Computational methods for the study of stochastic dynamics with small noise

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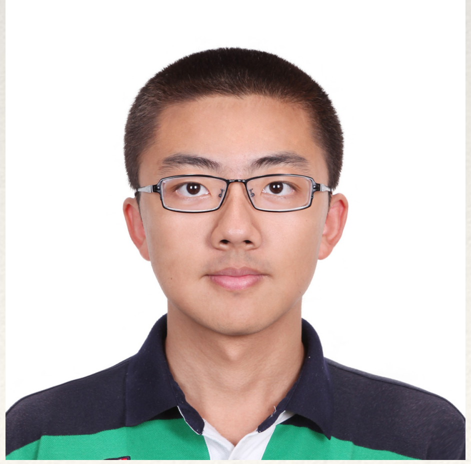
Joint work with ***Daisy Dahiya,*** ***Shuo Yang,*** *and* ***Samuel Potter***



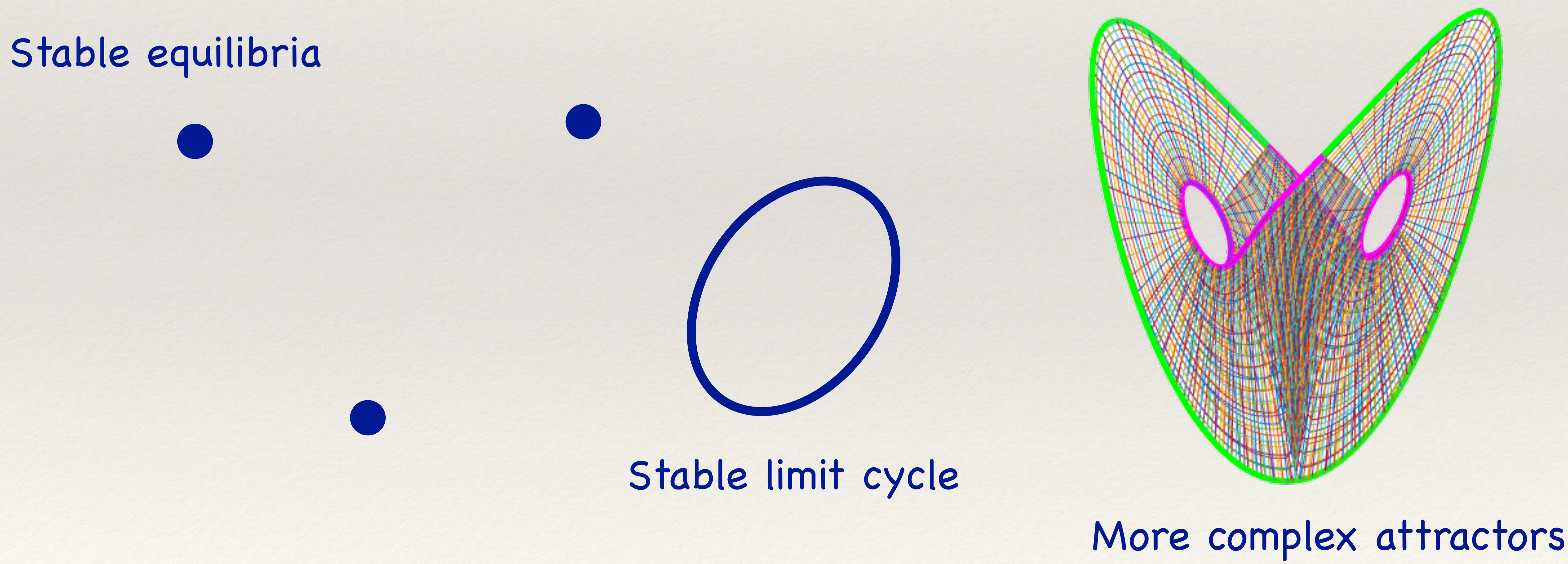
What are rare events?

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

$b(x)$: C^1 deterministic vector field

ϵ: small parameter

dw: Brownian motion

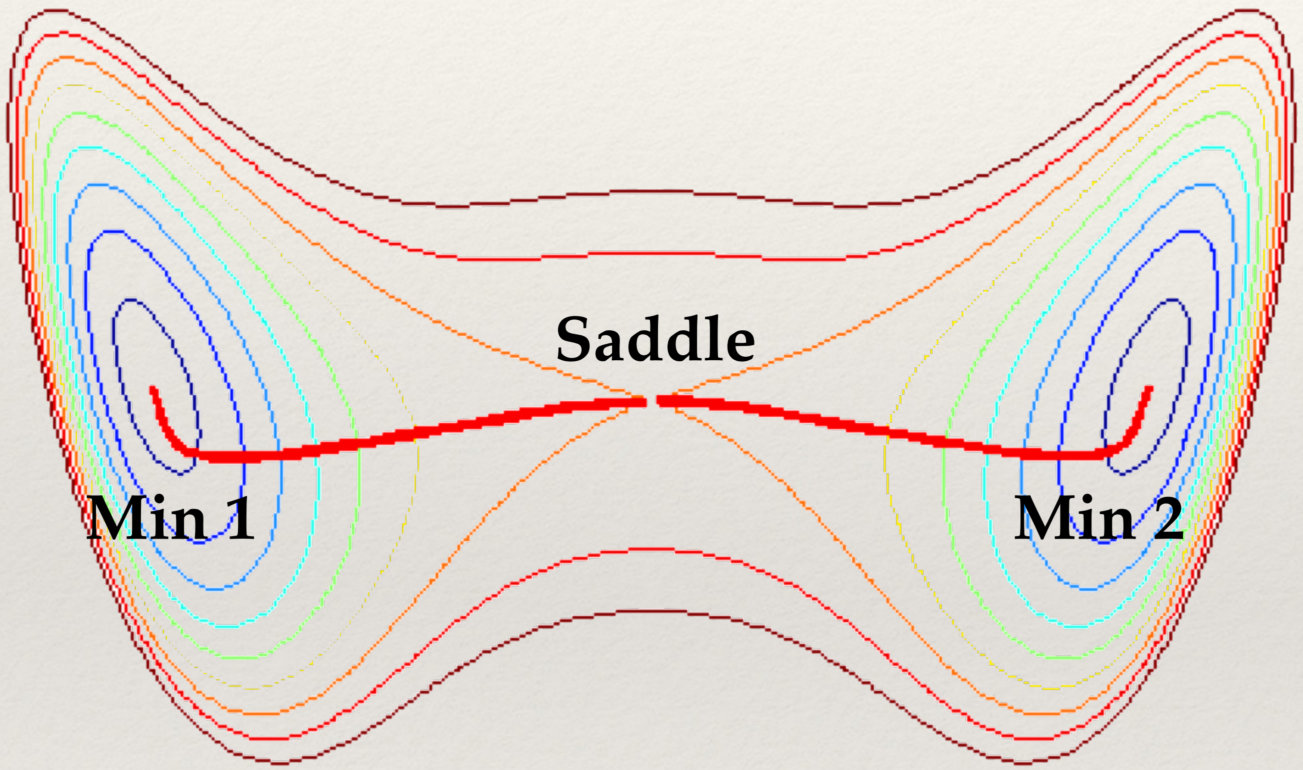


We want to estimate:

- expected escape times from the basins of attraction
- maximum likelihood escape paths
- quasi-invariant probability measures in the neighborhoods of attractors

Gradient SDEs

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



Arrhenius formula (1884):

$$Rate \propto e^{-(V_{sad}-V_{min})/(RT)}$$

Gibbs (1839- 1903) measure:

$$f(x) = Z^{-1}e^{-V(x)/k_B T}$$

Kramers' / Langer's formula:
1940 1969

$$Rate \approx \frac{|\lambda|}{2\pi}\sqrt{\frac{\det H_{min}}{|\det H_{sad}|}}e^{-\beta(V_{sad}-V_{min})}$$

Where nongradient SDE models come from

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

Large Deviation Theory

Freidlin and Wentzell, 1970s

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

Freidlin-Wentzell action functional

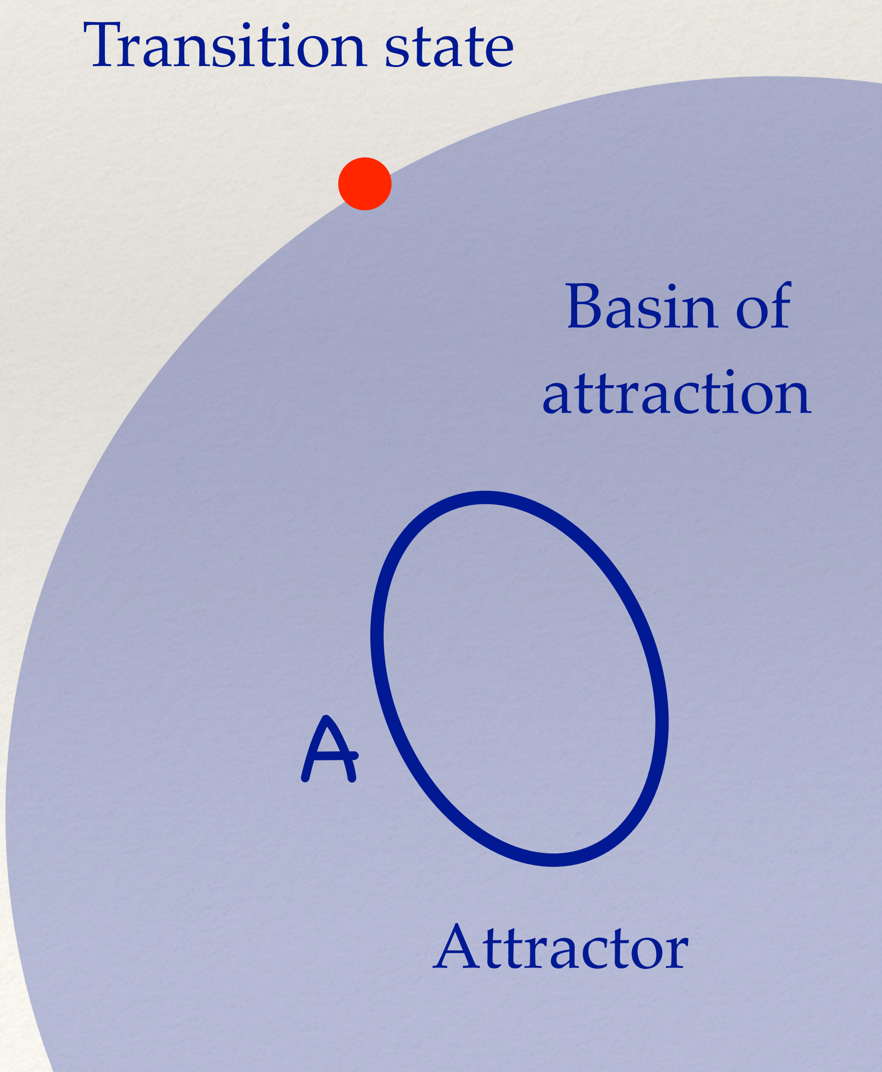
$$S_T(\phi) = \frac{1}{2}\int_0^T \|\dot{\phi} - b(\phi)\|^2 dt$$

Quasipotential

$$U_A(x) = \inf_{\phi, T}\{S_T(\phi) \mid \phi(0) \in A,\ \phi(T) = x\}$$

Expected escape time

$$\tau_A(D) \asymp \inf_{x \in \partial D} e^{U_A(x)/\epsilon}$$



Large Deviation theory for Gradient Case

$$dx = -\nabla V(x)dt + \sqrt{\epsilon}dw$$

Freidlin-Wentzell Action

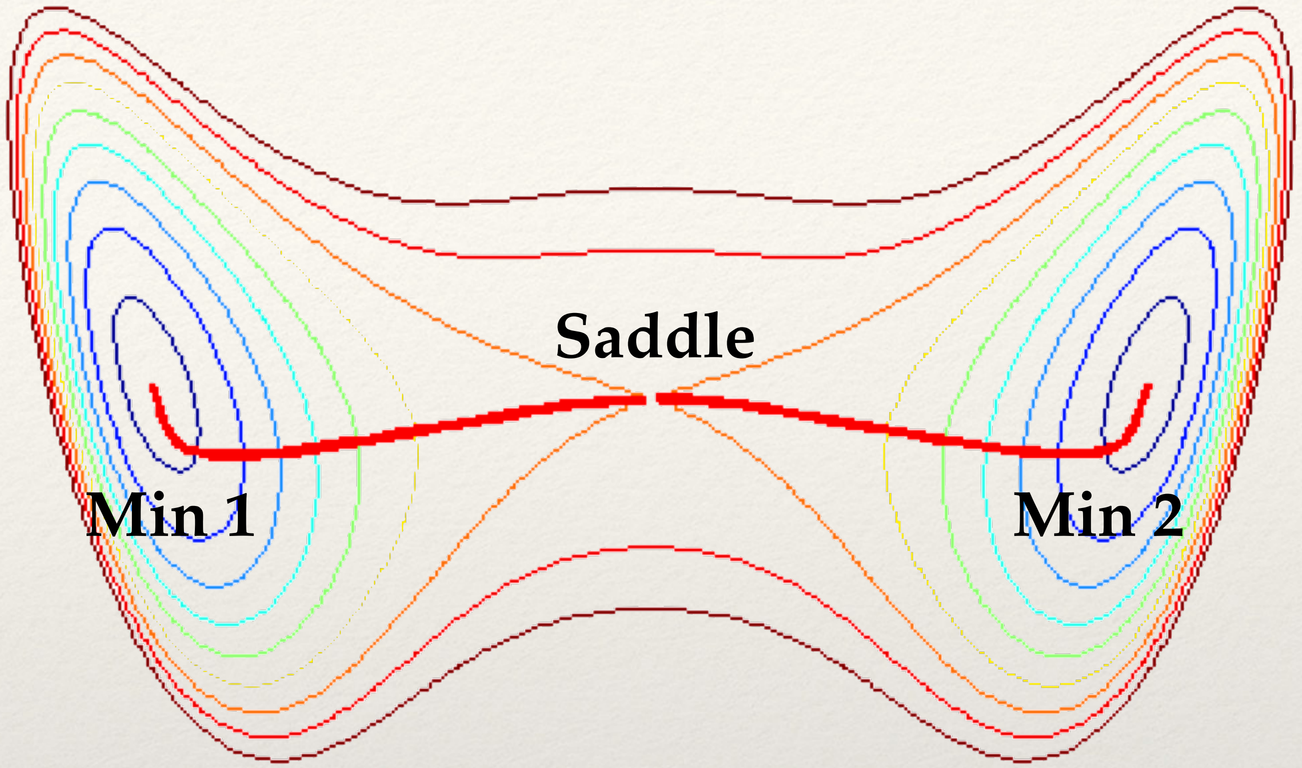
$$S_T(\phi) = \frac{1}{2}\int_0^T \|\dot{\phi} + \nabla V(\phi)\|^2 dt$$

Quasipotential

$$U_{\min 1}(x) = 2(V(x) - V_{\min 1})$$

Expected escape time

$$k_{12} \asymp e^{-2(V_{sad} - V_{\min 1})/\epsilon}$$



Minimum Action Path
(a.k.a. Maximum Likelihood Path
or instanton)

$$\|\dot{\phi}^*\| = \|b(\phi^*)\|$$

$$\dot{\phi}^* \parallel b(\phi^*)$$

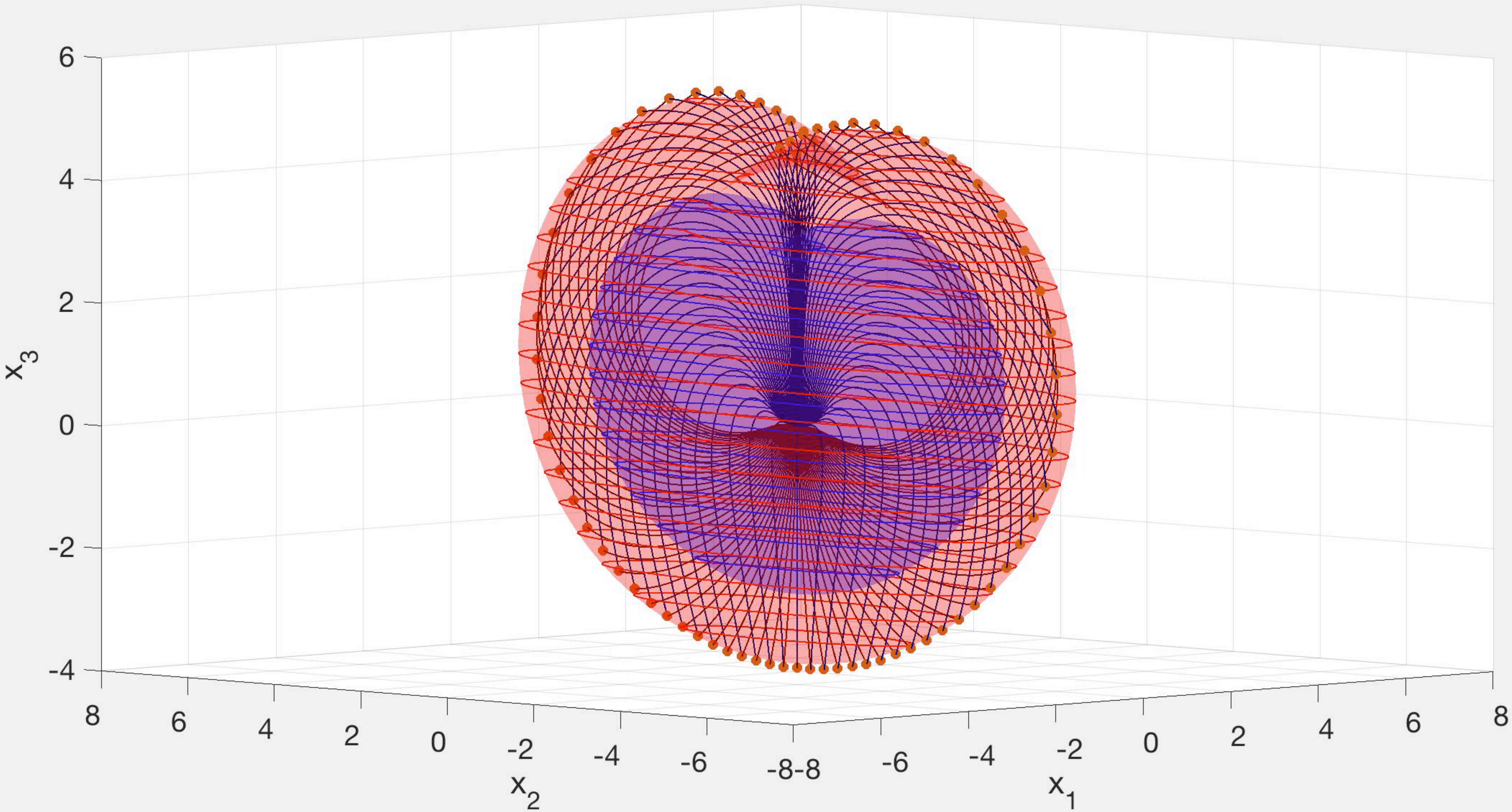
Nongradient case

Lorenz'63, $\sigma = 10$, $\beta = 8/3$, $\rho = 0.5$.

Surfaces: level sets of the quasipotential (U = 20, 40)

Indigo curves: trajectories

Dark red curves: MAPs



Nongradient Case

Hamilton-Jacobi-Bellman

PDE for the quasi-potential

$$\|\nabla U_A\|^2 + 2b(x)\cdot\nabla U_A = 0$$
$$U_A(x) = 0, \quad x \in A$$

The quasipotential is one of the solutions.
It is never unique!

$$S(\psi) = \int_0^L \|\psi'\|\|b(\psi)\| - \psi'\cdot b(\psi)ds$$
$$U(x) = \inf_{\psi}\{S(\psi) \mid \psi(0)\in A,\ \psi(L) = x\}$$

Minimization w.r.t. time can be done analytically leading to the geometric action
(FW, Heymann & Vanden-Eijnden)

Nongradient Case

Hamilton-Jacobi-Bellman

PDE for the quasi-potential

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$$U_A(x) = 0, \quad x \in A$$

Minimum Action Paths

$$(\psi^*)' \ \parallel \ \nabla U(\psi^*) + b(\psi^*)$$

Nongradient Case

Hamilton-Jacobi-Bellman

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Orthogonal decomposition

$$b(x) = -\frac{1}{2}\nabla U(x) + l(x)$$

$$l(x) := \frac{1}{2}\nabla U(x) + b(x)$$

$$l(x) \ \perp \ \nabla U(x)$$

Nongradient Case

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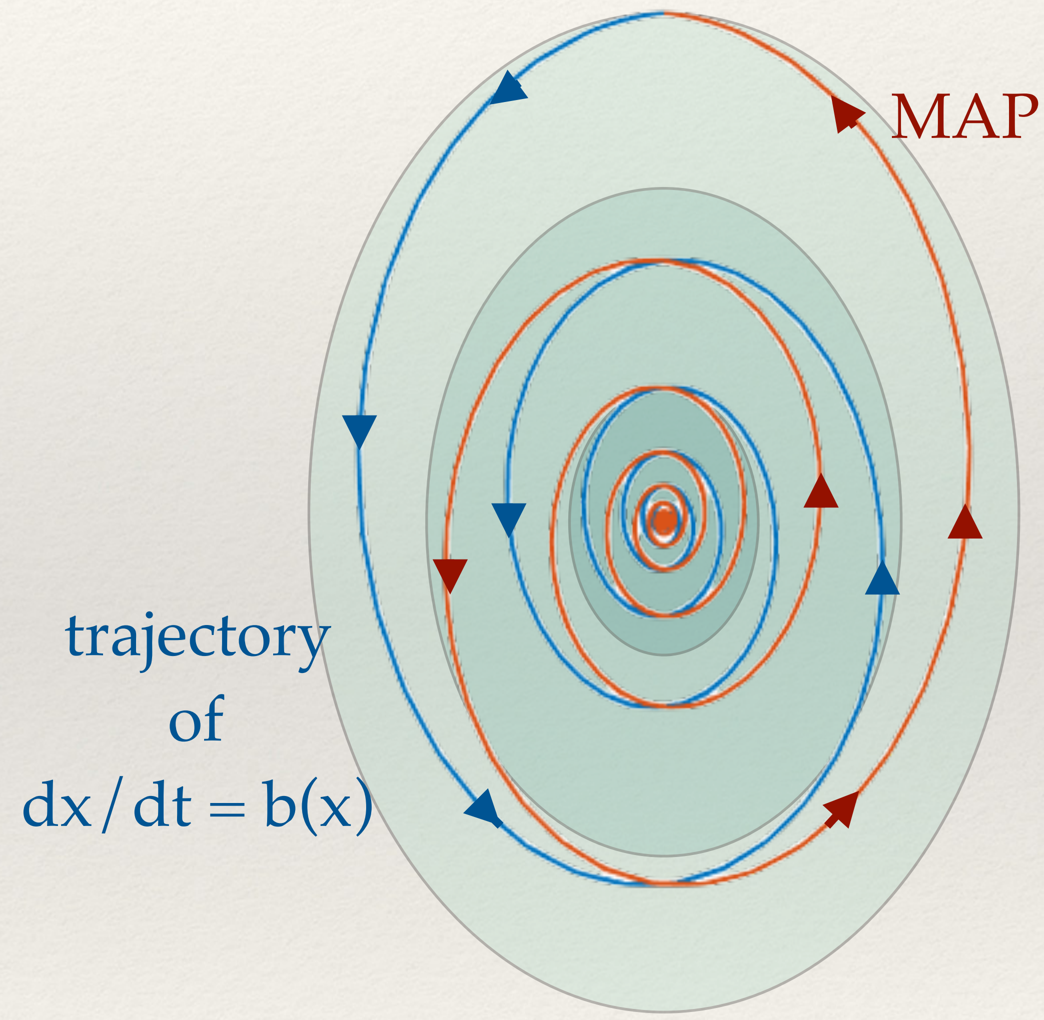


Goal

Develop numerical methods for computing

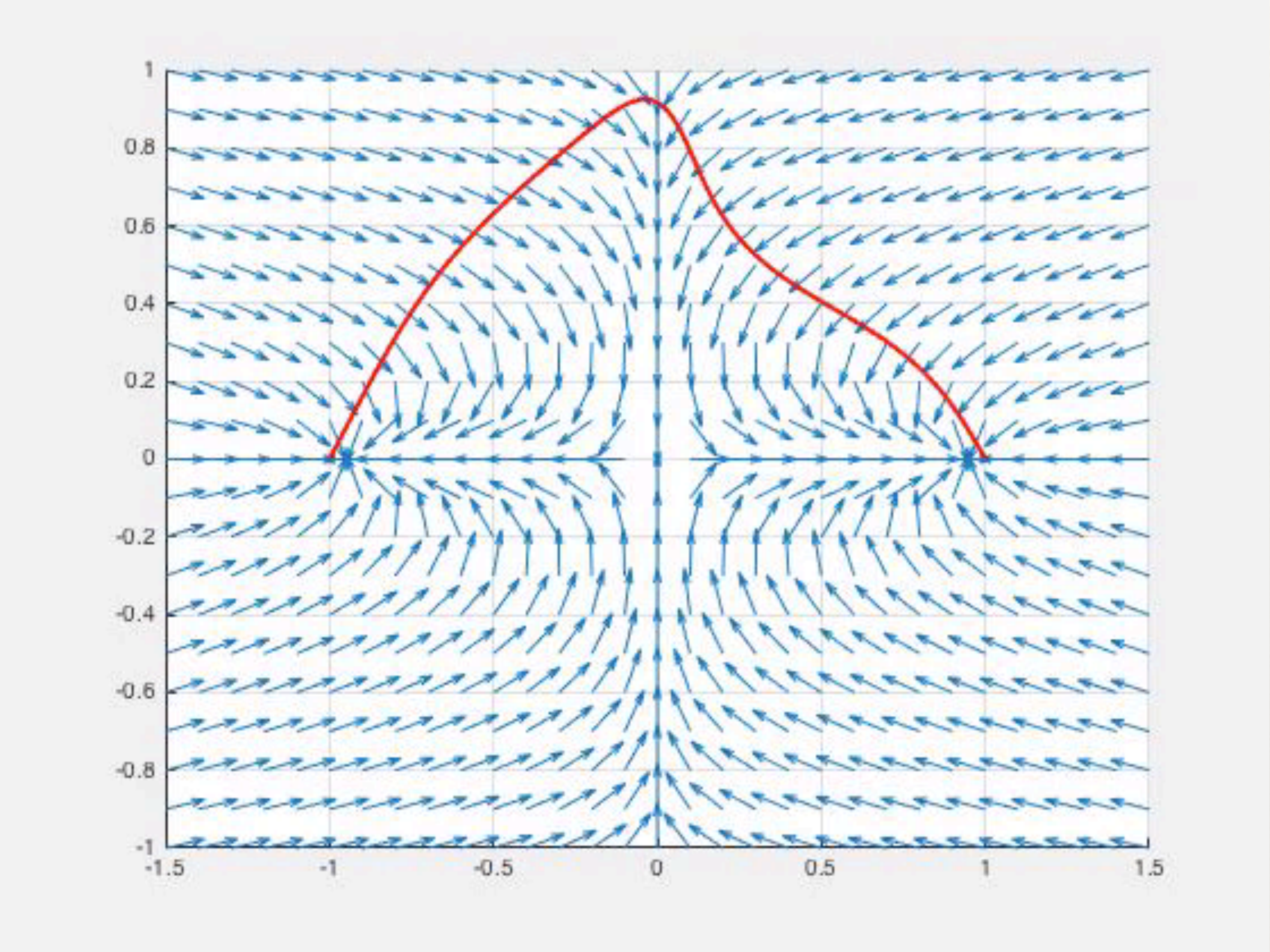
- Quasipotential
- Minimum Action Paths

Direction 1: Path-based methods

- E, Ren, Vanden-Eijnden: **MAM** (2004)
- Heymann and Vanden-Eijnden: **GMAM** (2008)

  (numerical minimization of the geometric action)

- Zhou, Ren, and E: **AMAM** (2008) (numerical minimization of the Freidlin-Wentzell action)



Maier-Stein model, 1990s

Direction 2: computing the quasipotential

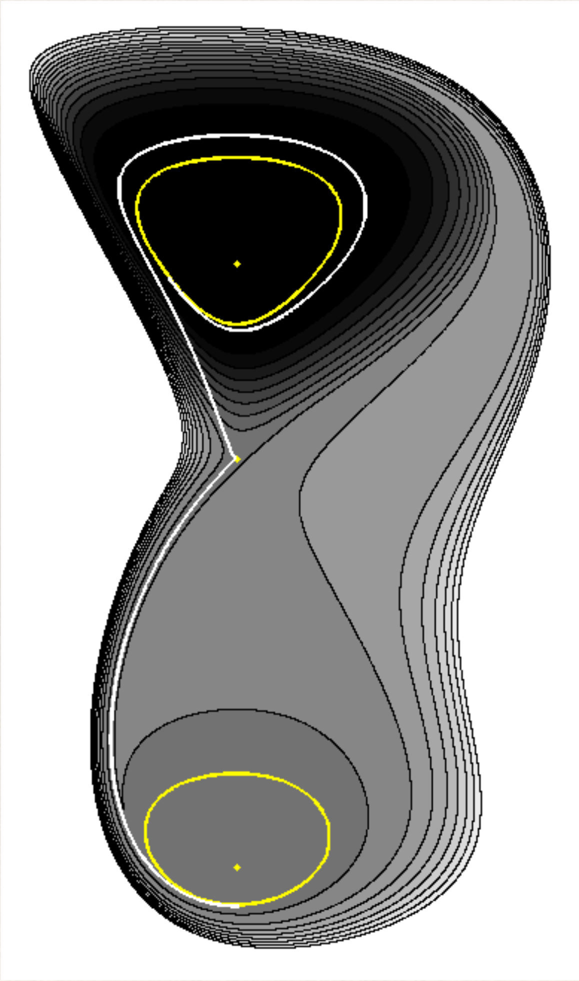
Cameron, 2012

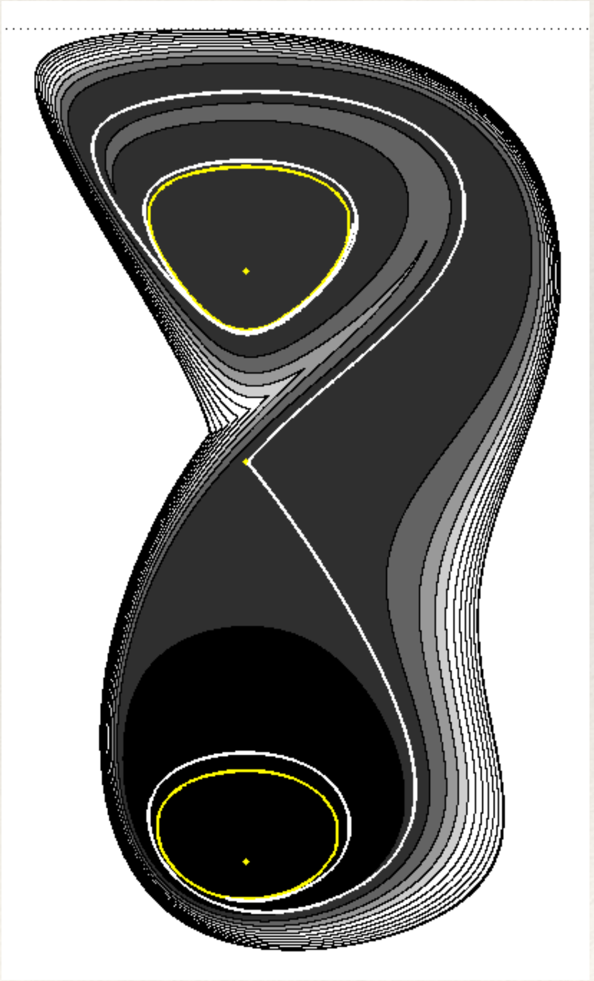
- *Compute the quasipotential on a mesh*
- *Find MAPs by numerical integration*
  x = target point
  A = attractor

$$dx = \frac{1}{\varepsilon}\left(x - \frac{x^3}{3} + y - \frac{y^3}{9}\right)dt + \sqrt{2\beta^{-1}}dw_1$$

$$dy = (x + 0.9)dt + \sqrt{2\beta^{-1}}dw_2$$

$$\psi' = -\frac{b(\psi) + \nabla U(\psi)}{\|b(\psi) + \nabla U(\psi)\|}$$





Computing the quasipotential on mesh

Motivation: ***Sethian and Vladimirsky*** (2001, 2003):
Ordered Upwind Method for solving HJ PDEs:

$$F(x,a)\|\nabla U(x)\| = 1$$

where

$$a := \frac{\nabla U}{\|\nabla U\|}$$

$$0 < F_{\min} \le F(x,a) \le F_{\max} < \infty$$

Key Idea:
Dynamical Programming Principle

Motivated by:
Sethian's **Fast Marching Method** (1996)
for solving the eikonal equation

$$F(x)\|\nabla U\| = 1$$

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The first quasipotential OUM-based solver

Cameron (2012): An adjustment of the **Ordered Upwind Method**

$$\|\nabla U\|^2 + 2b\cdot\nabla U = 0 \quad \Longrightarrow \quad \frac{1}{-2b\cdot a}\|\nabla U\| = 1$$

Unbounded!

The adjustment was
nontrivial
(will be explained later)

Applications and the Qpot R package

- B. C. Nolting and K. C. Abbot, Balls, cups, and quasi-potentials: quantifying stability in stochastic systems, Ecology, 97, 4, 850-864 (2016)
- B. Nolting, C. Moore, C. Stieha, M. Cameron, K. Abbott, QPot: An R package for stochastic differential equation quasi-potential analysis, R Journal 8, 2, 19-38 (2016)
- **https://cran.r-project.org/web/packages/QPot/index.html**
- Zhen Chen, Jinjie Zhu and Xianbin Liu, Crossing the quasi-threshold manifold of a noise-driven excitable system, Proc. R. Soc. A **473**: 20170058.

Ordered line integral methods (OLIMs)

Dahiya and C. (2017, J Sci Comp): 2D
Dahiya and C. (2018, Physica D): 2D, anisotropic diffusion
Yang, Potter, and C. (2018, *submitted*): 3D

Key differences:

- **Solve the minimization problem directly**:

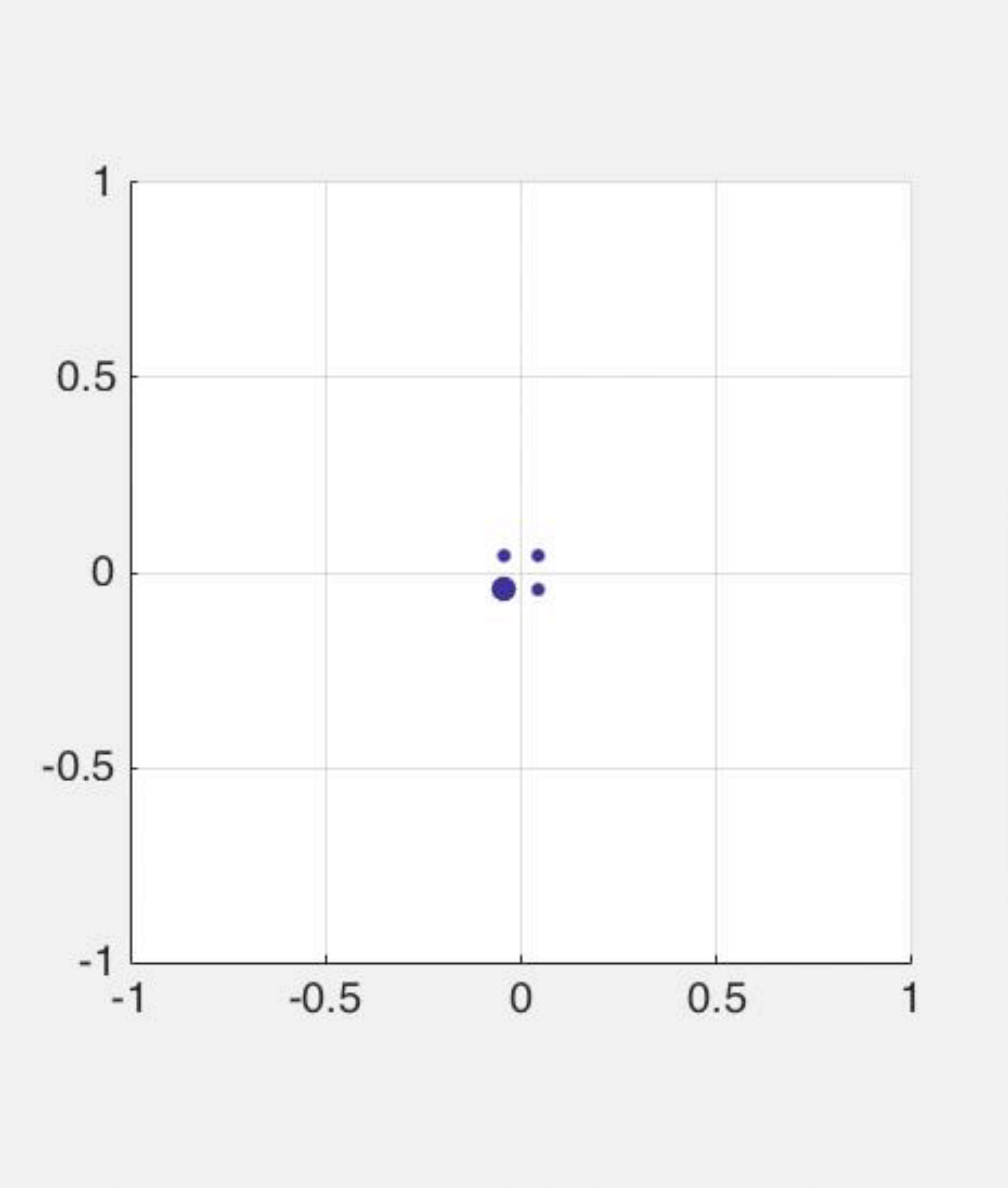
$$S(\psi) = \int_0^L \|\psi'\|\|b(\psi)\| - \psi' \cdot b(\psi) ds$$

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

The geometric action.
Minimization w.r.t. time
is done analytically

- **Technical innovations making the solver efficient**
  - A hierarchical update strategy
  - Use of the KKT constrained optimization theory to reject unnecessary simplex updates
  - Restricting the set of admissible simplexes and a fast search for them

Ordered Line Integral Methods



4 types of mesh points:

Unknown: U is not available

Considered: U is tentative

Accepted Front:
U is finalized,
has Considered nearest neighbors

Accepted: U is finalized,
no Considered nearest neighbors

Ordered Line Integral Methods

WHILE < boundary is not reached >

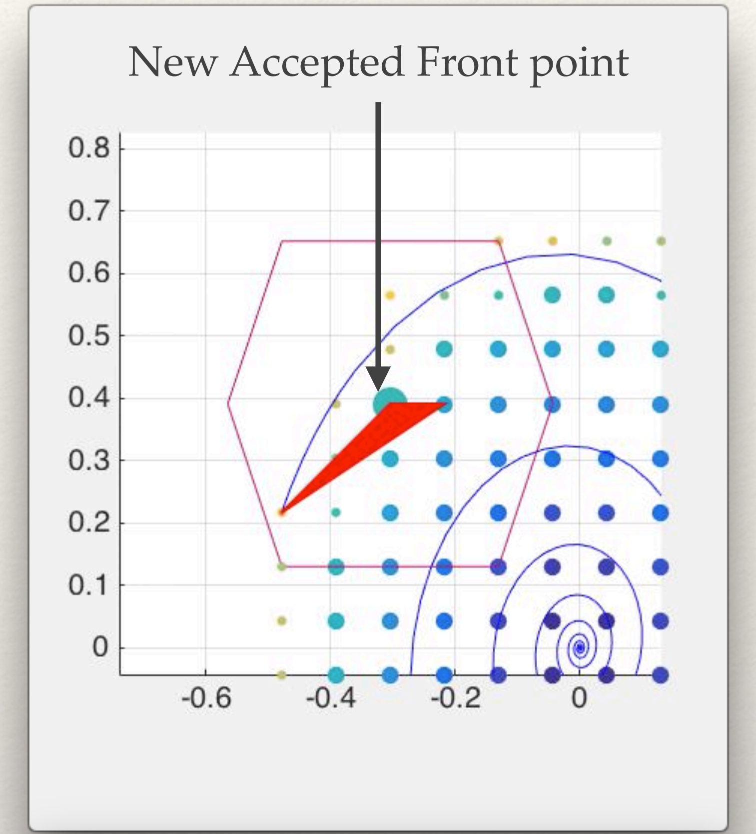
1. make the **Considered** point **x_0** with minimal U **Accepted Front**

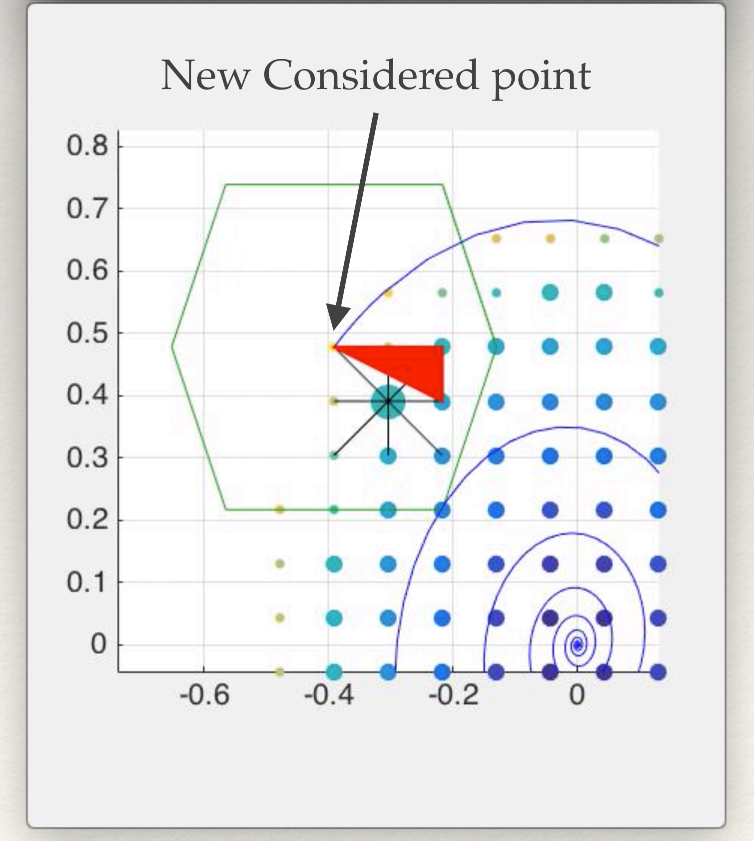
2. make **Accepted Front** points with no Considered NNs **Accepted**

3. update all **Considered** points within update radius from x_0 with **using x_0**

4. make all **Unknown** NNs of x_0 **Considered** and update them using Accepted Front points within update radius from them

END WHILE





One-point and triangle updates

The minimization problem for the quasipotential

$$S(\psi) = \int_0^L \|\psi'\|\|b(\psi)\| - \psi' \cdot b(\psi) ds$$

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

Approximate S(ψ) with a quadrature rule

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Approximate S(ψ) with a quadrature rule

$\mathcal{Q}(a, b)$ = quadrature rule:

Right-hand: OLIM-R

Midpoint: OLIM-MID

Trapezoid: OLIM-TR

Simpson: OLIM-SIM

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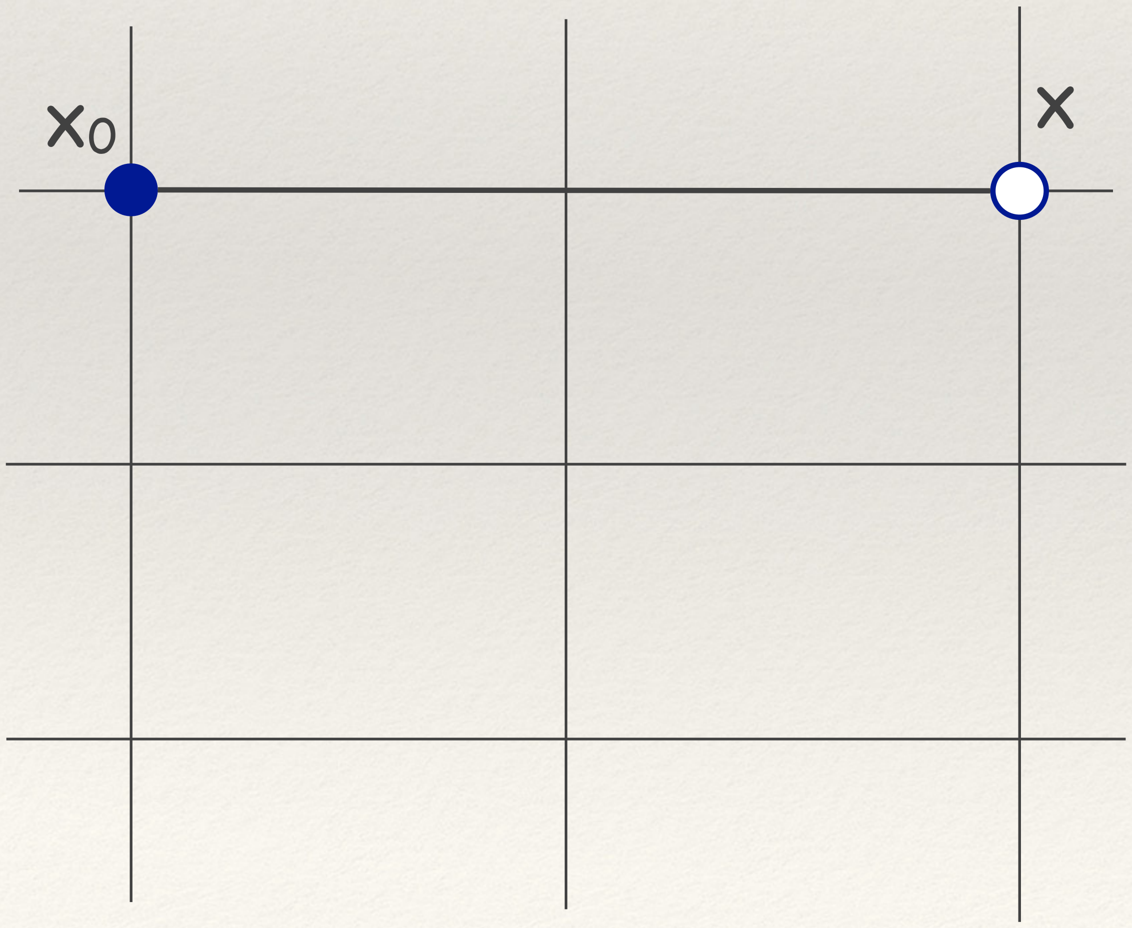

One-point update

$$\mathsf{Q}_{1pt}(x_0, x) = U(x_0) + \mathcal{Q}(x_0, x),$$
$$U(x) = \min\{\mathsf{Q}_{1pt}(x_0, x), U(x)\}.$$

One-point and triangle updates

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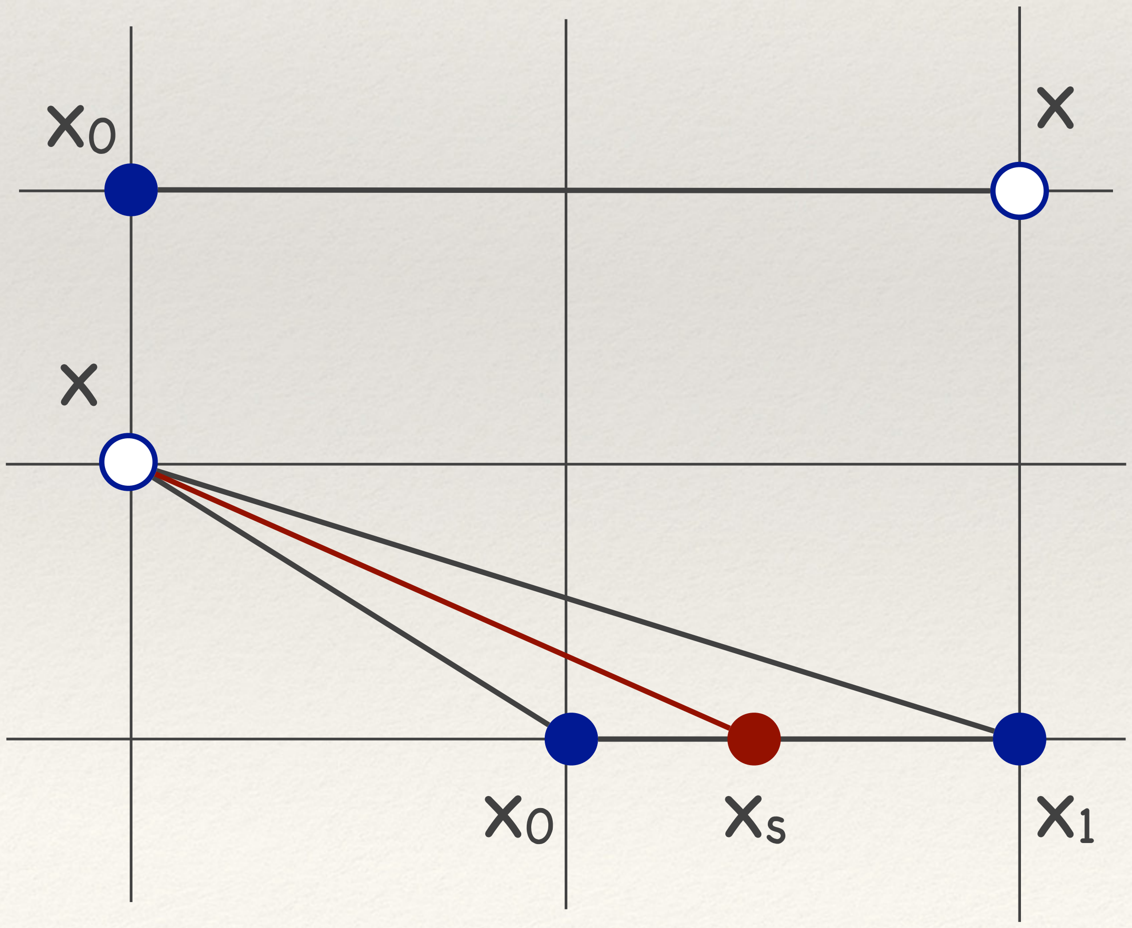

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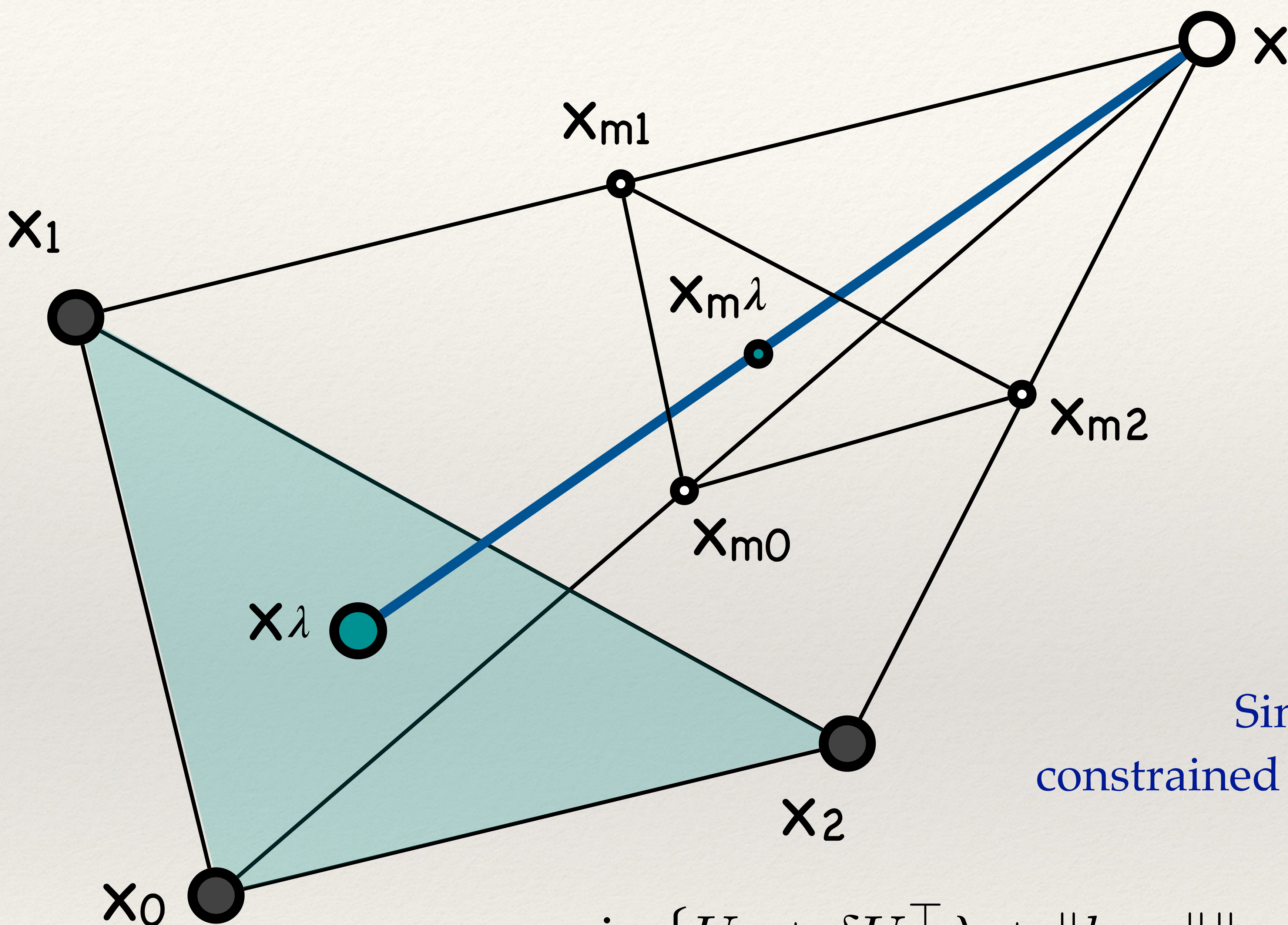
Triangle update

$$\mathsf{Q}_{2pt}(x_0, x_1, x) = \min_{s\in[0,1]}\{U_0 + s(U_1 - U_0) + \mathcal{Q}(x_s, x)\}$$

$$U(x) = \min\{\mathsf{Q}_{2pt}(x_0, x_1, x), U(x)\}$$

Simplex update



The midpoint rule
is optimal in balancing
CPU time and accuracy.

Simplex update
constrained minimization problem

$$\min \left\{ U_0 + \delta U^\top \lambda + \|b_{m\lambda}\| \|x - x_\lambda\| - b_{m\lambda}^\top (x - x_\lambda) \right\}$$

$$\text{subject to} \quad \lambda_1 \geq 0, \quad \lambda_2 \geq 0, \quad \lambda_1 + \lambda_2 \leq 1$$

Making the solver efficient

- **Hierarchical update strategy**

- **Use the KKT theory** to reject simplex updates that are unlikely to succeed in finding an inner point solution

- **Restrict the set of admissible simplexes** and devise a **fast search** for them

Making the solver efficient

- **Hierarchical update strategy**
  - Routine 1pt update
  - Minimizer of 1pt update —> triangle update
  - Successful 1pt update —> simplex update
- **Use the KKT theory** to reject simplex updates that are unlikely to succeed in finding an inner point solution
- **Restrict the set of admissible simplexes** and devise a **fast search** for them

Making the solver efficient

- **Hierarchical update strategy**
  - Routine 1pt update
  - Minimizer of 1pt update —> triangle update
  - Successful 1pt update —> simplex update
- **Use the KKT theory** to reject simplex updates that are unlikely to succeed in finding an inner point solution
  - Starting point = minimizer of a triangle update
  - Check sign of Lagrange multiplier,
  - Reject simplex update if the KKT criteria are met
- **Restrict the set of admissible simplexes** and devise a **fast search** for them

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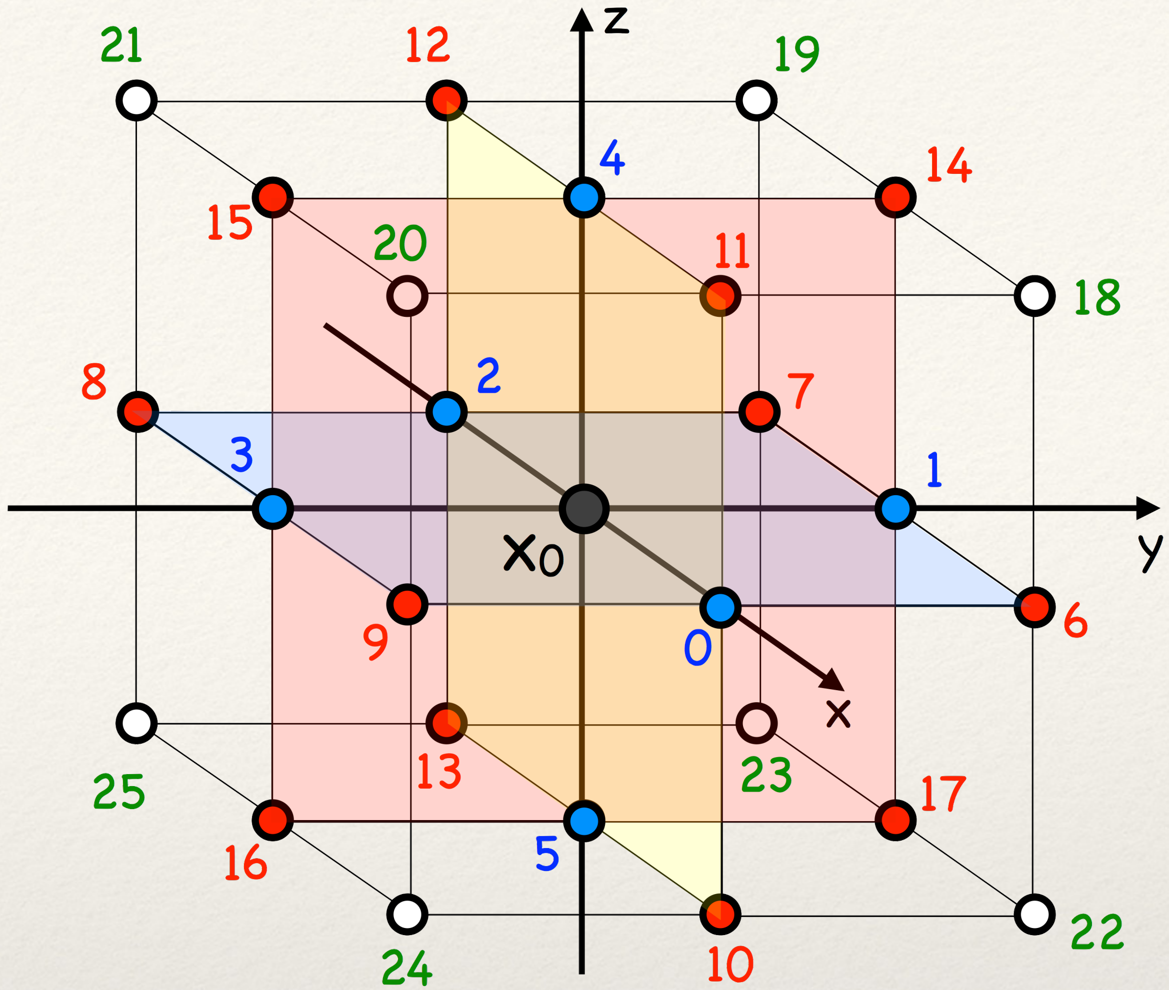
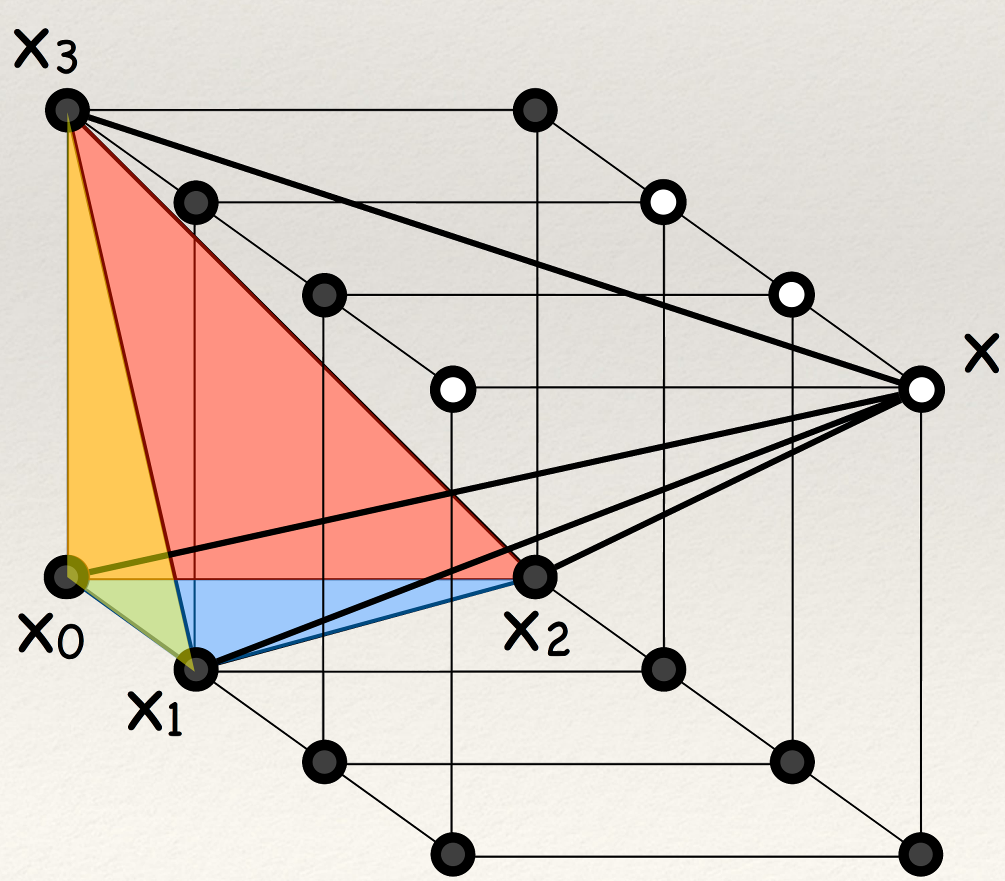
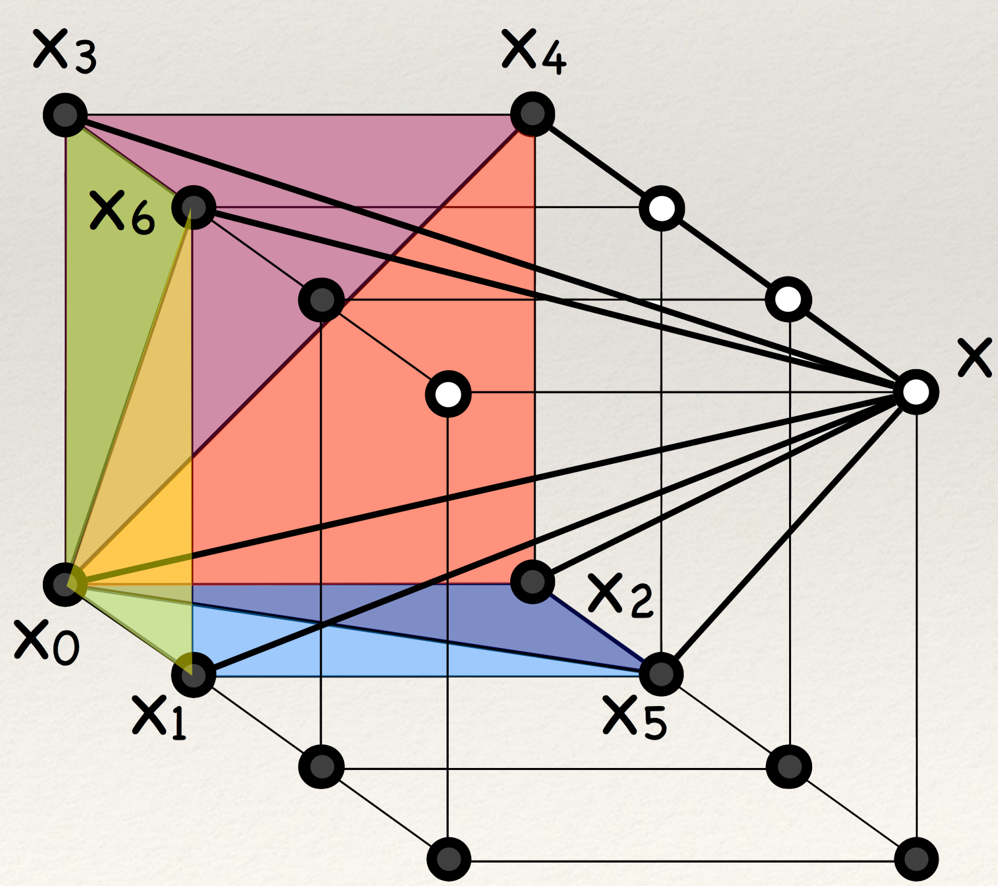






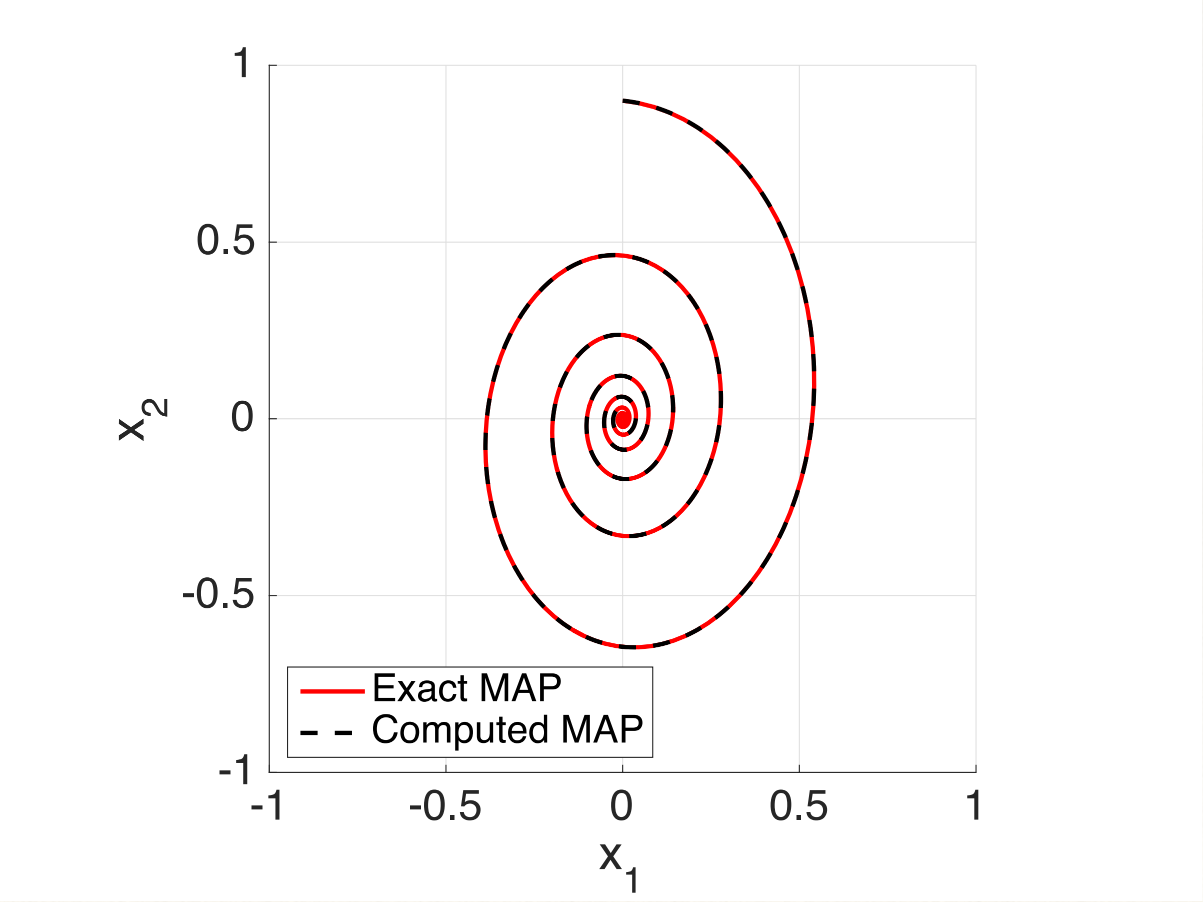
Performance tests

2D test problems

Linear

$$dx_1 = (-2x_1 - 10x_2)dt + \sqrt{\epsilon}dw_1$$
$$dx_2 = (20x_1 - x_2)dt + \sqrt{\epsilon}dw_2$$

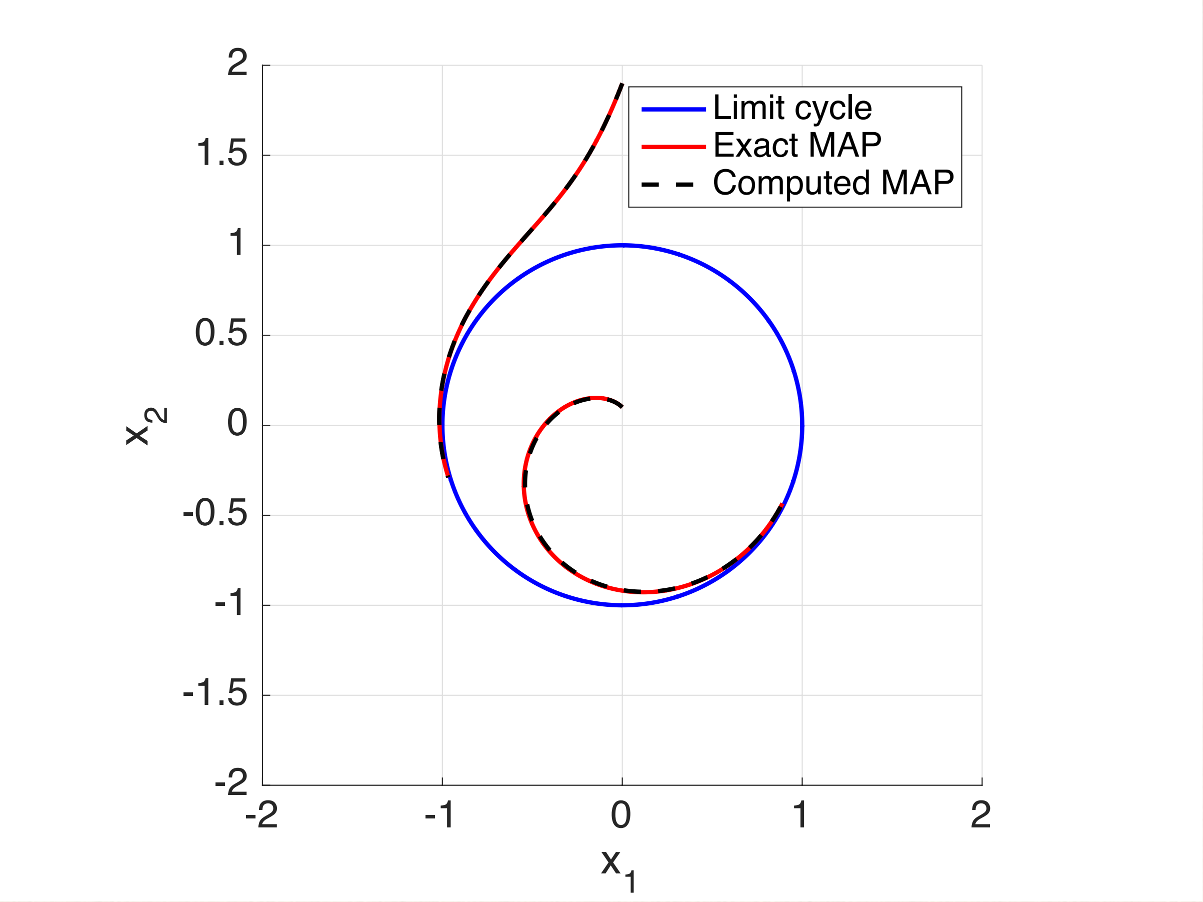
$$U(x_1, x_2) = 2x_1^2 + x_2^2$$



Circle

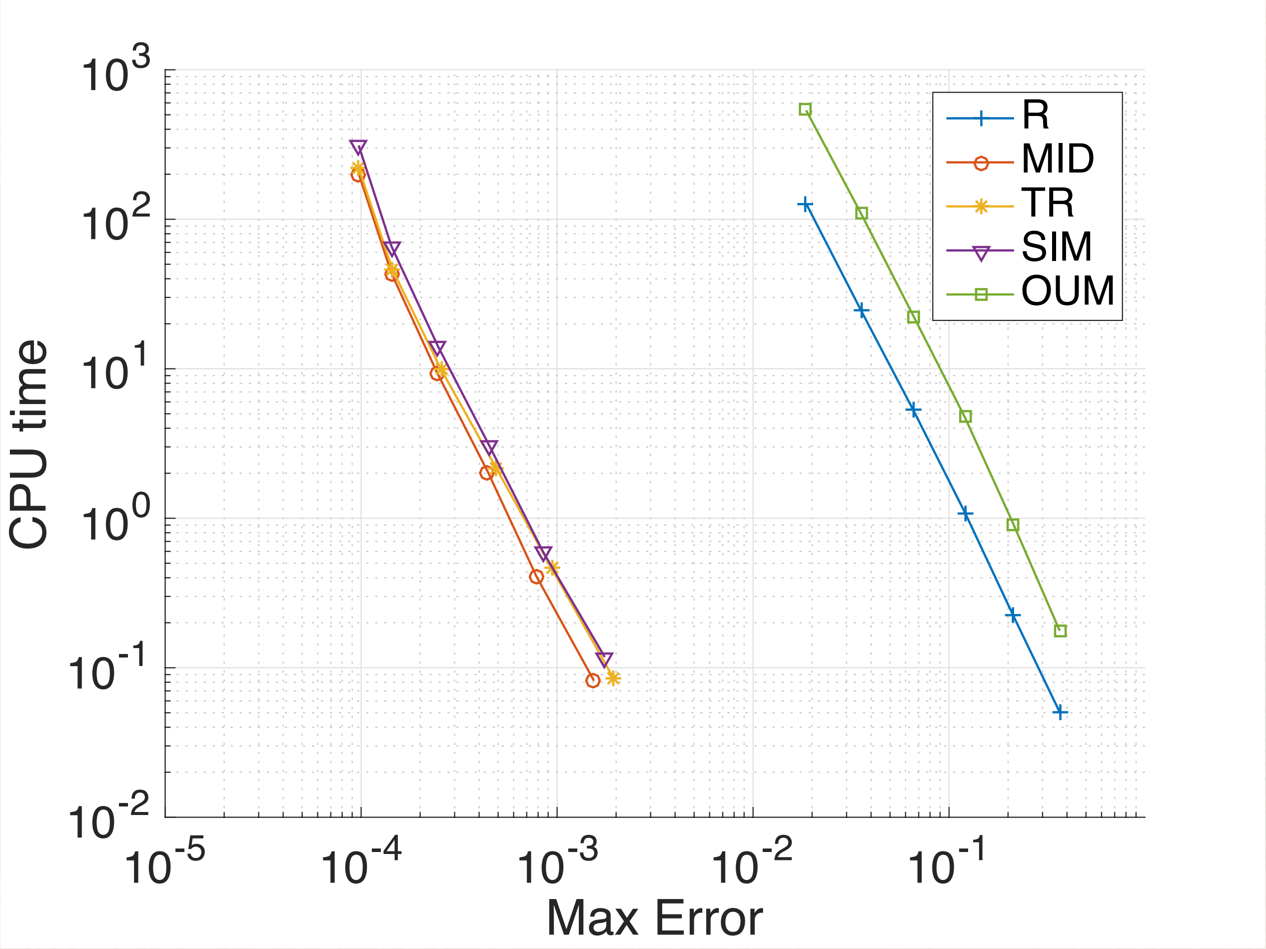
$$dx_1 = (x_2 + x_1(1 - r^2))dt + \sqrt{\epsilon}dw_1$$
$$dx_2 = (-x_1 + x_2(1 - r^2))dt + \sqrt{\epsilon}dw_2$$
$$r^2 := x_1^2 + x_2^2$$

$$U(x_1, x_2) = \frac{1}{2}(x_1^2 + x_2^2 - 1)^2.$$

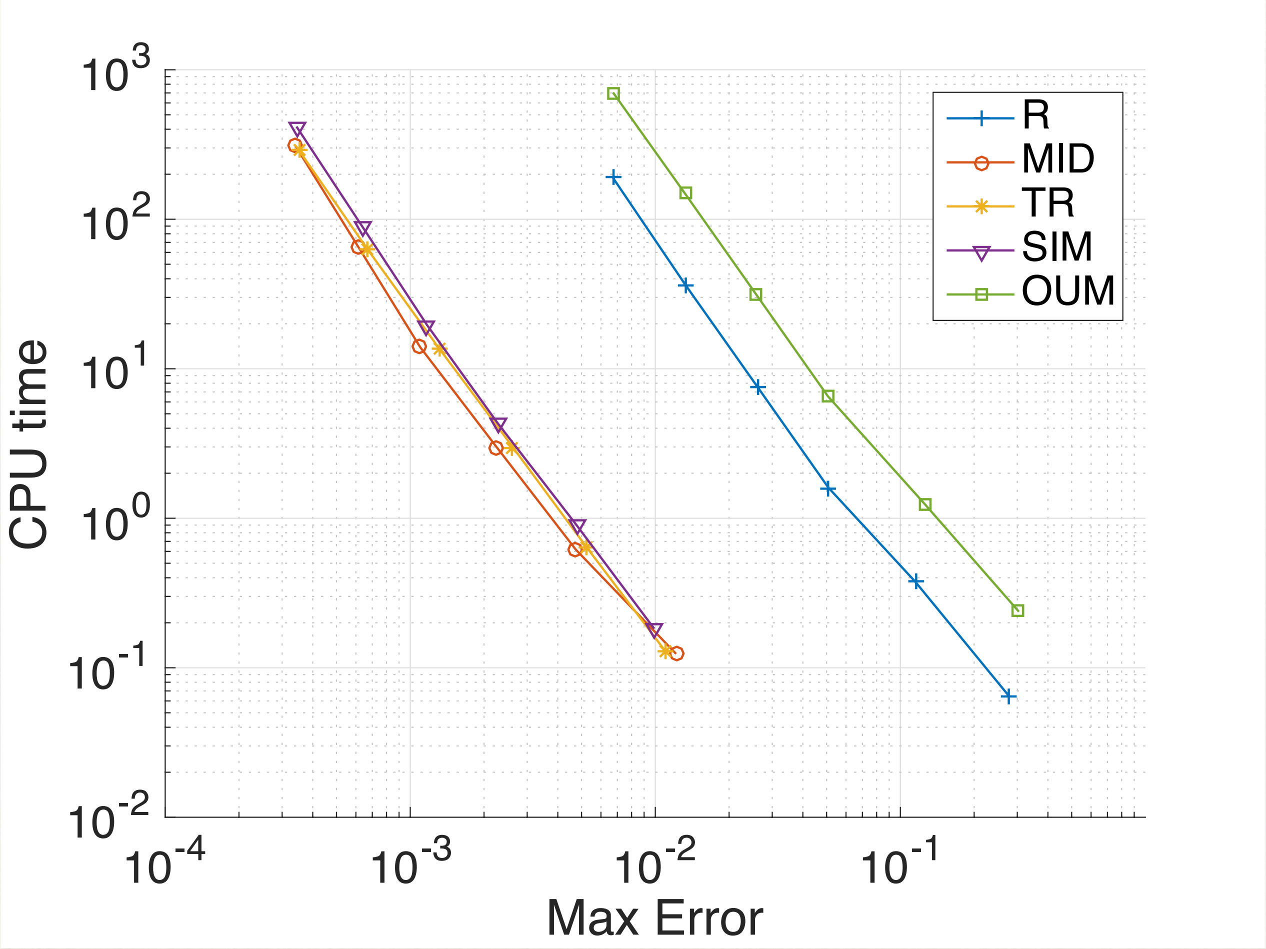


OLIMs vs OUM

Linear

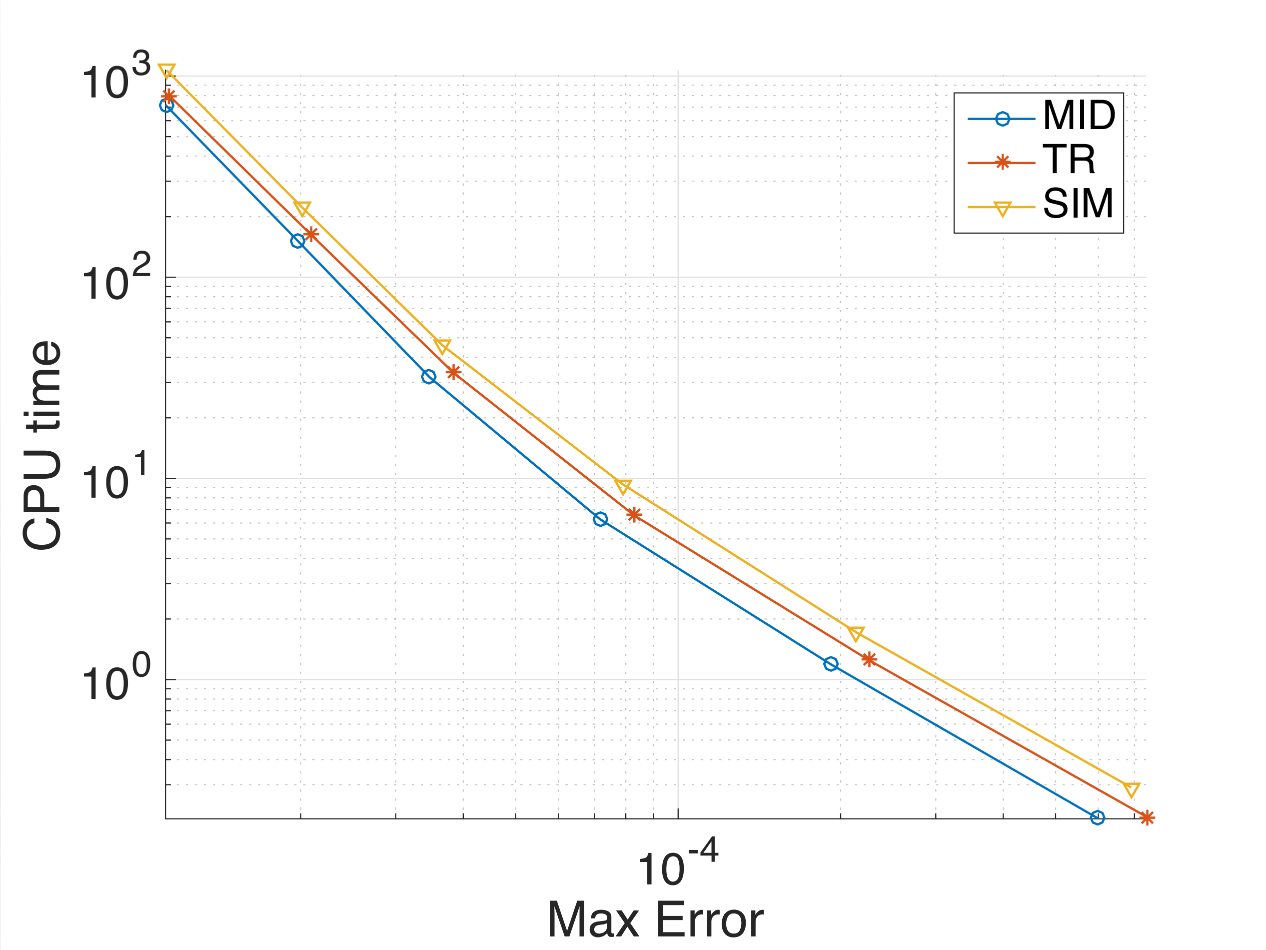


Circle

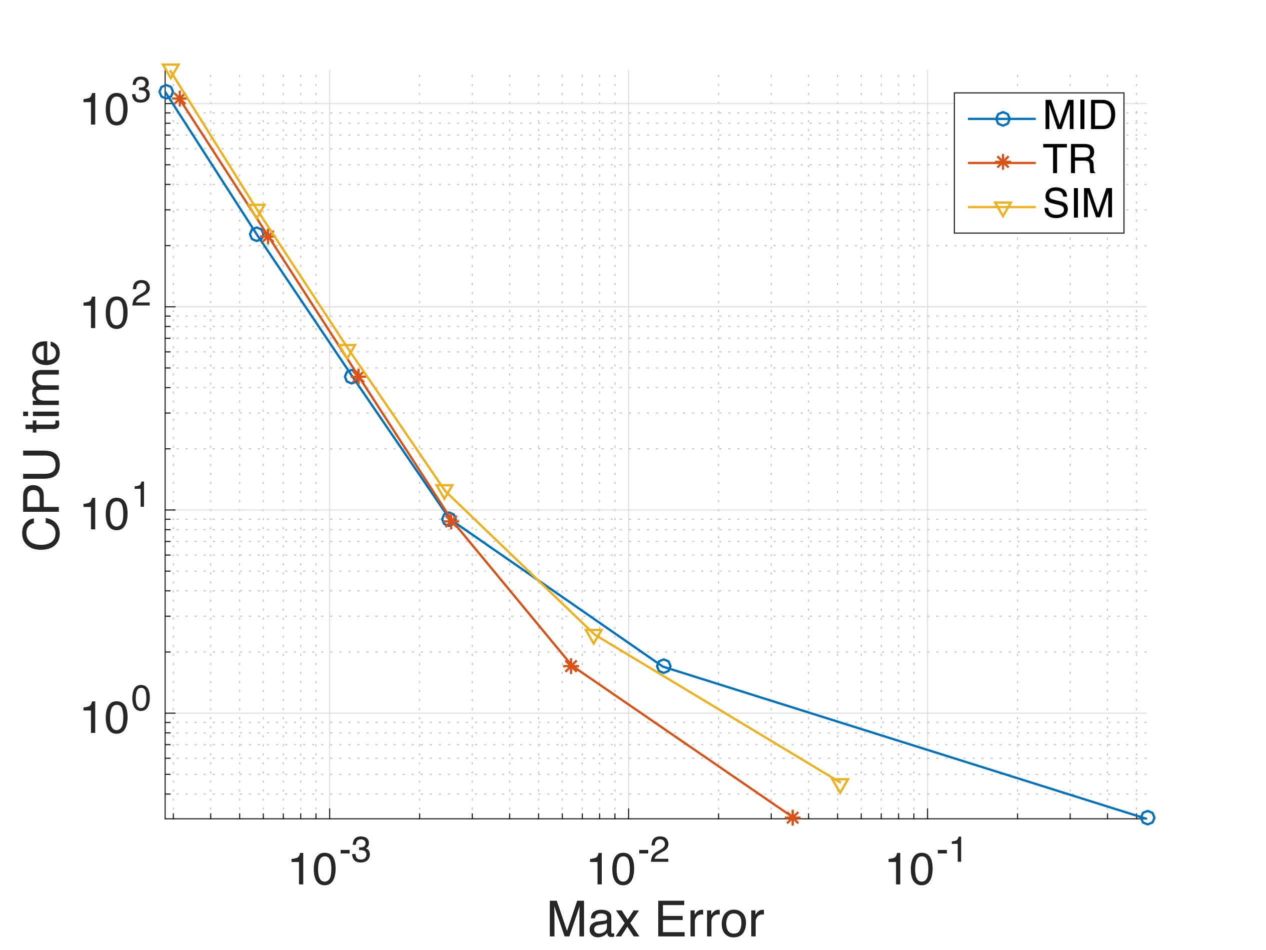


Comparison of OLIMs

Linear



Circle

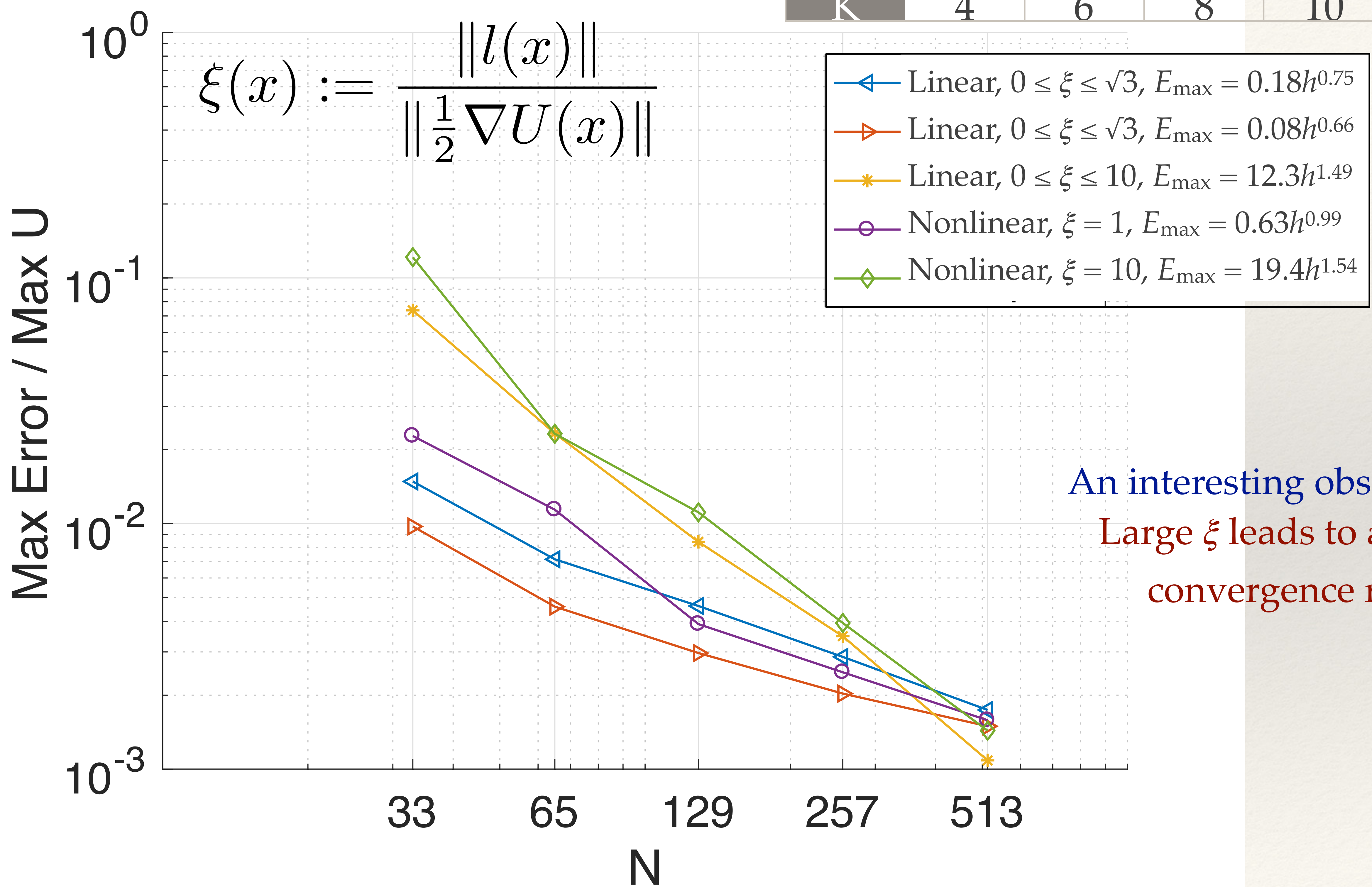


The winner is the midpoint rule!

3D performance test

Mesh size = N^3

N	33	65	129	256	513
K	4	6	8	10	14

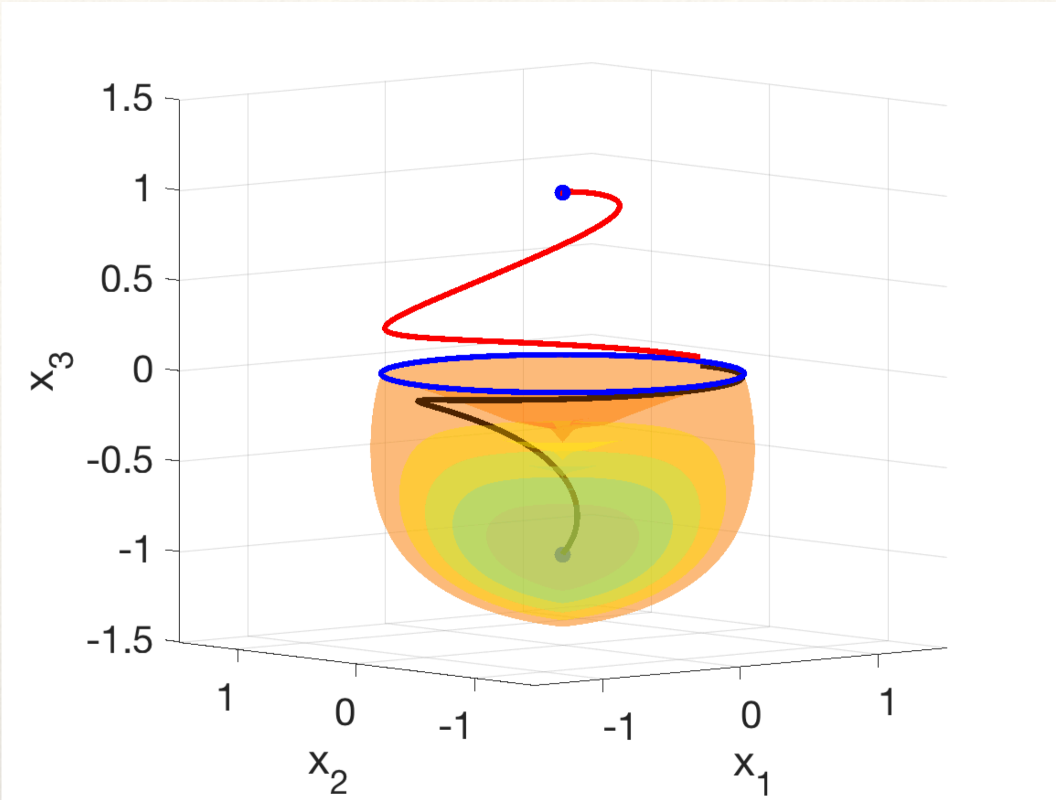


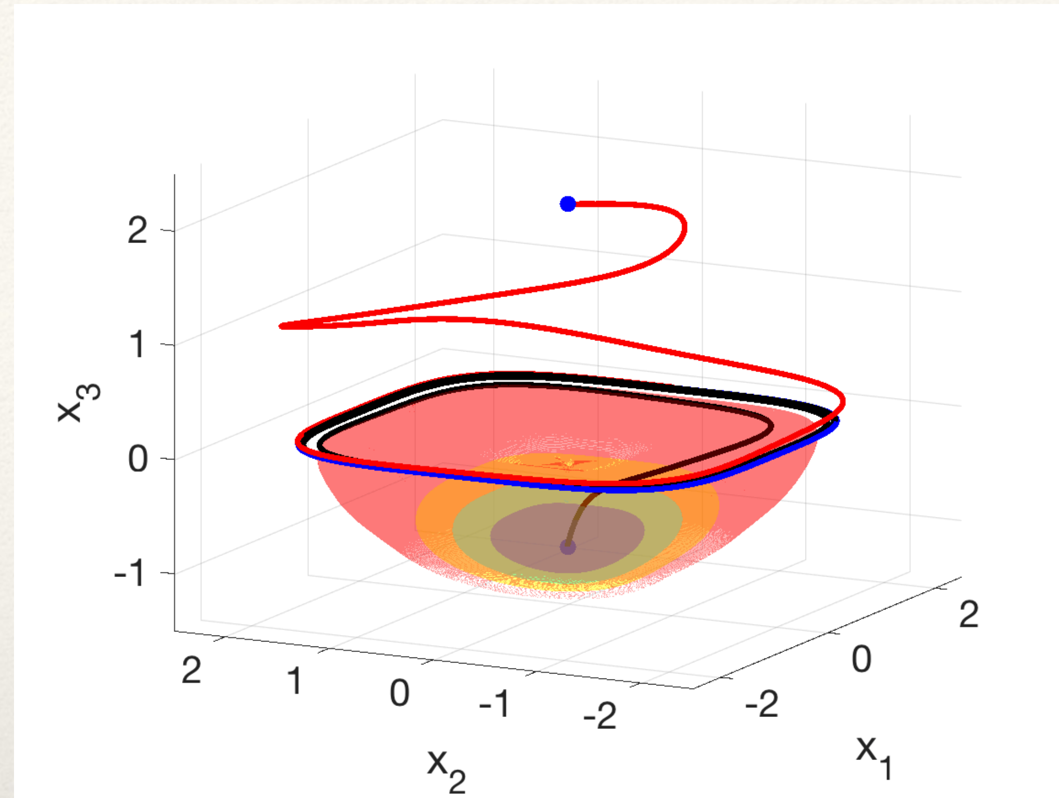
An interesting observation:
Large ξ leads to a faster convergence rate.

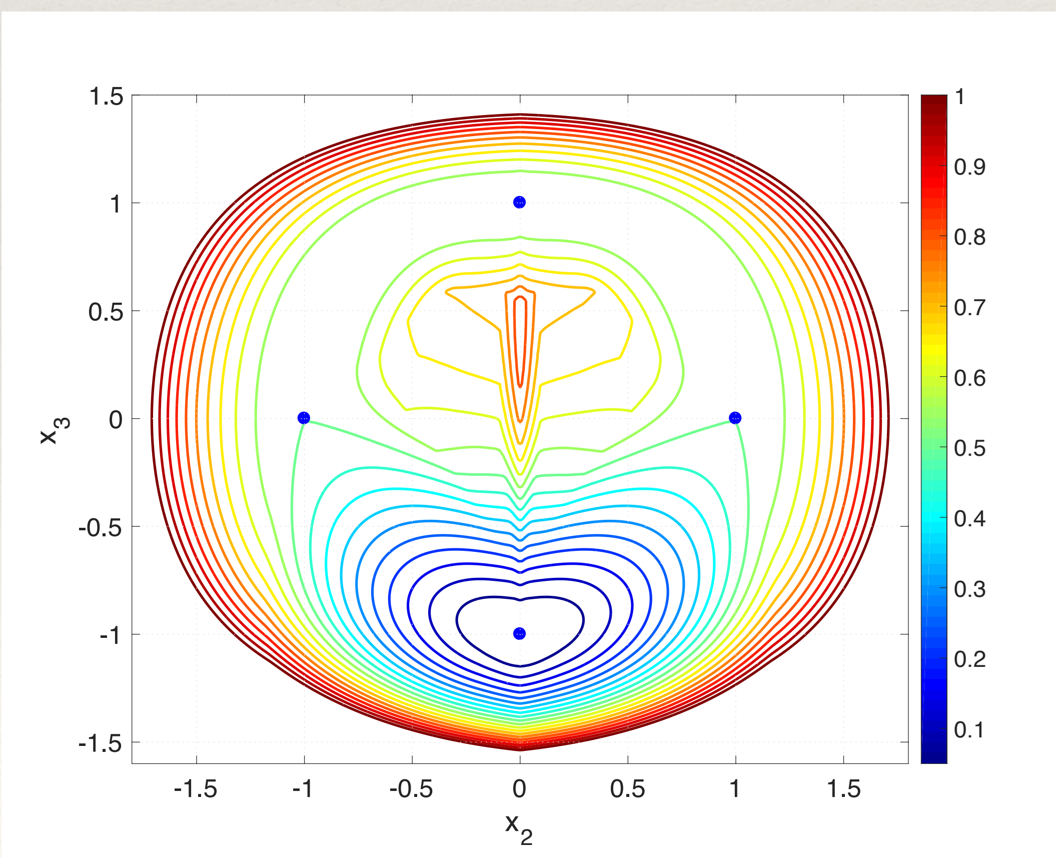
Applications

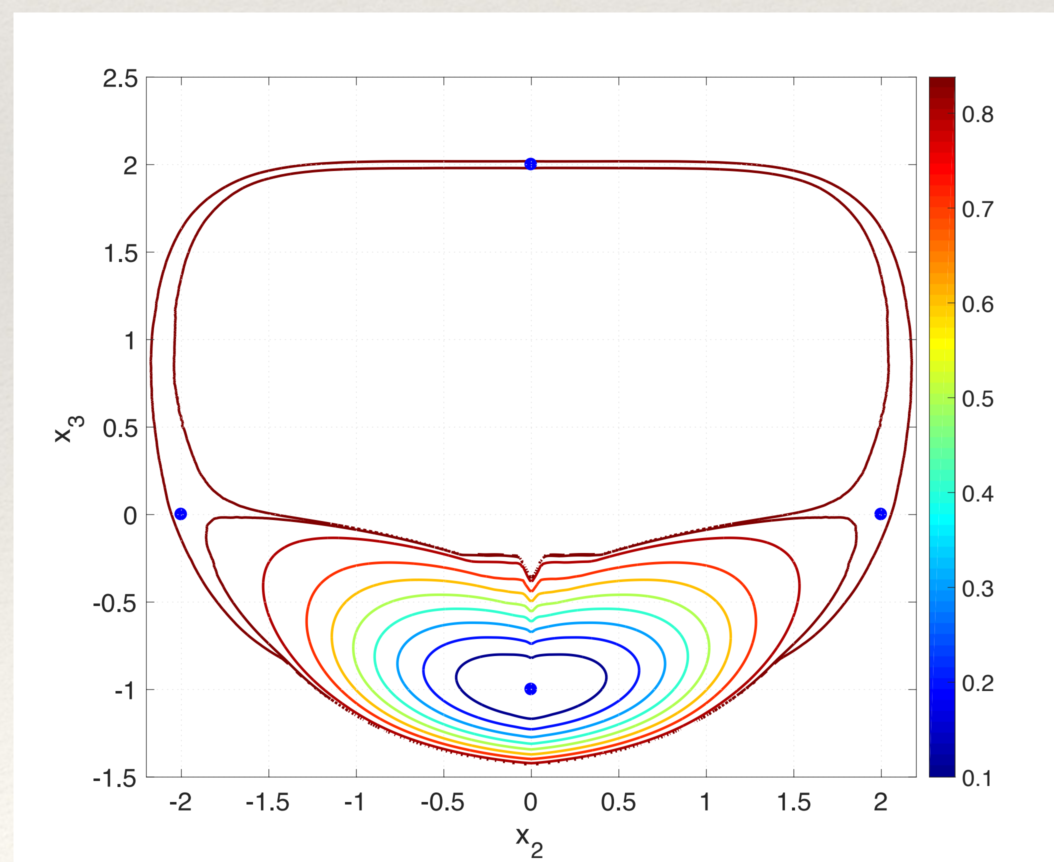
3D systems with hyperbolic periodic orbits

Tao’s examples, 2018





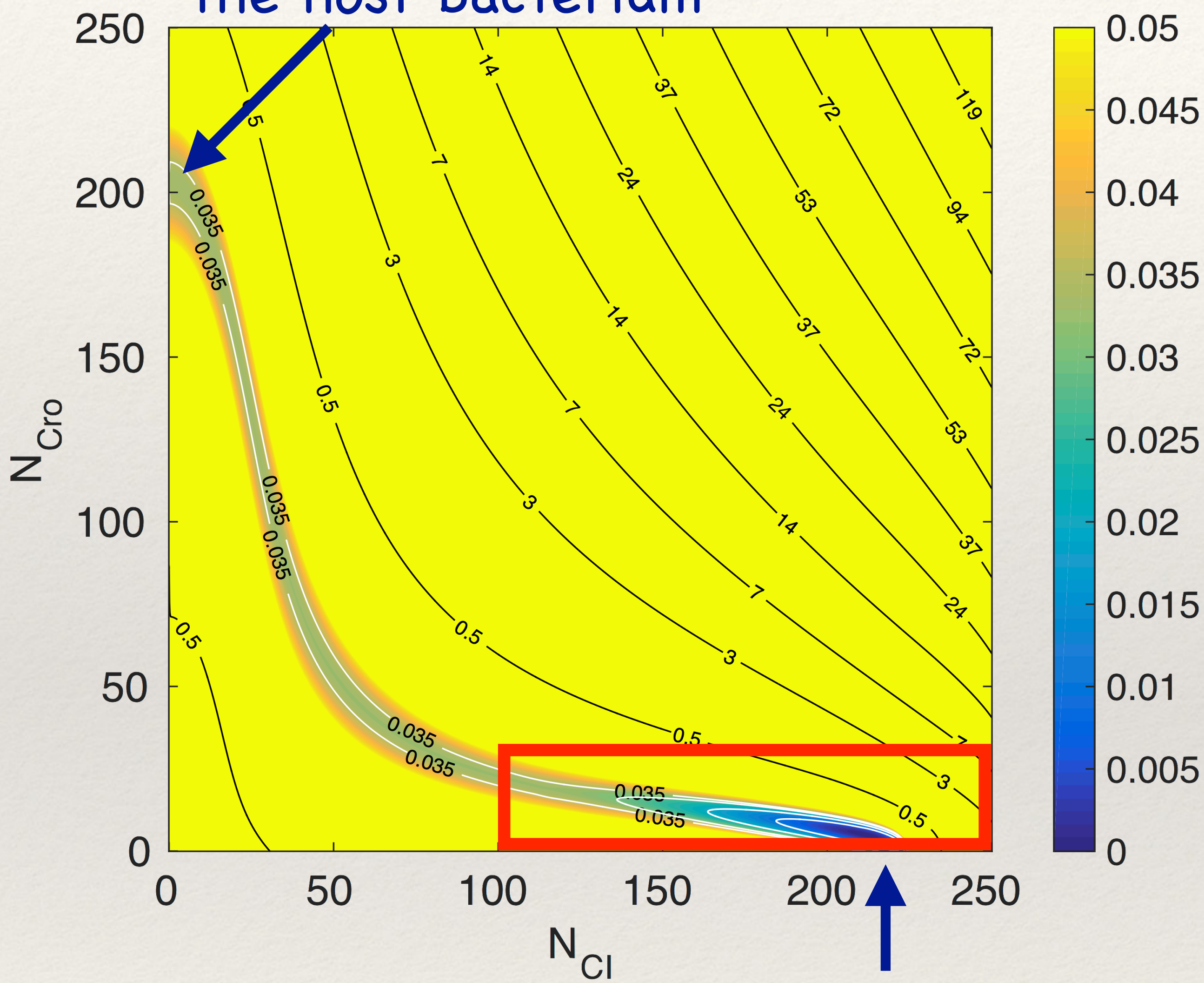




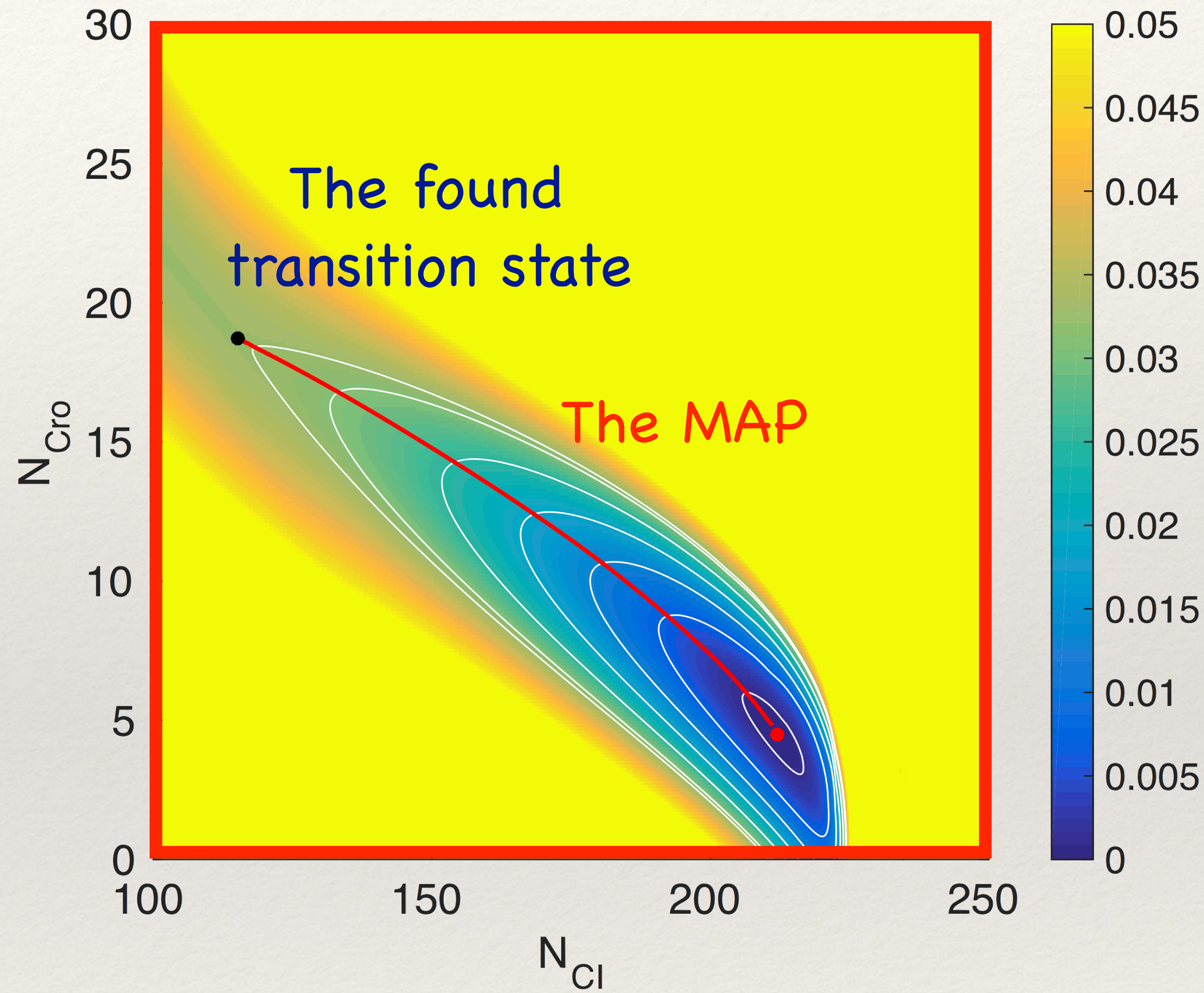
2D: Genetic switch in phage λ

SDE model: Aurell/Sneppel, 2002

Lytic state: phage λ kills the host bacterium



Lysogenic state: phage λ reproduces without killing the host bacterium

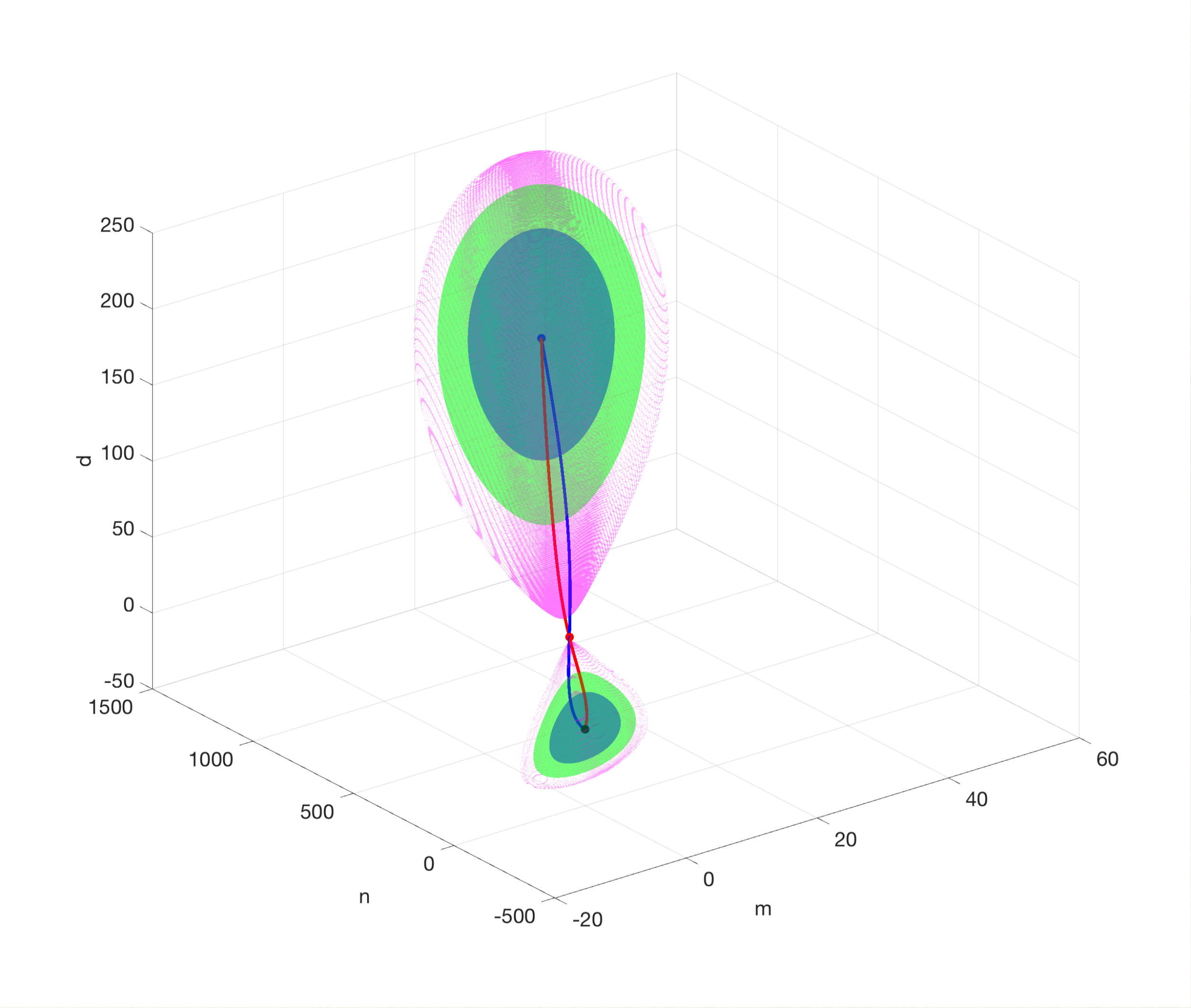


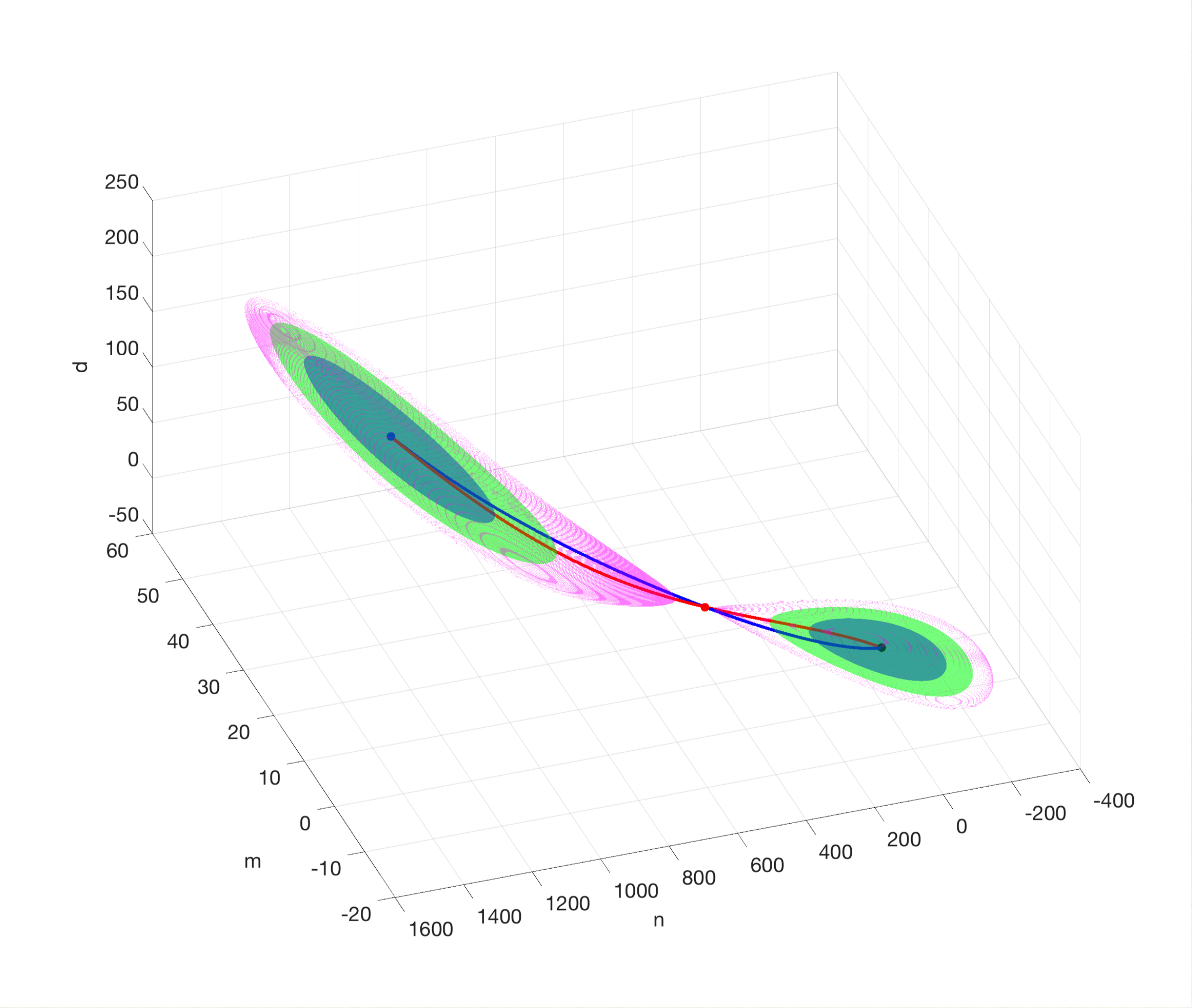
3D: Genetic switch model with a positive feedback

Lv, Li, Li, Li , 2014

$$
\begin{aligned}
d\mathsf{m} &= \left(\frac{a_0\gamma_0 + ak_0\mathsf{d}}{\gamma_0 + k_0\mathsf{d}} - \gamma_m\mathsf{m}\right) + \sqrt{\epsilon}dw_1,\\
d\mathsf{n} &= \left(b\mathsf{m} - \gamma_n\mathsf{n} - 2k_1\mathsf{n}^2 + 2\gamma_1\mathsf{d}\right) + \sqrt{\epsilon}dw_2,\\
d\mathsf{d} &= \left(k_1\mathsf{n}^2 - \gamma_1\mathsf{d}\right) + \sqrt{\epsilon}dw_3.
\end{aligned}
$$

m = #mRNA, n = #protein, d = #dimer





Lorenz'63

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} \sigma(y-x) \\ x(\rho - z) - y \\ xy - \beta z \end{bmatrix} dt + \sqrt{\epsilon} dw \qquad \sigma = 10, \quad \beta = 8/3, \quad 0 < \rho < \infty$$

Some critical values of ρ:

$\rho = 1$: the origin turned from a sink to a saddle, equilibria C_+ and C_- at $\left(\pm\sqrt{\beta(\rho-1)}, \pm\sqrt{\beta(\rho-1)}, \rho - 1\right)$ are born

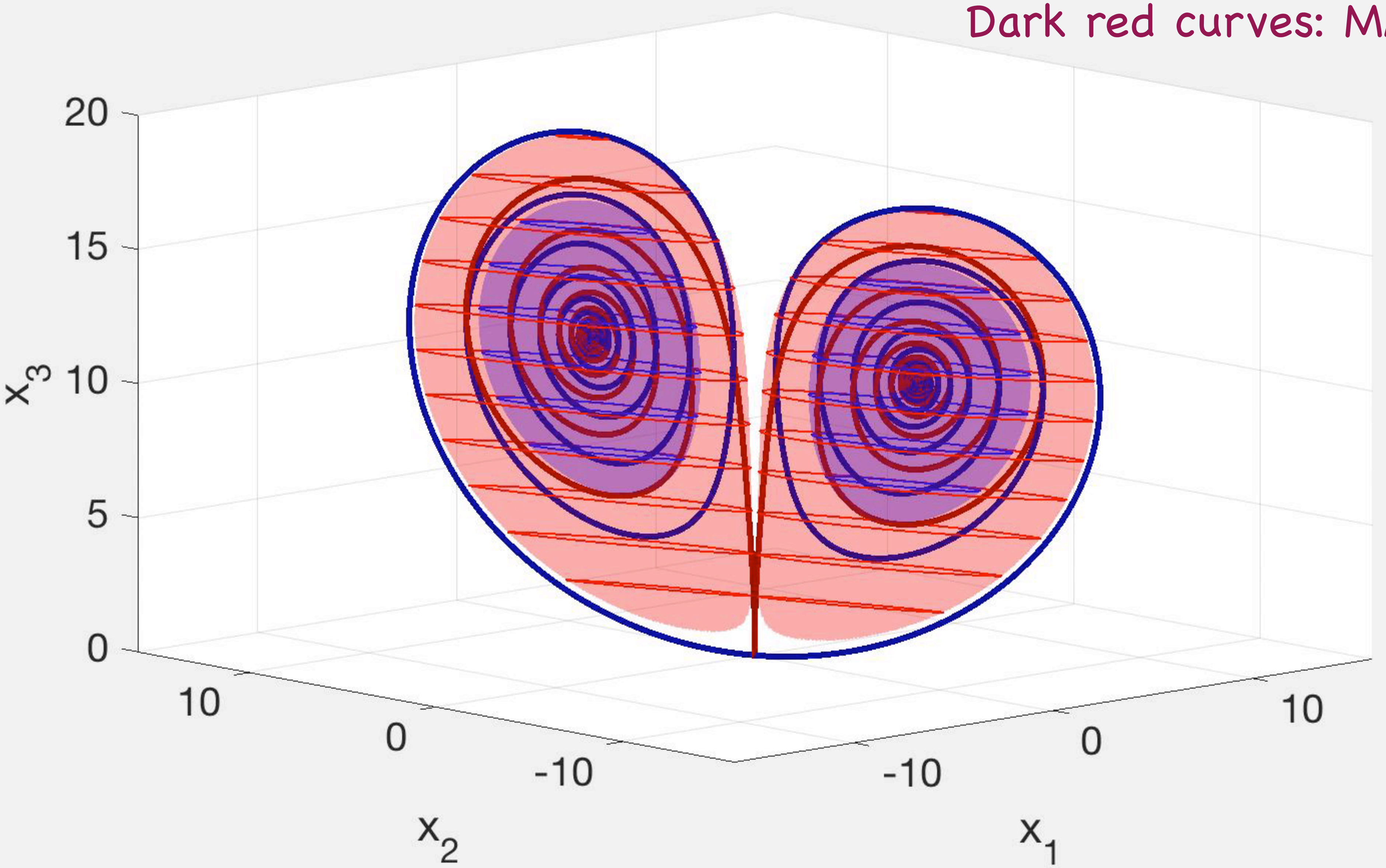
$\rho \simeq 13.926$: "preturbulence" starts (Kaplan & Yorke, 1979)

$\rho \simeq 24.06$: the strange attractor is born (Yorke & Yorke, 1979)

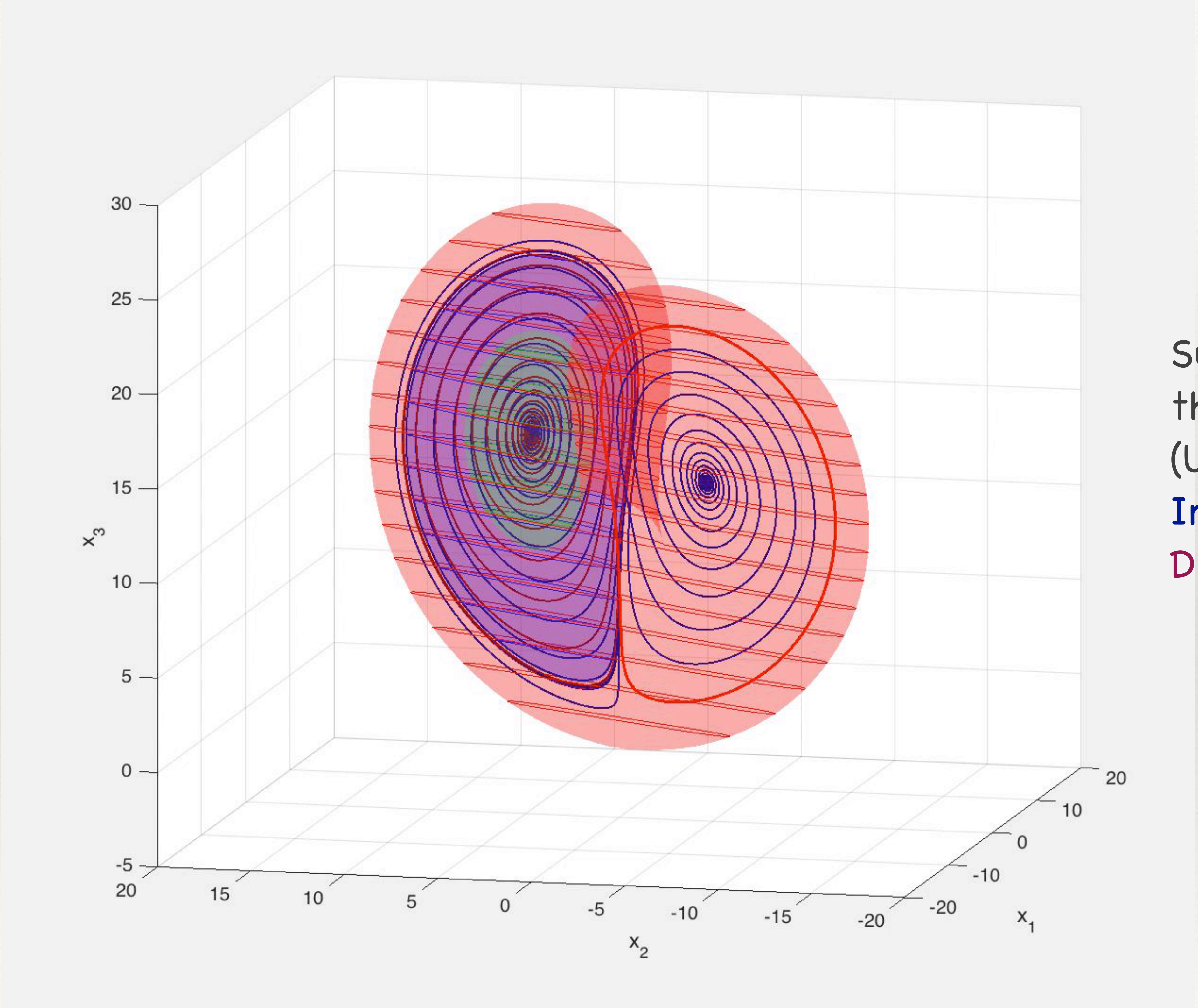
$\rho \simeq 24.74$: equilibria lose stability

$\rho = 12$

Surfaces: level sets of the quasipotential
(U = 10, U_{origin} - 0.05)
Indigo curves: trajectories
Dark red curves: MAPs



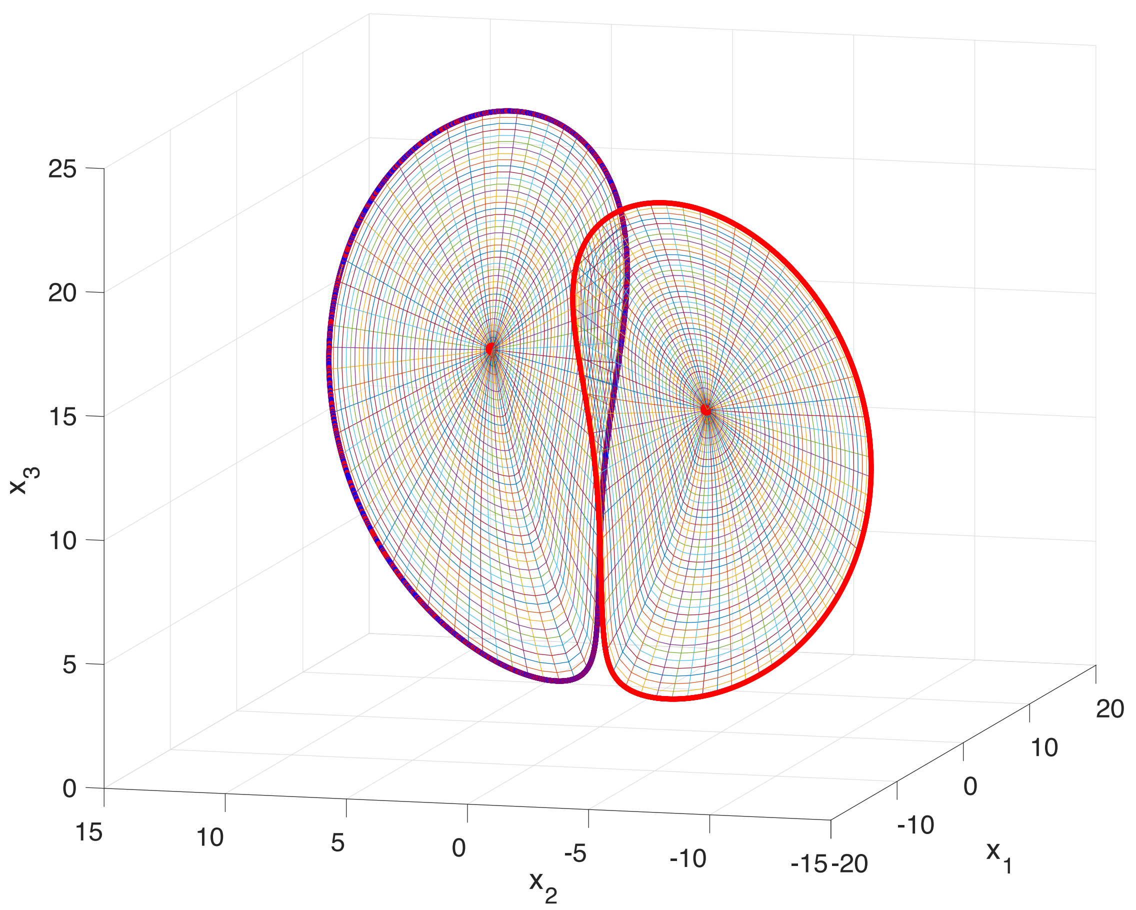
$\rho = 15$



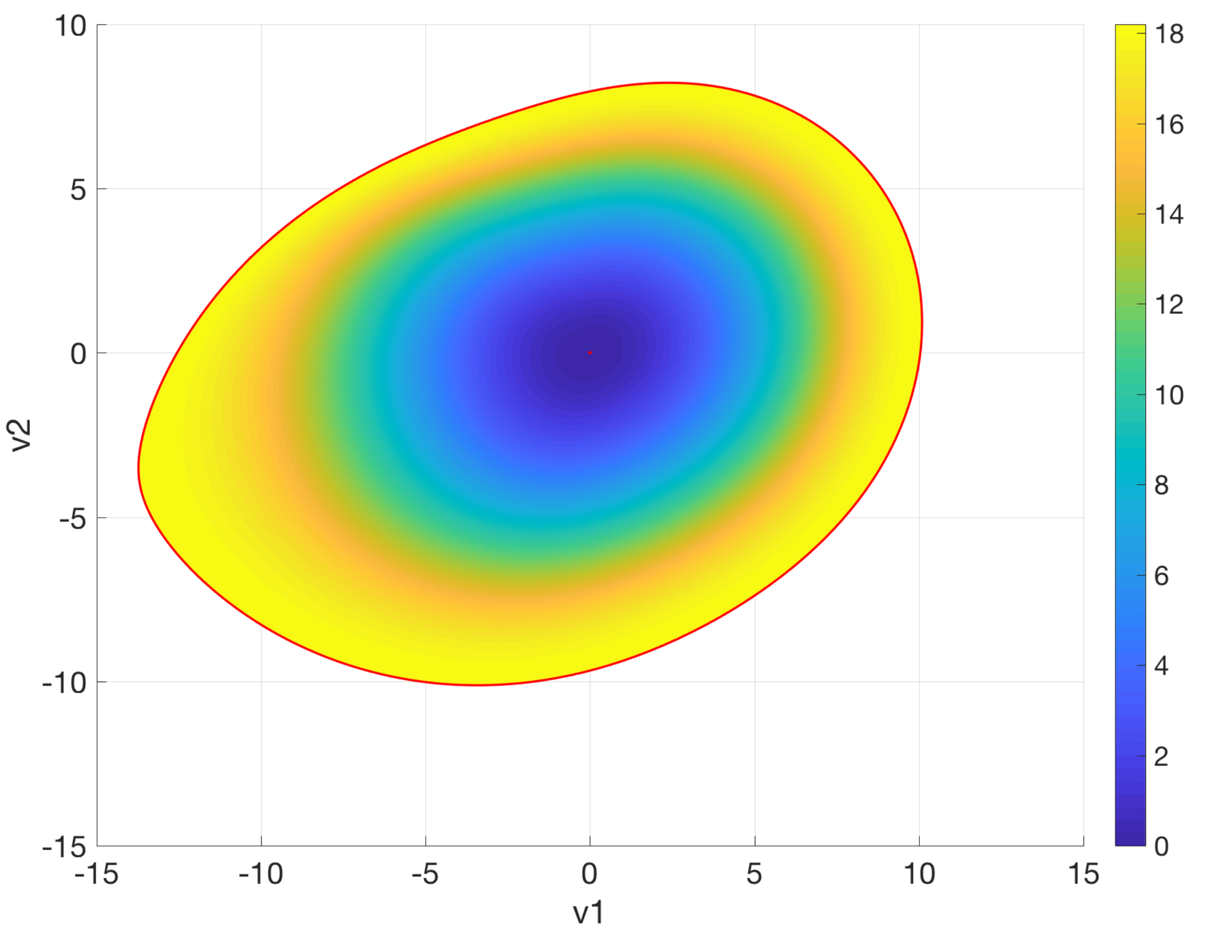
Surfaces: level sets of the quasipotential
(U = 8, $U_{\text{limit cycle}}$ - 0.01, 20)
Indigo curves: trajectories
Dark red curves: MAPs

$\rho = 15$

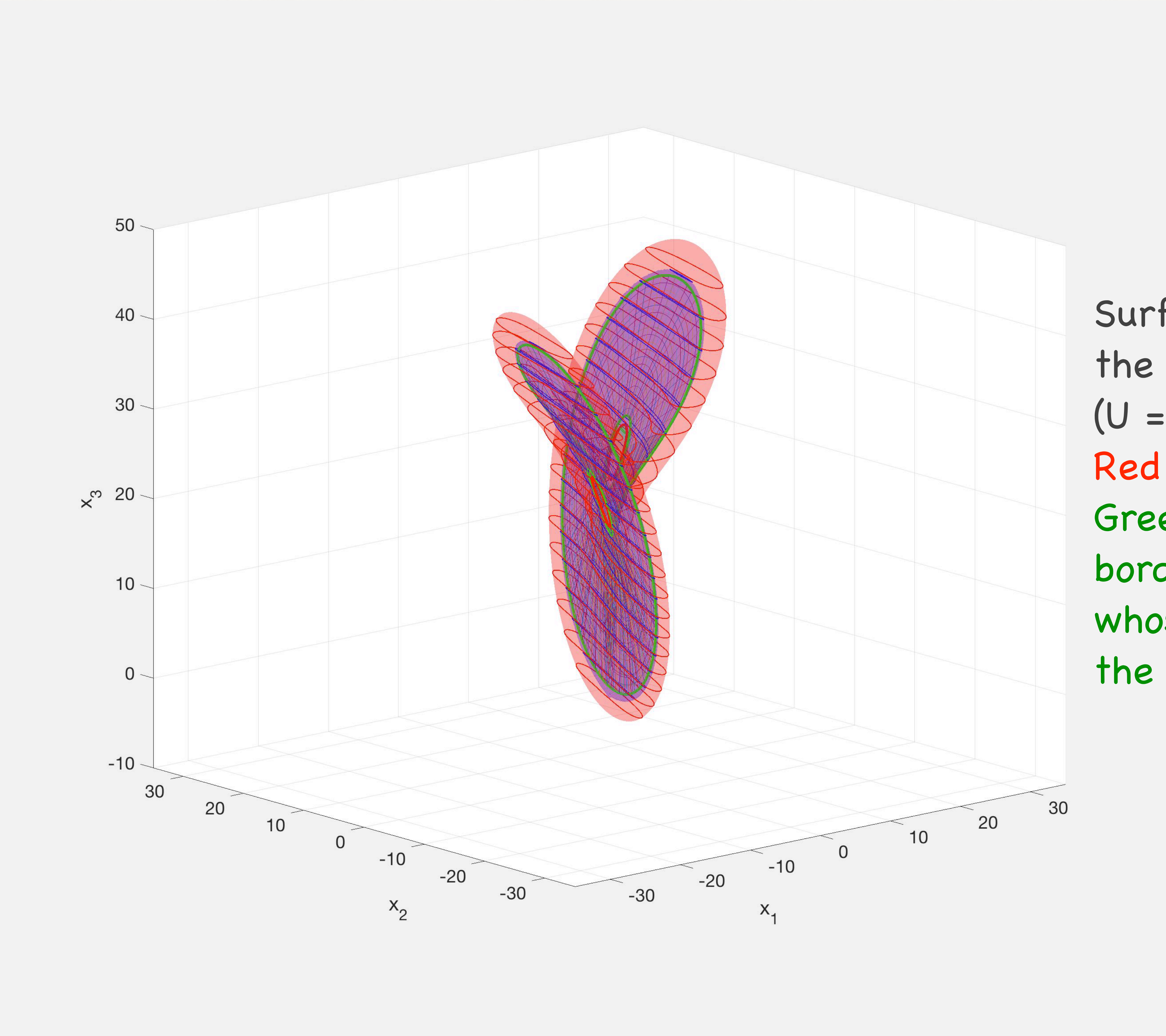
A 2D mesh on manifolds near which the dynamics are focused



The quasi potential computed on this 2D mesh

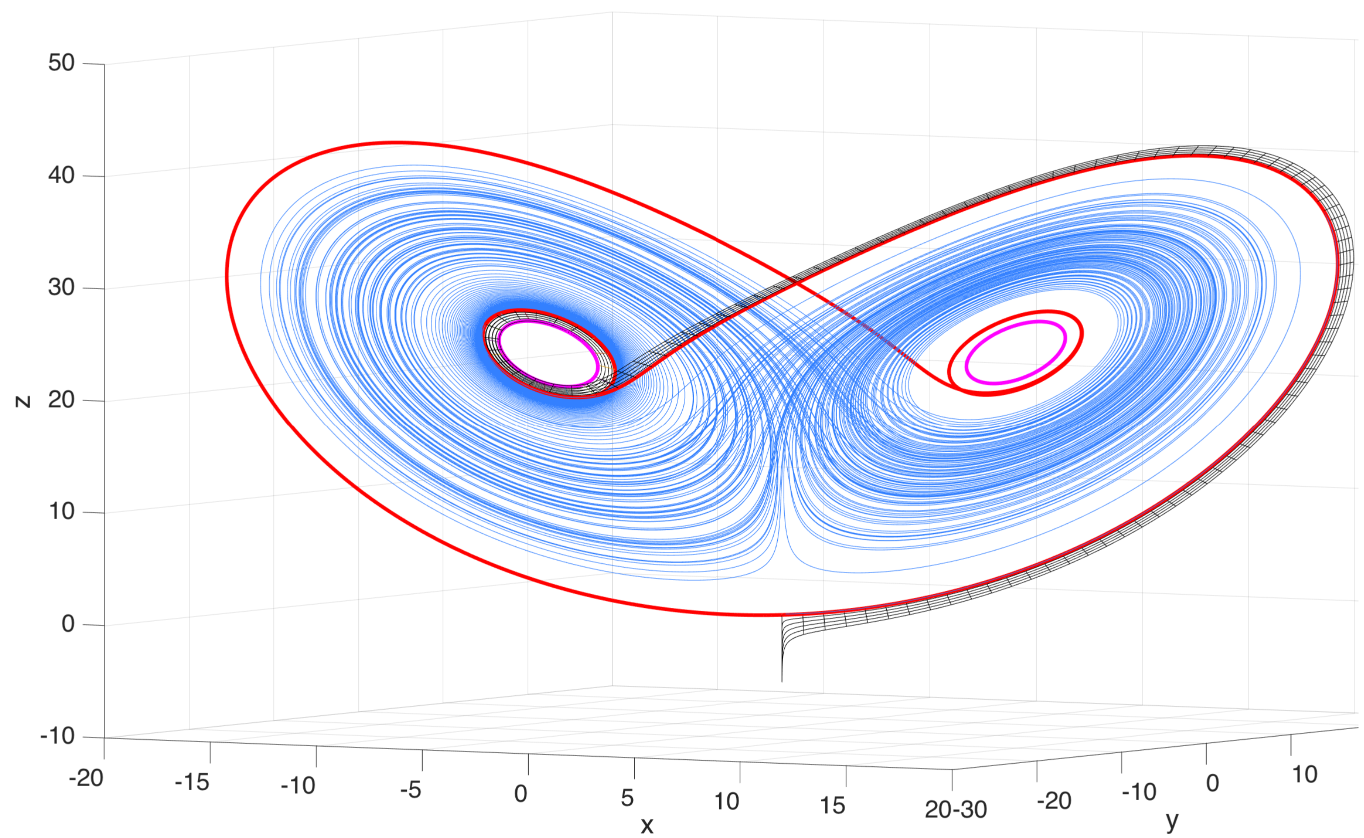


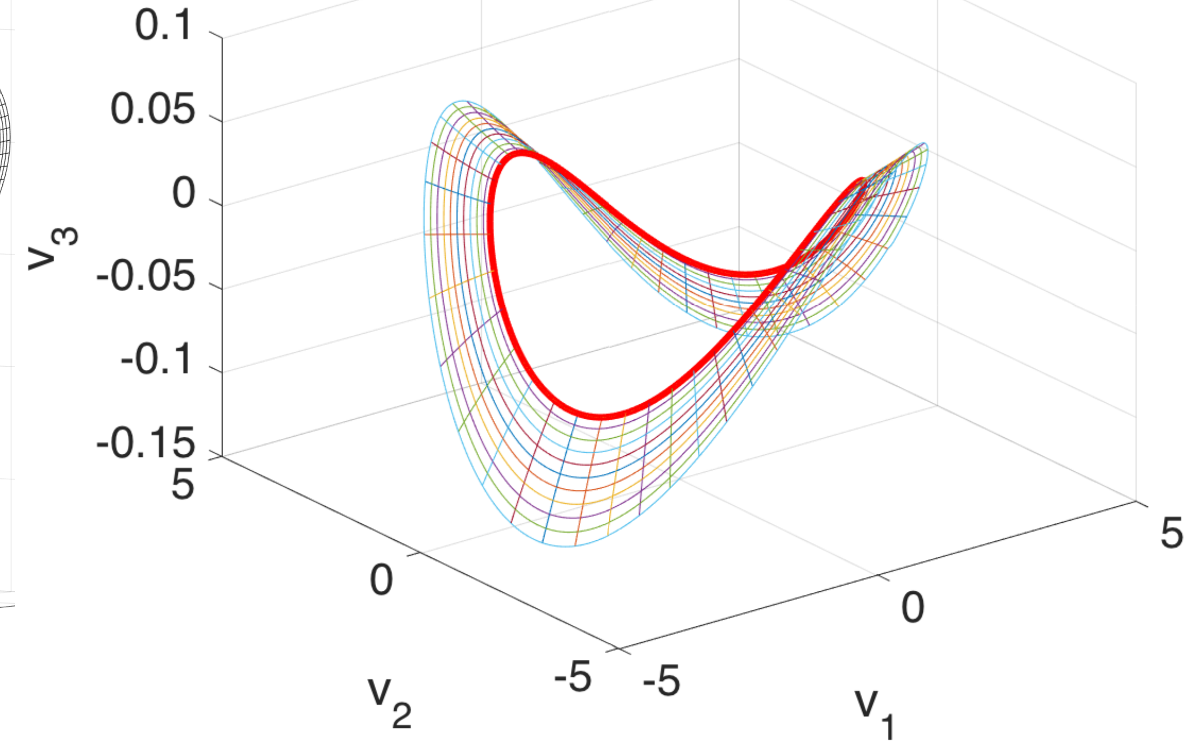
$\rho = 24.4$

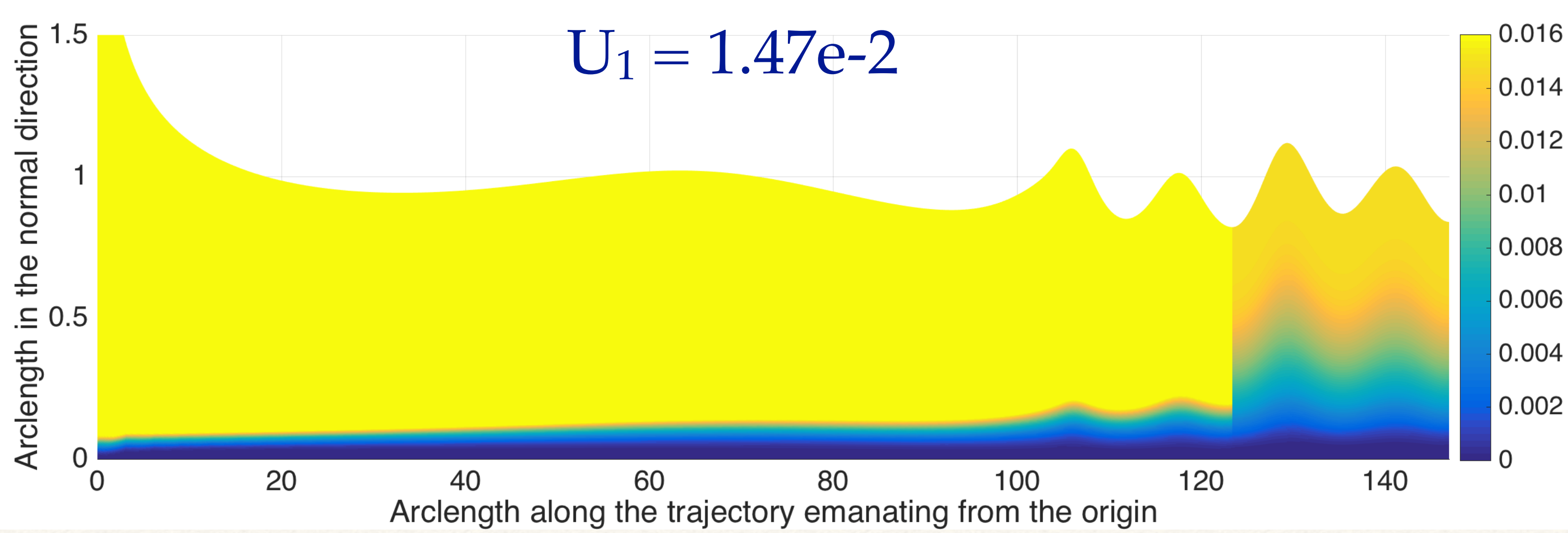


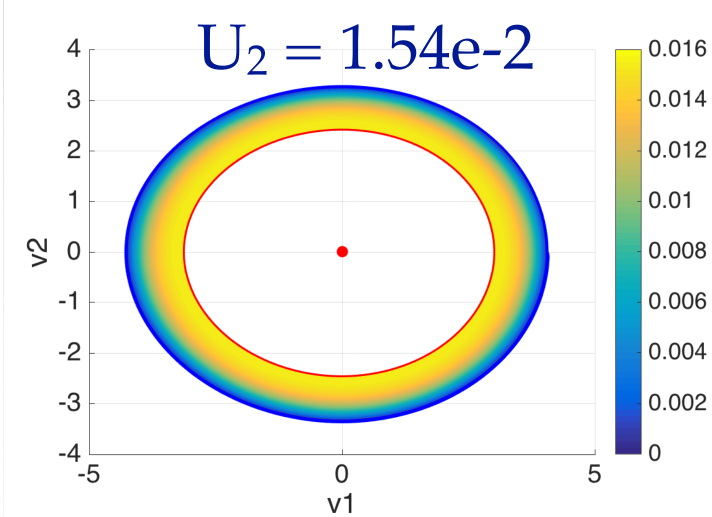
Surfaces: level sets of the quasipotential
($U = U_{limit\ cycle} - 0.01$, 2, 20)
Red loops: limit cycles
Green curves:
borders of manifolds whose union approximates the strange attractor

$\rho = 24.4$: from the strange attractor to stable equilibria: which way we go?









Conclusion

- The OLIM quasipotential solver is a numerical tool for analysis of dynamical systems perturbed by small noise
  - It **visualizes** the dynamics and allows us to find **maximum likelihood transition paths**, estimate **expected escape times**, and **invariant probability measure**
- Way to high dimensions: look for a low-dimensional manifold near which the dynamics are focused

References:

- Dahiya & C., Ordered line integral methods for computing the quasipotential, J. Sci. Comp., 75/3, 1351—1384 (2018), **arXiv: 1706.07509**
- Dahiya & C., An ordered line integral method for computing the quasipotential in the case of variable and anisotropic diffusion, Physica D (2018) *to appear*, **arXiv: 1806.05321**
- Yang, Potter, & C., Computing the quasipotential for nongradient SDEs in 3D, *submitted* (2018), **arXiv: 1808.00562**

- **C codes and user's guides:** http://www.math.umd.edu/~mariakc/index.html