Stability and Convergence of the String Method

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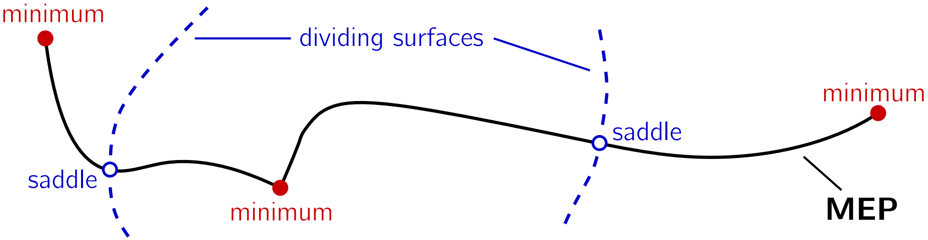
String Method and Minimum Energy Paths

String method [E, Ren, Vanden-Eijnden, 2002] and nudged elastic band [Henkelman, Jónsson, 2000] find minimum energy paths (MEPS).

Minimum Energy Path: Path ϕ between local minima of potential V with

$$\nabla V(\phi(\alpha))^{\perp} = \nabla V(\phi(\alpha)) - \left\langle \nabla V(\phi(\alpha)), \frac{\phi'(\alpha)}{\|\phi'(\alpha)\|} \right\rangle \frac{\phi'(\alpha)}{\|\phi'(\alpha)\|} = 0.$$

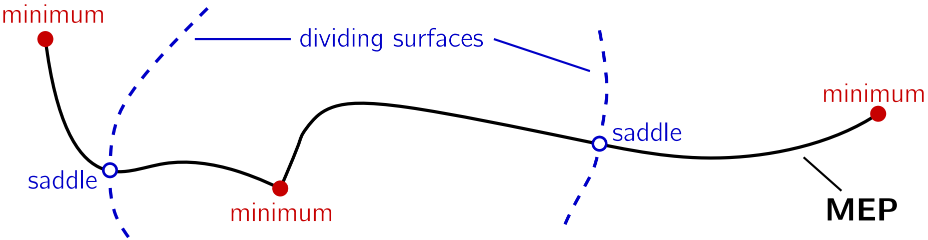


Why Minimum Energy Paths?

1. Relevant saddle point for transition state theory (TST) approximation of reaction rate is contained in MEP.
   Saddle of Index One: $x \in \mathbb{R}^d$ with $\nabla V(x) = 0$ and

$$\underbrace{\lambda_1 < 0 < \lambda_2 \leq \cdots \leq \lambda_d}_{\text{spectrum of } D^2 V(x)}.$$

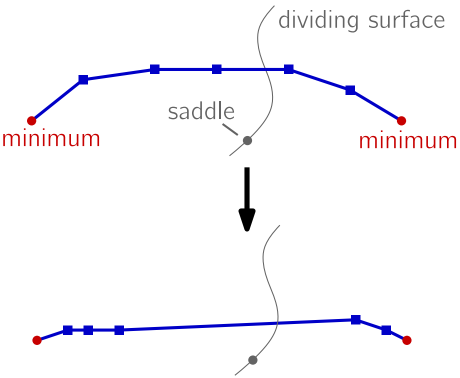
2. "Most probable reaction path for overdamped Langevin at low temperature" is an MEP, under certain conditions.



Simplified and Improved String Method

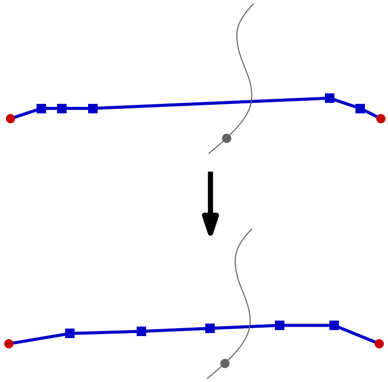
[E,Ren,Vanden-Eijnden, 2007]

Step 1: Evolve by Gradient Descent



After evolution, string is closer to saddle, but nodes are unevenly spaced.

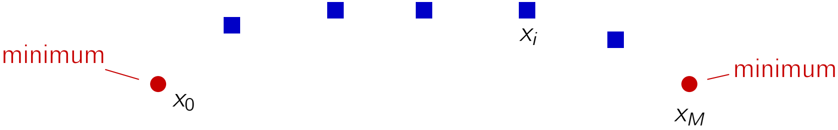
Step 2: Reparametrize



Reparametrization respaces nodes.

String Method: Terminology

A **String** $x \in \mathbb{R}^{(M+1)\times d}$ of $M+1$ **Images** $x_i \in \mathbb{R}^d$:



Numerical Flow Map $S_{\Delta t}$:

Let $S_{\Delta t}$ be a numerical integrator for gradient descent, e.g. Euler's method:

$$S_{\Delta t} x_i = x_i - \Delta t \nabla V(x_i).$$

Note: We let $S_{\Delta t}$ operate on strings as well as on images.

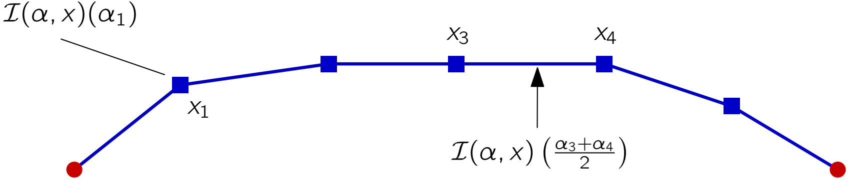
String Method: Interpolant

Linear Interpolant $\mathcal{I}(\alpha, x)$:

Given $x \in \mathbb{R}^{(M+1)\times d}$ and $\alpha_0 = 0 < \alpha_1 < \cdots < \alpha_M = 1$, let

$$\mathcal{I}(\alpha, x) : [0, 1] \to \mathbb{R}^d$$

be the linear interpolant of $\{(\alpha_i, x_i)\}_{i=0}^M$.



Note: Could use other interpolants, we choose linear for simplicity.

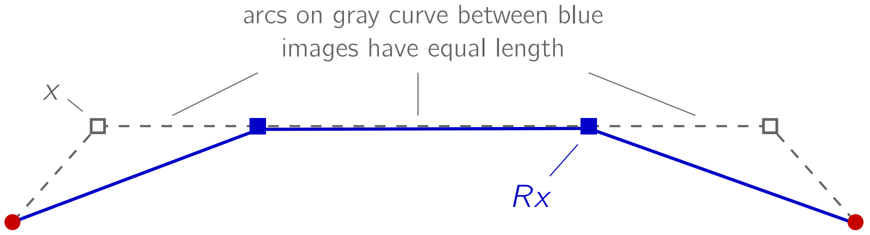
String Method: Reparametrization

Arc Length: Given $x \in \mathbb{R}^{(M+1)\times d}$, define $\ell(x) \in \mathbb{R}^{M+1}$ by

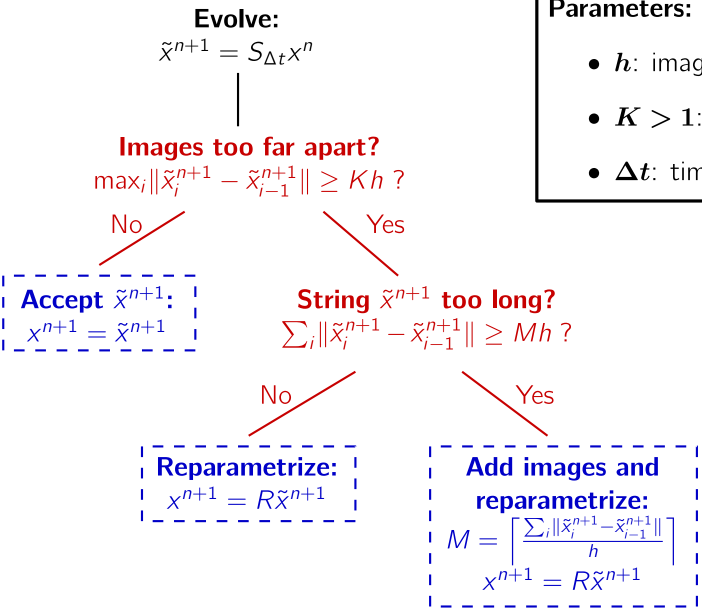
$$\ell_i(x) = \frac{\sum_{k=1}^{i} \|x_i - x_{i-1}\|}{\sum_{k=1}^{M} \|x_i - x_{i-1}\|}.$$

Reparametrization: $R : \mathbb{R}^{(M+1)\times d} \to \mathbb{R}^{(M+1)\times d}$ by

$$Rx_i = \mathcal{I}(\ell(x), x)\left(\frac{i}{M}\right)$$



Simplified and Improved SM [E,Ren,Vanden-Eijnden, 2007]



Parameters:

- $\boldsymbol{h}$: image spacing
- $\boldsymbol{K > 1}$: spacing tolerance
- $\boldsymbol{\Delta t}$: time step

Gradient Descent Dynamics on Curves (GDDC)

Flow for Gradient Descent: $\Phi_t : \mathbb{R}^d \to \mathbb{R}^d$ defined by

$$\Phi_t(x) = z(t) \text{ where } z'(s) = -\nabla V(z(s)) \text{ and } z(0) = x.$$

That is, **$\Phi_t(x)$ is the trajectory of gradient descent starting from x.**

Gradient Descent Dynamics on Curves:

Given path $\gamma_0 : [0,1] \to \mathbb{R}^d$ define a path γ_t by

$$\gamma_t(\alpha) = \Phi_t(\gamma_0(\alpha)) \text{ for } \alpha \in [0,1].$$

Note: MEPs are stationary points of GDDC, considered as a dynamics on *curves*.

Convergence of GDDC

Theorem [Cameron, Kohn, Vanden-Eijnden, 2011]: Suppose V has finitely many critical points, each of index ≤ 1. Under mild technical conditions, any trajectory of GDDC converges (in Hausdorff distance) to a MEP.

If there are saddles of index ≥ 2, may not converge to single MEP:

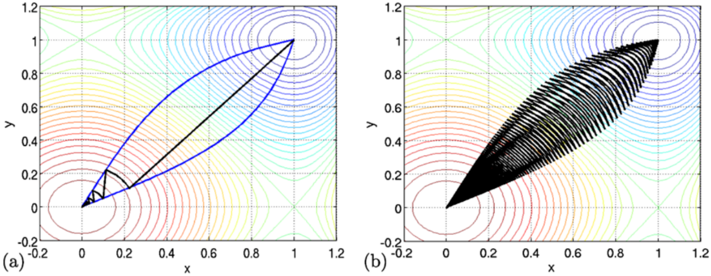


figure from [Cameron, Kohn, Vanden-Eijnden, 2011]

Here, the initial curve evolves under GDDC to fill a 2d region.

Numerical Analysis: Objectives

- *A Priori* **Existence and Convergence**:

  Given an MEP, show that SM converges to a path near the MEP, at least for x^0 sufficiently close to MEP and for $h, \Delta t$ sufficiently small.

  Show that as $h, \Delta t$ tend to zero, limit of SM converges to MEP.

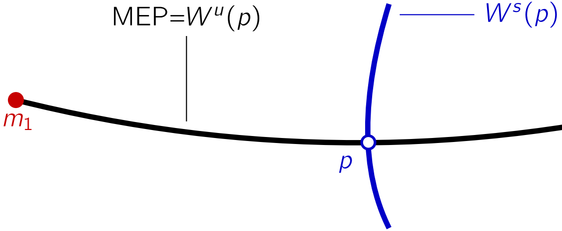
- *A Posteriori* **Existence**:

  Given a converged state of SM, show that there is an MEP nearby.

- Here, we address only the *a priori* part of the analysis.

Numerical Analysis: Assumptions

- Exactly two stable minima m_1, m_2 and one saddle p of index one.
- Stable manifold $W^s(p)$ of p separates basins of attraction of m_1, m_2.
  Note: $W^s(p) = \{x \in \mathbb{R}^d : \lim_{t\to\infty} \Phi_t(x) = p\}$.



- For now, also assume $S_{\Delta t} = \Phi_{\Delta t}$, i.e. ignore time discretization error.

Numerical Analysis: Stability

- [Cameron, Kohn, Vanden-Eijnden, 2011] $\Longrightarrow$ trajectories of GDDC converge in d_{H} to MEP under our assumptions.

- We need stronger stability properties to prove SM converges:

  1. **Uniform stability of MEP under GDDC**

  2. **Asymptotic stability of MEP with uniform convergence**

- Uniform & asymptotic stability

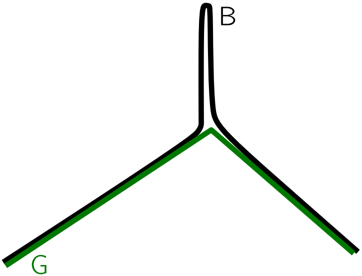
  $\Longrightarrow$ Lyapunov function for MEP under GDDC

  $\Longrightarrow$ error bounded in long time limit

Numerical Analysis: Measures of Distance

One-Sided Distance

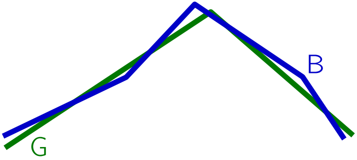
$d(G, B) = \max_{g \in G} \min_{b \in B} \|g - b\|$



Here, $d(G, B)$ is small,
but $d(B, G)$ is large.

Hausdorff Distance

$d_H(G, B) = \max\{d(G, B), d(B, G)\}$



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Numerical Analysis: Asymptotic Stability

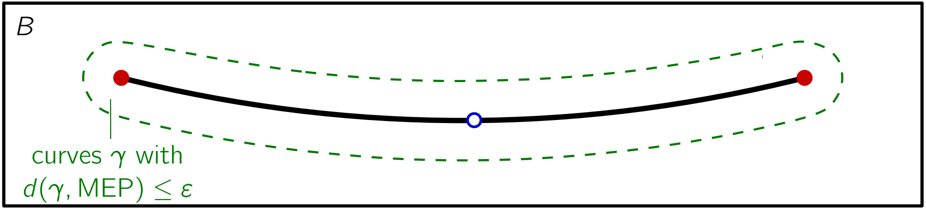
Definitions:

- $B \subset \mathbb{R}^d$: a bounded set containing MEP
- $C(m_1, m_2, B)$: set of continuous paths $\gamma : [0,1] \to B$ from m_1 to m_2.

Asymptotic Stability with Uniform Convergence on B:

For every $\varepsilon > 0$, there exists $T(\varepsilon, B) > 0$ so that

$$d_{\mathrm{H}}(\Phi_t(\gamma), \mathrm{MEP}) \leq \varepsilon \text{ for all } t > T(\varepsilon, B) \text{ and } \gamma \in C(m_1, m_2, B).$$



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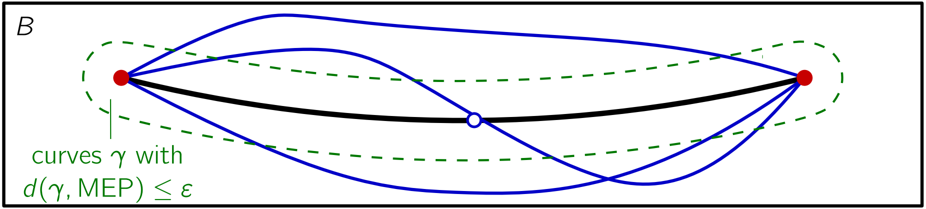

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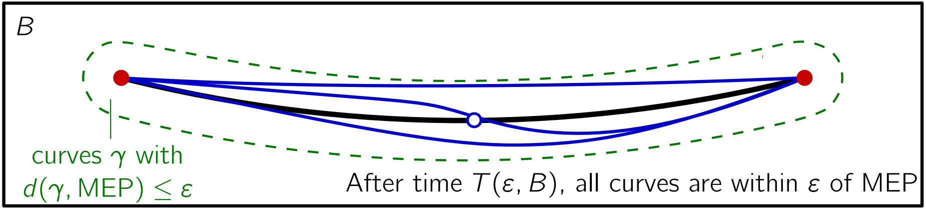

Numerical Analysis: Uniform Stability

Uniform Stability:

For every $\varepsilon > 0$ there exists a $\delta > 0$ so that

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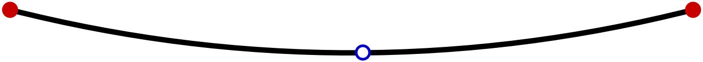

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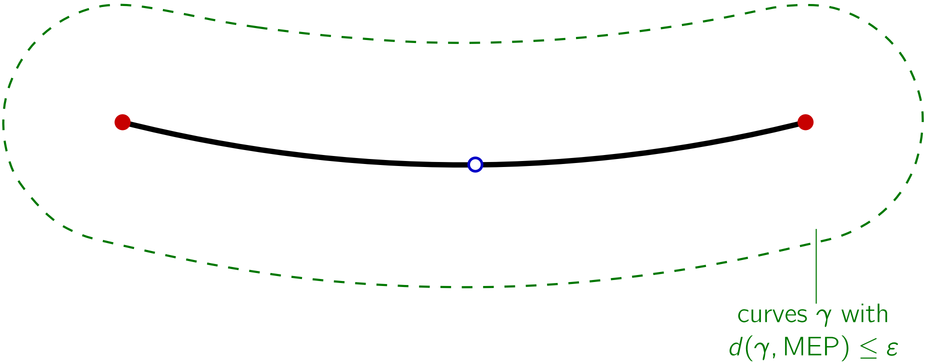

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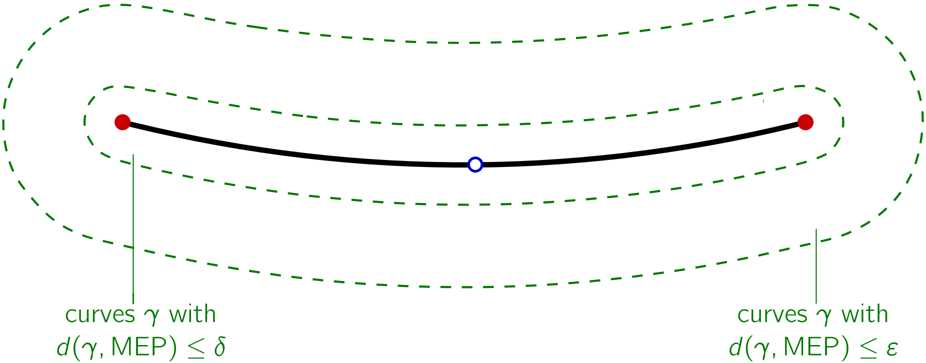

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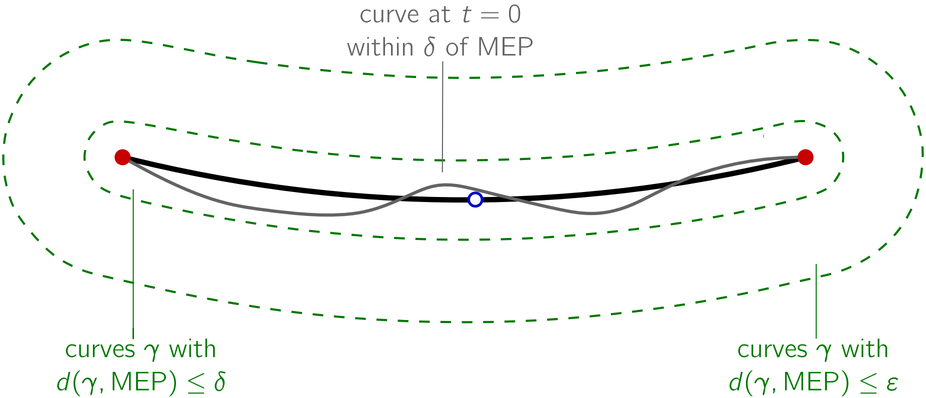

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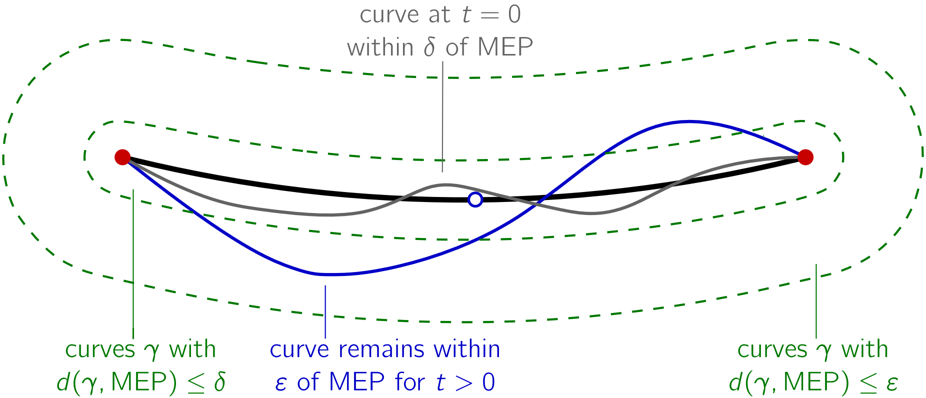
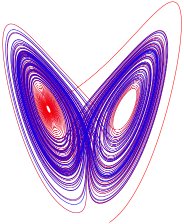


Why Uniform and Asymptotic Stability?

[Kloeden, Lorenz, 1986] $\Longrightarrow$ uniformly asymptotically stable sets are preserved under time discretization, e.g.



Lorenz attractor, figure from wikipedia

Theorem [Stuart, Humphries, 1996]: If a set A is uniformly asymptotically stable for an ODE, then for any one step discretization $S_{\Delta t}$, there exists a set $A_{\Delta t}$ which is uniformly asymptotically stable for $S_{\Delta t}$ such that

$$\lim_{\Delta t \to 0} d_{\mathrm{H}}(A, A_{\Delta t}) = 0.$$

Numerical Analysis: Lyapunov Function

Theorem [BvK, Luskin, 2017+]: Under our assumptions the MEP is uniformly stable, and it is asymptotically stable with uniform convergence on B for any bounded $B \supset$ MEP.

Modifying the proof of a similar result from [Yoshizawa, 1964] yields ...

Theorem [BvK, Luskin, 2017+]: There exists a Lyapunov function $W : C(m_1, m_2, B) \to [0, \infty)$ for the MEP such that

1. $W(\text{MEP}) = 0$
2. $W(\Phi_t(\gamma)) \leq \exp(-ct)W(\gamma)$ for some $c > 0$
3. $|W(\gamma) - W(\eta)| \leq d_\text{H}(\gamma, \eta)$
4. There exists a strictly increasing, continuous $\alpha : [0, \infty) \to [0, \infty)$ with $\alpha(0) = 0$ so that $\alpha(d_\text{H}(\gamma, \text{MEP})) \leq W(\gamma) \leq d_\text{H}(\gamma, \text{MEP})$.

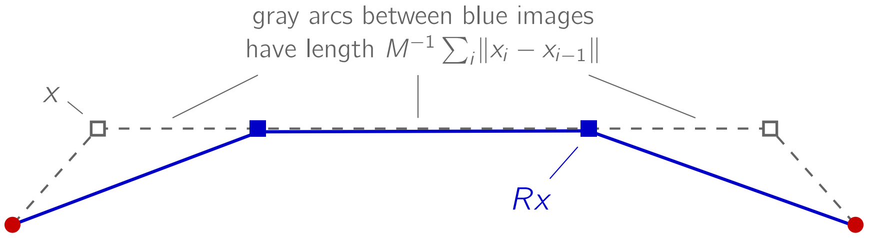
Numerical Analysis: Spatial Discretization Error I

Bound on Spacing: For $x^n \in \mathbb{R}^{(M+1)\times d}$ the n'th iterate of SM,

$$\max_i \|x_i^n - x_{i-1}^n\| \leq K \exp(\Delta t L) h,$$

where L is a Lipschitz constant for ∇V.

Why? Because $\max_i \|Rx_i - Rx_{i-1}\| \leq M^{-1} \times \overbrace{\sum_i \|x_i - x_{i-1}\|}^{\text{total length of } \mathcal{I}x} \leq h$:



Numerical Analysis: Spatial Discretization Error II

Notation: $\mathcal{I}x$ is linear interpolant of $x \in \mathbb{R}^{(M+1)\times d}$, understood as *curve*.

Spatial Discretization Error: For any $x \in \mathbb{R}^{(M+1)\times d}$,

$$d_{\mathrm{H}}(S_{\Delta t}\mathcal{I}x, \mathcal{I}S_{\Delta t}x) \leq C\Delta t \left(\max_i \|x_i - x_{i-1}\|\right)^2 .$$

Reparametrization Error: For any $x \in \mathbb{R}^{(M+1)\times d}$,

$$d_{\mathrm{H}}(\mathcal{I}x, \mathcal{I}Rx) \leq \frac{\max_i \|x_i - x_{i-1}\|}{2}.$$

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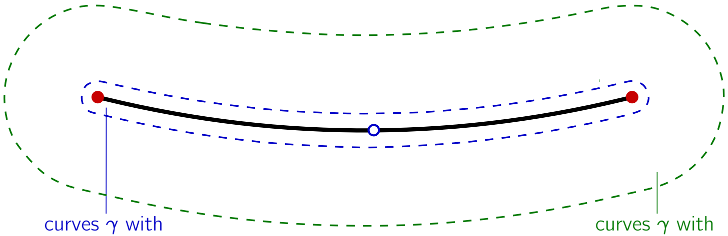
Reparametrization Frequency:

Evolve at least for time $\Delta t_{\min} := \frac{\log(K)}{L}$ between reparametrizations.

Convergence of String Method

"Trajectories of SM converge to a small neighborhood surrounding MEP; size of neighborhood shrinks as h tends to zero."

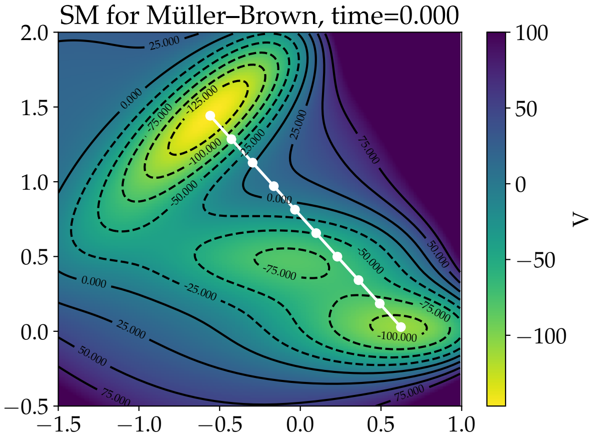


Theorem [BvK, Luskin, 2017+]: There exist $h_0 > 0$, $r_0 > 0$, $N_0 > 0$, and a function $e : (0, h_0) \to (0, \infty)$ with $\lim_{h \to 0} e(h) = 0$ such that if $d_{\mathrm{H}}(\mathcal{I}x^0, \mathrm{MEP}) < r_0$ and $h < h_0$, then

$$d_{\mathrm{H}}(\mathcal{I}x^n, \mathrm{MEP}) \leq e(h) \text{ for all } n > N_0.$$

Do Stronger Results Hold?

Run SM on Müller–Brown potential, $\Delta t = 0.0001$, *reparametrize every 10 time steps*, *plot results immediately after reparametrization.*



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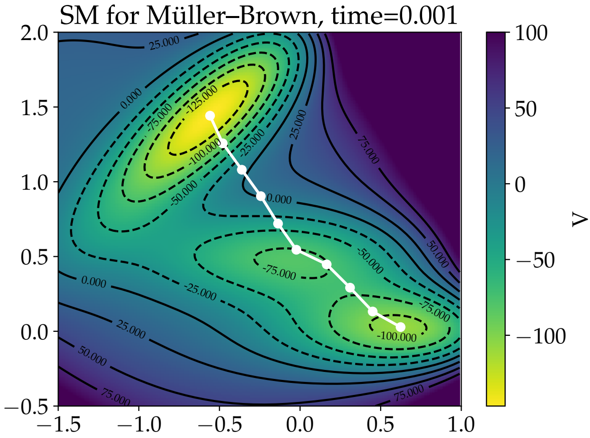

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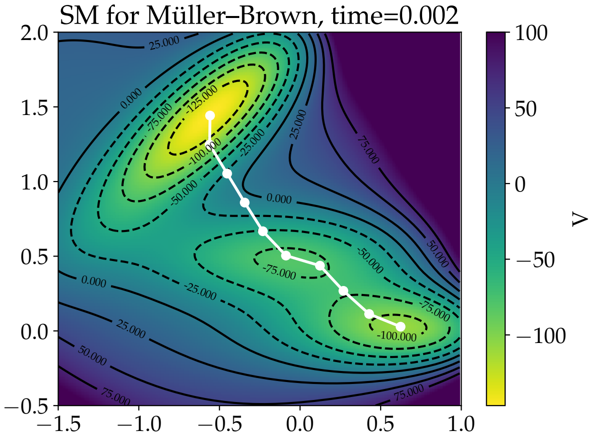

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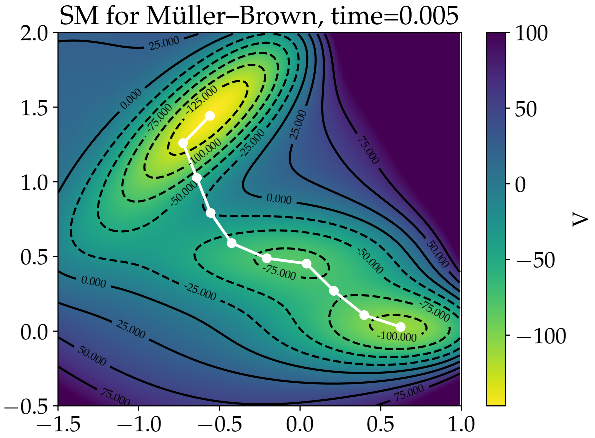

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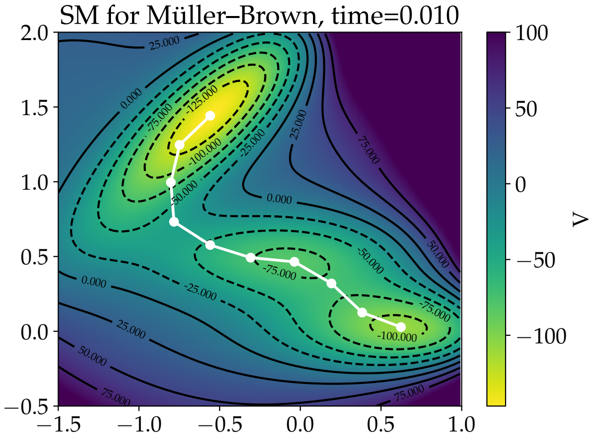

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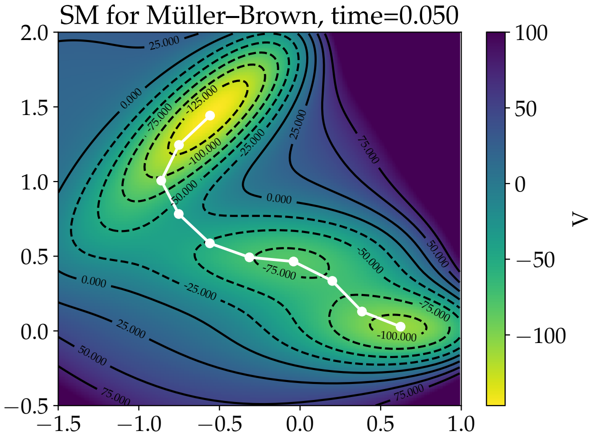

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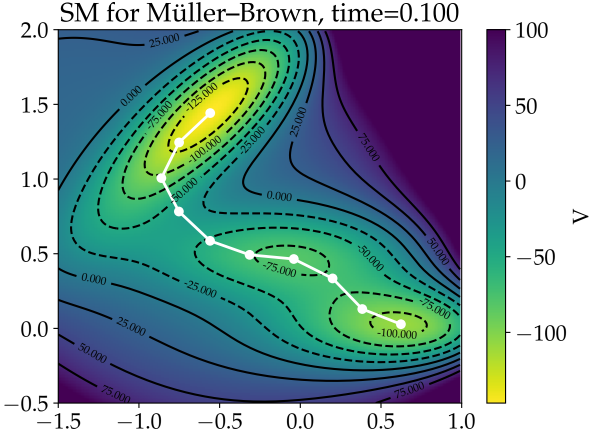
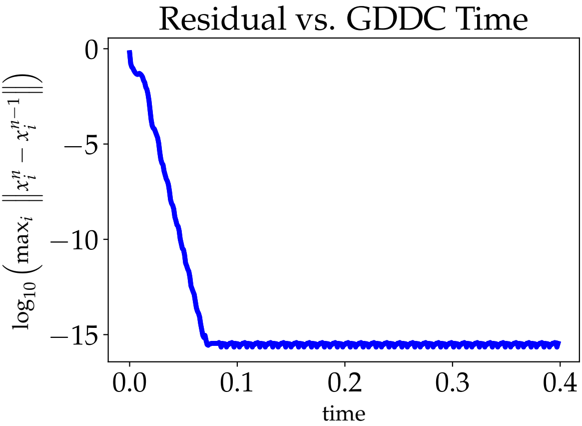


Do Stronger Results Hold?

Here, appears that SM converges to *single fixed point*:



Conclusions

Main Result [BvK, Luskin, 2017+]:

Using ideas from theory of dynamical systems, we prove convergence of simplified and improved SM to *a neighborhood of MEP whose size is* $o(1)$ *in* h, *under certain assumptions on* V.

Questions Not Addressed:

Does SM have a fixed point if reparametrization is performed after a fixed number of time steps?

Can one reparametrize after every time step, whether or not spacing of images is uneven?

Convergence of nudged elastic band, finite-temperature SM, SM in collective variables, variants of SM based on optimization, etc.