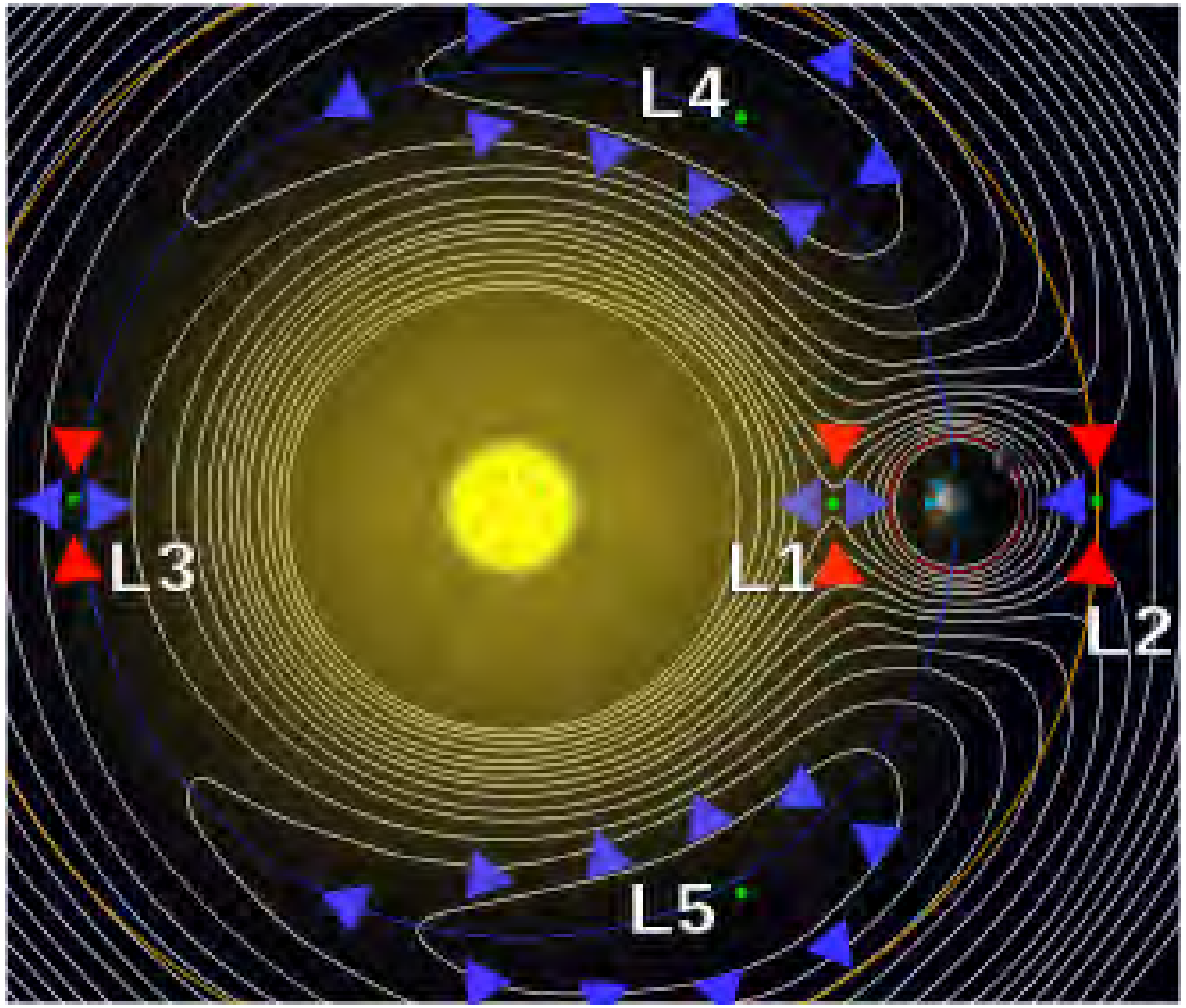
The SEP: unusually low current (a jam)



The x^2y^2 potential: regular islands



Lagrange Point



Effect of eccentricity and mass ratio