Most probable places of exit from a domain

Boris Nectoux (TU Wien)
Joint work with G. Di Gesù, T. Lelièvre, and D. Le Peutrec

- Overdamped Langevin process:

$$dX_t = -\nabla f(X_t)dt + \sqrt{h}\, dB_t.$$

- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain.
  - What are the **most probable places of exit** from Ω for the process $(X_t)_{t\geq 0}$?
  - What is the **exact repartition of probabilities** between these places ?
- Previous works of Day, Kamin, Perthame and Freidlin-Wentzell when $\partial_n f > 0$ on $\partial\Omega$ and f has only one critical point in Ω (which then is its global minimum in $\overline{\Omega}$).
- **Purpose of this work**: extend their result when f has several critical points in Ω and when $\partial_n f$ can change sign on $\partial\Omega$.
- Saddle points of f in Ω with a higher energy that $\min_{\partial\Omega} f$ can lead to significant changes in the concentration of the exit point distribution.

Efficient random walk for Wang-Landau algorithm in high dimensional spaces

Augustin Chevallier

September 18, 2018

Wang-Landau

- Wang-Landau, key features:
  - Stochastic algorithm to compute density of states
  - Asymptotic convergence well understood
  - Mild practical performances on real / complex systesm
- Novel ingredients:
  - Novel random walk using geometrical information (aka gradient)
    - counters some effects of measure concentration
  - Darting for multi-modal distributions
  - Test system: toy protein dialanine, dim $= 60$
    - One of the very first tests on biomolecules

Grégoire Ferré – CERMICS, ENPC

Consider an ergodic average of a diffusion

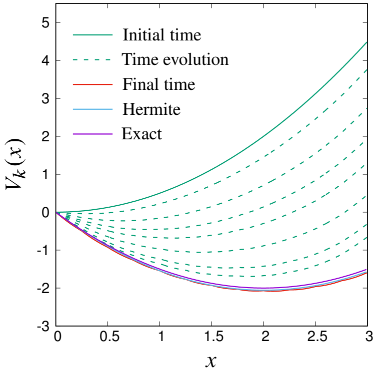
$$\frac{1}{t}\int_0^t f(X_s)\,ds \xrightarrow[t\to+\infty]{} \int_{\mathbb{R}^d} f\,d\mu.$$

Goal : compute the large deviations fluctuations

$$\mathbb{P}\left[\frac{1}{t}\int_0^t f(X_s)\,ds = a\right] \approx \mathrm{e}^{-tI(a)}.$$

Main strategies:

- importance splitting;
- *optimal control*.

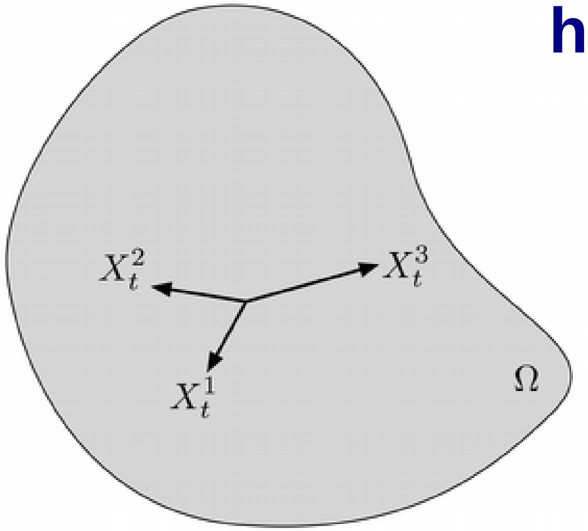


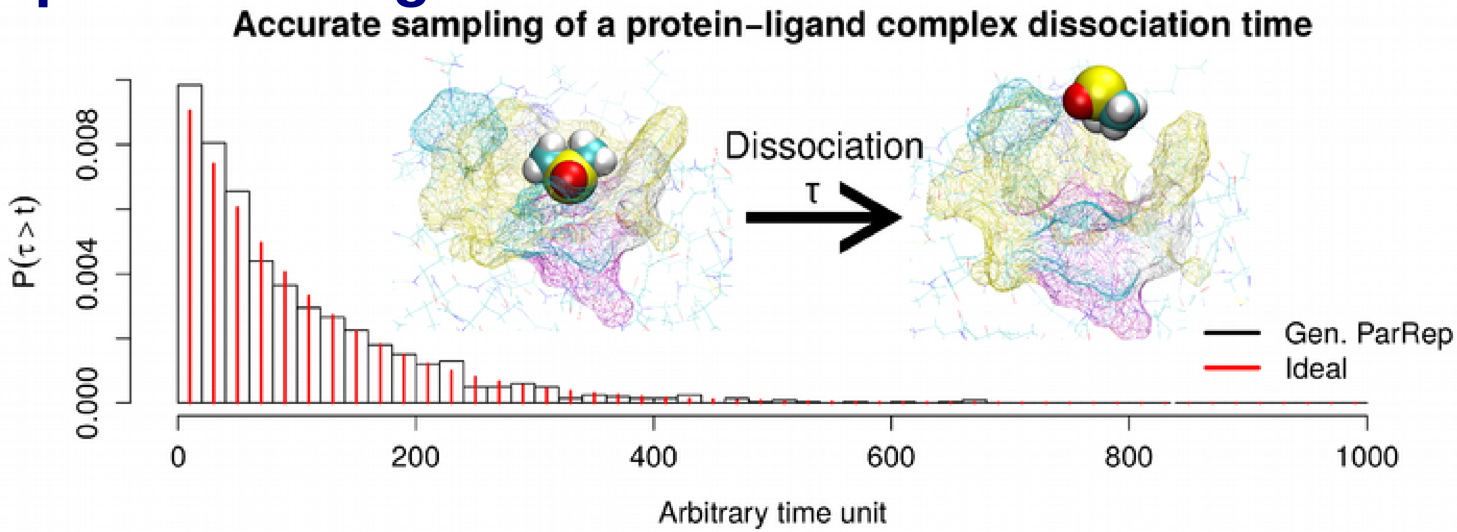
Poster: present an *adaptive algorithm* to learn the optimal bias and compute rare fluctuations. This is a joint work with H. Touchette (Stellenbosch).

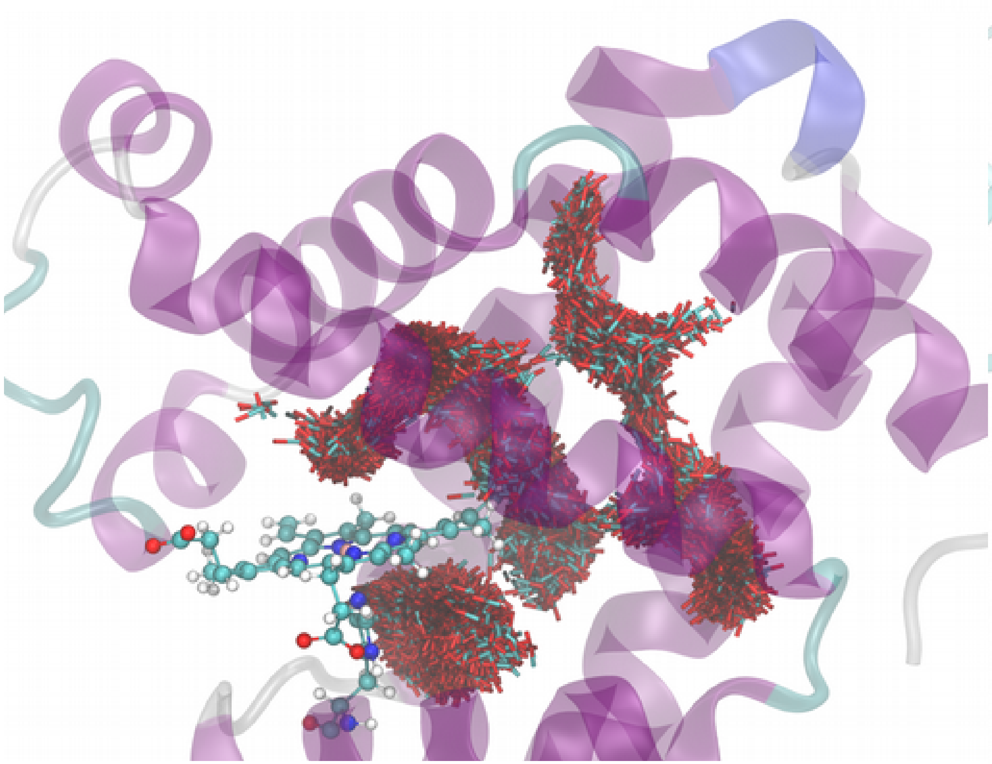
A new implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems

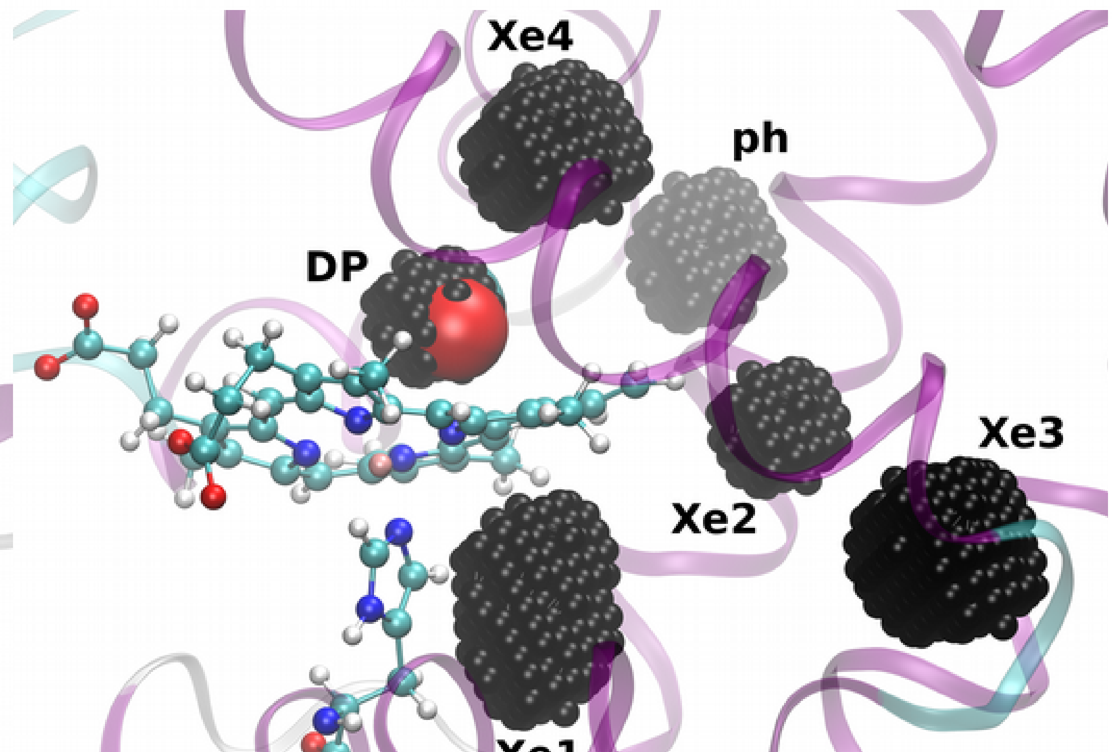
F. Hédin & T. Lelièvre, CERMICS ENPC

https://arxiv.org/abs/1807.02431







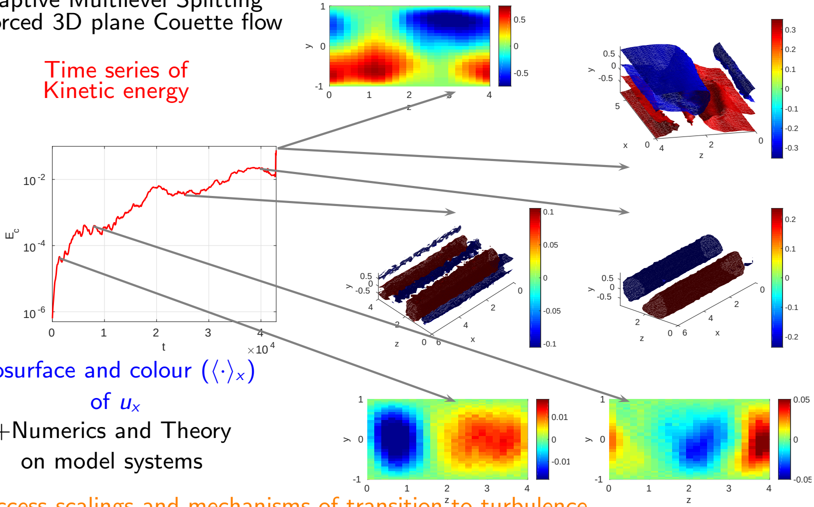


Using rare event methods to study multistability in models and simulations of wall flow transiting to turbulence

Joran Rolland, Laboratoire de Physique, ENS Lyon

Adaptive Multilevel Splitting
on forced 3D plane Couette flow

Time series of
Kinetic energy



Isosurface and colour $(\langle\cdot\rangle_x)$
of u_x
+Numerics and Theory
on model systems

$\Rightarrow$ Access scalings and mechanisms of transition to turbulence

Averaging and Conditional Expectations: Some Aspects of a Comparison

L. Neureither, U. Sharma, C. Hartmann

Brandenburgische Technische Universität Cottbus - Senftenberg

SFB 1114

Freie Universität Berlin

Slow-fast ($0 < \varepsilon \ll 1$) dynamics:
$$dX_t = (-X_t + Y_t)\,dt\,, \quad X_0 = x_0 \neq 0$$
$$dY_t = -\frac{1}{\varepsilon} Y_t\,dt + \frac{1}{\sqrt{\varepsilon}}\,dB_t\,, \ Y_0 = y_0.$$

Averaging $\quad \bar{X}_t = x_0 e^{-t} \quad \neq \quad X_t^{\mathrm{ce}} \equiv x_0 \quad$ Conditional Expectation

Questions:

- When does "Averaging = Conditional Expectation" hold?
- Under which conditions do we get convergence of the Conditional Expectation approach as $\varepsilon \to 0$?

Optimal importance sampling using stochastic control

Lorenz Richter, Carsten Hartmann

Freie Universität Berlin

SFB 1114

Brandenburgische Technische Universität Cottbus - Senftenberg

- **Goal**: compute $\gamma(x,t) = -\log \mathbb{E}_{\mathbb{P}}\left[\exp\left(-W(X_{t:T})\right)\middle| X_t = x\right]$

$$dX_s = b(X_s, s)\mathrm{d}s + \sigma(X_s)\mathrm{d}W_s, \qquad W(X_{t:T}) = \int_t^T f(X_s, s)\mathrm{d}s + g(X_T), \qquad f, g : \mathbb{R}^d \to \mathbb{R}$$

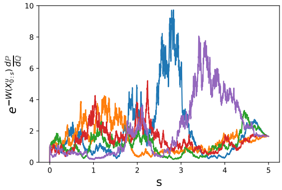
- Importance sampling: $\mathbb{E}_{\mathbb{Q}^u}\left[\exp\left(-W\right)\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{Q}^u}\right]$

- Duality between sampling and control:

$$\gamma(x,t) = \inf_{\mathbb{Q}^u \ll \mathbb{P}} \left\{\mathbb{E}_{\mathbb{Q}^u}\left[W\right] + \mathrm{KL}(\mathbb{Q}^u \| \mathbb{P})\right\}$$

  - zero-variance estimator

- Try to numerically approximate the optimal change of measure in path space
  - stochastic gradient descent
  - approximate dynamic programming



Constructing sampling schemes via coupling: Markov semigroups and optimal transport

Goal: Compute $\int_{\mathbb{R}^d} f \, \mathrm{d}\pi$, $\quad \pi \propto e^{-V} \, \mathrm{d}x \quad$ (via MCMC.)

$$\mathrm{d}X_t = -V'(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t^x,$$

$$\mathrm{d}Y_t = -V'(Y_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t^y, \qquad F(x,y) = \frac{1}{2}\left(f(x) + f(y)\right),$$

where $(W_t^x)_{t\geq 0}$ and $(W_t^y)_{t\geq 0}$ are not necessarily independent.

$(X_t, Y_t)_{t\geq 0}$ ergodic wrt. $\bar{\pi} \implies \bar{\pi}$ is a coupling of π_x and π_y
$\implies$ (nonstandard) **optimal transport problem**

$$\bar{\mathcal{L}}_\Gamma = \underbrace{-V'(x) + \partial_x^2}_{\mathcal{L}_x} \underbrace{-V'(y) + \partial_y^2}_{\mathcal{L}_y} + \Gamma,$$

Coupling operator: $\quad \Gamma = 2\alpha\partial_x\partial_y, \quad \alpha : \mathbb{R}^2 \to [-1, 1]$

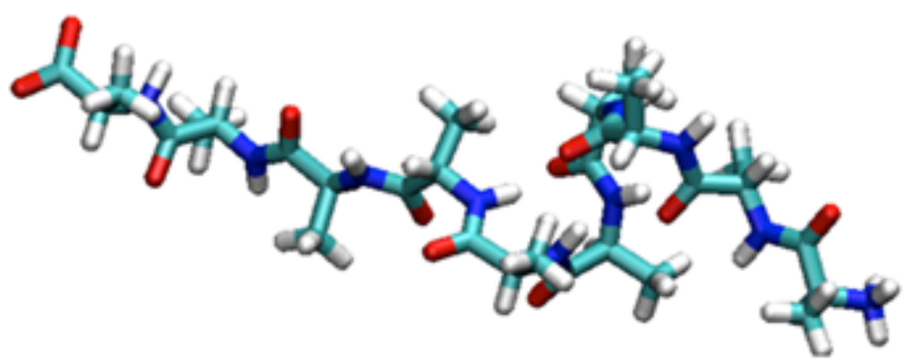
Effective Dynamics for SDEs

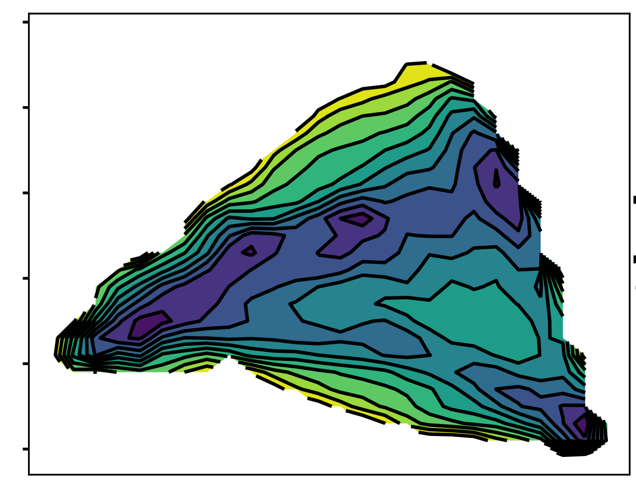
$Z = \xi(X)$

Original Dynamics → **Reduced Dynamics**

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

$$dZ_t = b^{\xi}(Z_t)dt + \sqrt{2\beta^{-1}}\sigma^{\xi}(Z_t)dW_t$$



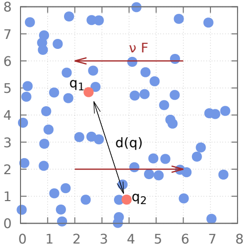


- Approximation Result for Slow Timescales
- Methods for Parameter Estimation
- Numerical Examples

A perturbative approach to control variates in molecular dynamics

Julien Roussel, Gabriel Stoltz, Cermics, ENPC and INRIA Paris

Dimer in a solvent under shearing



$$V(q) = V_{\mathrm{dimer}} + V_{\mathrm{solvent}}$$

$$V_{\mathrm{dimer}}(q) = v_{\mathrm{dimer}}(|q_1 - q_2|)$$

$$V_{\mathrm{solvent}} = \sum_{i \in \mathrm{all}} \sum_{j \in \mathrm{solvent}} v_{\mathrm{solvent}}(|q_i - q_j|)$$

$$\mathcal{L} = \mathcal{L}_0 + \left(-\nabla V_{\mathrm{solvent}}(q) - \nu F(q)\right)^\top \nabla$$

$$\mathrm{d}q_t = \left(-\nabla V(q_t) + \nu F(q_t)\right) \mathrm{d}t + \sqrt{2\beta^{-1}}\, \mathrm{d}W_t$$

Goal

Compute $\int_{\mathbb{T}^{2N}} |q_1 - q_2| \mathrm{d}\mu_\eta(\mathrm{d}q)$ (Nonequilibrium average).

A perturbative approach to control variates in molecular dynamics

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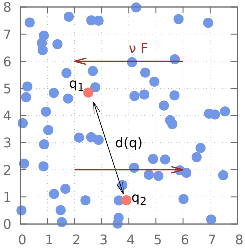
Dimer in a ~~solvent~~ under ~~shearing~~



$$V(q) = V_{\mathrm{dimer}} + \cancel{V_{\mathrm{solvent}}}$$

$$V_{\mathrm{dimer}}(q) = v_{\mathrm{dimer}}(|q_1 - q_2|)$$

$$\cancel{V_{\mathrm{solvent}} = \sum_{i \in \mathrm{all}} \sum_{j \in \mathrm{solvent}} v_{\mathrm{solvent}}(|q_i - q_j|)}$$

$$\mathcal{L} = \mathcal{L}_0 + \left(\cancel{-\nabla V_{\mathrm{solvent}}(q)} - \cancel{\nu F(q)}\right)^\top \nabla$$

$$\mathrm{d}q_t = \left(-\nabla V_{\mathrm{dimer}}(q_t) + \cancel{\nu F(q_t)}\right) \mathrm{d}t + \sqrt{2\beta^{-1}}\, \mathrm{d}W_t$$

Control variate method

1) Solve $-\mathcal{L}_0 u = |q_1 - q_2| - \mathbb{E}_0[|q_1 - q_2|]$ for u
2) Average $\zeta(q) = |q_1 - q_2| + \mathcal{L}_\eta u(q)$

An inequality connecting entropy distance, Fisher Information and large deviations

Upanshu Sharma

$L:$ generator of a Markov process on $\mathcal{X}$

Law of this process evolves according to forward Kolmogorov equation

$$\partial_t \rho = L^* \rho \qquad (*)$$

For two solutions ρ, μ :

$$\frac{d}{dt} H(\mu_t|\rho_t) = -R(\mu_t|\rho_t)$$

relative entropy Fisher Information

or in time-integrated form

$$H(\mu_T|\rho_T) - H(\mu_0|\rho_0) = -\int_0^T R(\mu_t|\rho_t)dt$$

What happens when μ is not a solution of $(*)$?

What is the error you make when you do not solve the equation?

Tobias Wöhrer, TU Vienna:

Sharp decay estimates in defective evolution equations

- Let $\mathsf{C} \in \mathbb{C}^{n\times n}$ be positive stable with spectral gap $\mu := \min\{\mathrm{Re}\,\lambda \mid \lambda \in \sigma(\mathsf{C})\} > 0$.

$$\dot{x}(t) = -\mathsf{C}x(t), \quad t \geq 0.$$

- Matrix C is defective in $\lambda_\mu :\iff$ algebraic multiplicity > geometric multiplicity of λ_μ
- **Construction of Lyapunov functional** $\|\cdot\|^2_{\mathsf{P}(t)}$ for sharp decay rate

$$\|x(t)\|_2^2 \leq c(1+t^{2M})e^{-2\mu t}, \qquad c = \frac{\lambda_{\max}^{\mathsf{P}(0)}}{\lambda_{\min}^{\mathsf{P}(0)}} c_M \beta.$$

- **Application to PDE:** Sensitivity analysis for $z \in \mathbb{R}$ of two-velocity BGK model ($x \in \mathbb{T}$)

$$\partial_t f_\pm(x,z) = \mp\partial_x f_\pm(x,z) \pm \frac{\sigma(z)}{2}(f_-(x,z) - f_+(x,z))$$

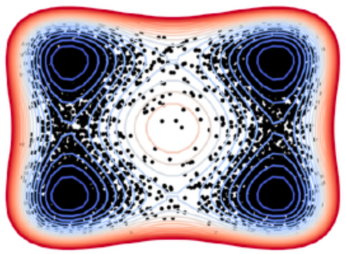
leads to defective ODE system for Fourier modes.

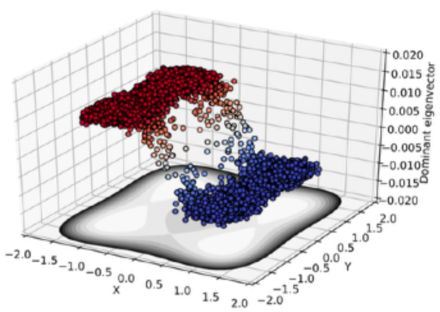
Diffusion maps: local and global tool for sampling of metastable systems

Z. Trstanova, B. Leimkuhler, T. Lelièvre

THE UNIVERSITY of EDINBURGH

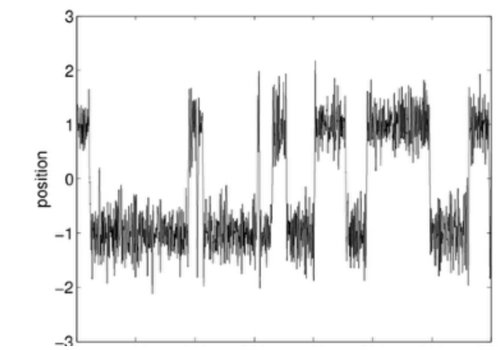
EPSRC Engineering and Physical Sciences Research Council





Diffusion maps
Manifold Learning

$$(L_{\varepsilon,\alpha}[f])_k \to \mathcal{L}f(x_k), \quad \mathcal{L} = -\nabla V \cdot \nabla + \beta^{-1}\Delta$$



$$dq_t = -\nabla V(q_t)dt + \sqrt{2/\beta}dW_t$$

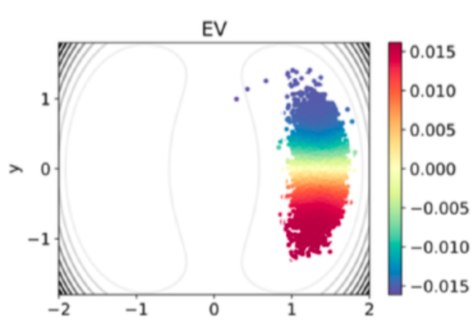
Langevin dynamics

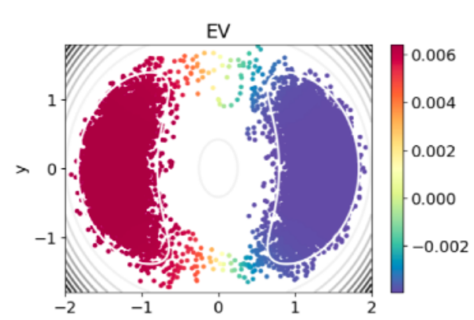
Local
Enhanced sampling & Automatically learned collective variables

$$\mathcal{L}_\Omega = \mathcal{L}_\pi + \nabla \ln(v) \cdot \nabla$$

Quasi-stationary distribution

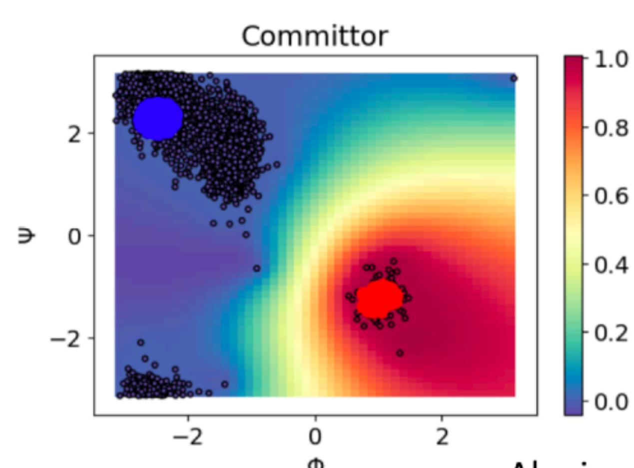
$$\forall x \in \Omega, \quad \nu(x) = \frac{v(x)e^{-\beta V(x)}}{\int_\Omega v(x)e^{-\beta V(x)}dx}.$$

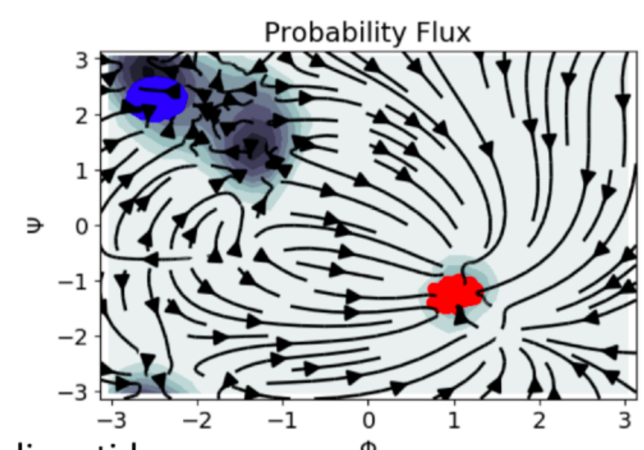




Global
Approximating Committors

$$\mathcal{L}q = 0, \text{ in } \Omega \setminus (A \cup B), q = 0, \text{ in } A, q = 1, \text{ in } B.$$

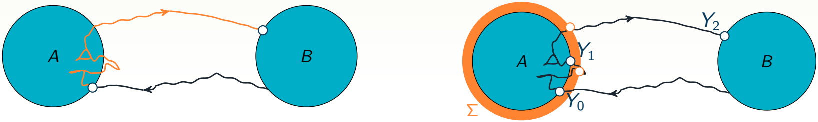




Alanine dipeptide

Time error estimation for metastable Markov processes

Manon Baudel



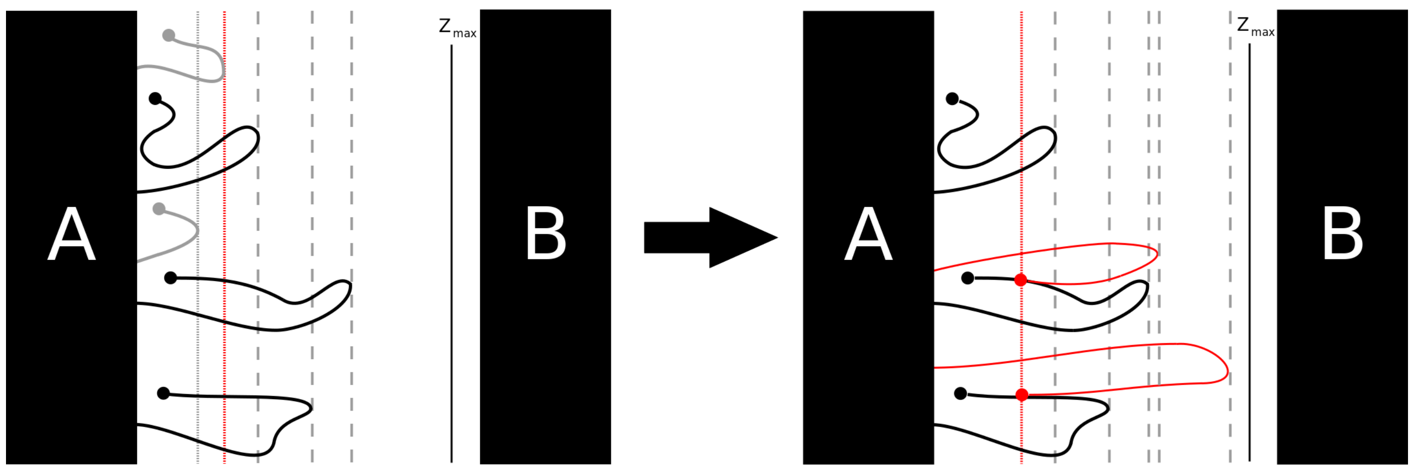
Mean transition time from A to B for equilibrium trajectories?

- Discrete-time continuous space Markov chain $(Y_n)_{n \geqslant 0}$
- Reactive entrance distribution vs Quasi-Stationary Distribution

Main tools: Trace process, Poisson boundary value problem, convergence to quasi-stationarity

Work in progress with Arnaud Guyader and Tony Lelièvre

Simulating rare events in molecular dynamics with the Adaptive Multilevel Splitting



Laura Lopes, Jérôme Hénin and Tony Lelièvre

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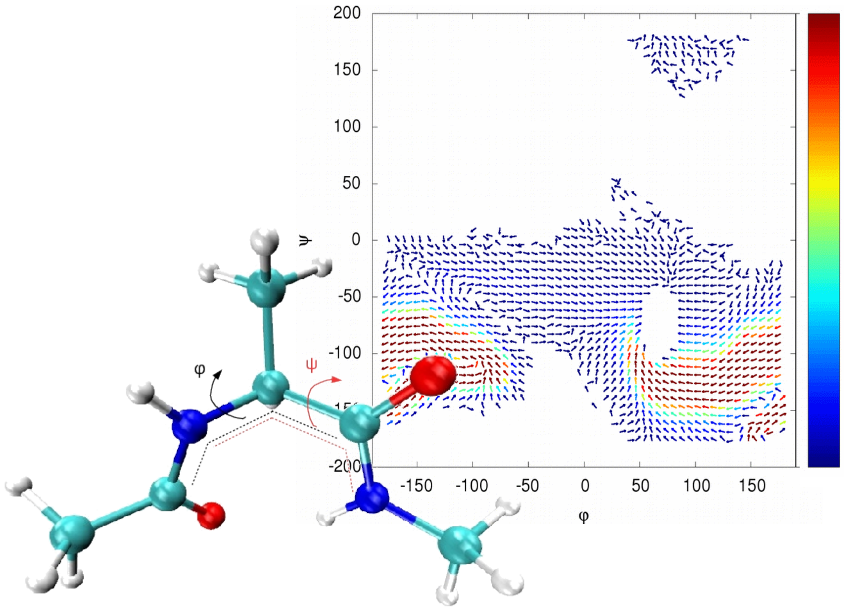
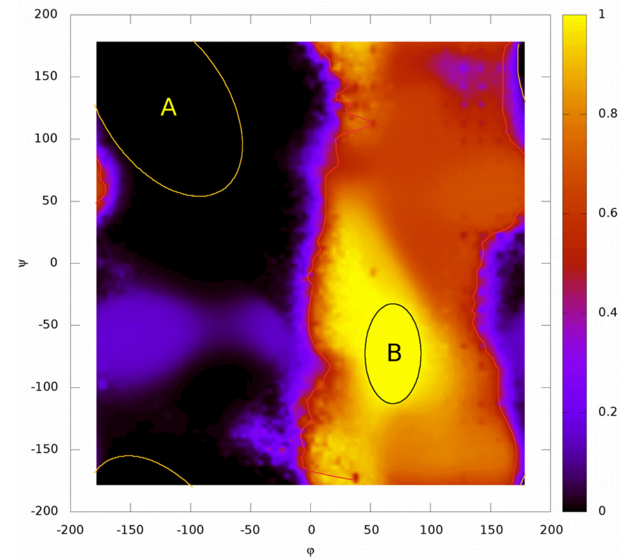
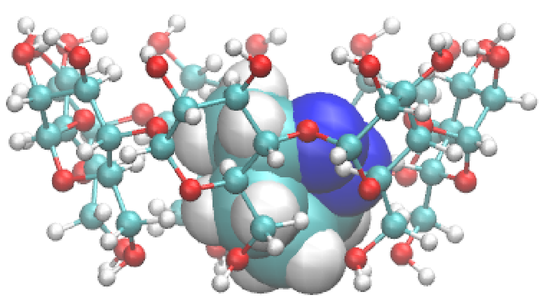
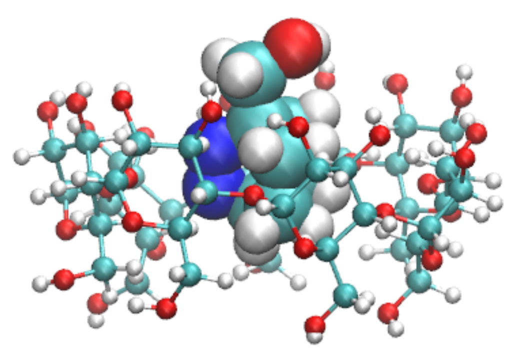
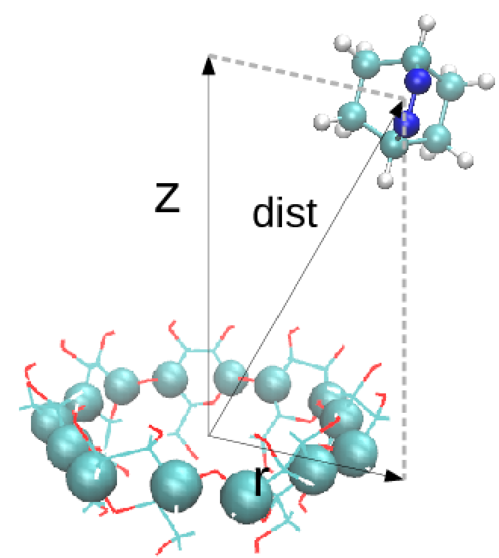




- Estimation of the probability of transition
- Estimation of the transition time
- Flux of reactive trajectories obtained with AMS
- Estimation of the committor function







Variance estimation for Adaptive Multilevel Splitting

Qiming Du[1]

joint work with Arnaud Guyader[2] and Tony Lelièvre [3]

[1]LPSM, Sorbonne Université

[2]LPSM, Cermics and ASPI

[3]CERMICS, Ecole des Ponts ParisTech

CIRM

19 September 2018, Marseille

AMS framework

1. **multinomial scheme:** All the particles do a multinomial selection before evolving to the next step. We only deal with the case where we kill a proportion of particles as $N \to \infty$
   - higher variance
   - higher computational cost
   - easy to analyse theoretically
2. **keep-survived scheme:** The survived particles stay at the same site during the selection procedure.
   - lower variance
   - lower computational cost
   - difficult to analyse

Our construction is based on the coalescent tree-typed occupation measures in the genealogy of the associated Interacting Particle System.

Three variance estimators

1. **multinomial scheme: asymptotic variance**
   - term-by-term estimator:
     - intuitive by construction
     - complex to calculate
     - consistent estimator
     - intermidiate estimator for the following one
   - disjoint ancestral line-based estimator:
     - same estimator proposed by Lee & Whiteley for Particle Filters
     - easy to calculate
     - consistent estimtator
2. **keep-survived scheme: non-asymptotic variance**
   - modified disjoint ancestral lines-based estimator:
     - available for almost all kinds of GAMS framework
     - easy to calculate
     - unbiased estimator
     - no consistency result (for now, heuristically, this would also be a consistent estimator under some regularity assumptions)