Data-driven methods and model reduction for the study of rare events in stochastic systems

The UMD REU Kick-off

Maria Cameron

June 12, 2023

Long-time behavior of systems governed by stochastic differential equations

Deterministic forcing

Stochastic forcing

SDE: $$dX_t = b(X_t)dt + \sqrt{\epsilon}\sigma(X_t)dW_t, \qquad X_t \in \mathcal{M} \subset \mathbb{R}^d$$

A smooth vector field

A small parameter

A smooth matrix function

The standard Brownian motion

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- b: A smooth vector field
- ϵ: A small parameter
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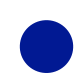
- W_t: The standard Brownian motion

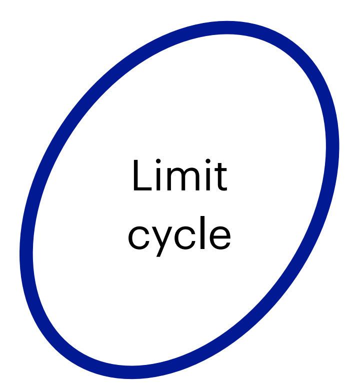
ODE: $$\frac{dx}{dt} = b(x)$$

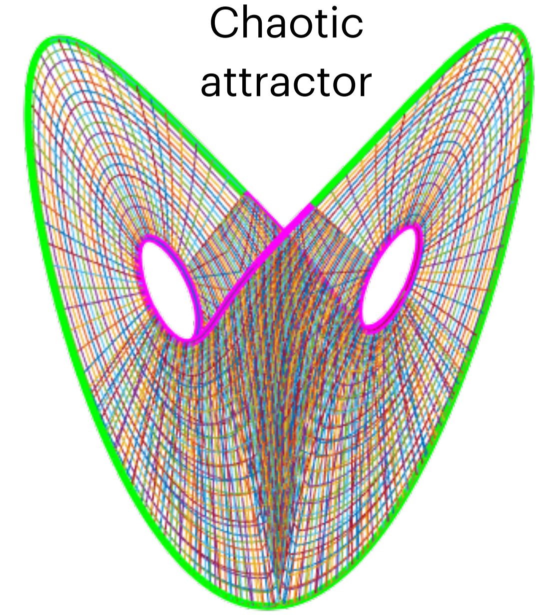
As $t \to \infty$, $x(t) \to$ an attractor

Attractors



Equilibrium point





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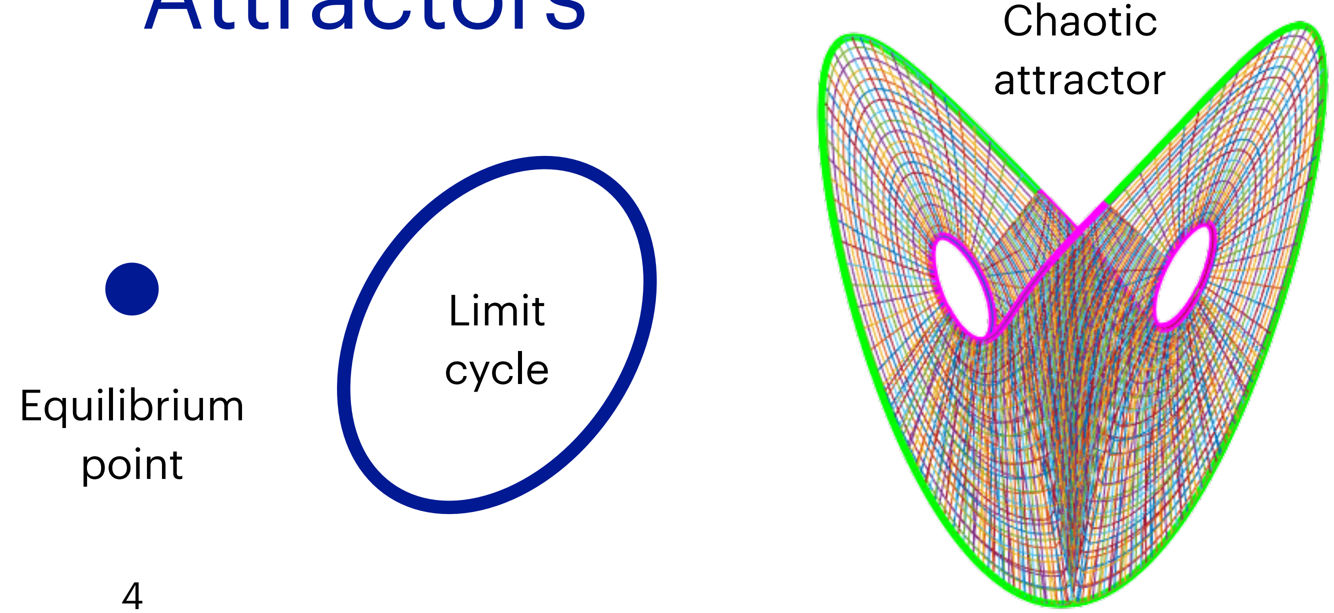
The stochastic term enables transitions between attractors!

We want to find:

- Maximum likelihood transition paths
- Transition rates

Attractors



Example 1: population dynamics

Consumer-resource model of plankton *x* and their consumers *y*

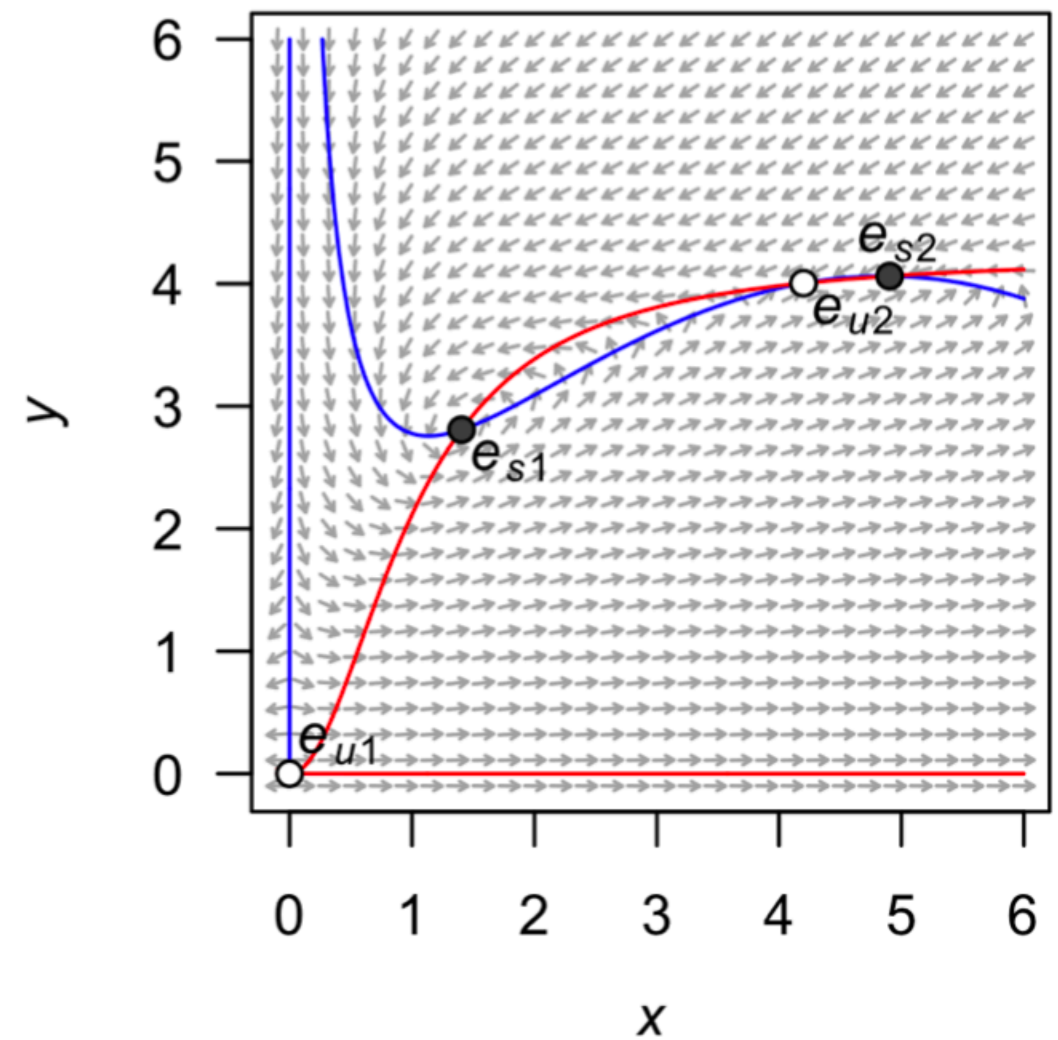
(Collie and Spencer, 1994; Steele and Henderson, 1981)

$$\begin{cases} dx = \left(\alpha x[1-\beta^{-1}x] - \frac{\delta x^2 y}{\kappa + x^2}\right) dt + \sigma dw_1 \\ dy = \left(\frac{\gamma x^2 y}{\kappa + x^2} - \mu y^2\right) dt + \sigma dw_2 \end{cases}$$

$$\alpha = 1.54,\ \beta = 10.14,$$
$$\gamma = 0.476,\ \delta = 1,$$
$$\kappa = 1,\ \mu = 0.112509$$

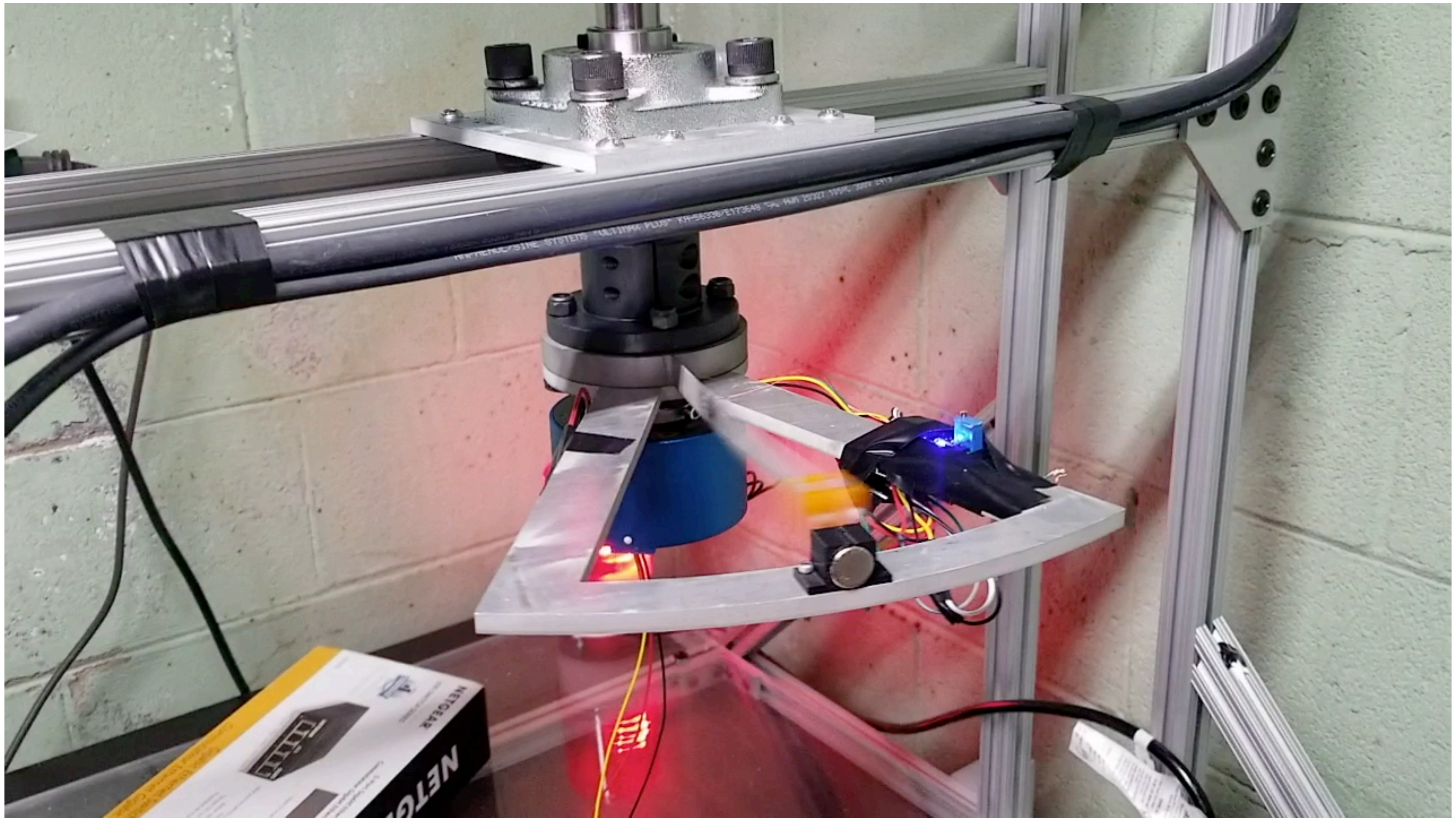
Two saddles and
two equilibrium point attractors

Source: https://journal.r-project.org/archive/2016/RJ-2016-031/RJ-2016-031.pdf



Example 2: nonlinear oscillator

A noise-driven transition from the high- to the low-amplitude attractor



Lautaro Cilenti,
Ph.D. Mech. Eng. UMD, 2022

System model: $x'' + ax' + c_1x + c_3x^3 = F\cos(\omega t) + \sigma\eta_t$

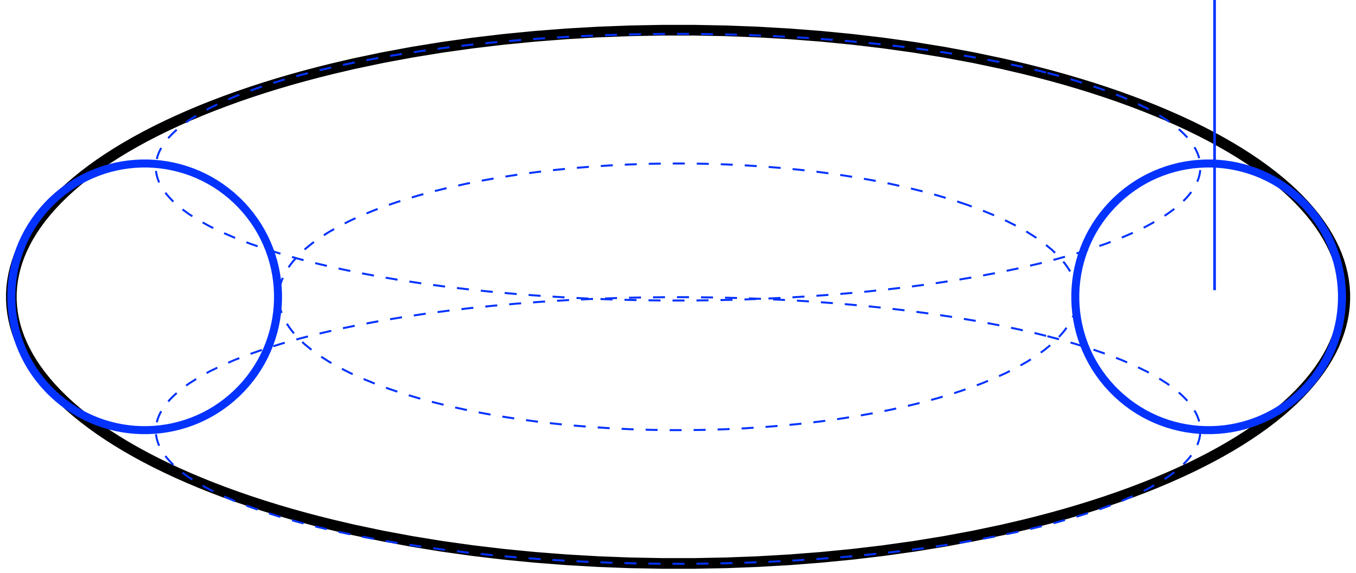
$$\begin{cases} \dot{x} = v \\ \dot{v} = -av - c_1x - c_3x^3 + F\cos(\omega\theta) + \sigma\eta(t) \\ \dot{\theta} = 1 \end{cases}$$

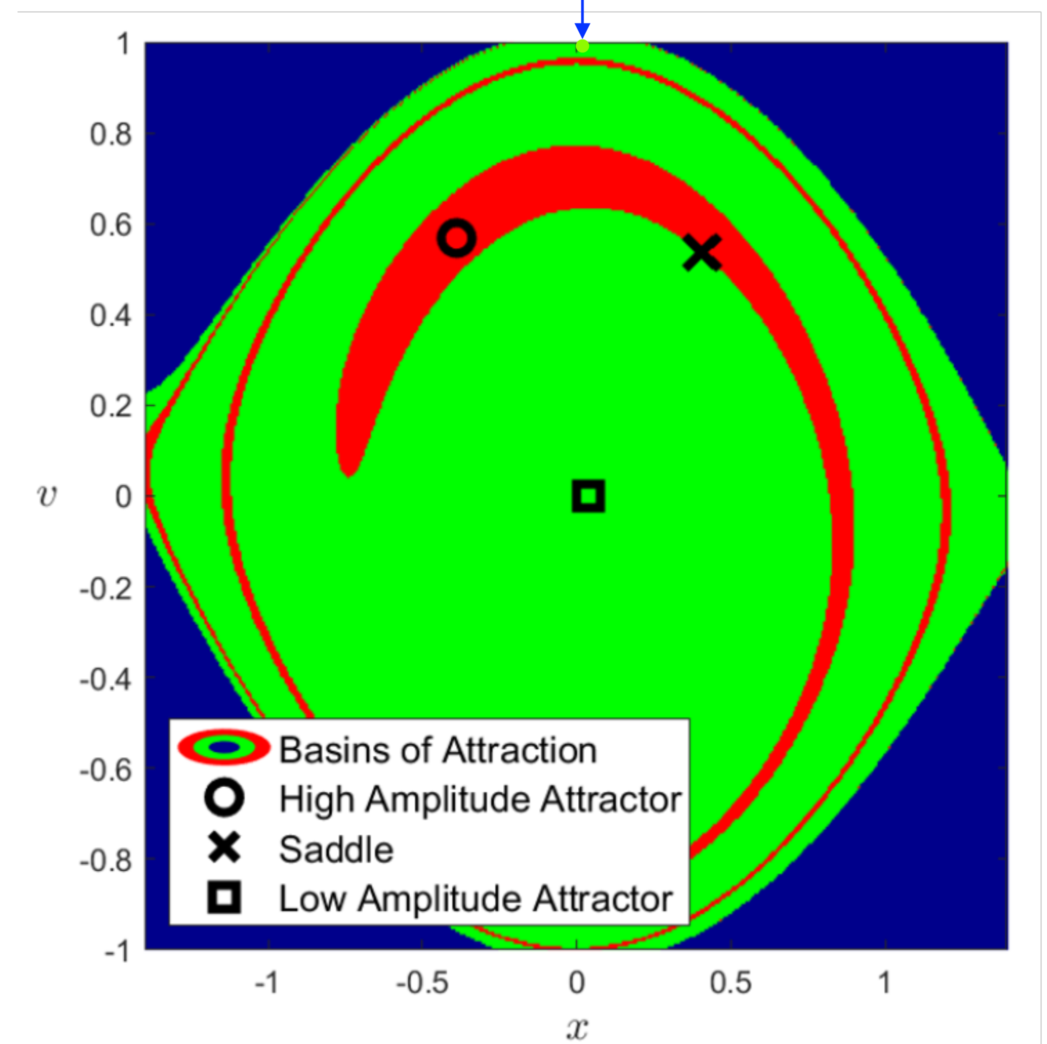
Example 2: nonlinear oscillator

System model: $x'' + ax' + c_1x + c_3x^3 = F\cos(\omega t) + \sigma\eta_t$

$$\begin{cases} \dot{x} = v, & x \in \mathbb{R} \\ \dot{v} = -av - c_1x - c_3x^3 + F\cos(\omega\theta) + \sigma\eta(t), & v \in \mathbb{R} \\ \dot{\theta} = 1, & \theta \in \mathbb{S}_{2\pi/\omega} \end{cases}$$

Phase space: $\mathbb{R}^2 \times \mathbb{S}_{2\pi/\omega}$

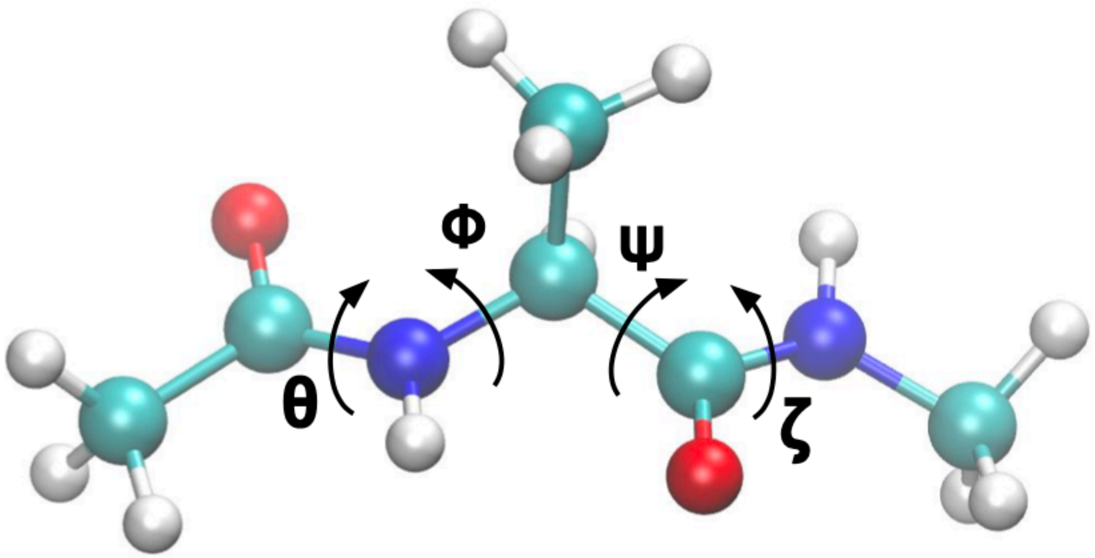




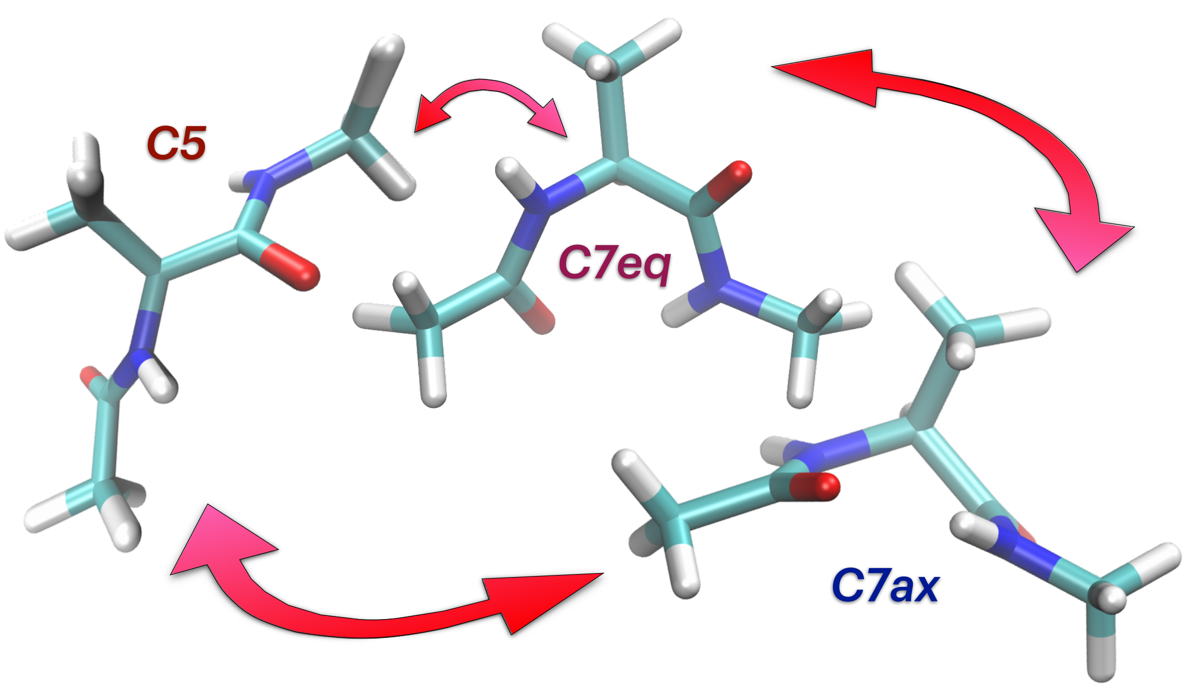
Example 3: molecular dynamics

Alanine dipeptide: 22 atoms

Phase space: $\mathbb{R}^{132}$



Three metastable configurations:



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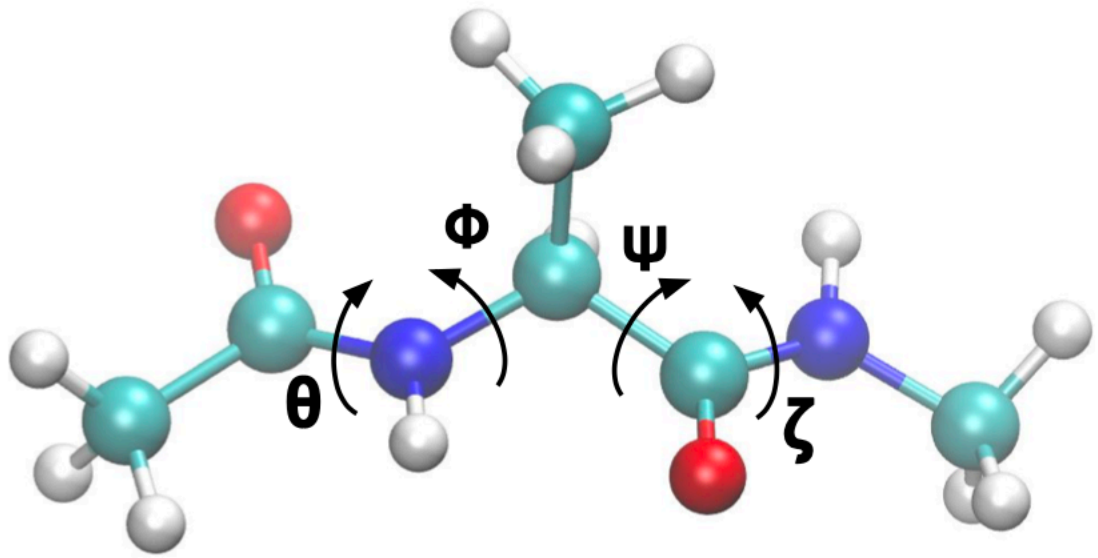

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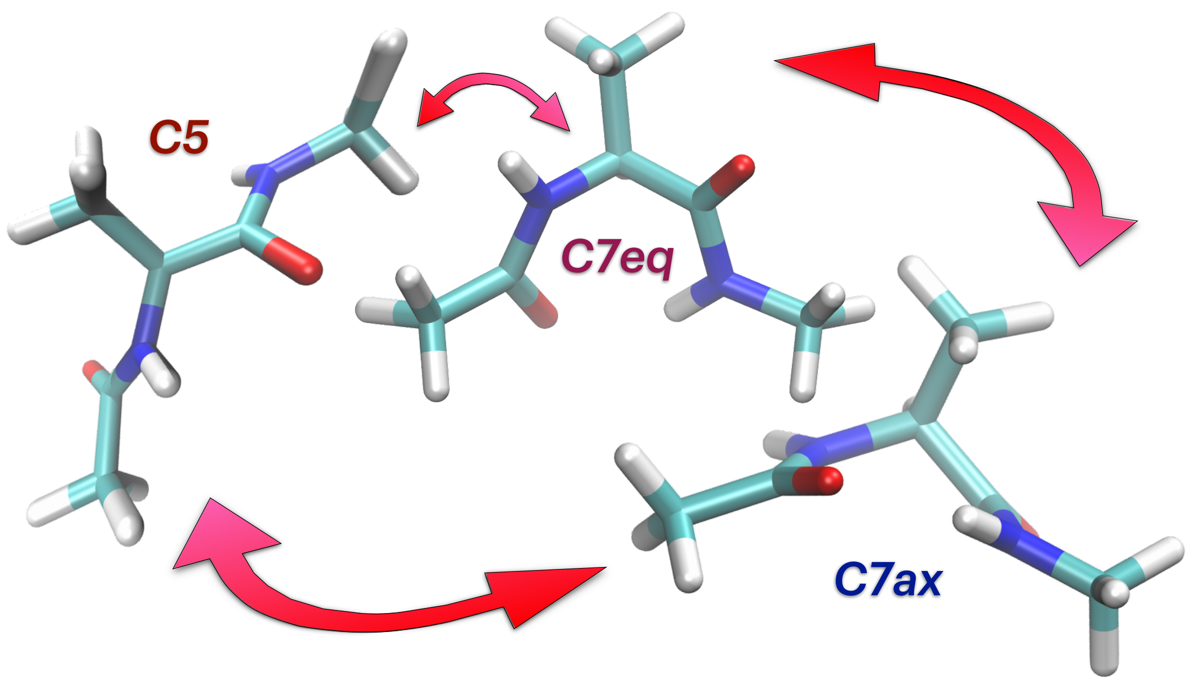
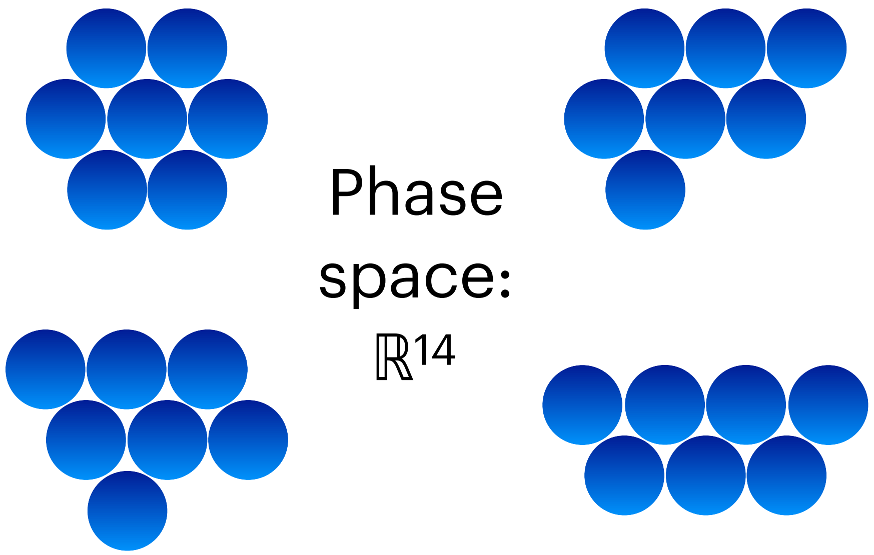


Lennard-Jones-7 in 2D,
overdamped Langevin dynamics



Phase space: $\mathbb{R}^{14}$

Example 3: molecular dynamics

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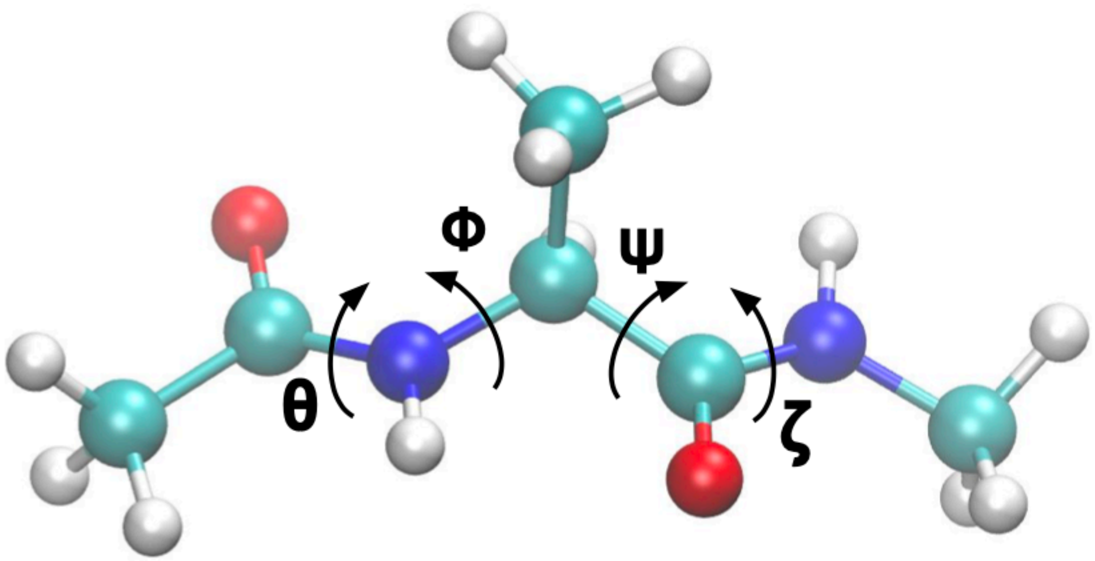

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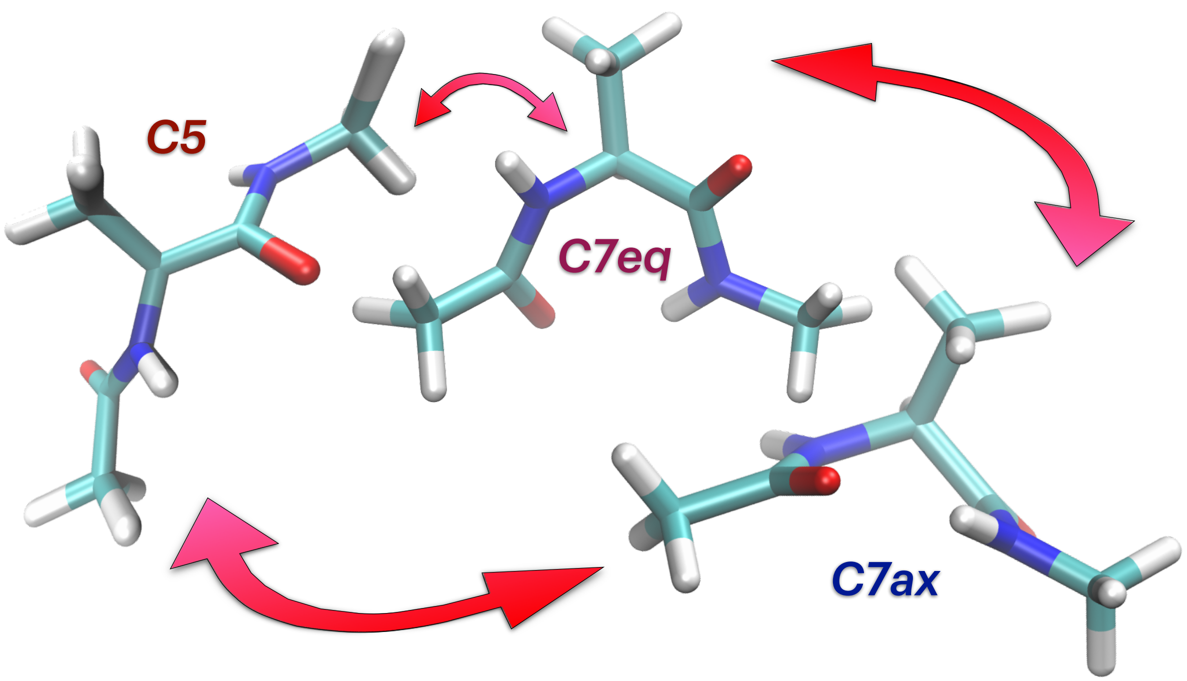

Lennard-Jones-7 in 2D,
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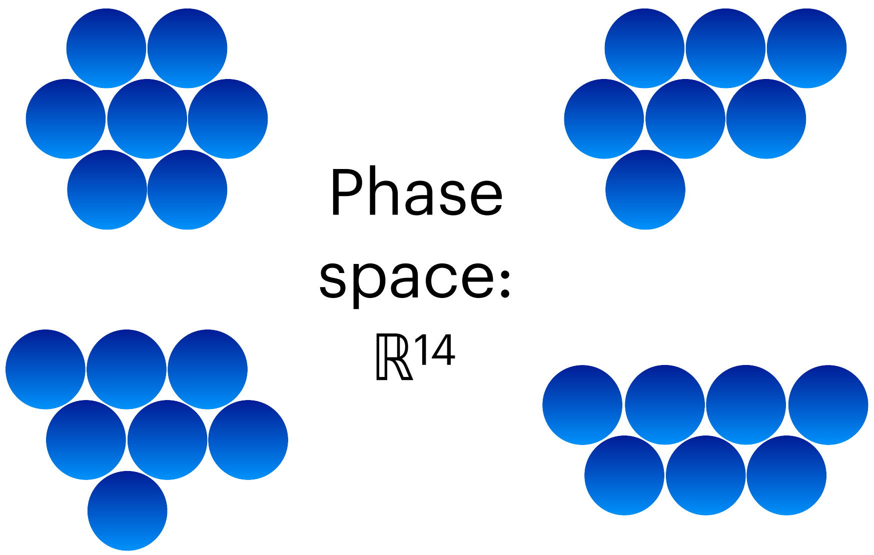
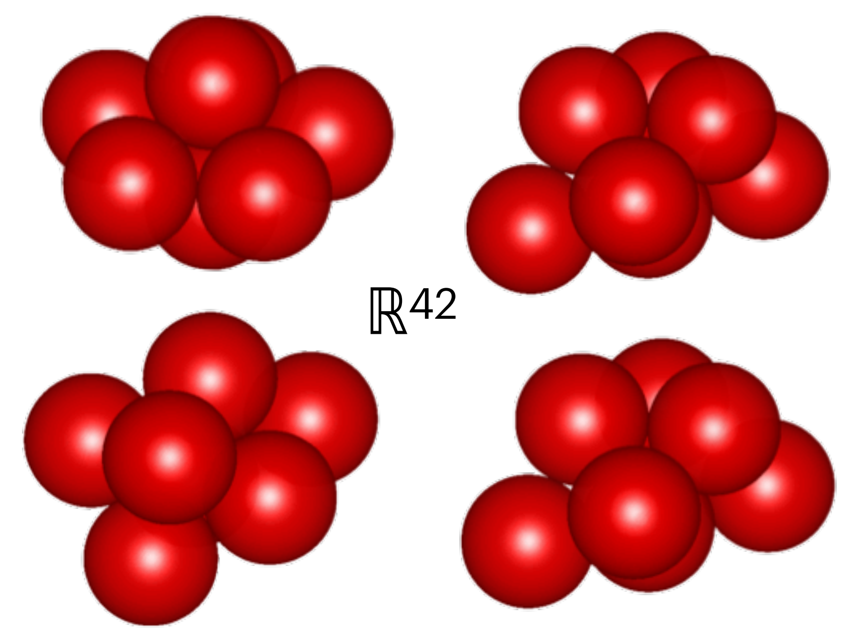


Phase space: $\mathbb{R}^{14}$

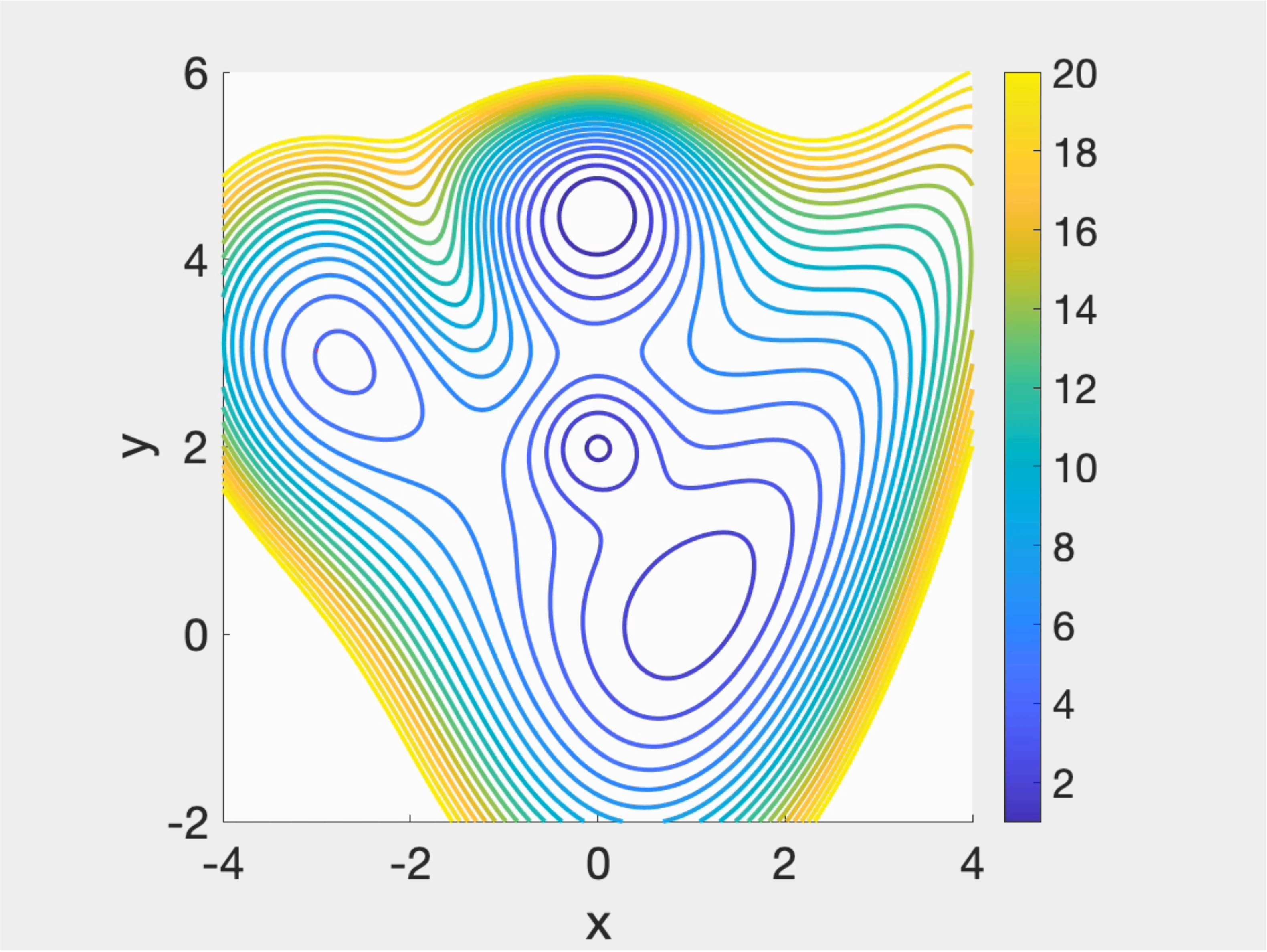
Lennard-Jones-7 in 3D,
Langevin dynamics



$\mathbb{R}^{42}$

An easy case: the overdamped Langevin dynamics in 2D

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dW_t$$



Invariant pdf is the Gibbs density:

$$\mu(x) = Z^{-1}e^{-\beta V(x)}$$

Expected exit time from the basin of $x_{\min}$:

$$\mathbb{E}[\tau_{\partial B_{x_{\min}}}] \approx C e^{\beta(V(x_{\text{saddle}})-V(x_{\min}))}$$

Transition path theory

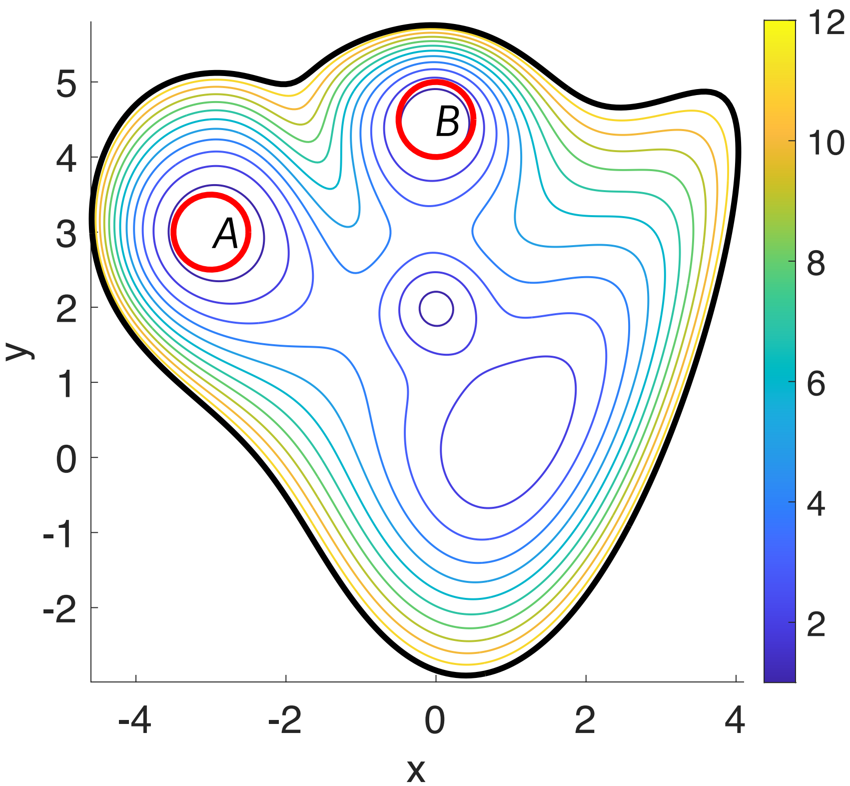
(A mathematical framework for quantifying transition processes)

W. E and E. Vanden-Eijnden, 2006

The ***committor*** is the probability that the process starting at *x* will reach region *B* prior to reaching region *A*

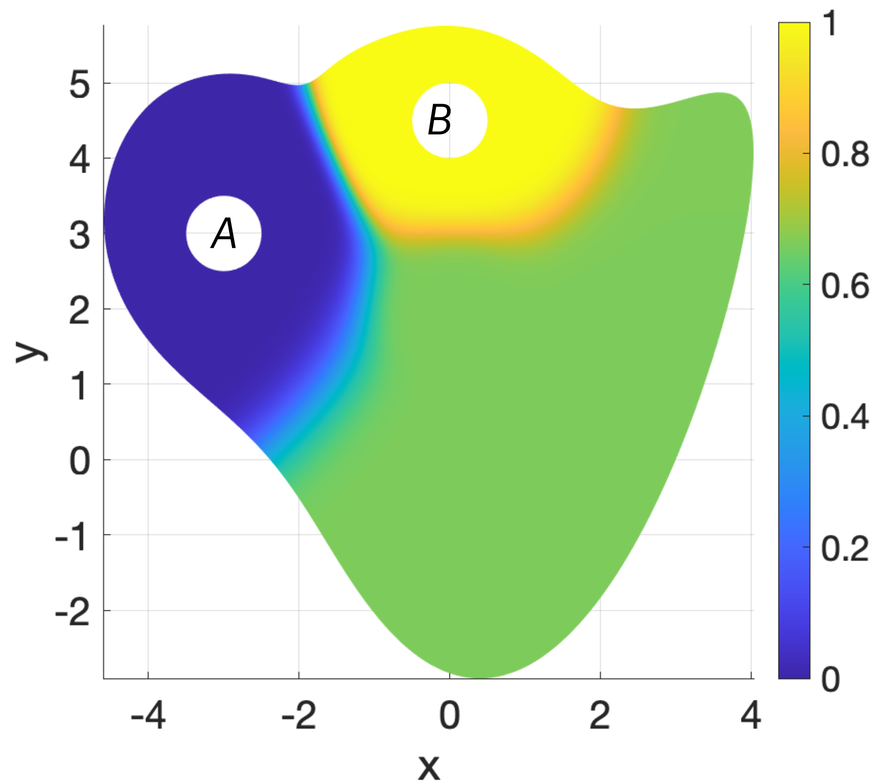
$$q(x) := \mathrm{Prob}_x(\tau_B < \tau_A)$$

The potential function

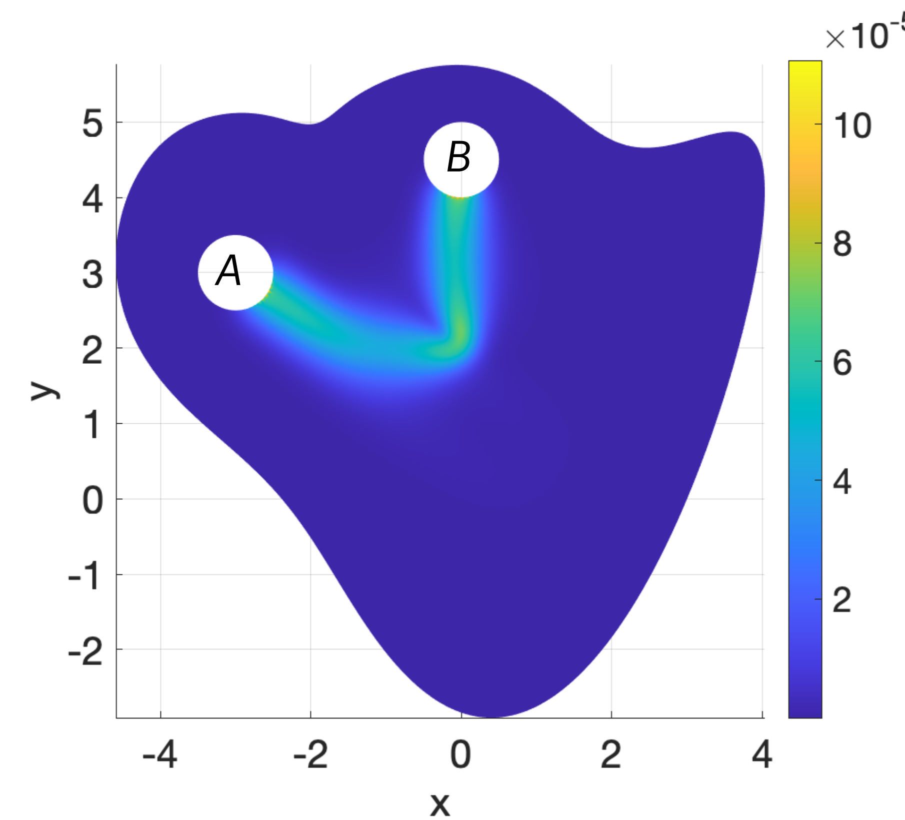


$$\mu(x) = Z^{-1} e^{-\beta V(x)}$$

The committor



The reactive current



$$J(x) = \beta^{-1} \mu \nabla q(x)$$

The transition rate:

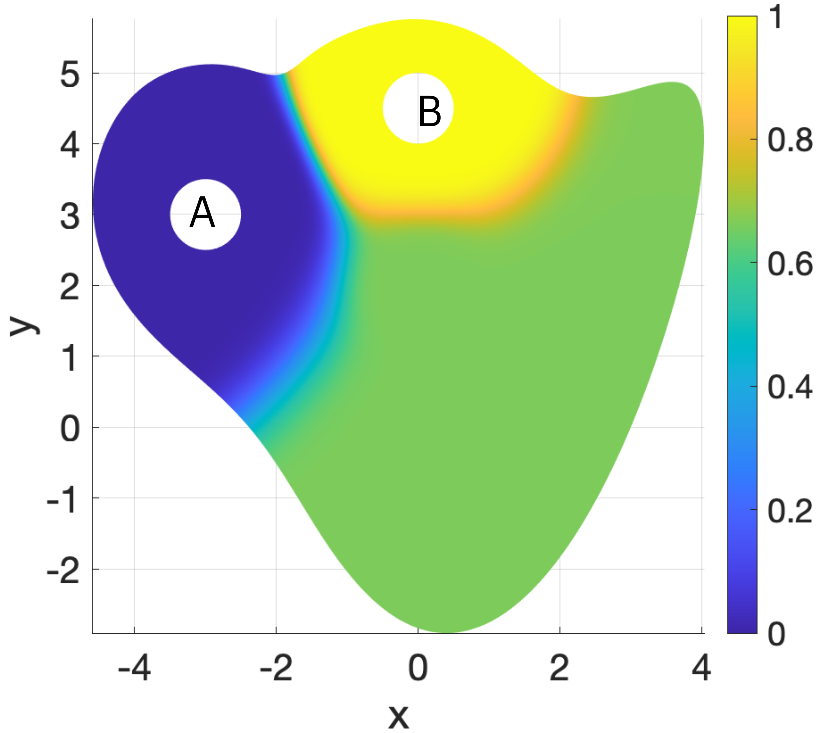
$$\nu_{AB} = \beta^{-1} \int_{\Omega_{AB}} \|\nabla q\|^2 \mu dx$$

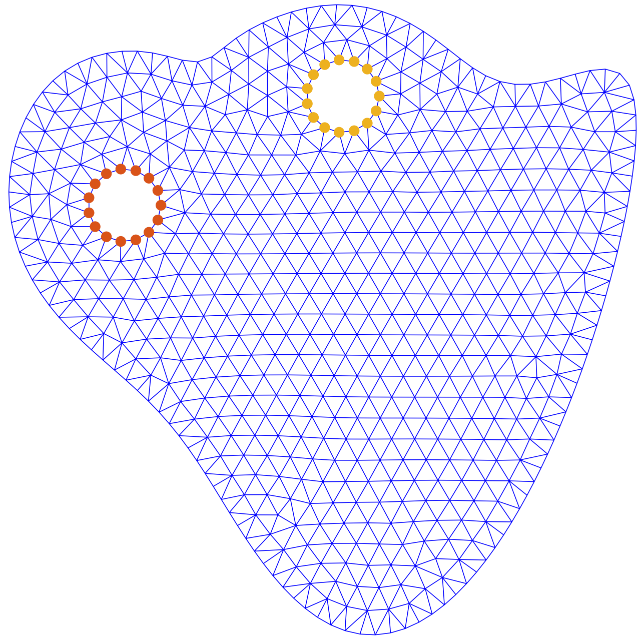
Solving the committor problem

$$\begin{cases} \mathcal{L}q = \beta^{-1} e^{\beta V} \nabla \cdot \left(e^{-\beta V} \nabla q \right) = 0 \\ q(\partial A) = 0, \quad q(\partial B) = 1 \end{cases}$$

Approach 1:

finite element method





Good for dim = 2 or 3

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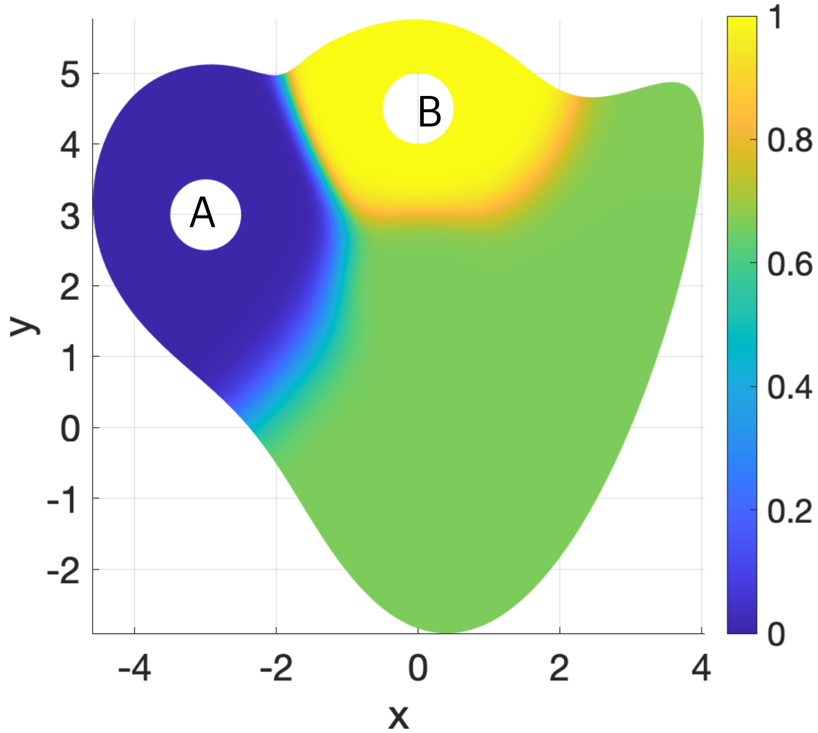
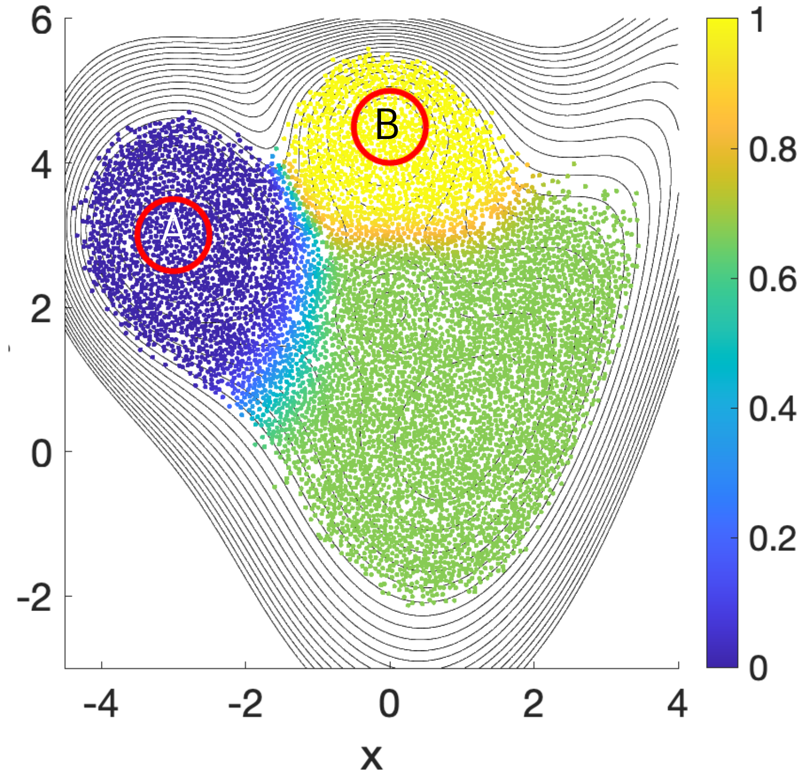
Approach 1:

finite element method

Approach 2:

Target-measure diffusion map





Good for dim = 2 or 3

Good for low intrinsic dimension
The ambient space can be high-dimensional

Solving the committor problem

$$\begin{cases} \mathcal{L}q = \beta^{-1}e^{\beta V}\nabla\cdot\left(e^{-\beta V}\nabla q\right) = 0 \\ q(\partial A) = 0, \quad q(\partial B) = 1 \end{cases}$$

Approach 1:

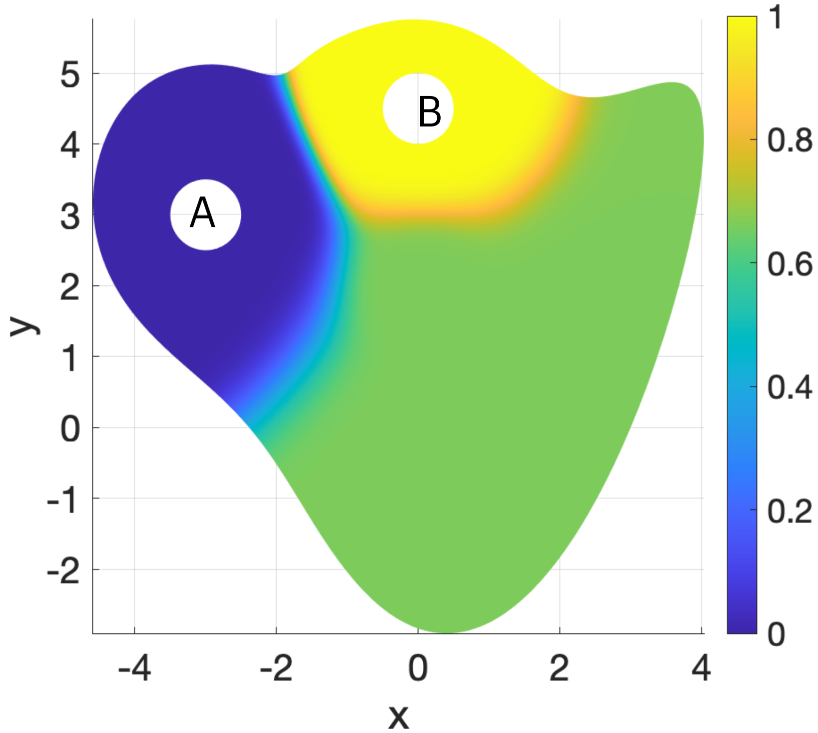
finite element method

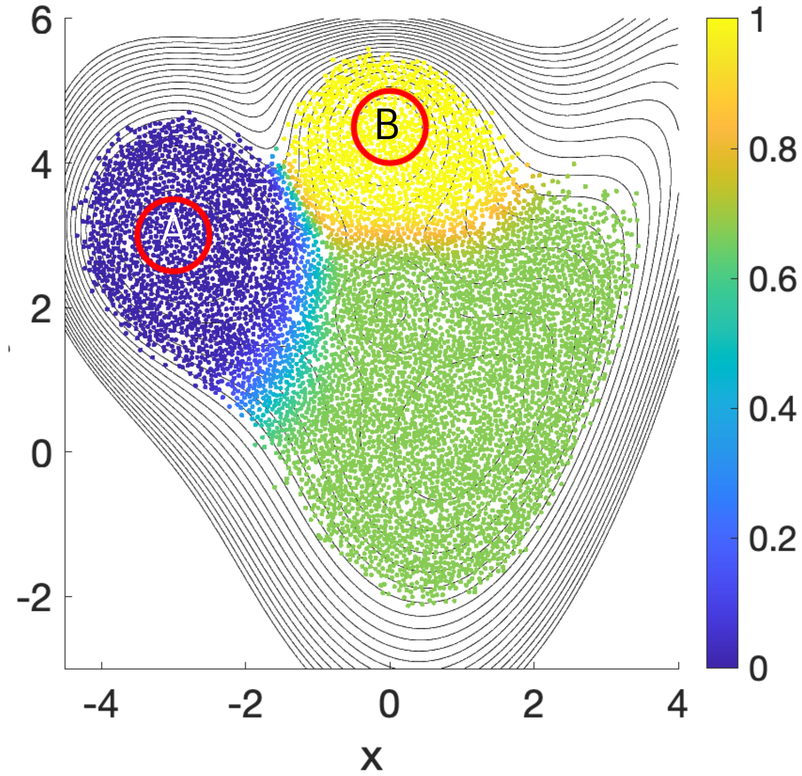
Approach 2:

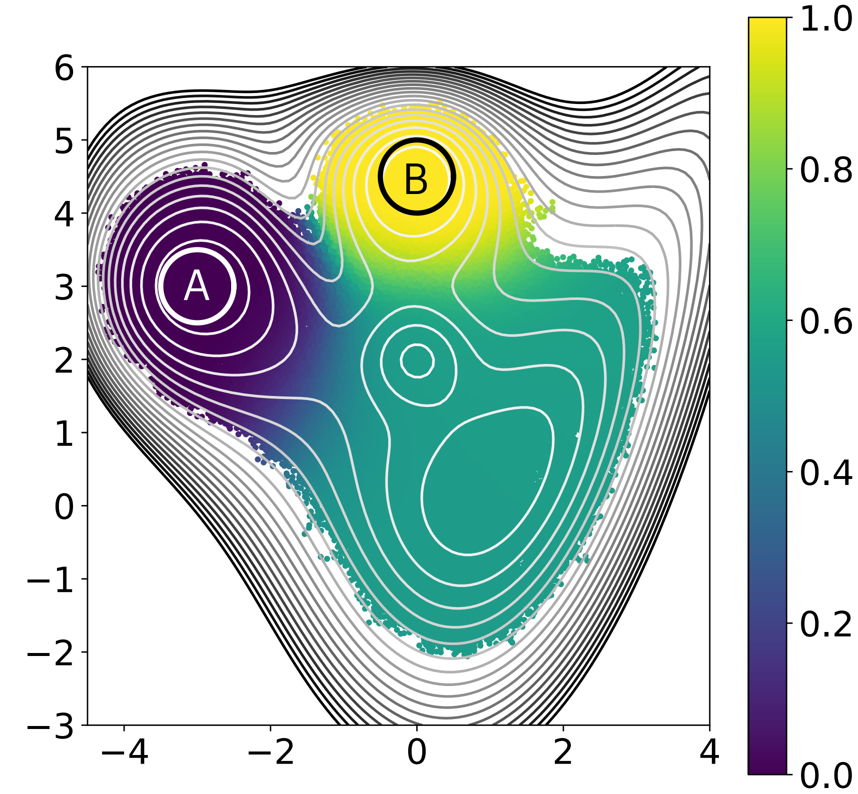
Target-measure diffusion map

Approach 3:

Neural network-based solvers







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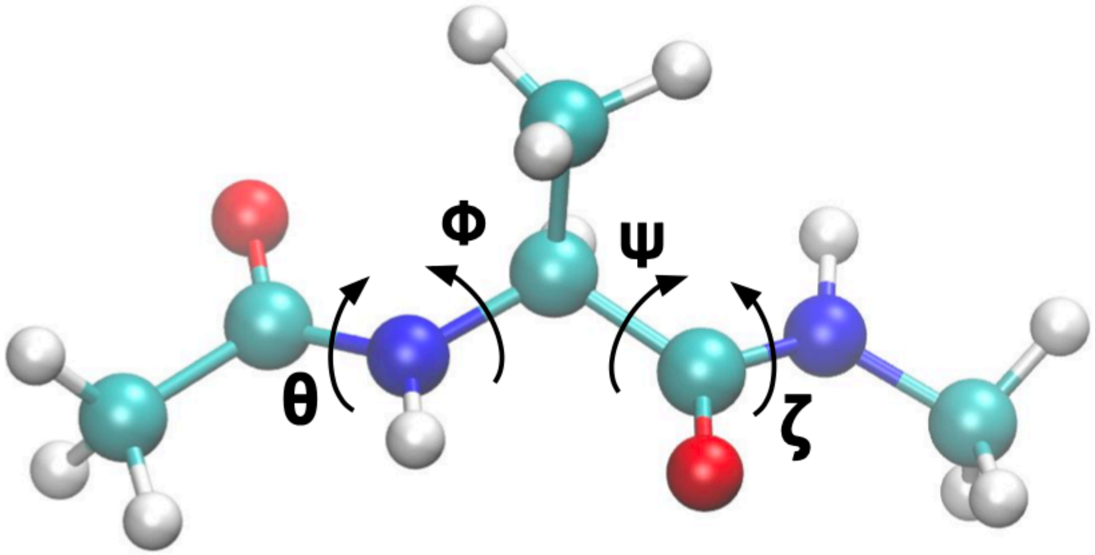
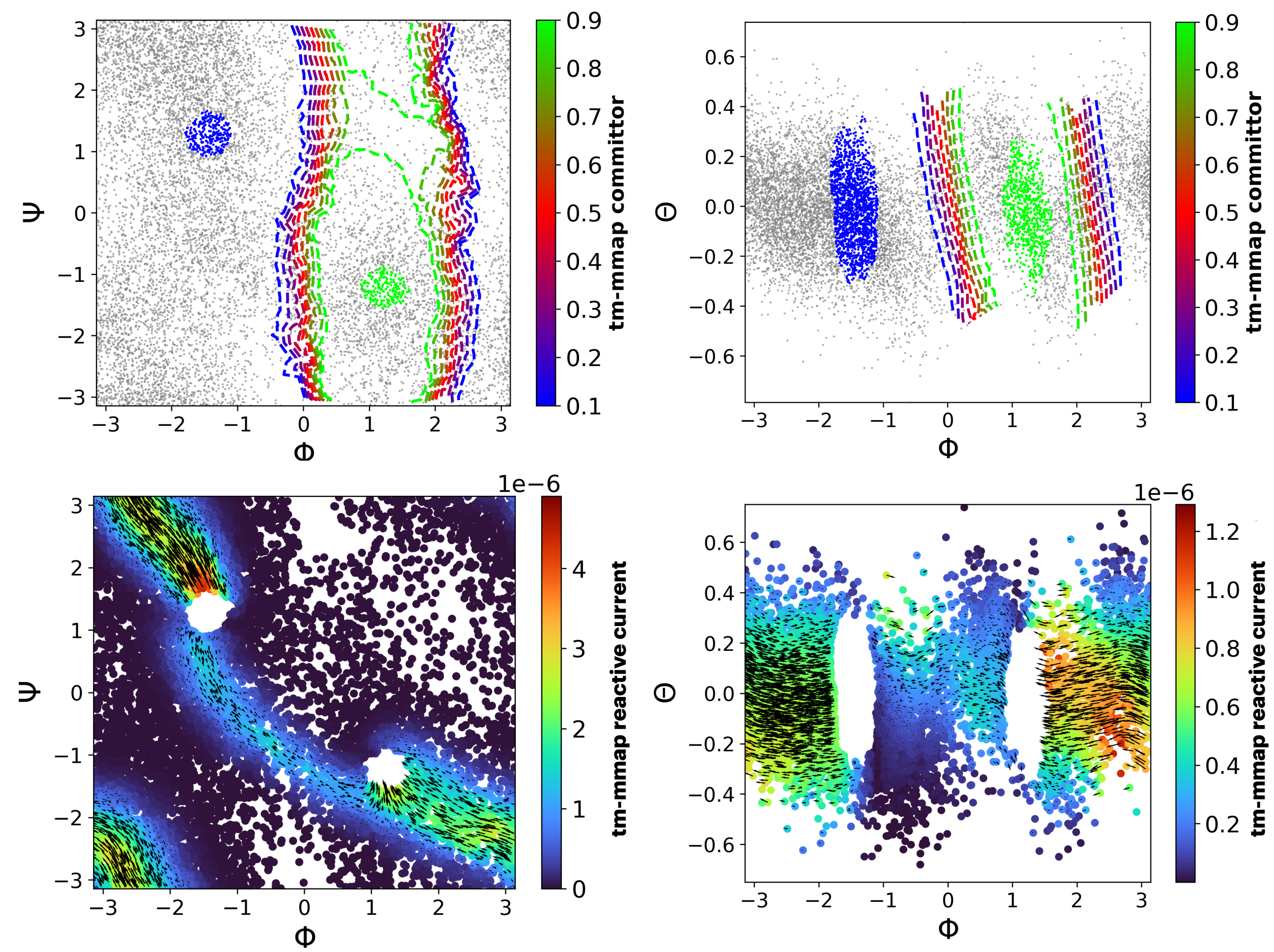
Model reduction via physically motivated collective variables





$$dX_t = [-M(X_t)\nabla F(X_t) + \beta^{-1}\nabla \cdot M(X_t)]dt + \sqrt{2\beta^{-1}}M(X_t)^{1/2}dw_t$$

Phase space: $\mathbb{T}^4$

Method: target-measure Mahalanobis diffusion map (Evans, MC, Tiwary, 2022)

$\texttt{tmmmap} + \texttt{deltanet}$:

$2.0 \cdot 10^{-6}\ \mathrm{ps}^{-1}$

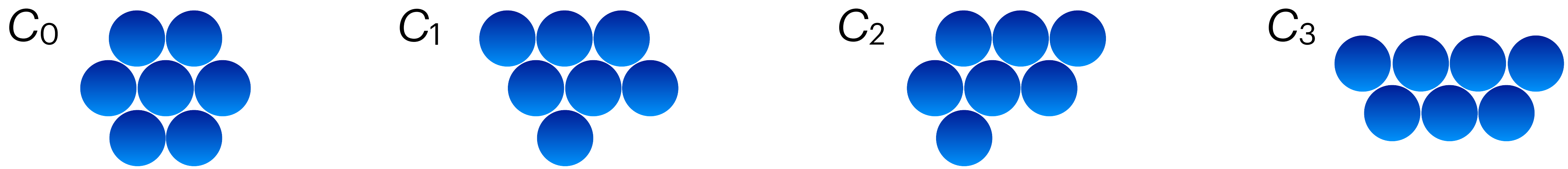
long trajectory :

(Vani, Weare, Dinner, 2022)

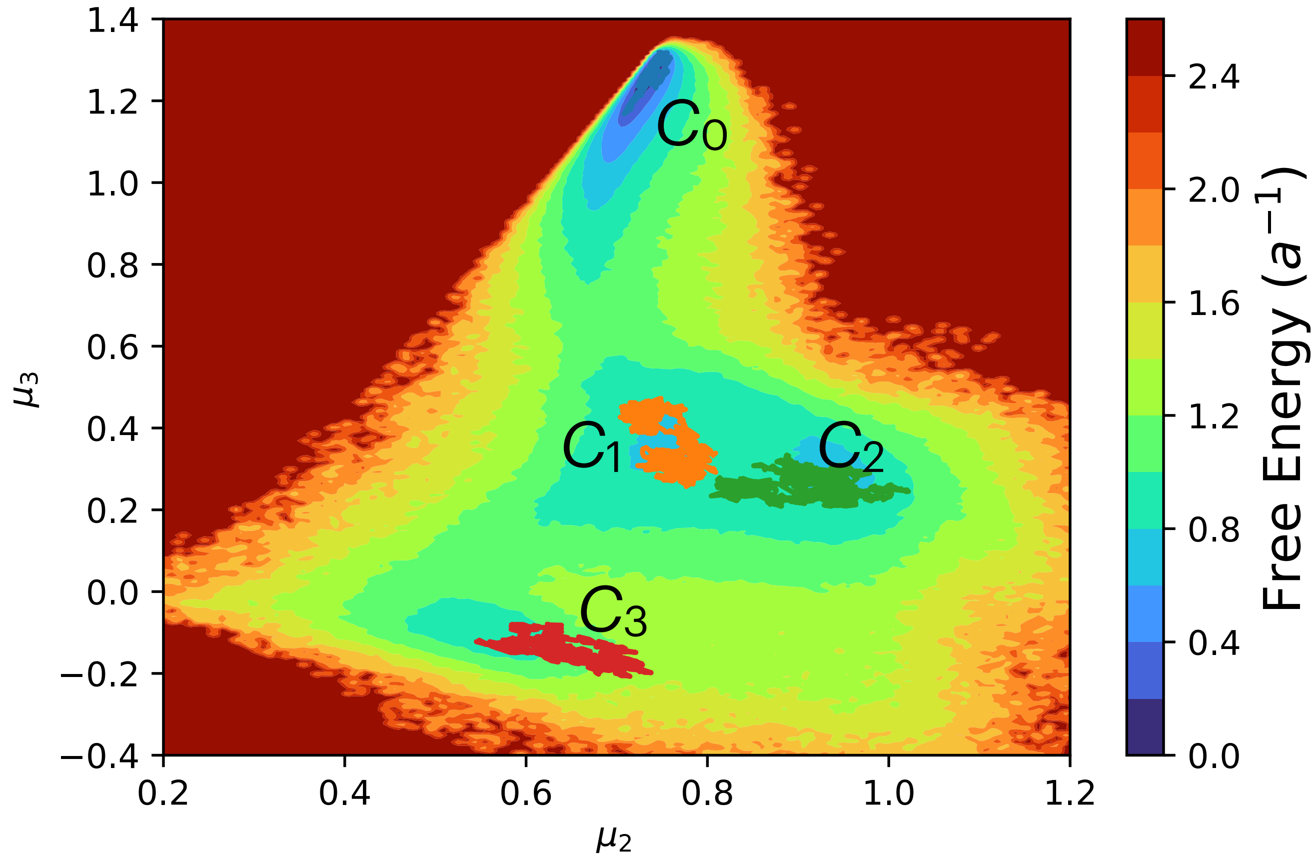
$1.4 \cdot 10^{-6}\ \mathrm{ps}^{-1}$

Model reduction via machine-learned collective variables

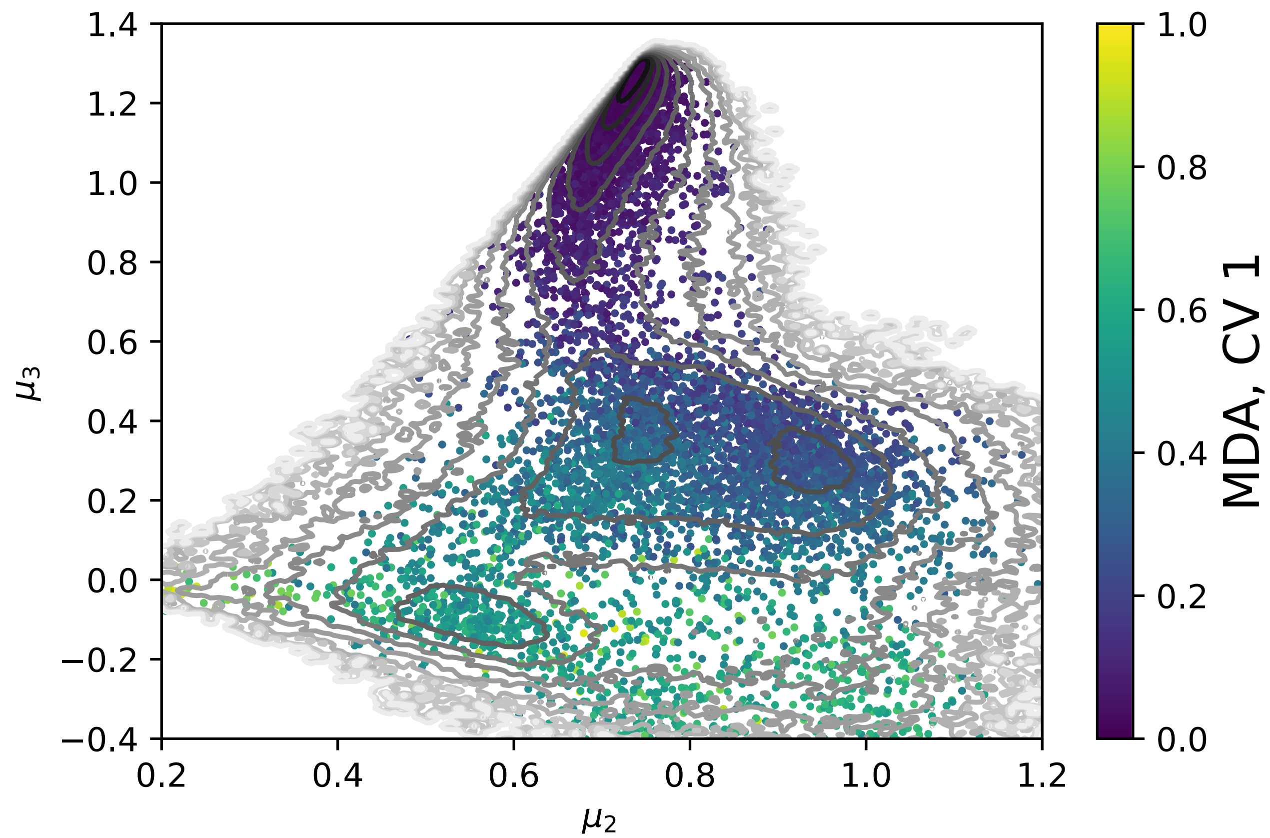
Linear discriminant analysis (LDA)



Physically motivated collective variables and labeled data

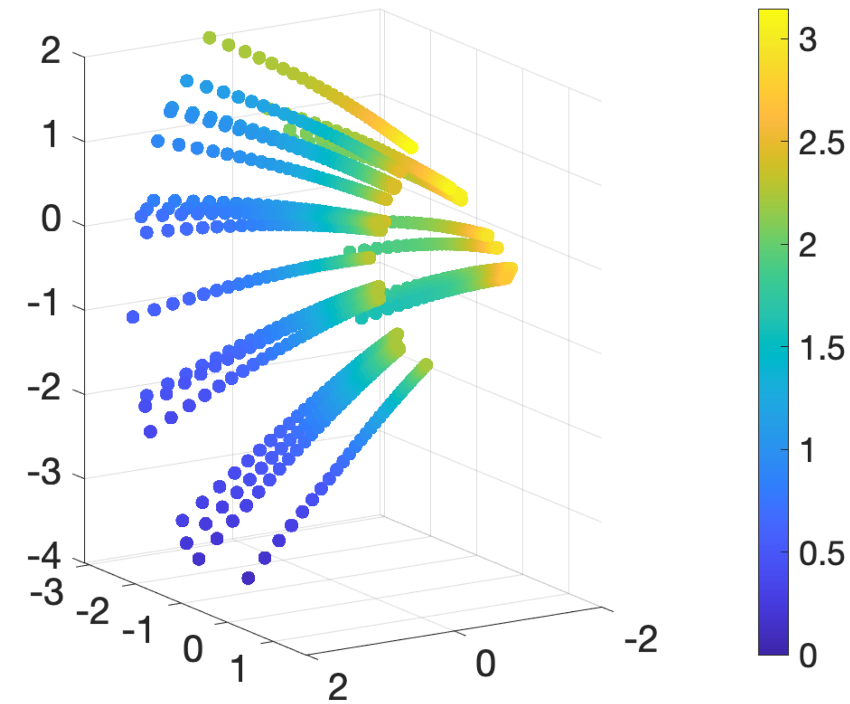


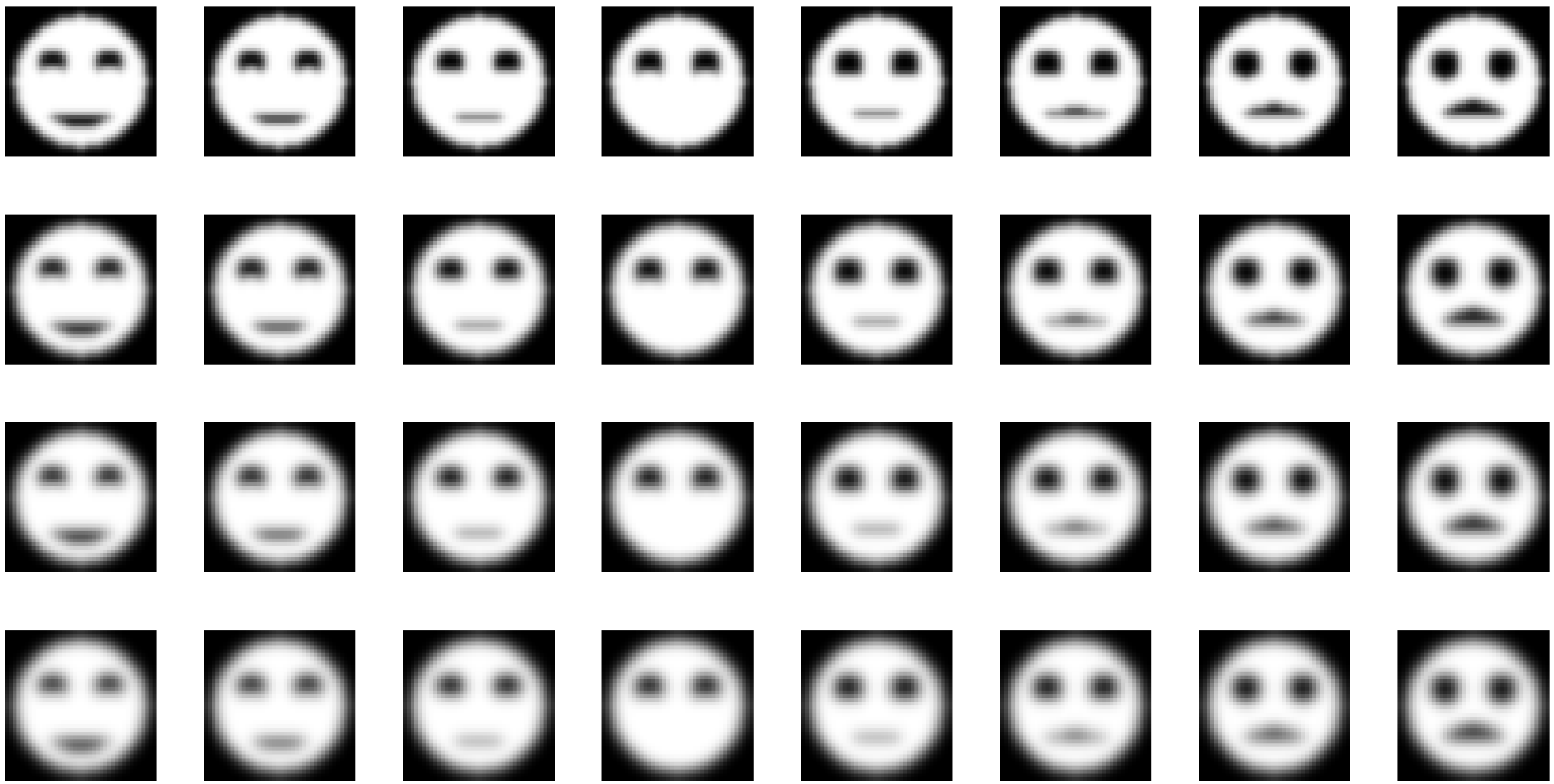
The collective variable learned by the LDA



Model reduction via diffusion maps

Coifman and Lafon, 2006

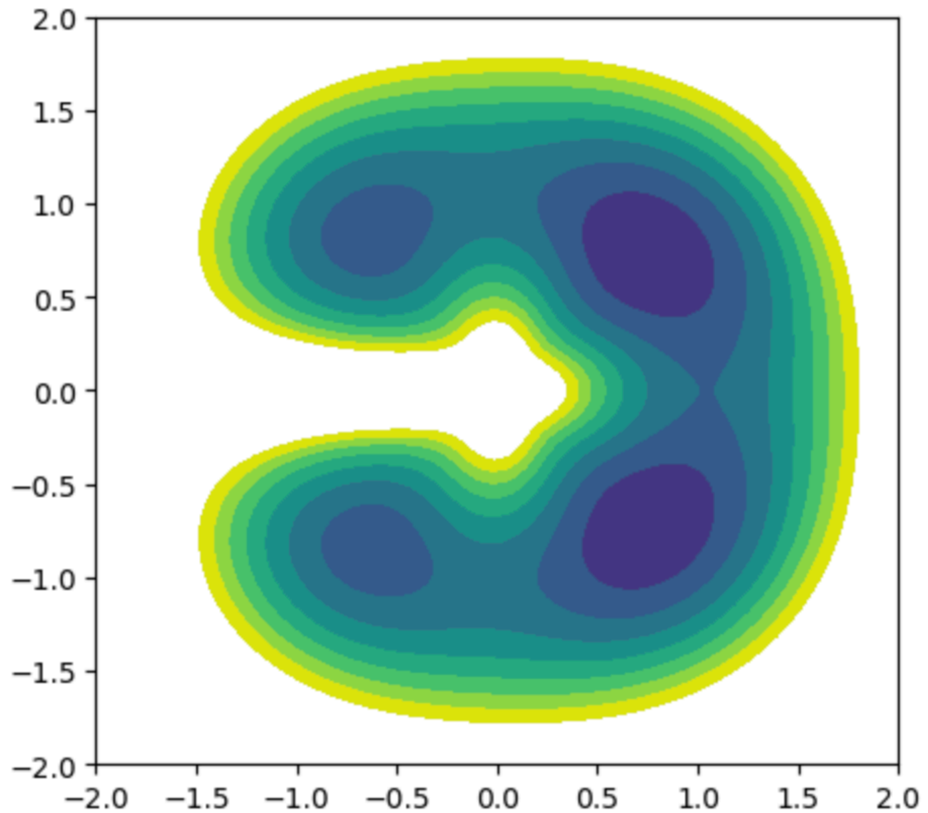


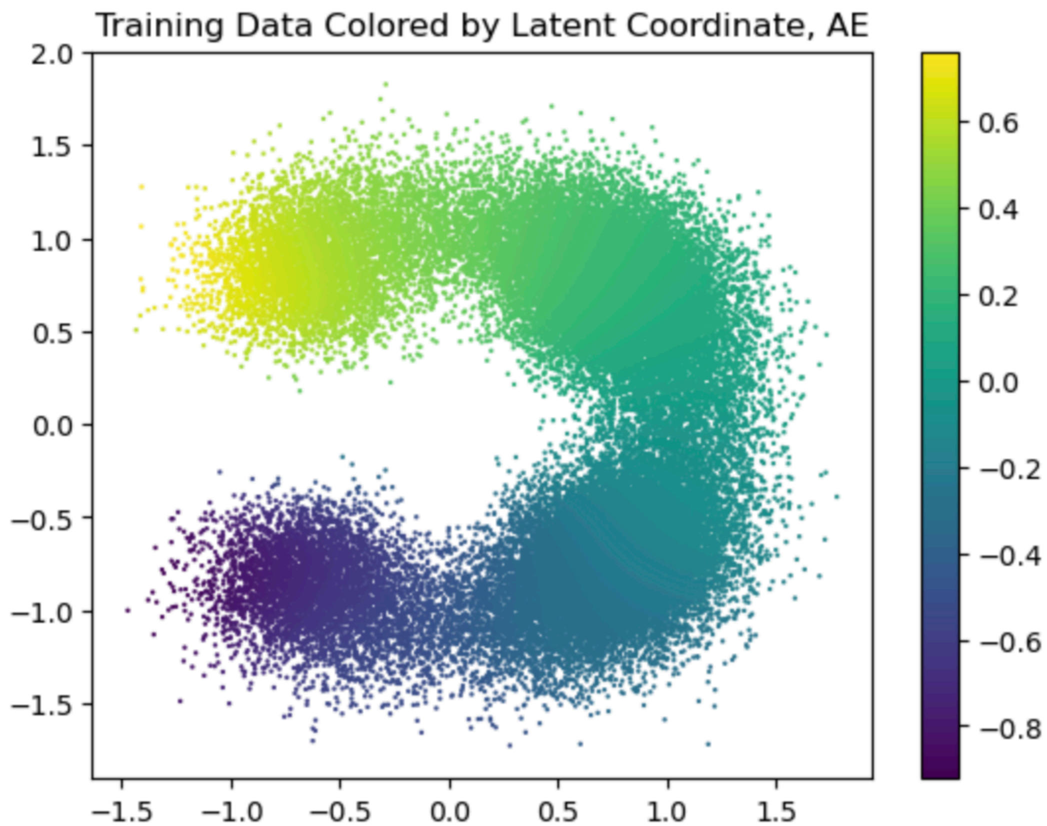


Model reduction via machine-learned collective variables

Autoencoders
Tutorial:
https://deeptime-ml.github.io/latest/notebooks/tae.html
implementation by L. Evans)

Lemon Slice Potential
https://www.mdpi.com/1099-4300/23/2/134

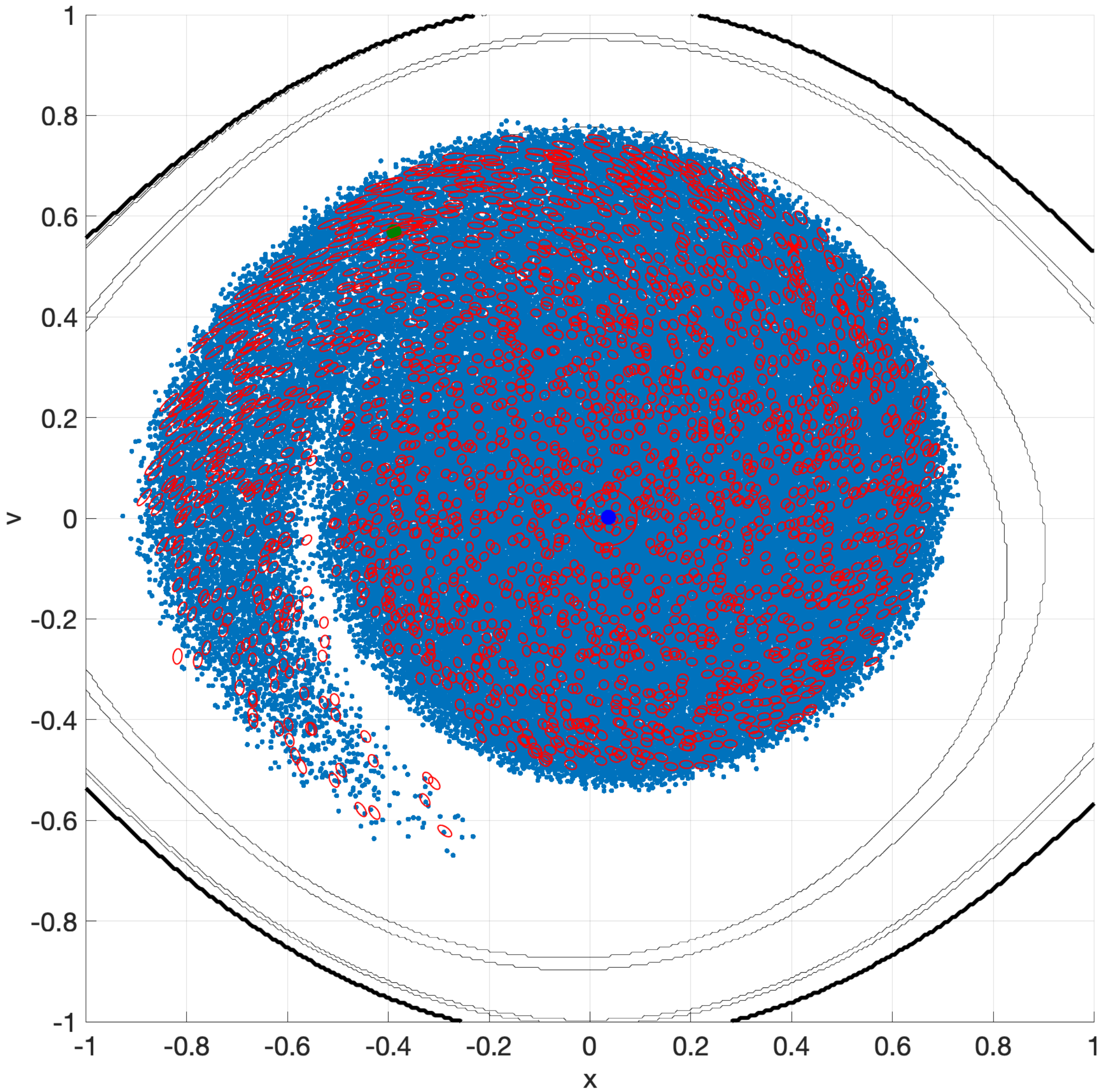


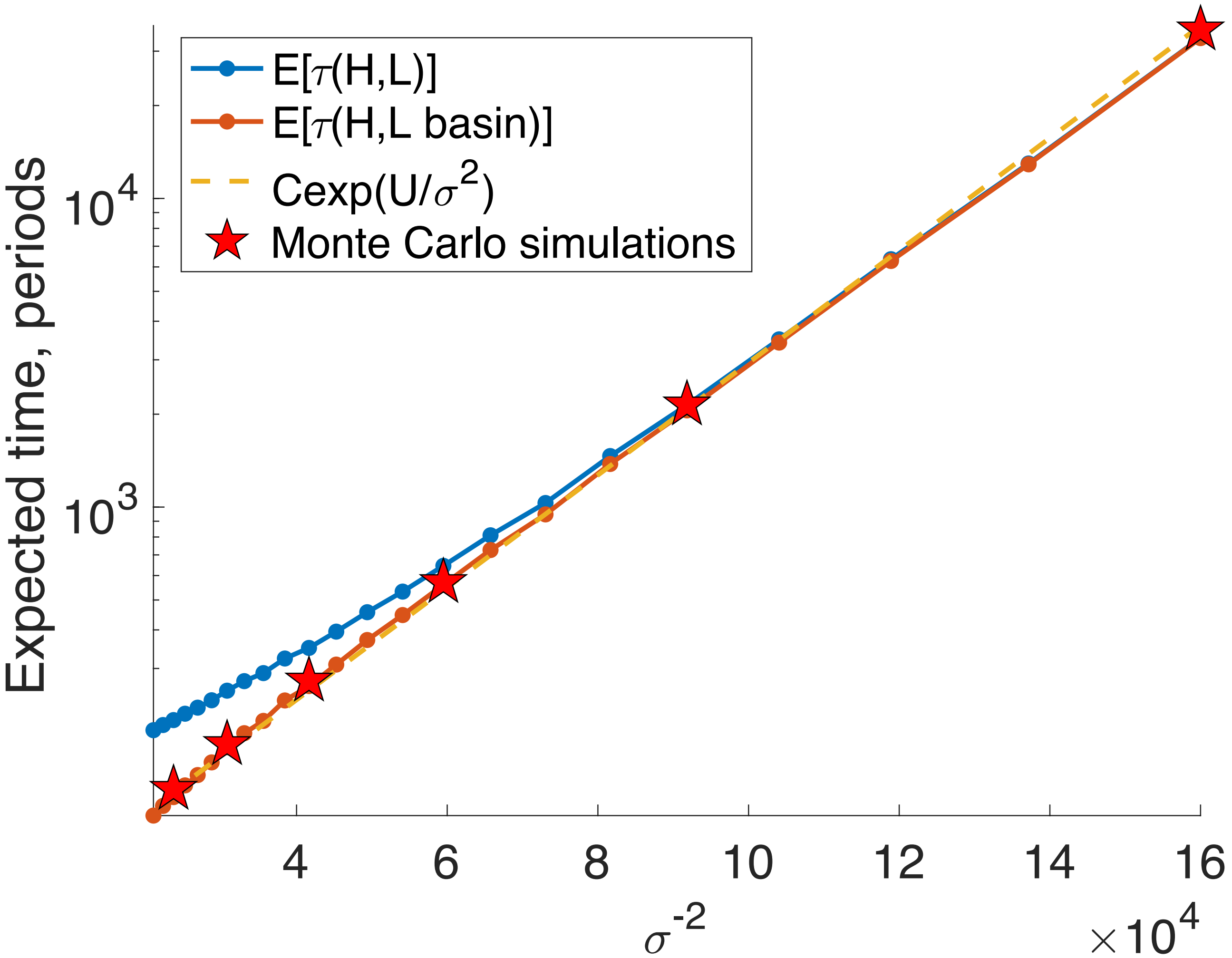


Model reduction via Markov chain

Noisy nonlinear oscillator with periodic forcing

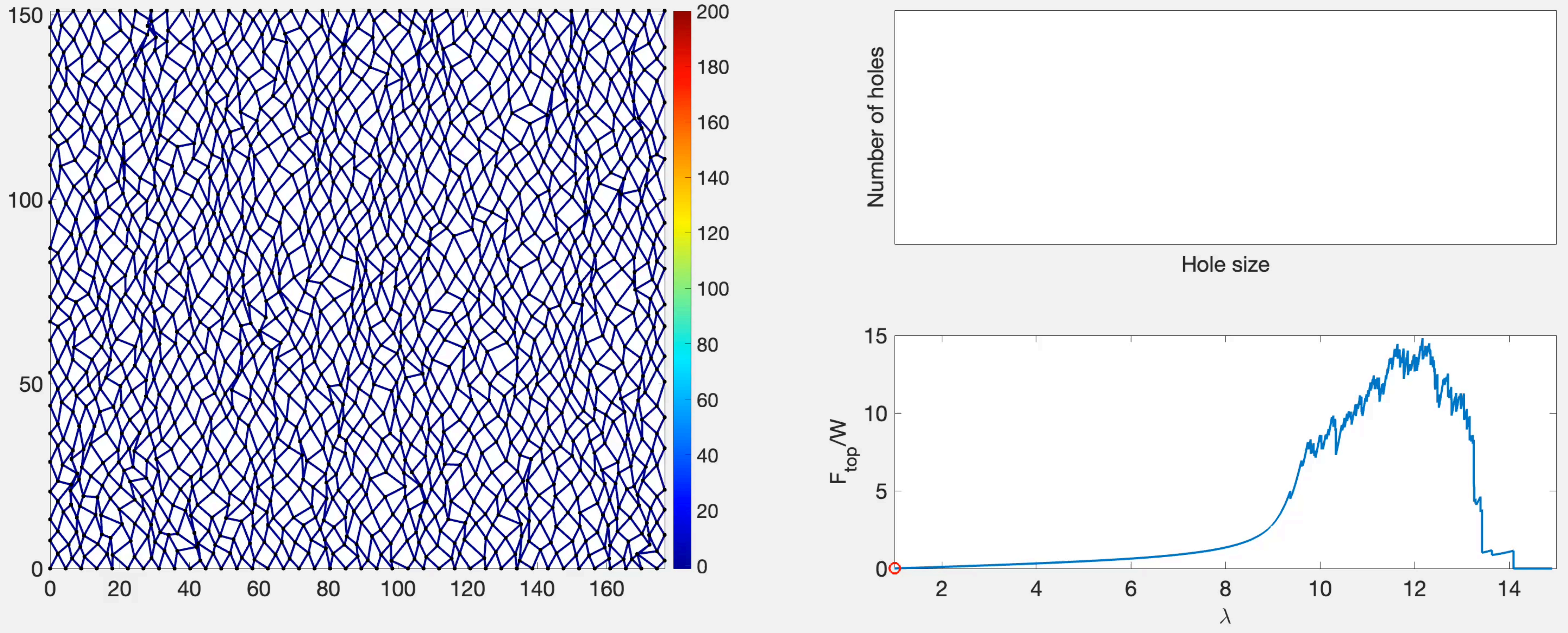
$$x'' + ax' + c_1x + c_3x^3 = F\cos(\omega t) + \sigma\eta_t$$





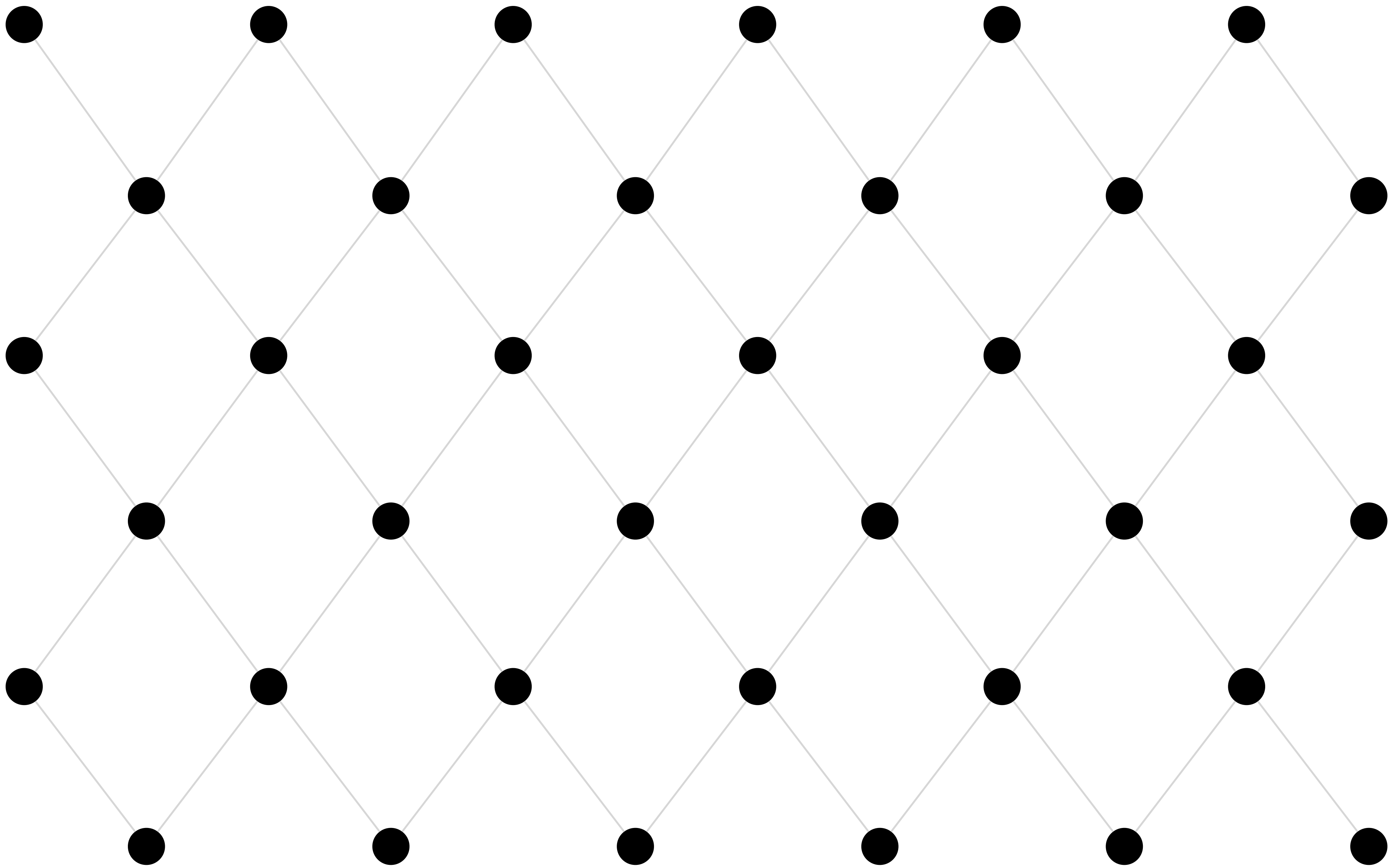
Polymer network fracture and random graphs

Manyuan Tao, work in preparation



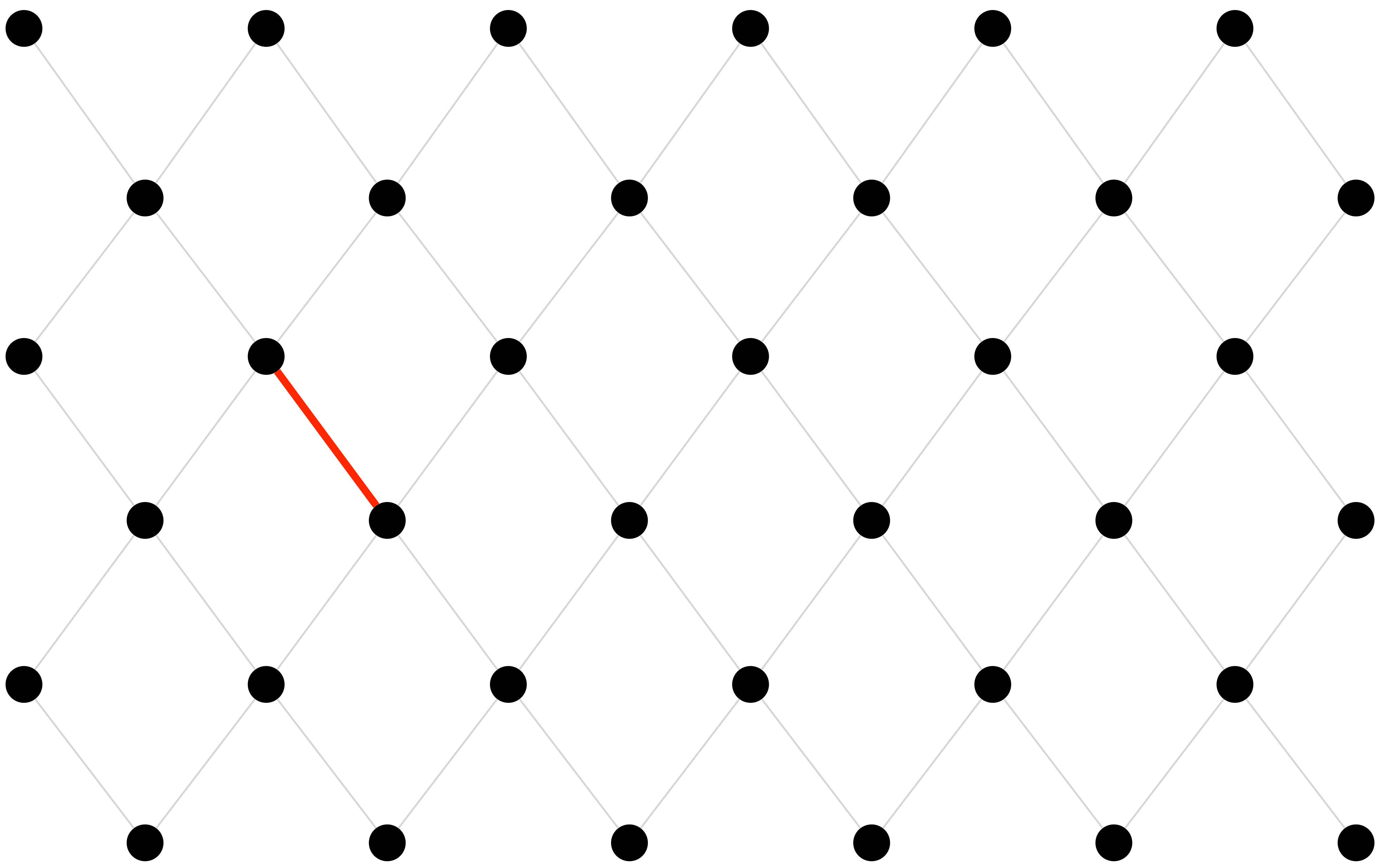
Goal: develop a random graph model describing the evolution of holes

Vertices = the network cells. Initially, there are no holes, hence no edges



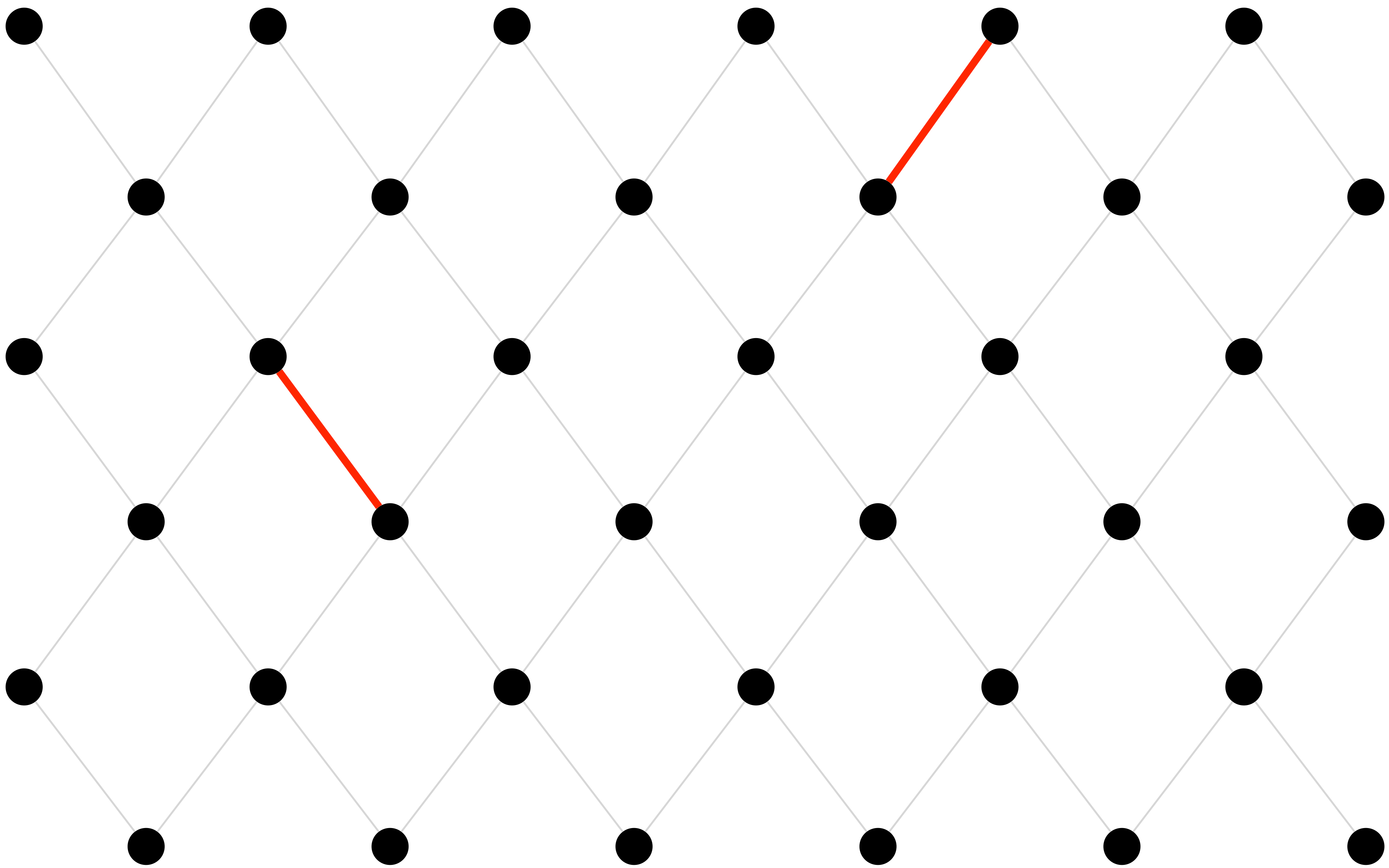
Goal: develop a random graph model describing the evolution of holes

Time = 1: add one edge at random



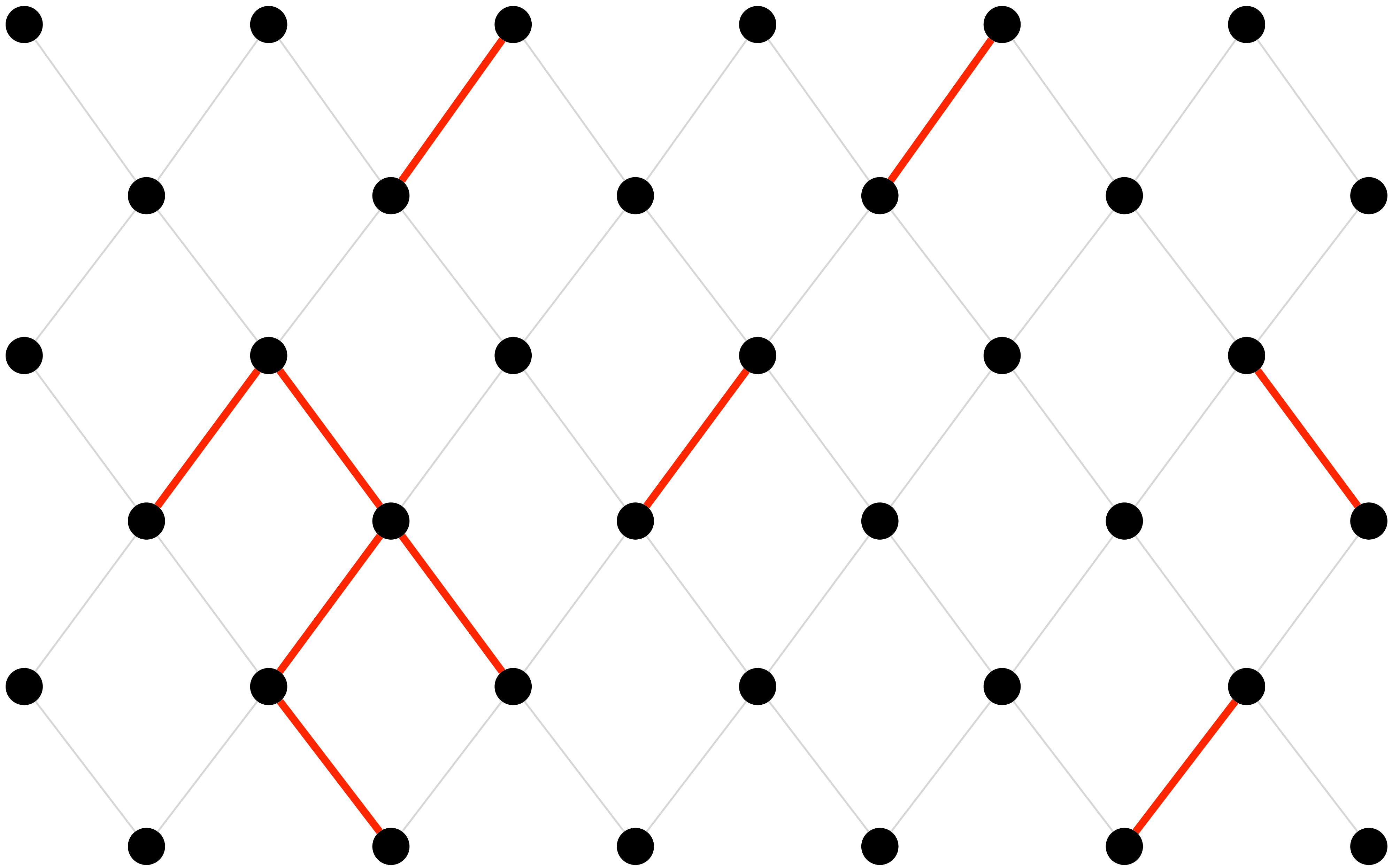
Goal: develop a random graph model describing the evolution of holes

Time = 2: add one edge at random



Goal: develop a random graph model describing the evolution of holes

Time = j: j edges



Goal: develop a random graph model describing the evolution of holes

Research plan and research questions

- Assume that the network is N-by-N where N is large.
- Start with the assumption that the edges are added uniformly at random.
- Predict the size distribution of connected components at time t.
- Predict time at which the giant component arises.
- Predict the time or complete fracture for the polymer network.
- Compare with the experimental data.
- Assume a preferential attachment model for adding edges.
- Predict the component size distribution, the time at which the giant component arises, and the time of fracture of the polymer network.