# Theoretical and computational approaches to parallel replica dynamics

Mitchell Luskin

School of Mathematics
University of Minnesota

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Collaborators C. Le Bris (CERMICS), T. Lelievre (CERMICS), D. Perez (LANL), G. Simpson (UMN), A.F. Voter (LANL), A. Binder (UMN)

# Outline

# The Parallel Replica Algorithm

The Parallel Replica Algorithm proposed by A.F. Voter in 1998 is a method to accelerate a "coarse-grained projection" of a dynamics. We consider the overdamped Langevin dynamics:

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

and we assume that we are given a smooth mapping

$$\mathcal{S} : \mathbb{R}^d \to \mathbb{N}$$

which to a configuration in $\mathbb{R}^d$ associates a state number (e.g., a numbering of the wells of the potential $V$).

The goal of the parallel replica dynamics is to generate very efficiently a trajectory $(S_t)_{t\geq 0}$ which has (almost) the same law as $(\mathcal{S}(X_t))_{t\geq 0}$.

# The Parallel Replica Algorithm

Initialization: Consider an initial condition $X_0^{ref}$ for a reference walker, the associated initial state $S_0 = \mathcal{S}(X_0^{ref})$, and a simulation time counter $T_{simu} = 0$.

One iteration of the algorithm goes through three steps.

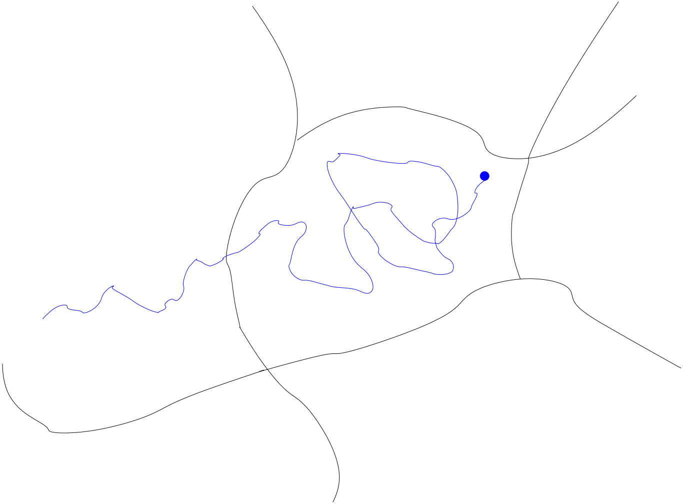
- The decorrelation step: Let the reference walker $(X_{T_{simu}+t}^{ref})_{t \geq 0}$ evolve over a time interval $t \in [0, \tau_{corr}]$. Then,
  - If the process leaves the well during the time interval (*i.e.*, $\exists t \leq \tau_{corr}$ such that $\mathcal{S}\left(X_{T_{simu}+t}^{ref}\right) \neq \mathcal{S}\left(X_{T_{simu}}^{ref}\right)$) advance the simulation clock by $\tau_{corr}$ and restart the decorrelation step ;
  - otherwise, advance the simulation clock by $\tau_{corr}$ and proceed to the dephasing step.

# The Parallel Replica Algorithm

The reference walker enter a new state

# The Parallel Replica Algorithm

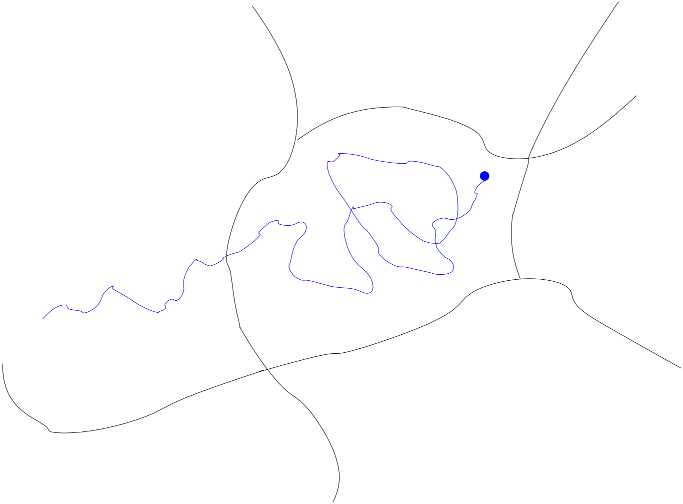
Decorrelation step: wait for a time $\tau_{corr}$.



- The dephasing step: Duplicate the walker $X^{ref}_{T_{simu}}$ into $N$ replicas. Let these replicas evolve independently and in parallel over a time interval of length $\tau_{dephase}$. If a replica leaves the well during this time interval, restart the dephasing step for this replica. Throughout this step, the simulation counter is stopped.

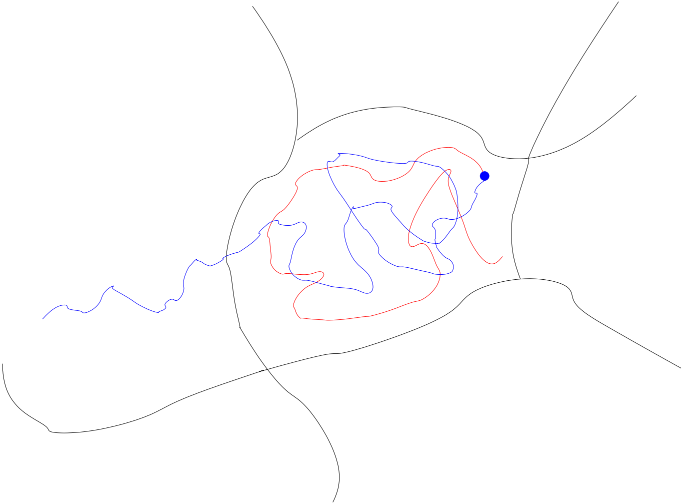
# The Parallel Replica Algorithm

Dephasing step.



# The Parallel Replica Algorithm

Dephasing step: generate new initial conditions in the state.



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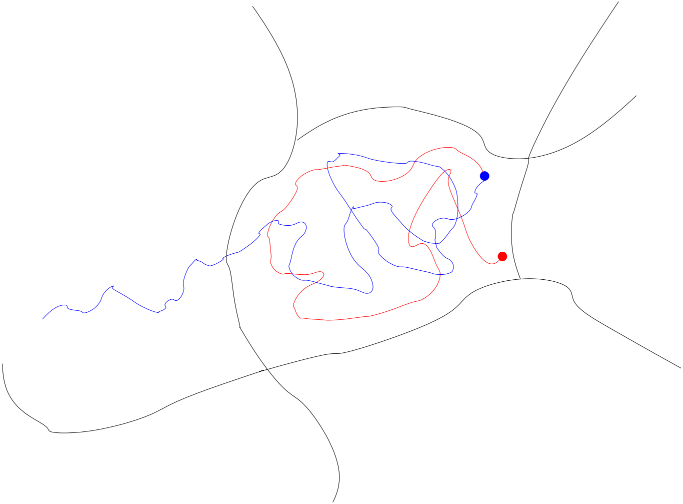

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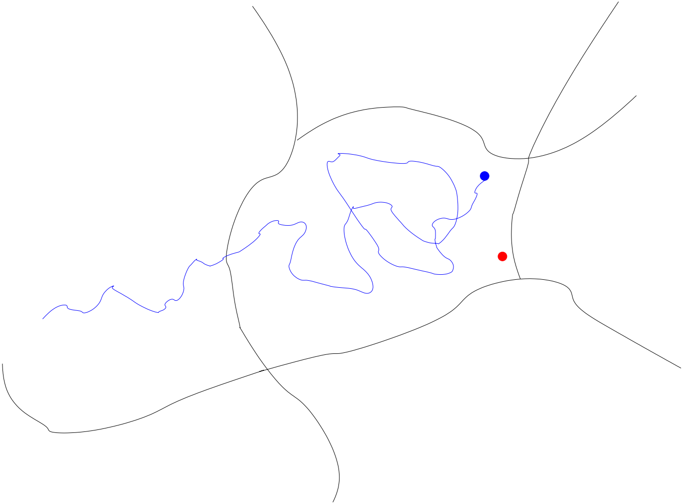

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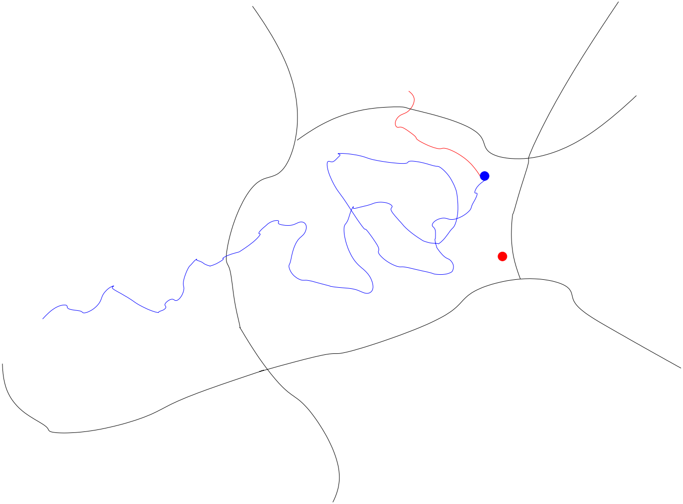

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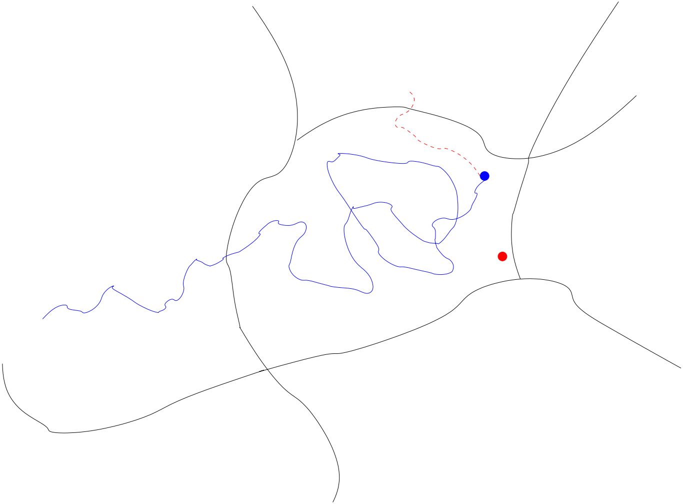

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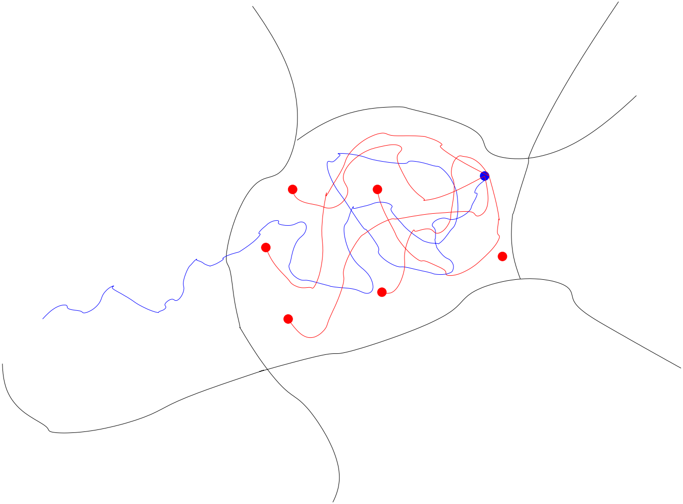

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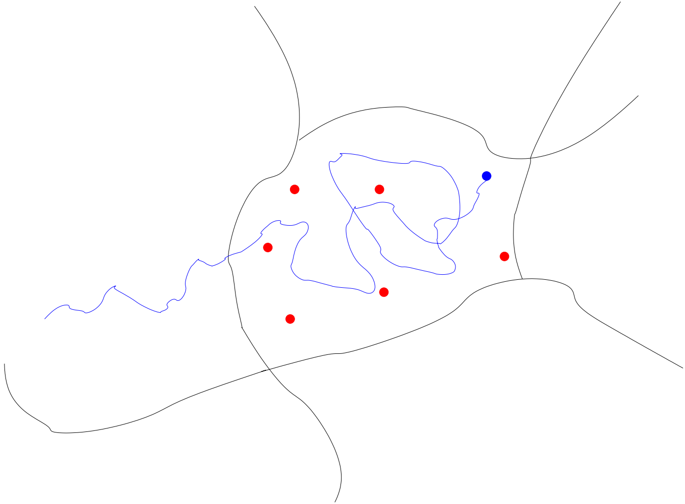


- The parallel step: Let all the replicas evolve independently and track the first escape event:

$$T = \inf_k T_W^k = T_W^{K_0},$$

where $K_0 = \arg\inf_k T_W^k$ and

$$T_W^k = \inf\{t \geq 0, \mathcal{S}(X_{T_{simu}+t}^k) \neq \mathcal{S}(X_{T_{simu}}^k)\}$$

is the first time the $k$-th replica leaves the well. Then:

$$T_{simu} = T_{simu} + NT \text{ and } X_{T_{simu}+NT}^{ref} = X_{T_{simu}+T}^{K_0}.$$

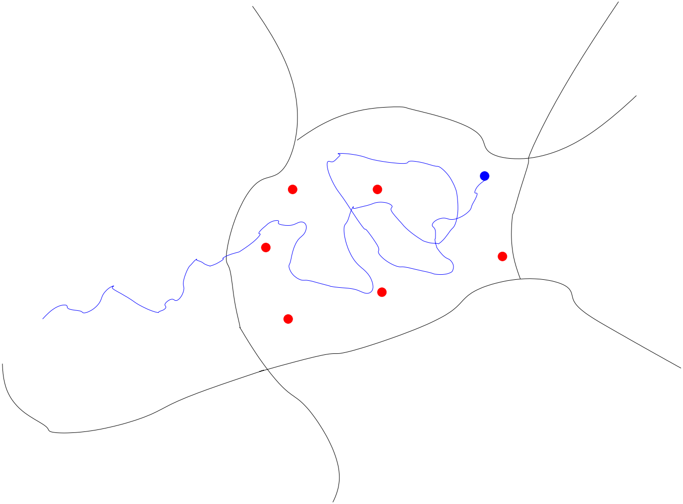
Moreover, over $[T_{simu}, T_{simu} + NT]$, the state dynamics $S_t$ is constant and defined as:

$$S_t = \mathcal{S}(X_{T_{simu}}^1).$$

Then, go back to the decorrelation step...

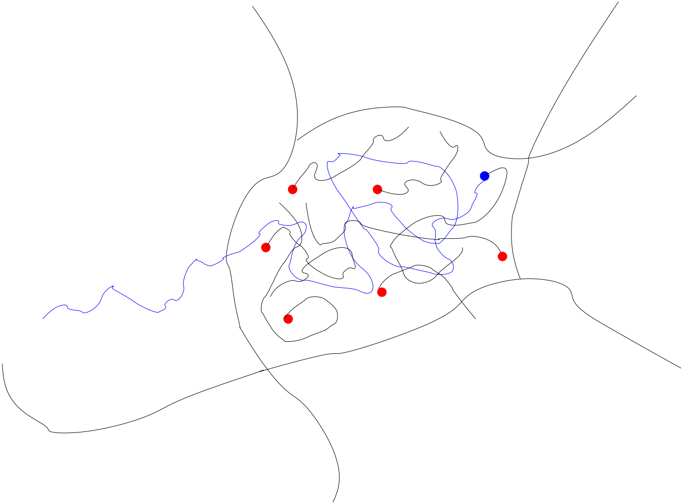
# The Parallel Replica Algorithm

Parallel step.



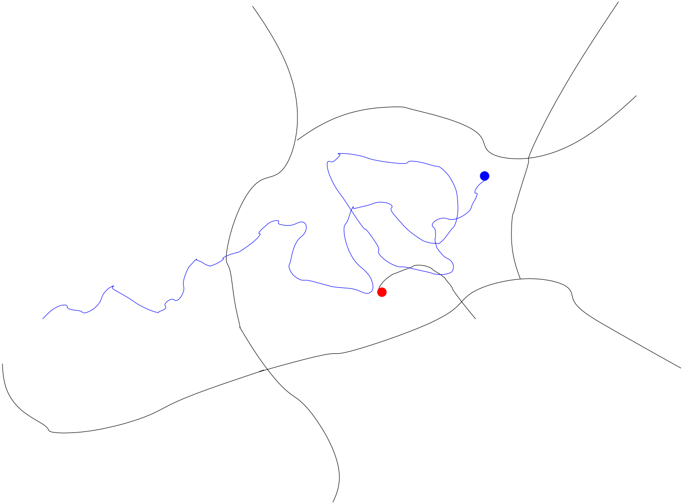
# The Parallel Replica Algorithm

Parallel step: run independent trajectories in parallel...



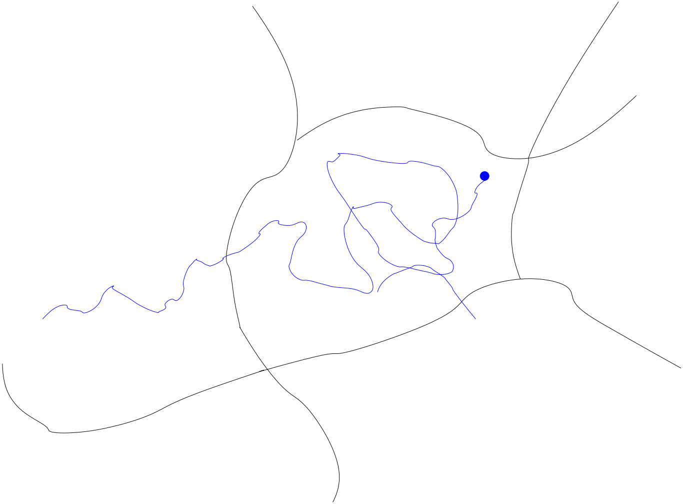
# The Parallel Replica Algorithm

Parallel step: ... and detect the first transition event.



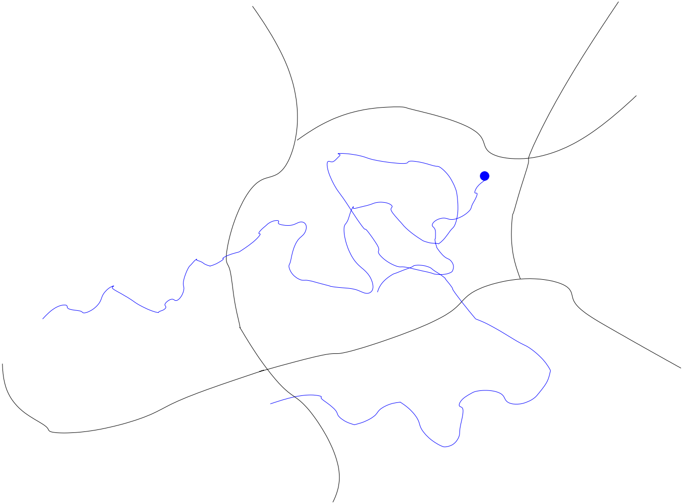
# The Parallel Replica Algorithm

Parallel step: update the time clock: $T_{simu} = T_{simu} + NT$.



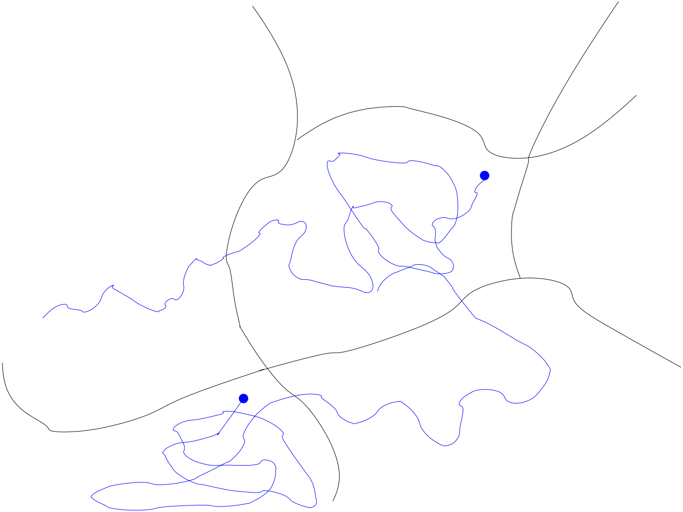
# The Parallel Replica Algorithm

A new decorrelation step starts...



# The Parallel Replica Algorithm

New decorrelation step



# Error analysis for the Parallel Replica Algorithm

The parallel step would introduce no error if

- the escape time $T_W^1$ was exponentially distributed
- and independent of the next visited state.

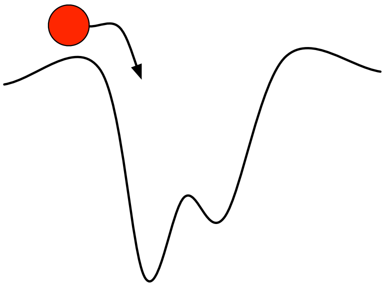
How can we analyze the error introduced by the algorithm ?

# Parallel Replica Dynamics – Steps

## Escaping a Single Well

1. Decorrelation Step – Let a reference process sample a well for some time
2. Dephasing Step – Simultaneously create independent replicas that further sample the well
3. Parallel Step – Run the replicas until one exits the well

# Decorrelating the Reference Process



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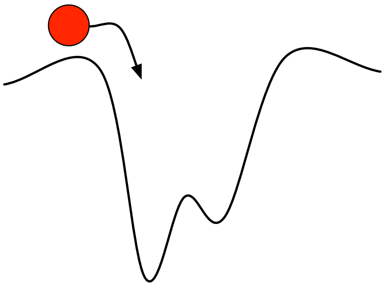

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- Run for $t \leq t_{\rm corr}$

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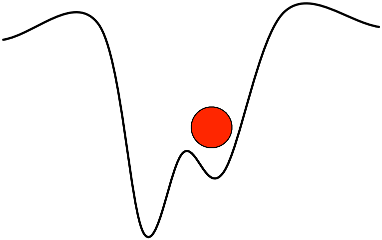

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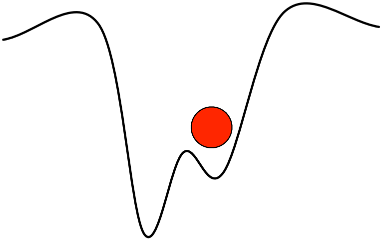

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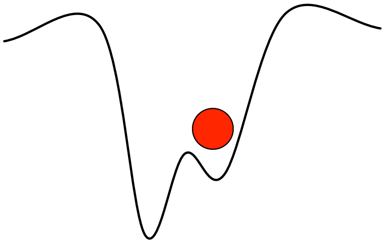

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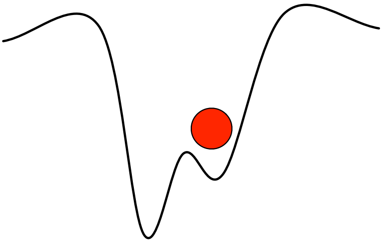

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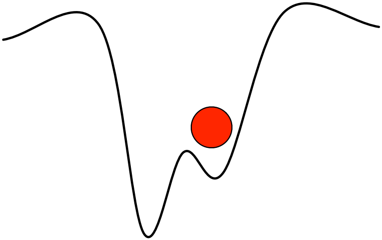

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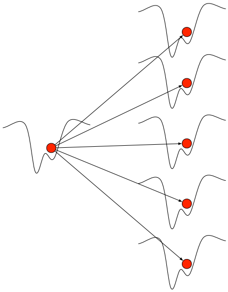
- $t_{\mathrm{corr}}$ is one of the user parameters
- Simulation clock is advanced by $t_{\mathrm{corr}}$

# Dephasing by Direct Simulation



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- Replicas begin running at $t_{\mathrm{launch}} < t_{\mathrm{corr}}$ ($t_{\mathrm{launch}}$ can be zero, as in the previous Par Rep version)

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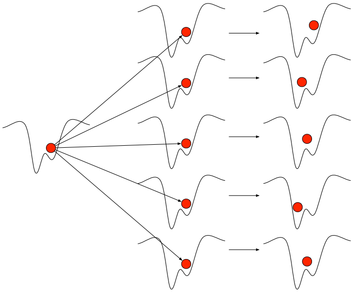

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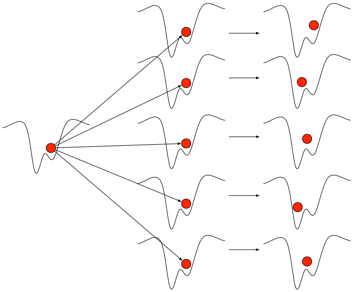

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- If $X_t^k$ leaves the well, restart it

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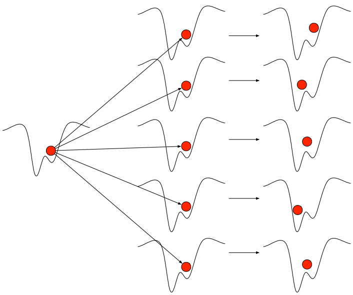

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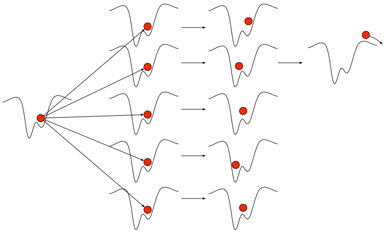
- If $X_t^k$ leaves the well, restart it
- $t_{\text{launch}}$ and $t_{\text{phase}}$ are other user parameters



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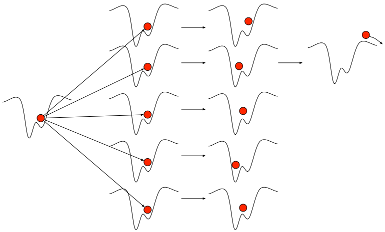
- The first process $k_*$ to leave the well, at time $T_{\rm exit} := T_{k_*}$, becomes the new reference process, and the algorithm restarts



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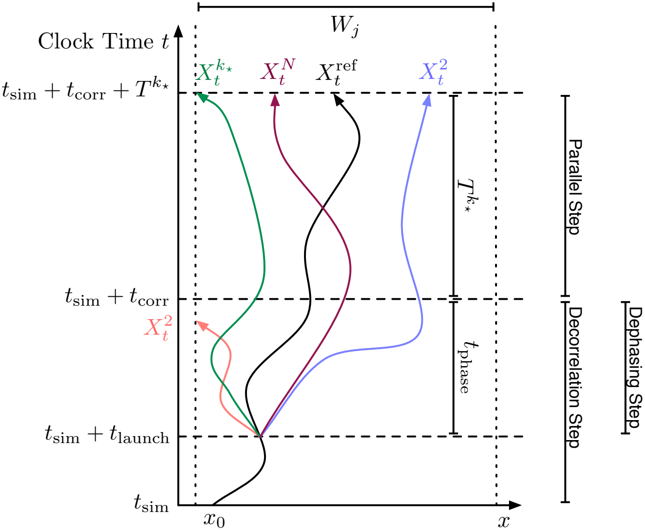
- The simulation clock is advanced by $NT_{\mathrm{exit}}$

# Parallel Replica Dynamics – Recap



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- Given that we begin in well $W \subset \mathbb{R}^n$, determine the properties of $T_{\mathrm{exit}}$, the first exit time from $W$
- What is the distribution for $T_{\mathrm{exit}}$?
- What are the properties of $X_{T_{\mathrm{exit}}}$, the first hitting point distribution?
- Can we estimate the accuracy of ParRep?
- Can we optimize the efficiency of ParRep?

# Fokker-Planck Equation

The Fokker-Planck Equation for the overdamped Langevin equation $dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dB_t$ and absorbing boundary conditions:

$$\frac{\partial \rho}{\partial t} = L^* \rho := \nabla \cdot \left[ (\nabla V)\, \rho + \beta^{-1} \nabla \rho \right] \qquad \forall x \in W, \ t \geq 0,$$

$$\rho(x,t) = 0 \qquad \forall x \in \partial W, \ t \geq 0,$$

$$\rho(x,0) \geq 0 \quad \forall x \in W, \qquad \int_W \rho(x,0)\, dx = 1,$$

is given by the series expansion

$$\rho(x,t) = \sum_1^\infty a_j e^{-\lambda_j t} \psi_j(x),$$

for eigenvalues $0 < \lambda_1 < \lambda_2 \leq \cdots$ and eigenfunctions $\psi_j(x)$ of

$$L^* \psi_j = \nabla \cdot \left[ (\nabla V)\, \psi_j + \beta^{-1} \nabla \psi_j \right] = -\lambda_j \psi_j \qquad \forall x \in W,$$

$$\psi_j = 0 \qquad \forall x \in \partial W.$$

# The Exit Density

The exit density through the boundary point $x \in \partial W$ at time $t \geq 0$ is

$$\beta^{-1} \frac{\partial \rho}{\partial n}(x, t),$$

the first exit time density is

$$\int_{\partial W} \beta^{-1} \frac{\partial \rho}{\partial n}(x, t)\, dx,$$

and the first hitting point density is

$$\int_0^\infty \beta^{-1} \frac{\partial \rho}{\partial n}(x, t)\, dt.$$

# The Quasistationary Distribution (QSD)

The renormalized density $\rho(x,t)$ converges to $\psi_1(x)$ at rate $\lambda_2 - \lambda_1$ (where $\psi_1(x) > 0$ is normalized by $\int_W \psi_1(x,t)\,dx = 1$):

$$\frac{\rho(x,t)}{\int_W \rho(x,t)\,dx} = \psi_1(x) + O\left(e^{-(\lambda_2-\lambda_1)t}\right) \quad \text{as } t \to \infty.$$

The Fokker-Planck solution $\rho(x,t) = \psi_1(x)e^{-\lambda_1 t}$ has exit density

$$\beta^{-1}\frac{\partial \psi_1}{\partial n}(x)\,e^{-\lambda_1 t} \qquad \forall x \in \partial W,\ \ t \geq 0,$$

with independent exit time and hitting point.

# The Quasistationary Distribution (QSD)

The first exit time density of $\rho(x,t) = \psi_1(x) e^{-\lambda_1 t}$ is exponential:

$$\int_{\partial W} \beta^{-1} \frac{\partial \psi_1}{\partial n}(x)\, e^{-\lambda_1 t}\, dx = \lambda_1 e^{-\lambda_1 t},$$

and independent of the hitting point density:

$$\int_0^\infty \beta^{-1} \frac{\partial \psi_1}{\partial n}(x)\, e^{-\lambda_1 t}\, dt = \frac{1}{\lambda_1 \beta} \frac{\partial \psi_1}{\partial n}(x).$$

# The Quasistationary Distribution (QSD)

### Definition

On well $W$, a QSD is a distribution $\nu$ such that for all $A \subset W$ and $t \geq 0$,

$$\nu(A) = \int_W \mathbb{P}^x \left[X_t \in A \mid t < T_{\text{exit}}\right] d\nu(x). \tag{1}$$

The dephasing stage of the Par Rep Method converges to the QSD as $t_{\text{phase}} \to \infty$. (1) states that the QSD is invariant for the dephasing step.

### Theorem

*$\psi_1(x)\,dx$ is a QSD where $\psi_1(x) > 0$ is the unique ground state of the Fokker-Planck operator with eigenvalues* $0 < \lambda_1 < \lambda_2 \leq \ldots$

$$L^*\psi_j = \nabla \cdot \left[(\nabla V)\,\psi_j + \beta^{-1}\nabla\psi_j\right] = -\lambda_j\psi_j \qquad \forall x \in W,$$
$$\psi_j = 0 \qquad \forall x \in \partial W.$$

# Utility of the QSD

**Theorem**

*Let $X_t^k$ be $N$ i.i.d. processes in the well $W$, and assume:*

- $T_{\mathrm{exit}}^k$ *are exponentially distributed,*
- *Exit time is independent of hitting point.*

*If*

$$T_{\mathrm{exit}} \equiv T_{\mathrm{exit}}^{k_\star}, \quad X_{T_{\mathrm{exit}}} \equiv X_{T_{\mathrm{exit}}^{k_\star}}^{k_\star}, \quad k_\star \equiv \mathrm{argmin}_k\, T_{\mathrm{exit}}^k,$$

*then $NT_{\mathrm{exit}}$ has the same law as $T_{\mathrm{exit}}^k$, and $X_{T_{\mathrm{exit}}}$ is independent of first hitting time.*

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## QSD and ParRep

Goal of the decorrelation/dephasing step: Produce $N$ processes distributed as close as possible to $\nu$.

# Decorrelation Result

### Theorem

*Let $X_0$ be distributed by $\mu_0$ on $W$, then for any observable $f$*

$$\left|\mathbb{E}^{\mu_t}\left[f(T, X_T)\right] - \mathbb{E}^{\nu}\left[f(T, X_T)\right]\right| \lesssim d(\mu_0, \nu)\, \|f\|_{L^\infty}\, e^{-(\lambda_2-\lambda_1)t}.$$

*where*

$$d\mu_t(x) := \frac{\rho(x,t)\,dx}{\int_W \rho(x,t)\,dx}.$$

- $d(\mu_t, \nu)$ measures the difference between $\mu_t$ and $\nu$; vanishes as $t \to \infty$.

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- $d(\mu_t, \nu)$ measures the difference between $\mu_t$ and $\nu$; vanishes as $t \to \infty$.
- Exponential convergence with decorrelation time scale is

$$\frac{1}{\lambda_2 - \lambda_1}$$

- ParRep is efficient when the decorrrelation time scale is much less than the mean first exit time

# Decorrelation Example

- We have

$$\left|\mathbb{E}^{\mu_{t_{\mathrm{corr}}}}\left[f(T, X_T)\right] - \mathbb{E}^{\nu}\left[f(T, X_T)\right]\right| \lesssim d(\mu_0, \nu)\left\|f\right\|_{L^\infty} e^{-(\lambda_2-\lambda_1)t_{\mathrm{corr}}}$$

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# Decorrelation Example

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- For any $t \geq 0$, to obtain an error estimate for the exit point distribution, let $f(\tau, \xi) = \phi(\xi)$; then

$$\left|\mathbb{E}^{\mu_{\mathrm{corr}}}\left[\phi(X_T) \mid T > t\right] - \int_{\partial W} \phi d\rho\right| \lesssim d(\mu_0, \nu) e^{-(\lambda_2-\lambda_1)t_{\mathrm{corr}}}$$

# Parallel Step Error

## Theorem

*Assume at time $t_{\mathrm{corr}}$, there are $N$ processes $X^k_{t_{\mathrm{corr}}}$ distributed according to $\mu_{\mathrm{corr}}$ and such that*

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*Then for any $\phi : \partial W \to \mathbb{R}$, smooth,*

$$\left|\mathbb{P}^{\mu_{\mathrm{corr}}}\left[T^{k_*} > t\right] - e^{-N\lambda_1 t}\right| \lesssim N\epsilon_{\mathrm{corr}},$$

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# Toy Problem

## Set Up

- $$V(x) = -k\cos(\pi x).$$
- Wells boundaries at odd integers, centered at even integers.
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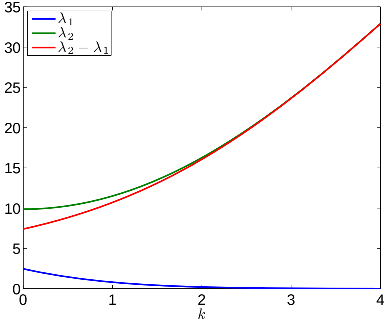
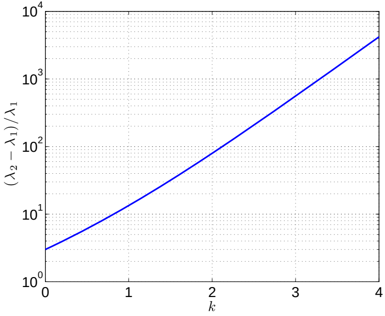
- How well does ParRep perform?

# Time Scale Separation

$V(x) = -k\cos(\pi x)$



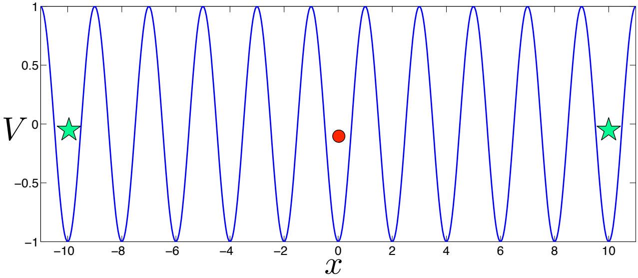

- Scale separations exist

# Rapid Convergence to the QSD

(Loading...)

- $V(x) = -2\cos(\pi x)$, $\beta = 1$.
- $W = (-1, 1)$.
- Initial distribution is $\delta_0(x)$.

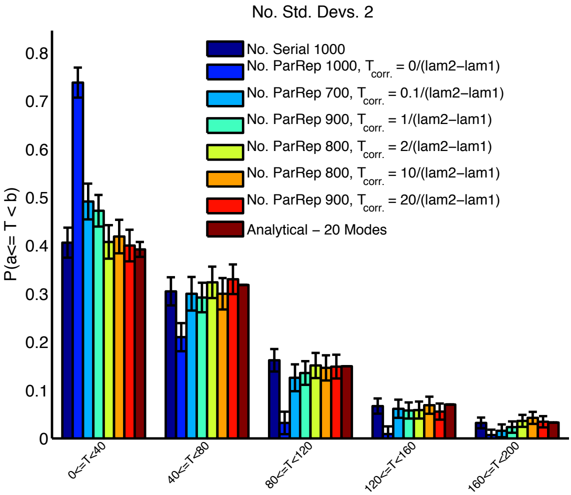
# First Exit Problem – Many Wells




- Process ends if $X_t$ enters either well at $\pm 10$.
- Run a full step of ParRep (Decorrelation, Dephasing, Parallel) every time a new well is entered.
- Dephasing is conducted "analytically" from the QSD.

# Hitting Time Distribution, $k = 1$

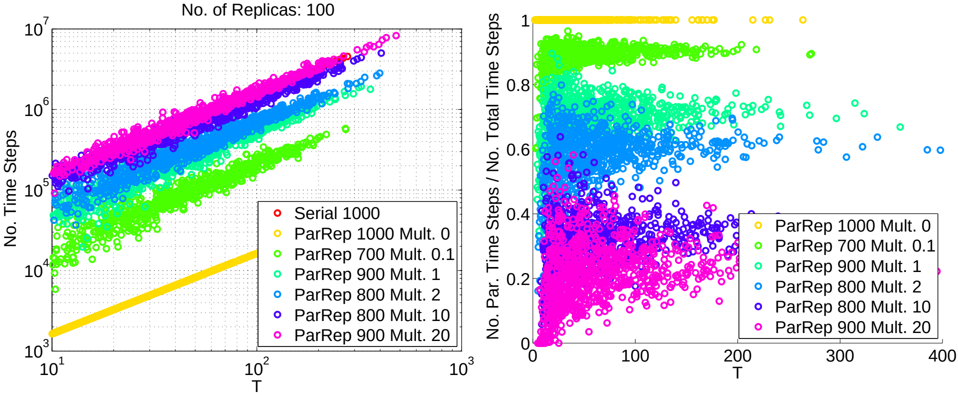
## $V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$




- Time scale separation $\sim 10$
- Cases with $t_{\mathrm{corr}} < 2/(\lambda_2 - \lambda_1)$ give poor results

# Performance, $k = 1$

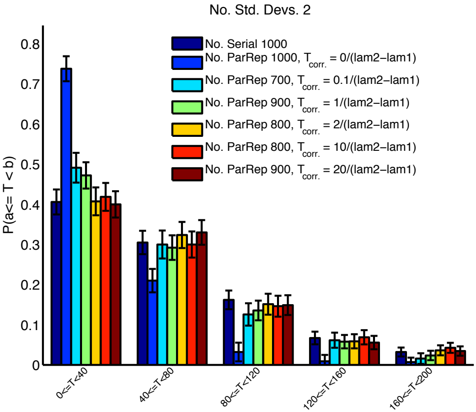
## $V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$

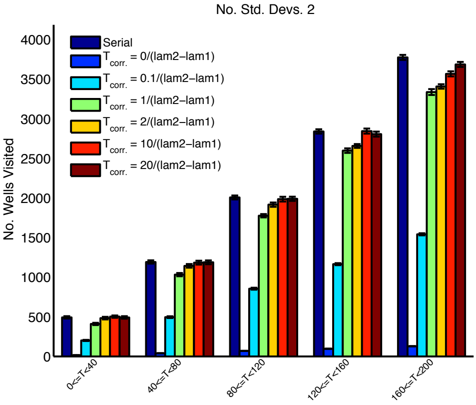



- For small separation of time scales, $\sim 10$, minimal speedup

# Number of Wells Visited, $k = 1$

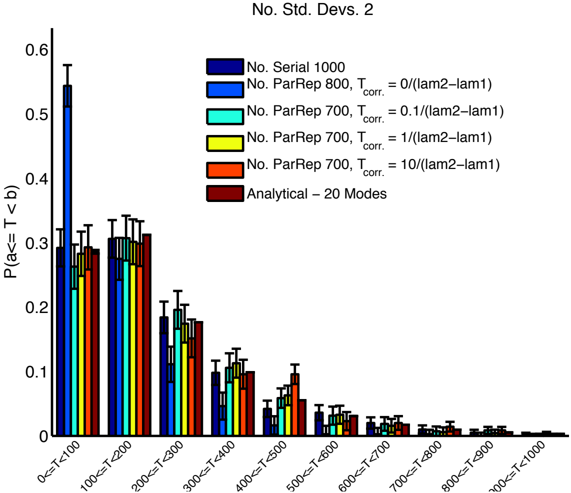
## $V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$



# Hitting Time Distribution, $k = 2$

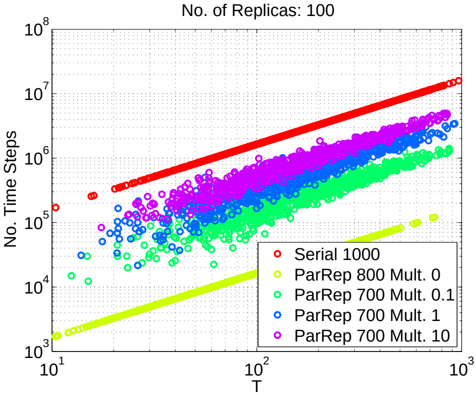
## $V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$

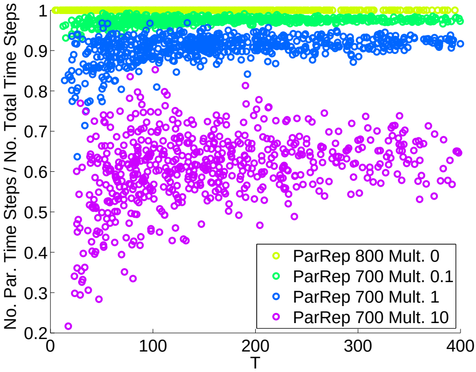



- Time scale separation $\sim 80$
- Only $T_{\mathrm{corr}} = 0$ gives poor results

# Performance, $k = 2$

$V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$

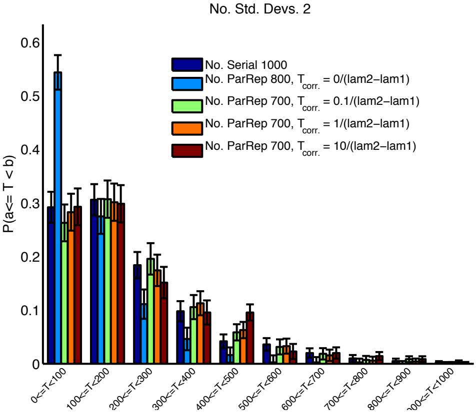


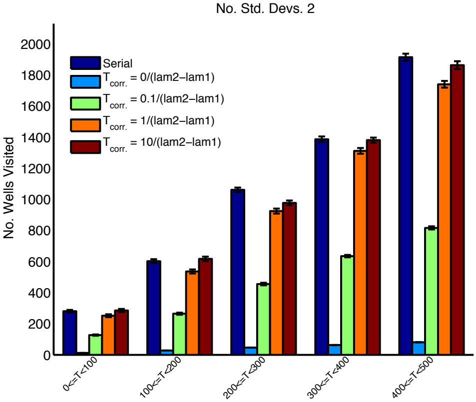




- For larger separation of time scales, $\sim 80$, speedup approaches theoretical factor of $N = 100$.

# Number of Wells Visited, $k = 2$

## $V(x) = -k\cos(\pi x)$, Target Wells $\pm 10$




- Despite agreement in the exit time distributions, there may be disagreements in the distribution in the number of wells visited

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# References


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