Computational methods for modeling rare events

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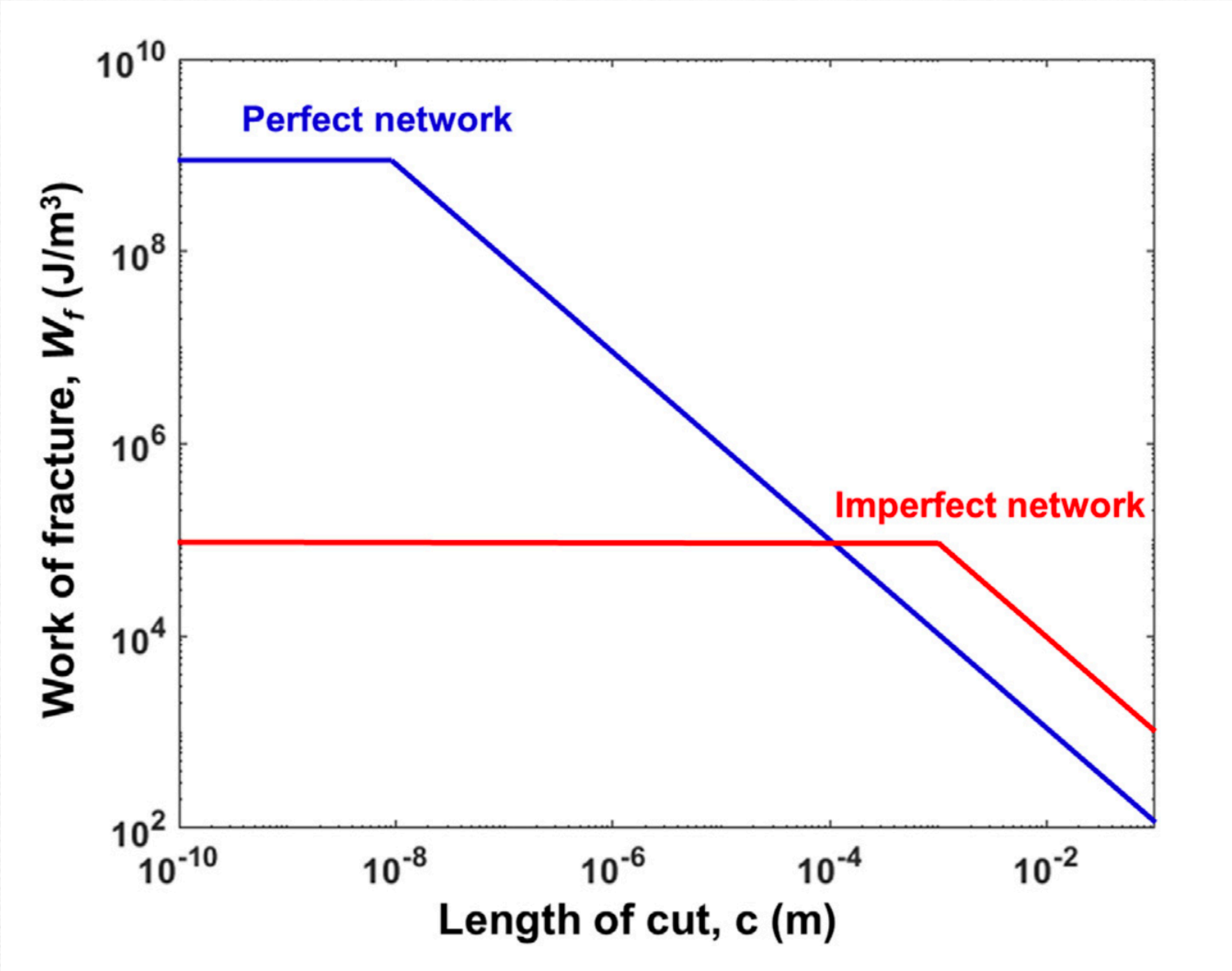
Agenda

- Microscopic models for material fracture (joint project with Z. Suo's group)
- Model reduction for chemical reaction networks (joint project with E. Reed's group)
- Systems of interacting particles: aggregation, dissociation, cluster rearrangements
- Computing quasipotentials, escape paths and expected escape times in nongradient SDEs

The fracture quest

Joint work with Z. Suo's group



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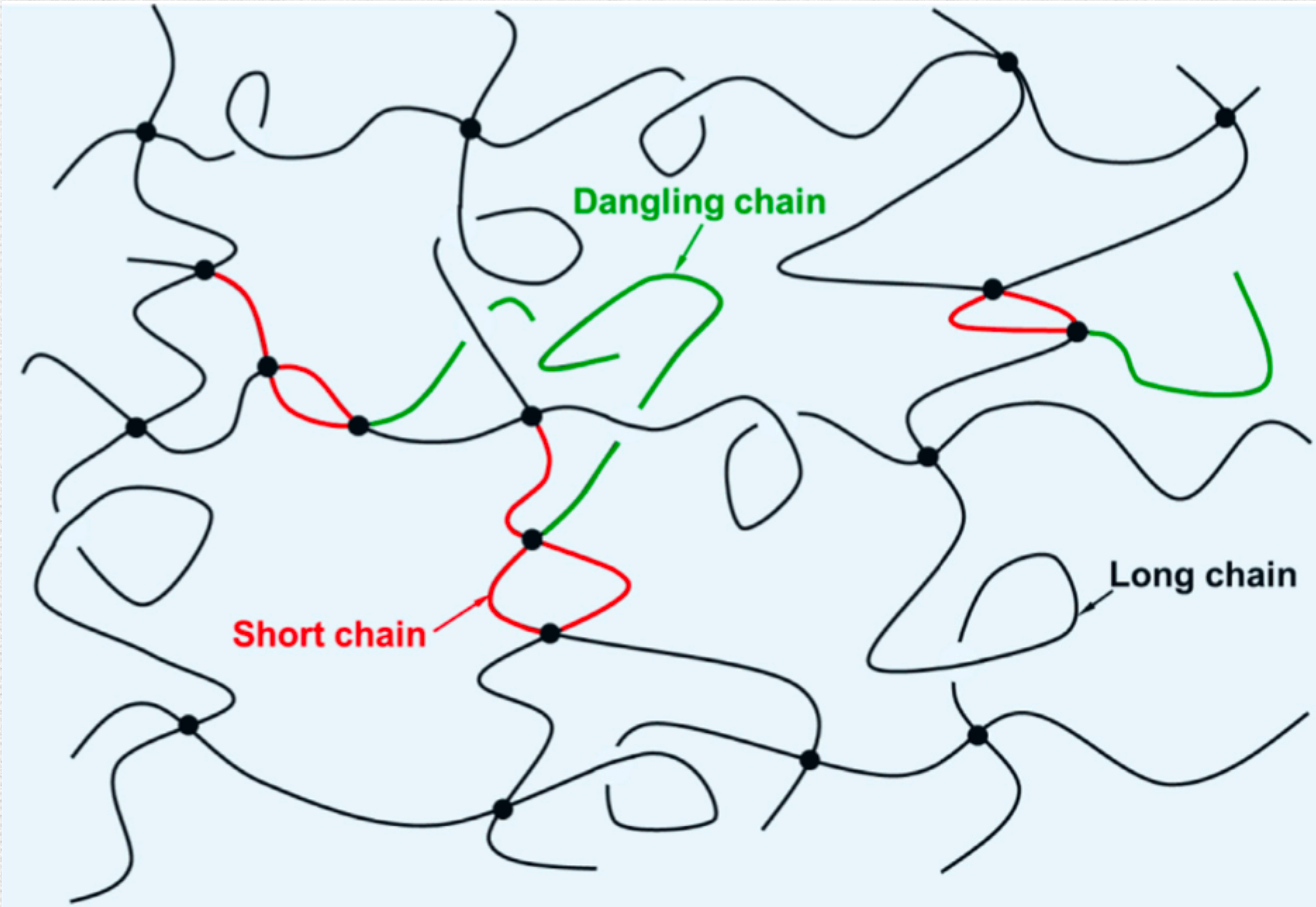
What is going on?



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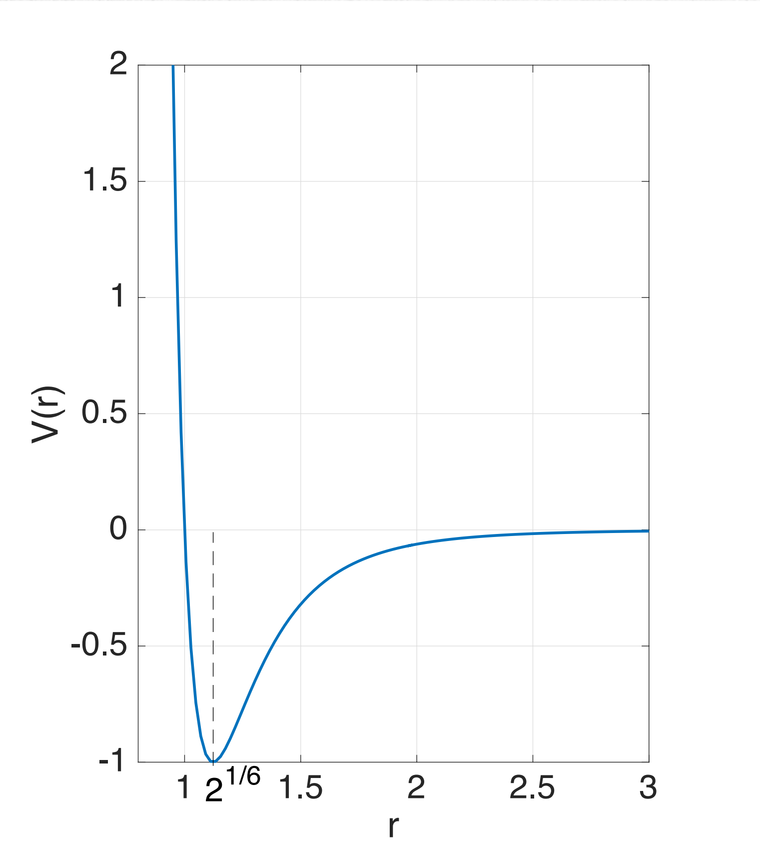
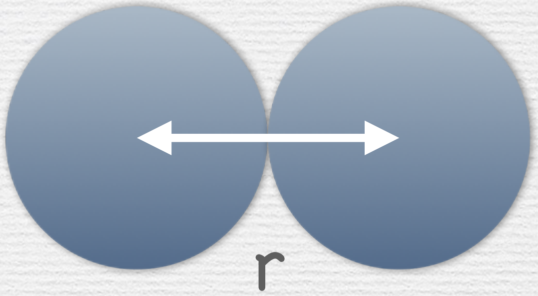
Aggregation and dynamics of Lennard-Jones clusters

$$V(r) = 4(r^{-12} - r^{-6})$$





Adequate for rare gases:
Ar, Kr, Xe, Rn

Often used for modeling interaction of other spherical particles.

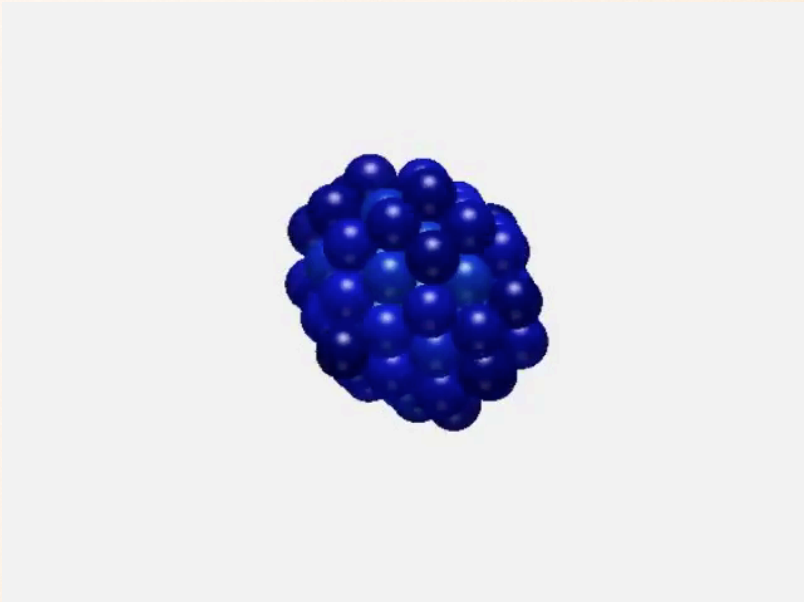
Large datasets are available thanks to Wales's group (Cambridge, UK).

DIFFICULTIES IN MODELING THE DYNAMICS OF LJ CLUSTERS

- High dimensionality:
  3n coordinates, 3n momenta

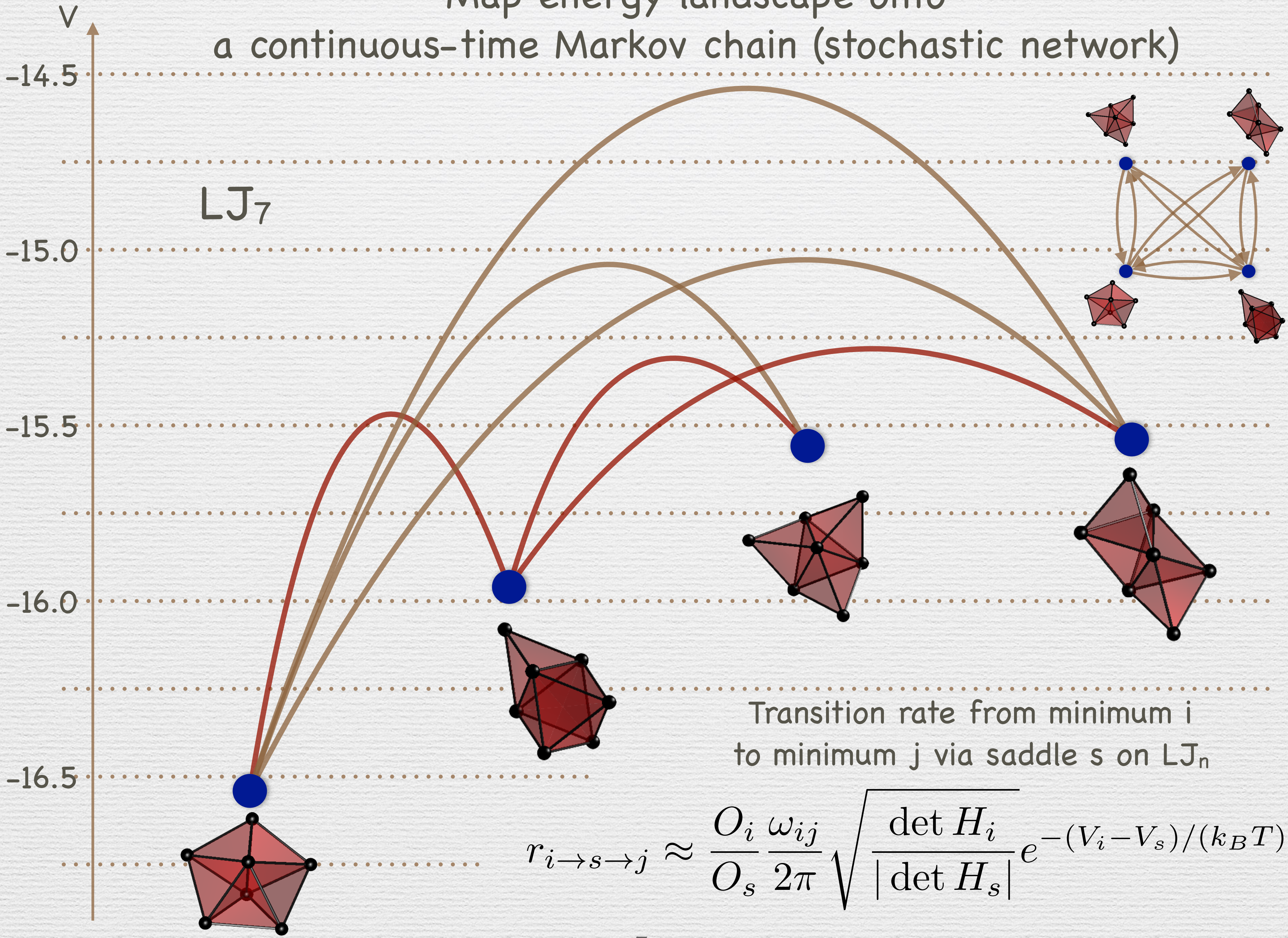
- Long waiting time in direct simulations:
  structural transitions occur rarely on the timescale of the system

- Large range of timescales for various transition processes



LJ_{75}

Map energy landscape onto a continuous-time Markov chain (stochastic network)



Transition rate from minimum i to minimum j via saddle s on LJ_n

$$r_{i\to s\to j} \approx \frac{O_i}{O_s}\frac{\omega_{ij}}{2\pi}\sqrt{\frac{\det H_i}{|\det H_s|}}e^{-(V_i-V_s)/(k_BT)}$$

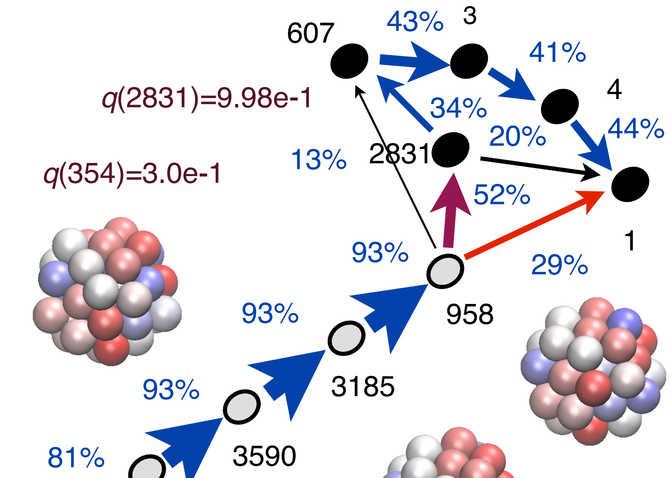
Joint work with E. Vanden-Eijnden, 2014

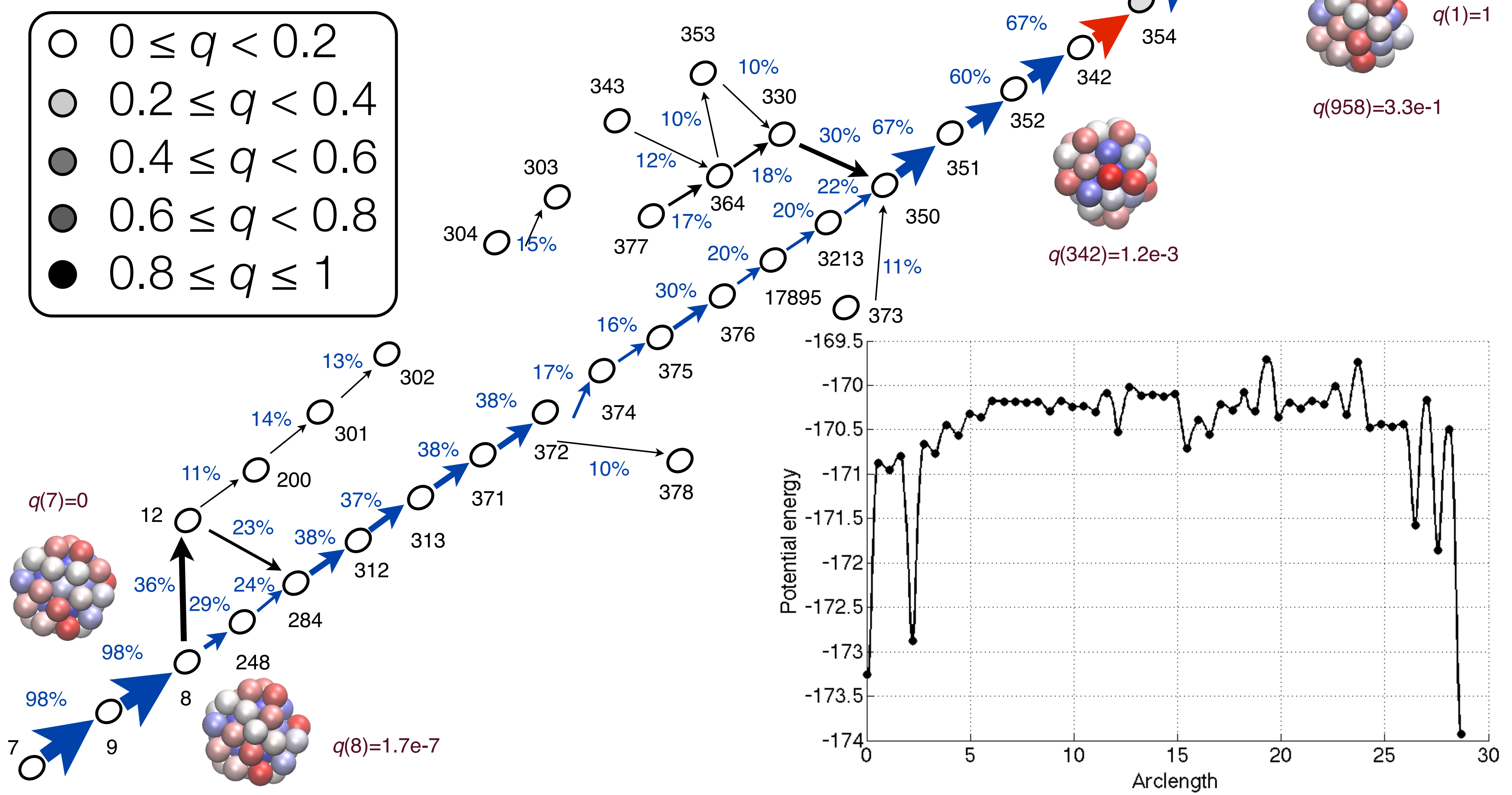
LJ38

Cartoon of the transition process at T=0.06:

Still good agreement with the LDT prediction:

The **dominant representative pathway** coincides with the **minimax pathway**

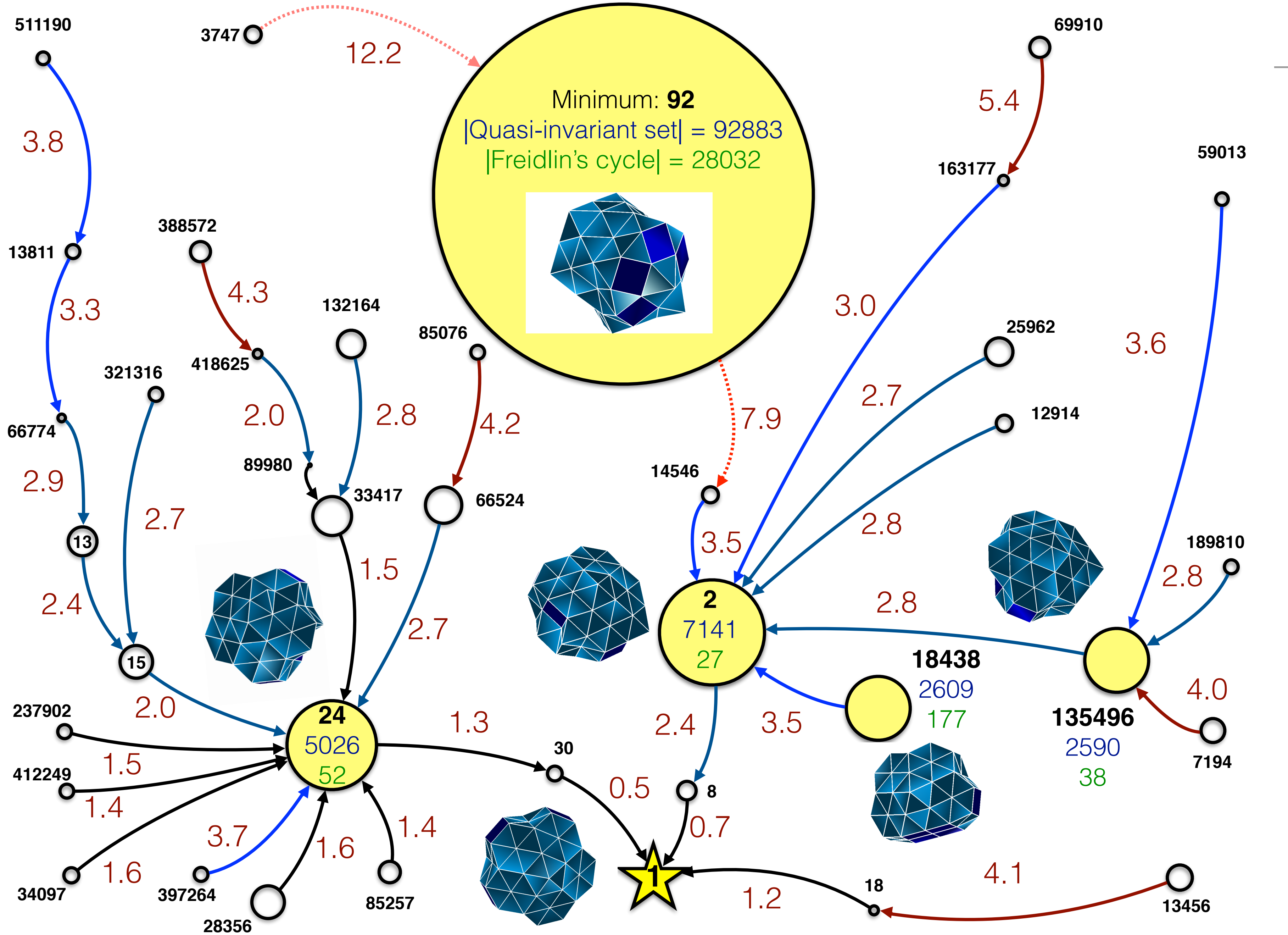




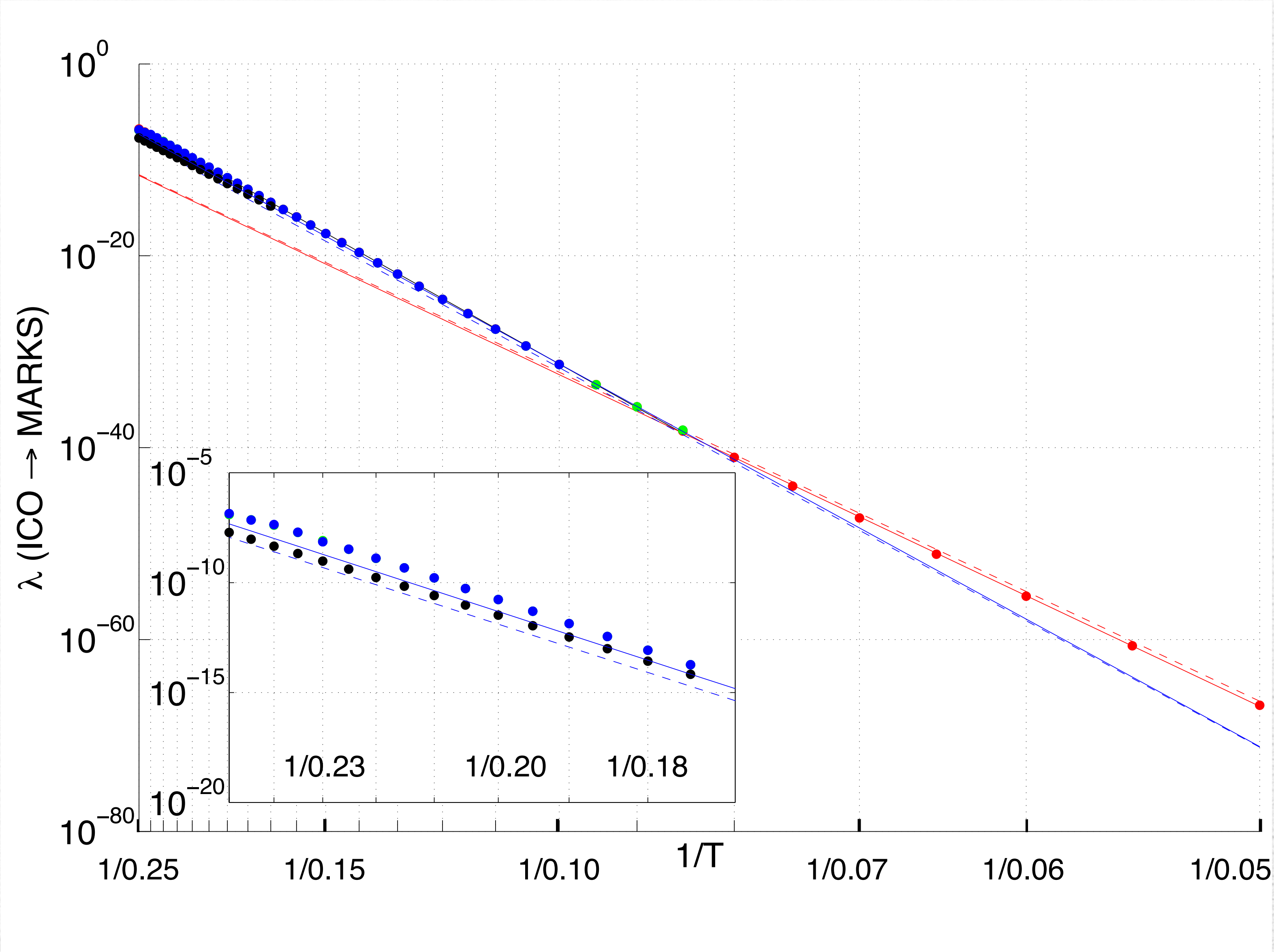
LJ75

Joint work with T. Gan, 2016

Largest quasi-invariant sets (> 100 local minima)



Asymptotic spectral analysis and finite temperature continuation



Joint work with T. Gan, 2016

Van de Waal's hypothesis

Mass spectrography by electron or X-ray diffraction (since 1980s)

Results: clusters with < ~1500 atoms have icosahedral packing; larger clusters have FCC packing

Van de Waal, PRL, 1996

No Evidence for Size-Dependent Icosahedral —> FCC Structural Transition in Rare-Gas Clusters

Faulty face-centered cubic layers grow on icosahedral core

Experimental confirmation:

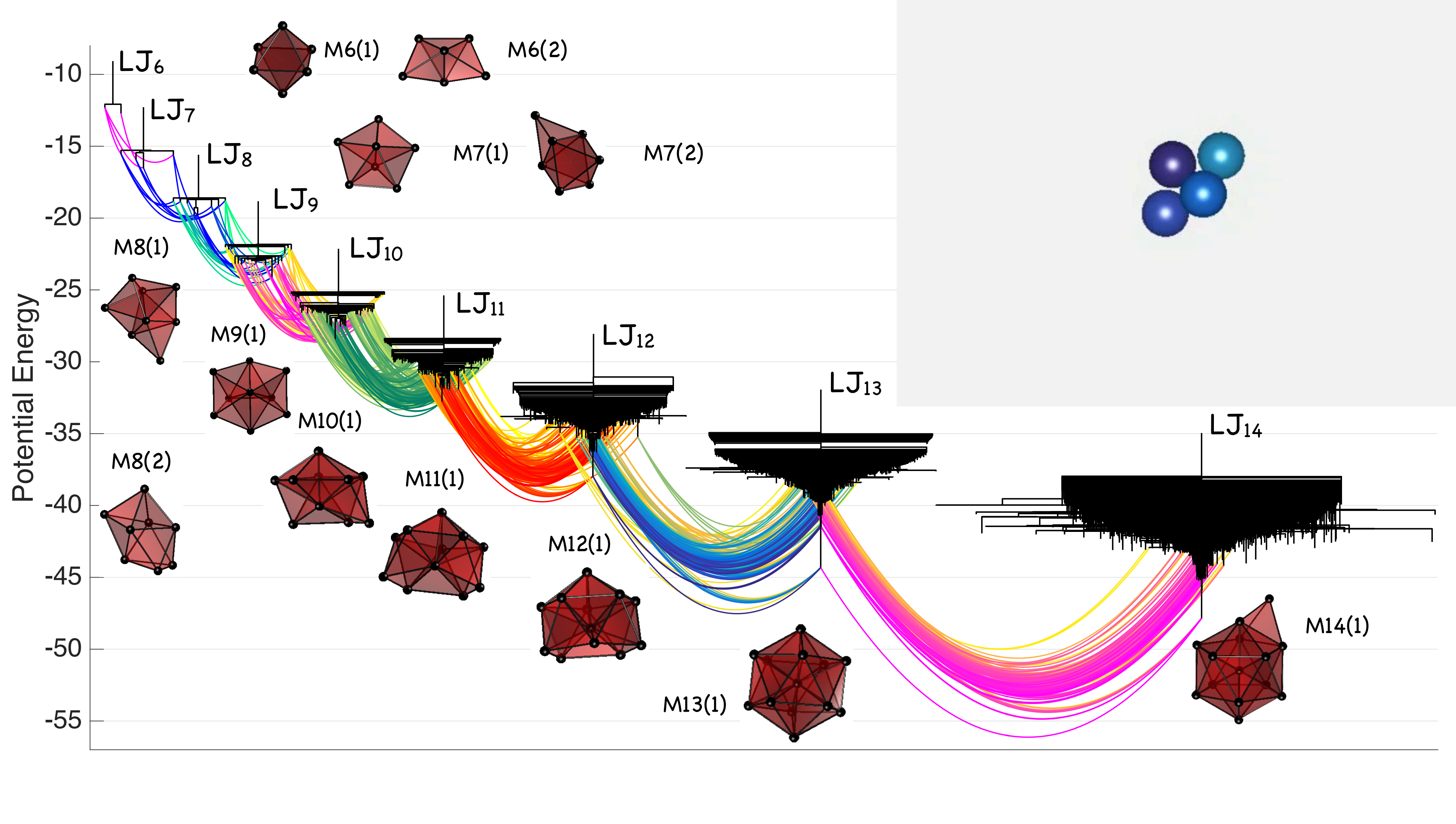
Kovalenko, Solnyshkin, Verkhovtseva, Low Temp Phys, 2000

On the mechanism of transformation of icosahedral rare-gas clusters into FCC aggregations

The experimental results correlate with the calculation if it is assumed that the clusters have a face-centered cubic structure with a constant number of intersecting stacking faults.

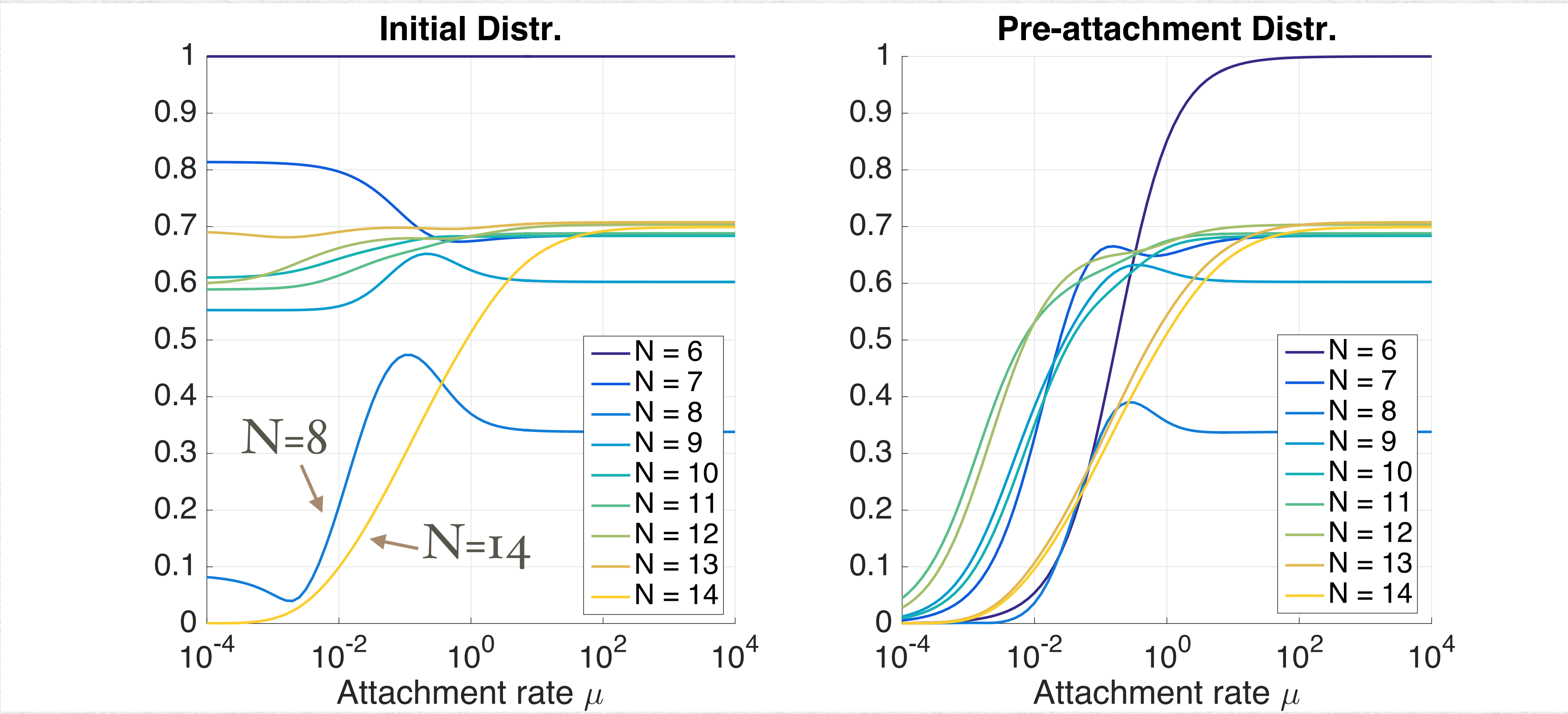
LJ6 – 14 aggregation/deformation network

Y. Forman, S. Sousa and M. Cameron (REU 2016)



Attachment does mixing

A normalized RMS deviations from the invariant distributions



β^{-1} = 0.10

Perspectives

- Adapt the developed techniques to coarse-graining of chemical reaction networks
- Importance sampling of configurations
- Allowing dissociations of particles from clusters
- Other kinds of interacting particles, e.g. sticky particles

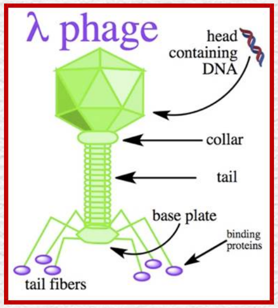
Computational methods for analysis of large deviations in SDEs

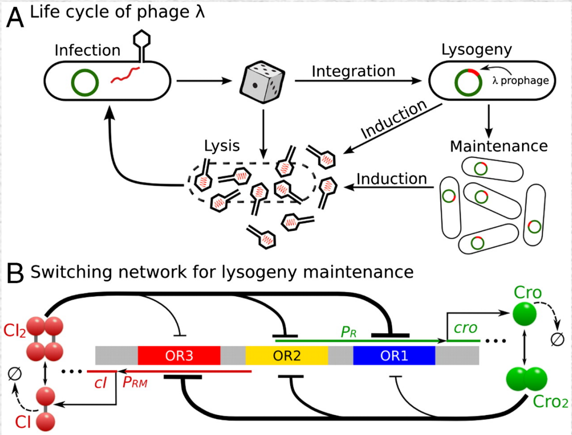
Quasipotential for nongradient SDEs

$$dx = b(x)dt + \sigma(x)\sqrt{\epsilon}dw$$

Biological and ecological models

- Genetic switches
  - Lambda Phage (Shea et al. (1980s), Aurell and Sneppel (2002)), 2D
  - Two-state gene expression model with positive feedback (Lv et al. 2014), 3D



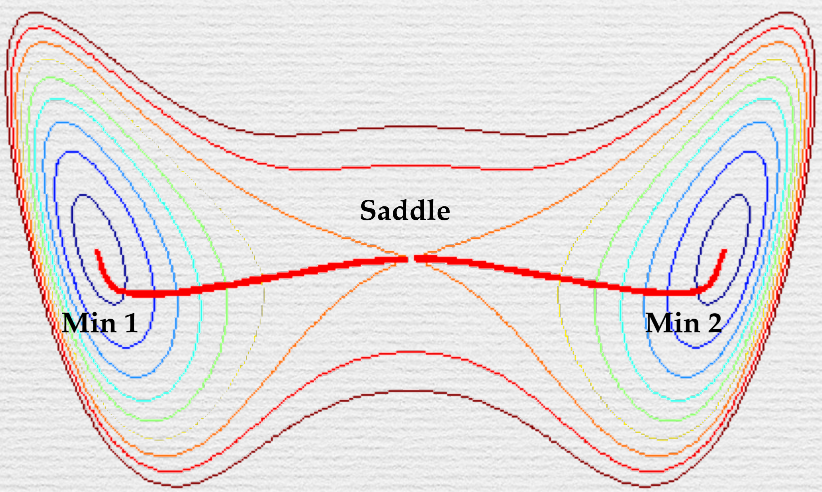


- Population dynamics
  - Dynamics of savanna landscapes (Touboul et al. 2017), 3D or 4D
  - Consumer-resource model (Collie & Spencer (1994), Steele and Henderson (1981)), 2D

Gradient vs nongradient SDEs

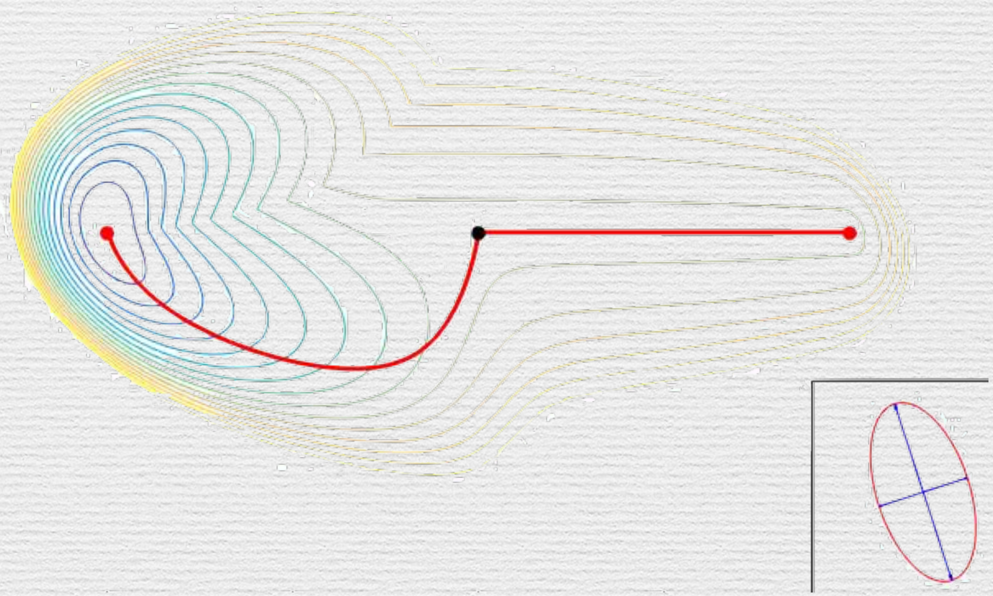
$$dx = -\nabla V(x)dt + \sqrt{2\beta^{-1}}dw$$

Potential $V(x)$ is given. It allows us to predict max likelihood transition paths and rates.



$$dx = b(x)dt + \sigma(x)\sqrt{\epsilon}dw$$

Potential $V(x)$ does not exist. We compute the ***quasipotential*** and predict escape path and rates.



Approach

Solve the optimal control problem on mesh:

$$U_A(x) = \inf_{\psi}\{S(\psi) \mid \psi(0) \in A, \psi(L) = x\} \text{ where}$$

$$S(\psi) = \int_0^L \|b(\psi)\|\Sigma^{-1}(\psi)\|\psi'\|\Sigma^{-1}(\psi) - \langle \psi', b(\psi)\rangle_{\Sigma}^{-1}(\psi)ds,$$

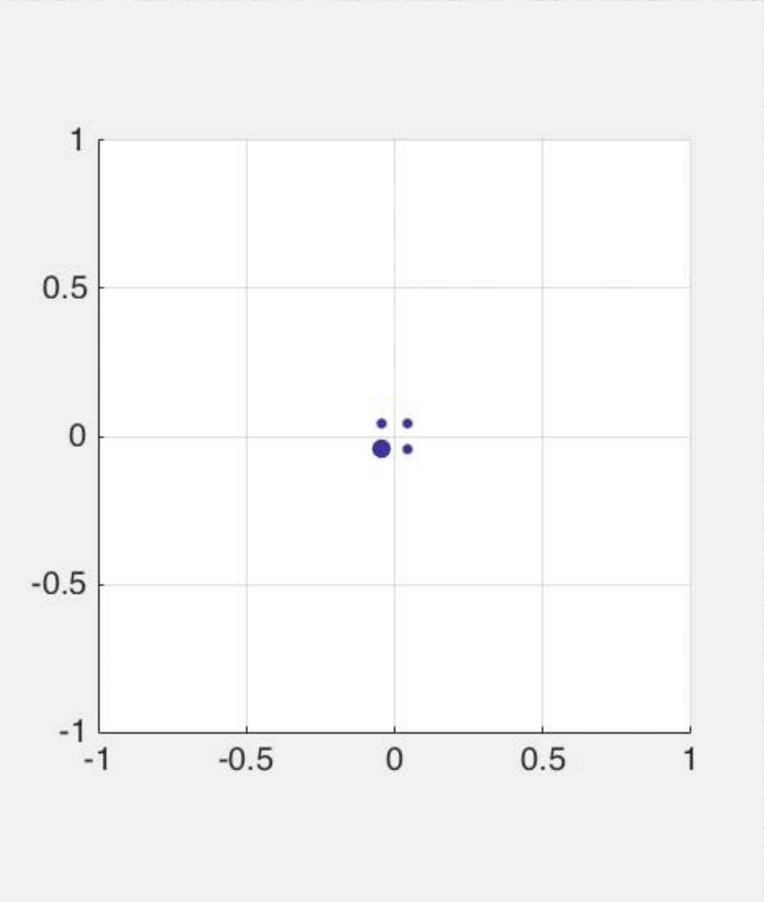
$$\Sigma(\psi) = \sigma(\psi)\sigma(\psi)^\top$$

Ordered line integral methods (OLIMs)

(Joint work with Dahiya, Yang, Potter, 2017—2019)

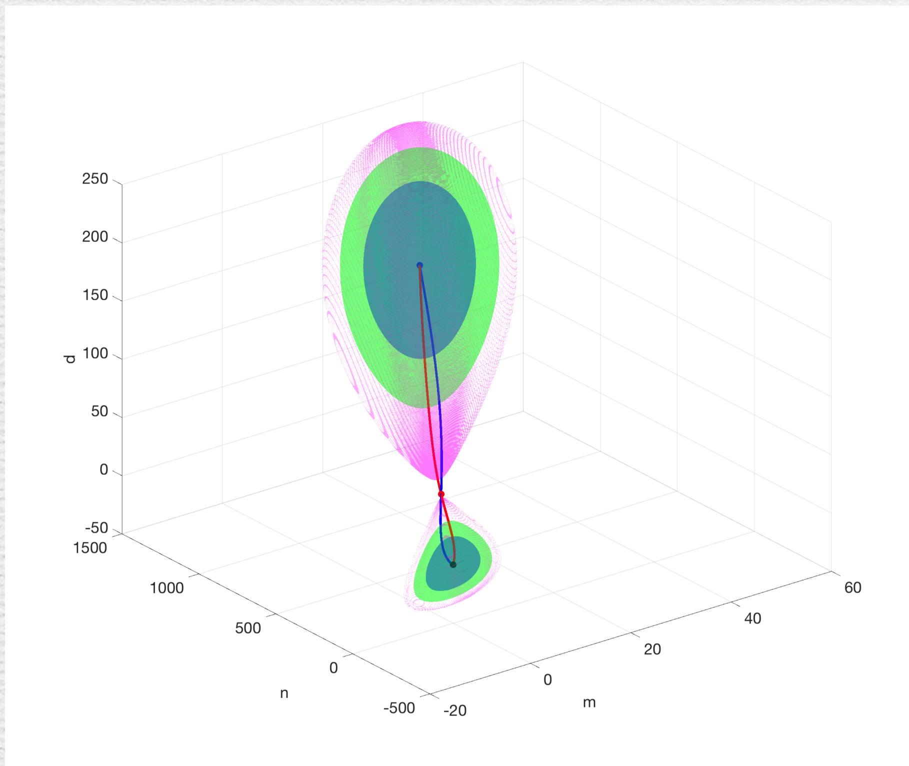
Take $\nabla U_A(x)$, shoot max likelihood escape paths.

$$\psi' = b(\psi) + \Sigma(\psi)\nabla U(\psi)$$

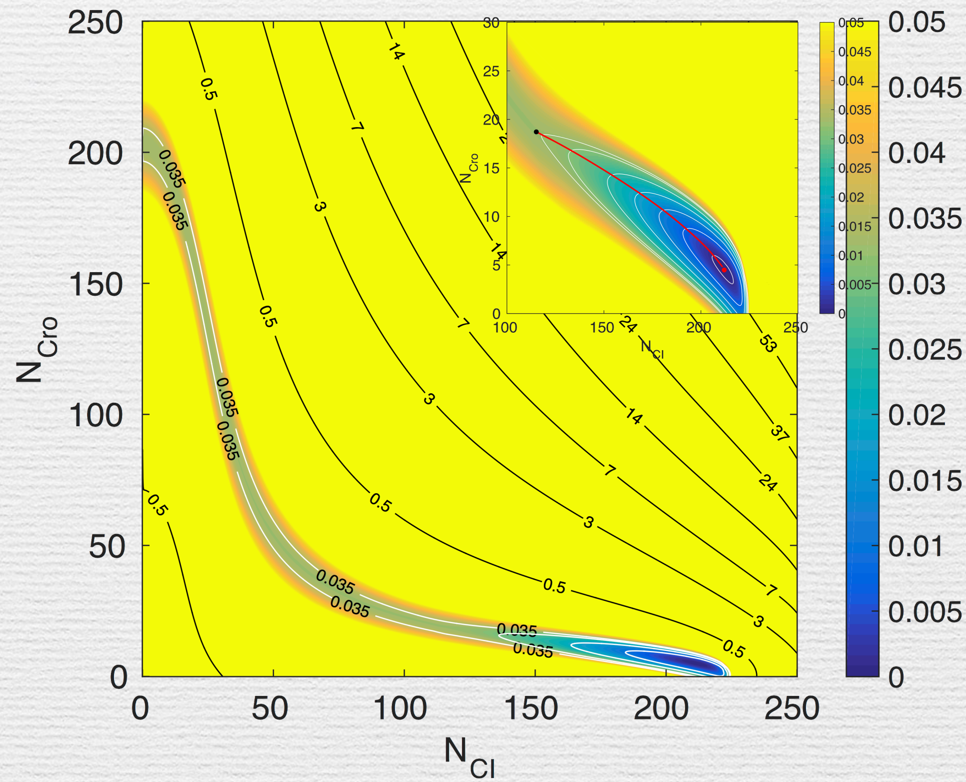


Flagship examples

3D genetic switch model with positive feedback (Li et al, 2014)

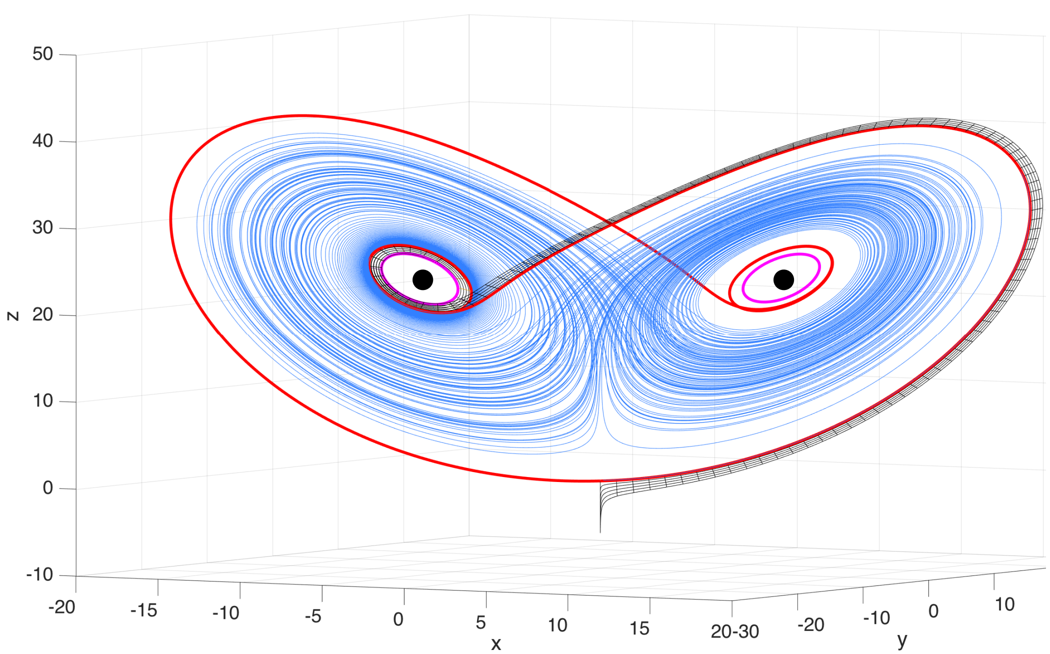


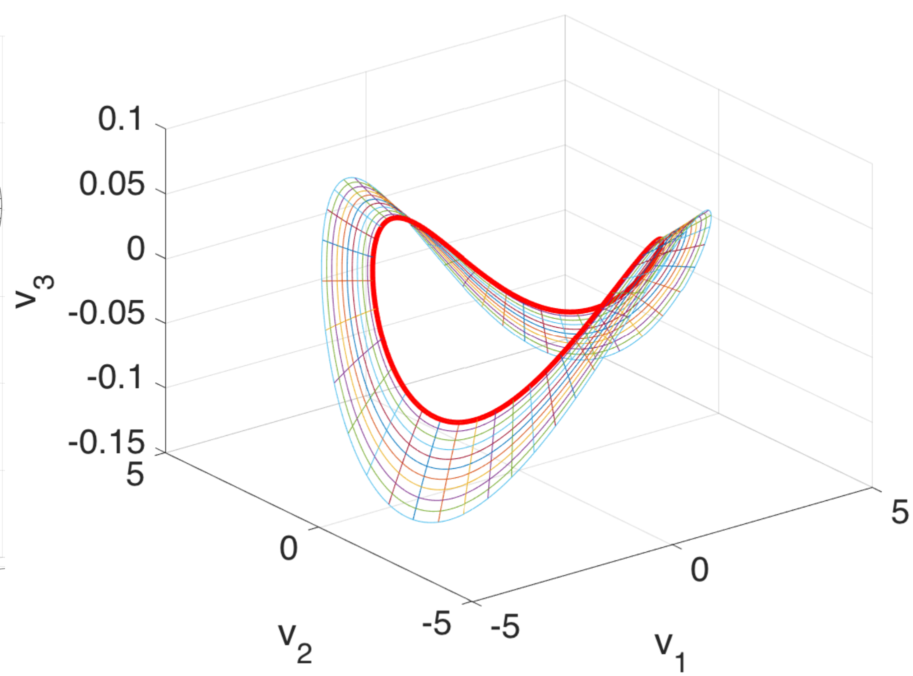
Genetic switch in λ phage (Aurell-Sneppel, 2002)

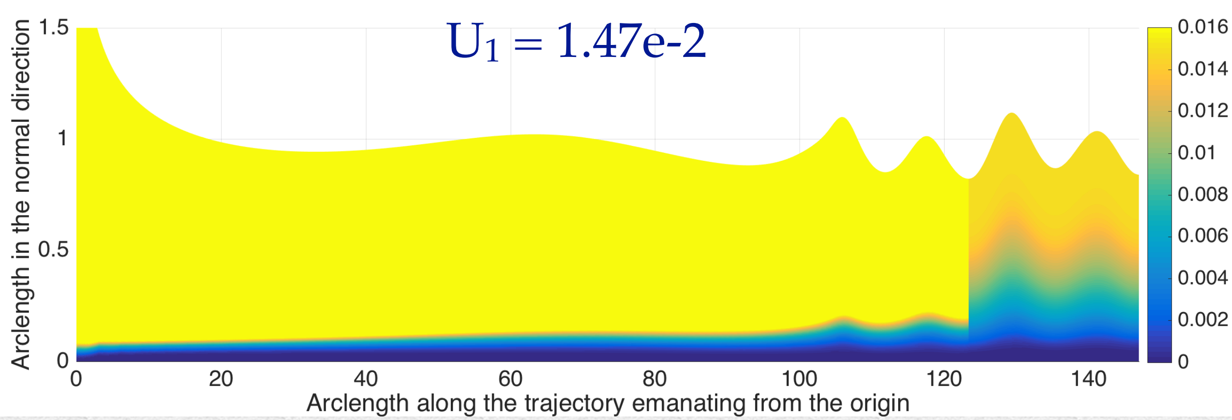


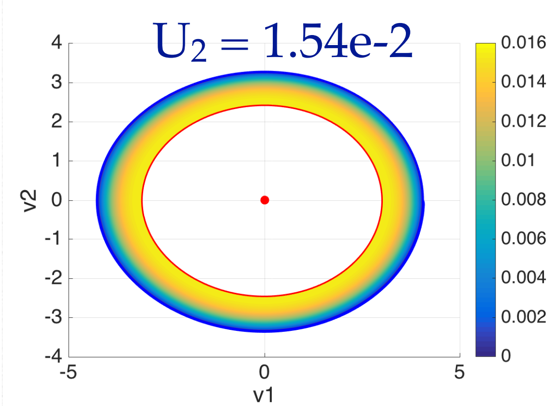
Lorenz'63 with small white noise. $\rho = 24.4$

From the strange attractor to stable equilibria: which way we go?









Perspectives

- Further enhancement of quasipotential solvers (work in progress)
- Mechanical systems: inertia, weak external periodic forcing, small white noise (or bounded magnitude noise)
- Going to higher dimensions. Approach: neural networks, point clouds.
- Applications

My research group

- PhD students
  - Manyuan Tao (started to work on the fracture project)
  - Luke Evans (currently working on computing committors by means of diffusion maps in the context of chemical physics applications; will be involved into chemical network model reduction project)
  - Nicholas Paskal (enhancement of quasipotential solvers: adaptive stencil refinement + Hermite interpolation), will graduate in Summer 2021
- Postdoc
  - Christopher Moakler (UNC, Physics, advisor K. Newhall, PhD May 2021 expected, will join my group in August 2021)
- Acknowledgement: MURI FA9550-20-1-0397