The parallel replica method for simulating long trajectories of Markov chains

David Aristoff\textsuperscript{a⋆}, Tony Lelièvre\textsuperscript{b}, and Gideon Simpson\textsuperscript{c}

\textsuperscript{a}School of Mathematics, University of Minnesota
\textsuperscript{b}CERMICS, École des Ponts ParisTech
\textsuperscript{c}Department of Mathematics, Drexel University

Abstract: The parallel replica dynamics method, originally developed by A.F. Voter, can efficiently simulate very long trajectories of Langevin dynamics in the presence of metastability. In this work, we extend the algorithm to discrete in time Markov processes. We give a mathematical analysis of the algorithm which relies on the properties of quasistationary distributions. One application of the algorithm is the correction of time step discretization errors for the original parallel replica dynamics applied to Langevin dynamics.

KEY WORDS Markov chains, parallel computing, Parallel Replica Dynamics, quasistationary distributions, metastability

1 Introduction

In this article we consider the problem of efficiently simulating long trajectories of time homogeneous Markov chains. In many problems there may be subsets of the state space where the Markov chain typically remains for a long time before leaving. Such subsets are called metastable states. Such metastable states often arise in molecular dynamics simulations, such as time discretized Langevin dynamics, or in Markov State or kinetic Monte Carlo models.

For Markov chains with metastable states, efficiently computing long trajectories is a difficult and important problem. We propose adapting A.F. Voter’s parallel replica dynamics\textsuperscript{12,13} (ParRep) to this setting. ParRep was originally developed to efficiently compute transitions between metastable states of a Langevin model for molecular dynamics, namely a continuous in time stochastic process satisfying:

\begin{align*}
\frac{dq_t}{dt} &= M^{-1}p_t \, dt, \\
\frac{dp_t}{dt} &= -\nabla V(q_t) \, dt - \gamma M^{-1}p_t \, dt + \sqrt{2\gamma \beta^{-1}} \, dW_t.
\end{align*}

The process \((q_t, p_t)\) takes values in \(\mathbb{R}^{3N \times 3N}\), with \(q_t\) (resp. \(p_t\)) denoting the positions (resp. the momenta) of \(N\) particles, interacting through potential \(V : \mathbb{R}^{3N} \to \mathbb{R}\). The mass matrix \(M\), the friction parameter \(\gamma\) and the inverse temperature \(\beta = (k_B T)^{-1}\) are the other parameters of the model. Such dynamics are used to describe the evolution of a molecular system at a fixed temperature, with applications in molecular biology or material sciences. In many cases, the process \((q_t, p_t)\) can become trapped for long intervals in metastable states. This is closely related to the vast separation between the atomistic time scale of femtoseconds and macroscopic time scale of microseconds, or more.

The original ParRep algorithm uses many replicas of the process, simulated in parallel asynchronously, to rapidly find a transition pathway out of metastable states. The gain in efficiency over direct simulation comes from the distribution of work across many processors, parallelizing the problem in time. The cost of this gain is that the trajectory becomes coarse-grained, evolving in the set of metastable states instead of the original state space. Broadly speaking, the original algorithm is of interest in that it efficiently replicates the coarse-grained dynamics without any assumptions on the energy barriers between metastable states or on the temperature being sufficiently small. Moreover, the dynamics need not be reversible. See\textsuperscript{8,11} for analyses of ParRep in the original continuous in time setting.

Inspired by Voter’s work, we adapt ParRep to discrete in time Markov processes. This is somewhat a generic problem since, in practice, continuous in time dynamics must be discretized. So in practice it is always the discrete in time dynamics that are simulated. The continuous in time algorithm does not have a straightforward

\*Correspondence to: daristof@umn.edu

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extension to the discrete in time case, since the exit laws from metastable regions change from exponential (in continuous time) to geometric (in discrete time). Taking into account this change in exit law, we propose a new algorithm for the discrete in time case. The discrete in time algorithm can be applied so long as the Markov chain can be simulated and a partition of the state space into metastable states is available. After presenting the algorithm, we give a mathematical analysis of it which follows ideas from [8]. In particular, the analysis is based on the association of a quasistationary distribution (QSD) to each metastable state.

This paper is organized as follows. In Section 2, we define the QSD. In Section 3, we introduce the new ParRep algorithm. In Section 4, we show that, subject to certain idealizing assumptions, our algorithm produces coarse-grained trajectories that are exact; see Theorem 4.5 below. In Section 5, we demonstrate the algorithm for a few problems.

2 The quasistationary distribution

Throughout this paper \((X_n)_{n \geq 0}\) will be a time homogeneous Markov chain in state space \(\Omega\) with a given transition kernel \(k(x,dy)\). For a random variable \(X\) and probability measure \(\mu\), we write \(X \sim \mu\) to indicate \(X\) is distributed according to \(\mu\). For random variables \(X\) and \(Y\), we write \(X \sim Y\) when \(Y\) is a random variable with the same law as \(X\). We write \(X^n\) to denote the random variable \(X\), given that \(X_0 \sim \mu\), and we write \(X^n\) if \(X_0 \sim \delta_x\). If we do not wish to specify an initial distribution we simply write \(X^n\).

To formulate and apply ParRep, we first need to identify the metastable states.

**Definition 2.1.** Let \(S\) be the collection of metastable states, which we assume are disjoint bounded measurable subsets of \(\Omega\). We write \(S\) for a generic element of \(S\), and \(\Pi: \Omega \rightarrow \Omega / S\) for the (quotient) map identifying the states.

As we will be concerned with when the chain exits metastable states, we define the first exit time from \(S\) starting from a measure \(\mu\).

**Definition 2.2.** Given a probability measure \(\mu\) with support in \(S \in S\), we set

\[
\tau^\mu = \min \{ n \geq 0 : X^n \notin S \}.
\]

Much of the algorithm and analysis depends on the properties of the QSD, which we now define.

**Definition 2.3.** A probability measure \(\nu\) with support in \(S\) is a QSD if for all measurable \(A \subset S\) and all \(n \in \mathbb{N}\),

\[
\nu(A) = \mathbb{P}(X^n \in A | \tau^\nu > n).
\]

Of course \(\nu\) depends on \(S\), but for ease of notation we do not indicate this explicitly. The QSD can be seen as a local equilibrium reached by the Markov chain, conditioned on the event that the process remains in the state. Indeed, it is easy to check that if \(\nu\) is a measure with support in \(S\) such that,

\[
\nu(A) = \lim_{n \rightarrow \infty} \mathbb{P}(X^n \in A | \tau^\mu > n),
\]

then \(\nu\) is the QSD, which is then unique. In Section 4.1 below, we give sufficient conditions for existence and uniqueness of the QSD and for the convergence (3) to occur (see Theorem 4.2 in Section 4.1). We refer the reader to [4,5,8–10] for properties of the QSD and additional details.

3 The ParRep algorithm

Using the notation of the previous section, the aim of the ParRep algorithm is to efficiently generate a trajectory \((\tilde{X}_n)_{n \geq 0}\) evolving in \(\Omega / S\) which has (almost) the same law as \((\Pi(X_n))_{n \geq 0}\). We can now formulate the ParRep algorithm we propose for Markov chains. As in the original algorithm, a decorrelation time \(T_{corr}\) and a dephasing time \(T_{phase}\) are associated to each subset \(S\) (see the remarks below). Again we omit the dependence of \(T_{corr}\) and \(T_{phase}\) on \(S\).

**Algorithm 3.1.** Initialize a reference trajectory \(X_{ref} \in \Omega\). Let \(N\) be a fixed number of replicas and \(T_{poll}\) a polling time at which the replicas resynchronize. Set the simulation clock to zero: \(T_{sim} = 0\). A coarse-grained trajectory \((\tilde{X}_n)_{n \geq 0}\) evolving in \(\Omega / S\) is obtained by iterating the following:

1. Initialize a reference trajectory \(X_{ref} \in \Omega\).
2. Let \(N\) be a fixed number of replicas and \(T_{poll}\) a polling time at which the replicas resynchronize.
3. Set the simulation clock to zero: \(T_{sim} = 0\).
4. Iterate the following:
   a. Sample a replica \(X_0 \sim \mu\).
   b. Simulate \(X^n\) for a time \(T_{corr}\), where \(T_{corr}\) depends on the subset \(S\).
   c. Simulate \(X^{\nu}\) for a time \(T_{phase}\), where \(T_{phase}\) also depends on the subset \(S\).
   d. Update the replica distribution by taking \(\Pi(X_0)\) and \(\Pi(X^n)\) as initial distributions for \(X^{\nu}\) and \(X^{\nu}\), respectively.
5. Repeat steps 4a-d for \(N\) replicas.
6. Repeat steps 4-5 for a time \(T_{poll}\).
7. Update \(T_{sim}\) by \(T_{sim} = T_{sim} + T_{poll}\), and repeat steps 4-6 for \(N\) replicas.
8. When \(T_{sim}\) has reached a pre-defined final time, stop the simulation.
**Decorrelation Step:** Evolve the reference trajectory \((X_n^{\text{ref}})_{n \geq 0}\) until it spends \(T_{\text{corr}}\) consecutive time steps in some state \(S \in S\). Then proceed to the dephasing step. Through this step, the simulation clock \(T_{\text{sim}}\) is running and the coarse-grained trajectory is given by

\[
\dot{X}_{T_{\text{sim}}} = \Pi(X_{T_{\text{sim}}}^{\text{ref}}). \tag{4}
\]

**Dephasing Step:** The simulation clock \(T_{\text{sim}}\) is now stopped and the reference and coarse-grained trajectories do not evolve. Evolve \(N\) independent replicas \(\{X_n^j\}_{j=1}^N\) starting at some initial distribution with support in \(S\), such that whenever a replica leaves \(S\) it is restarted at the initial distribution. When a replica spends \(T_{\text{phase}}\) consecutive time steps in \(S\), stop it and store its end position. When all the replicas have stopped, reset each replica’s clock to \(n = 0\) and proceed to the parallel step.

**Parallel Step:** Set \(M = 1\) and iterate the following:

1. Evolve all \(N\) replicas \(\{X_n^j\}_{j=1}^N\) from time \(n = (M - 1)T_{\text{poll}}\) to time \(n = MT_{\text{poll}}\). The simulation clock \(T_{\text{sim}}\) is not advanced in this step.
2. If none of the replicas leaves \(S\) during this time, update \(M = M + 1\) and return to 1, above.
   Otherwise, let \(K\) be the smallest number \(j\) such that \(X_n^j\) leaves \(S\) during this time, let \(\tau^K\) be the corresponding (first) exit time, and set

\[
X_{\text{acc}} = X_{\tau^K}^K, \quad T_{\text{acc}} = (N - 1)(M - 1)T_{\text{poll}} + (K - 1)T_{\text{poll}} + \tau^K.
\]

Update the coarse-grained trajectory by

\[
\dot{X}_n = \Pi(S) \quad \text{for} \quad n \in [T_{\text{sim}}, T_{\text{sim}} + T_{\text{acc}} - 1], \tag{5}
\]

and the simulation clock by \(T_{\text{sim}} = T_{\text{sim}} + T_{\text{acc}}\). Set \(X_{T_{\text{sim}}}^{\text{ref}} = X_{\text{acc}}\), and return to the decorrelation step.

The idea of the Parallel step is to compute the exit time from \(S\) as the sum of the times spent by the replicas up to the first exit observed among the replicas. More precisely, if we imagine the replicas being ordered by their indices (1 through \(N\)), this sum is over all \(N\) replicas up to the last polling time, and then over the first \(K\) replicas in the last polling time, if the first of the replicas to exit during this time was the \(K\)th. See Figure 1 for a schematic of the parallel step.

The continuous in time algorithm cannot be directly applied to the discrete in time setting because the exit time from a metastable region in the continuous in time case is exponentially distributed, while it is geometrically distributed in the discrete in time case. Thus the usual time correction, based on the stability of the exponential time from a metastable region in the continuous in time case is exponentially distributed, while it is geometrically distributed in the discrete in time case. The usual time correction, based on the stability of the exponential law under minimization – \(N\) \(\min(T_1, \ldots, T_N)\) has the same law as \(T_1\), if the \(T_i\)’s are i.i.d. exponential random variables – does not apply. A few remarks are in order (see also [8,11] for additional comments on the continuous in time algorithm):

**The Decorrelation Step.** In this step, the reference trajectory is allowed to evolve until it spends a sufficiently long time in a single state. At the termination of the decorrelation step, the distribution of the reference trajectory should be, according to (3), close to that of the QSD (see also Theorem 4.2 in Section 4.1). The evolution of the reference trajectory is exact in the decorrelation step, and so the coarse-grained trajectory is also exact in the decorrelation step.

**The Dephasing Step.** The purpose of the dephasing step is to generate \(N\) samples from the QSD. While we have described a simple rejection sampling algorithm, other techniques are available, involving branching and interacting particle processes related to the Fleming-Viot process. See [1,2,5,7,10] for studies of these algorithms.

In our rejection sampling we have flexibility on where to initialize the replicas. One could use the position of the reference chain at the end of the decorrelation step, or any other point in \(S\).

**The Decorrelation and Dephasing Times.** The times \(T_{\text{corr}}\) and \(T_{\text{phase}}\) should be chosen large enough so that the distributions of both the reference process and the replicas are as close as possible to the QSD, without exhausting computational resources. \(T_{\text{phase}}\) and \(T_{\text{corr}}\) play similar roles, and they both depend on the initial distribution of the processes in \(S\).

In practice, these times can be obtained by using the Fleming-Viot process mentioned above [3], or postulated from some \textit{a priori} knowledge, such as the barriers between the metastable states.
The Polling Time. The purpose of the polling time is to permit for periods of asynchronous computation of the replicas in a distributed computing environment. For the accelerated time to be correct, it is essential that all replicas have run for at least as long as replica $K$. Ensuring this requires resynchronization; we propose to handle this via a polling time.

If communication amongst the replicas is cheap or there is little loss of synchronization of time stepping, one can take $T_{\text{poll}} = 1$.

The Efficiency of the Algorithm. For the algorithm to be efficient, one needs the metastates states to be chosen appropriately: the typical time to reach the QSD in a metastable state ($T_{\text{corr}}$ and $T_{\text{phase}}$) should be much shorter than the typical time to leave the state. Indeed, this can be considered the definition of a metastable state. One interesting aspect of the algorithm is it does not actually require the metastable states to be chosen according to the consideration above; any partition of the state space into subsets may be used. However, if the partition is not reasonably defined, it will be difficult to obtain any gain in efficiency with ParRep. Defining a partition of the state space into metastable states requires some a priori knowledge on the system described by the model. In the original ParRep algorithm applied to Langevin dynamics, the metastable states are defined as the basins of attraction of the gradient dynamics $\dot{x} = -\nabla V(x)$. One could also think of defining these regions in terms of some collective variables known to correctly describe the macroscopic configuration of the system.

4 Mathematical analysis of ParRep

The main result of this section, Theorem 4.5, shows that the coarse-grained trajectory simulated in ParRep is exact if the QSD has indeed been reached in the decorrelation and dephasing steps.

4.1 Properties of the quasistationary distribution

Before examining ParRep we give a condition under which the QSD exists and is unique.

Assumption 4.1. Assume the following holds for each $S \in S$. For every $x \in S$,

$$\mathbb{P}(X_1^x \in S) > 0.$$
Also, there exists \( m \geq 1 \) and \( \delta \in (0,1) \) such that for all \( x,y \in S \) and all bounded, non-negative, measurable functions \( f : S \to \mathbb{R} \),
\[
\mathbb{E} \left[ f(X^x_m) 1_{\{\tau^y > m\}} \right] \geq \delta \mathbb{E} \left[ f(X^y_m) 1_{\{\tau^x > m\}} \right].
\]

The following is proved in [6, Theorem 1]:

**Theorem 4.2.** Under Assumption 4.1, there exists a unique QSD \( \nu \) in place of \( n \)

where the replicas in the dephasing step to be close to the QSD in total variation norm, one may take \( T^{n/m} \) where \( n \) independent random variables. Furthermore, \( \tau \) measurable functions \( f \)

Also, there exists \( f \) such that for all \( \nu \) and any bounded measurable function \( f : S \to \mathbb{R} \),
\[
\mathbb{E} \left[ f(X^x_n) \left| \tau^\nu > n \right. \right] = \int_S f(x) \nu(dx) \leq \left( \sup_{S} |f| \right) 4 \delta^{-1} (1 - \delta^2)^{n/m} \]
where \( [n/m] \) denotes the integer part of \( n/m \).

We see in Theorem 4.2 that for the distributions of the reference process in the decorrelation step and of the replicas in the dephasing step to be close to the QSD in total variation norm, one may take \( T^{corr} \) and \( T^{phase} \), in place of \( m \), in [6] sufficiently large so as to make the right hand side small.

Next we prove a property of the QSD which will be essential to our mathematical analysis of ParRep.

**Theorem 4.3.** Assume there is a QSD \( \nu \) in \( S \) associated to the Markov chain \((X_n)_{n \geq 0}\). Then \( \tau^\nu \) and \( X^\nu_{\tau^\nu} \) are independent random variables. Furthermore, \( \tau^\nu \) is a geometric random variable:
\[
\mathbb{P}(\tau^\nu > n) = (1 - p)^n
\]
where \( p = \mathbb{P}(X^\nu_1 \notin S) \).

**Proof.** Recall that \( k(x,dy) \) denotes the transition kernel of the underlying Markov chain. For any bounded measurable \( f : \Omega \to \mathbb{R} \), observe that
\[
\mathbb{E} \left[ f(X^\nu_{\tau^\nu}) \right| \tau^\nu = n] = \frac{\mathbb{E} \left[ f(X^\nu_{\tau^\nu}) 1_{\{\tau^\nu = n\}} \right]}{\mathbb{E} \left[ 1_{\{\tau^\nu = n\}} \right]}
\]
\[
= \frac{\mathbb{E} \left[ 1_{\{\tau^\nu > n\}} \int_{S \setminus S} f(y)k(X^\nu_{n-1},dy) \right]}{\mathbb{E} \left[ 1_{\{\tau^\nu > n\}} \right]}
\]
\[
= \frac{\mathbb{E} \left[ \int_{S \setminus S} f(y)k(X^\nu_{n-1},dy) \right]}{\mathbb{E} \left[ \int_{S \setminus S} k(X^\nu_{n-1},dy) \right]}
\]
\[
= \frac{\int_{S} \left( \int_{S \setminus S} f(y)k(x,dy) \right) \nu(dx)}{\int_{S} \left( \int_{S \setminus S} k(x,dy) \right) \nu(dx)}
\]
where the second to last equality above comes from equation (2). Since the last line is independent of \( n \), the first part is proven.

To establish the second part of the theorem, compute
\[
\mathbb{P}(\tau^\nu > n) = \mathbb{P}(\tau^\nu > n|\tau^\nu > n - 1) \mathbb{P}(\tau^\nu > n - 1)
\]
and
\[
\mathbb{P}(\tau^\nu > n|\tau^\nu > n - 1) = \frac{\mathbb{E} \left[ 1_{\{\tau^\nu > n\}} \right]}{\mathbb{E} \left[ 1_{\{\tau^\nu > n-1\}} \right]}
\]
\[
= \frac{\mathbb{E} \left[ 1_{\{\tau^\nu > n\}} \int_{S} k(X^\nu_{n-1},dy) \right]}{\mathbb{E} \left[ 1_{\{\tau^\nu > n-1\}} \right]}
\]
\[
= \frac{\mathbb{E} \left[ \int_{S} k(X^\nu_{n-1},dy) \right]}{\mathbb{E} \left[ \int_{S} k(x,dy) \right]}
\]
\[
= \mathbb{P}(X^\nu \in S).
\]
where the second to last line again comes from equation (2). Thus one obtains
\[ P(\tau^n > n) = P(X^n_1 \in S)P(\tau^n > n - 1), \]
and, by induction,
\[ P(\tau^n > n) = [P(X^n_1 \in S)]^n = (1 - p)^n. \]

4.2 Analysis of the exit event

We are now ready to prove our main result, Theorem 4.5 below. Throughout, we assume that (3) holds for each \( S \in \mathcal{S} \) and thus that there is a unique QSD in each metastable state. We refer to the previous section for a sufficient condition.

We will show that ParRep (Algorithm 3.1) is exact under the following idealizing assumption:

**Assumption 4.4.** Assume that:

(A1) After spending \( T_{\text{corr}} \) consecutive time steps in \( S \), the process \( (X_n)_{n \geq 0} \) is exactly distributed according to the QSD \( \nu \) in \( S \). In particular, at the end of the decorrelation step, \( X_{\text{ref}}^T \sim \nu \).

(A2) At the end of the dephasing step, all \( N \) replicas are i.i.d. with law exactly given by \( \nu \).

To analyze the error due to finite decorrelation and dephasing times, one must specify the system under consideration; convergence to the QSD is related to the spectral properties of the semigroup induced by the process. For the continuous in time problem, see [8,11]. The purpose of this work is mainly to adapt the parallel step to the discrete in time setting, not to analyze the error induced by a particular choice of parameters, so we will not consider this error.

**Theorem 4.5.** Let Assumption 4.4 hold. Then ParRep is exact: the trajectory generated by ParRep has the same probability law as the true coarse-grained chain:
\[ (\hat{X}_n)_{n \geq 0} \sim (\Pi(X_n))_{n \geq 0}. \]

Observe that the evolution of the coarse-grained trajectory is exact in the decorrelation step, and the coarse-grained trajectory is not updated during the dephasing step, so the error in Algorithm 3.1 can arise only in the parallel step. In light of this, (A1) and Theorem 4.3 Theorem 4.5 is a corollary of the following proposition which analyzes the exit event.

**Proposition 4.6.** Assume 4.4-(A2). Then the parallel step of Algorithm 3.1 is exact. That is, the following holds:

(i) \( T_{\text{acc}} \) is a geometric random variable with parameter \( p = P(X^n_1 \notin S) \),

(ii) \( T_{\text{acc}} \) is independent of \( X_{\text{acc}} \), and

(iii) \( X_{\text{acc}} \) and \( X_{\tau^n} \) have the same law: \( X_{\text{acc}} \sim X_{\tau^n} \).

Before proving Proposition 4.6, we need the following lemma:

**Lemma 4.7.** Let \( \tau^1, \tau^2, \ldots, \tau^N \) be i.i.d. geometric random variables with parameter \( p \): for \( t \in \mathbb{N} \cup \{0\} \),
\[ P(\tau^j > t) = (1 - p)^t. \]

Define
\[ M = \min\{m \geq 1 : \exists j \in \{1, \ldots, N\} \text{ s.t. } \tau^j \leq mT_{\text{poll}}\} \]
\[ K = \min\{j \in \{1, \ldots, N\} : \tau^j \leq MT_{\text{poll}}\} \]
\[ \xi = (N - 1)(M - 1)T_{\text{poll}} + (K - 1)T_{\text{poll}} + \tau^K. \]

Then \( \xi \) has the same law as \( \tau^1 \).
Proof. Notice that $\xi$ can be rewritten as
\[ \xi = N(M - 1)T_{\text{poll}} + (K - 1)T_{\text{poll}} + [\tau^K - (M - 1)T_{\text{poll}}]. \]

Observe moreover that any natural number $z$ can be uniquely expressed as $z = N(m - 1)T_{\text{poll}} + (k - 1)T_{\text{poll}} + t$ where $m \in \mathbb{N} \setminus \{0\}$, $k \in \{1, \ldots, N\}$ and $t \in \{1, 2, \ldots, T_{\text{poll}}\}$. For such $m$, $k$ and $t$ we compute
\[
\mathbb{P}[\xi = N(m - 1)T_{\text{poll}} + (k - 1)T_{\text{poll}} + t] = \mathbb{P}[M = m, K = k, \tau^K = t]
\]
\[
= \mathbb{P}[\tau^1 > mT_{\text{poll}}, \ldots, \tau^{k-1} > mT_{\text{poll}}, \tau^k = (m - 1)T_{\text{poll}} + t, \tau^{k+1} > (m - 1)T_{\text{poll}}, \ldots, \tau^N > (m - 1)T_{\text{poll}}]
\]
\[
= \mathbb{P}[\tau^1 > mT_{\text{poll}}] \mathbb{P}[\tau^k = (m - 1)T_{\text{poll}} + t] \mathbb{P}[\tau^{k+1} > (m - 1)T_{\text{poll}}] \ldots \mathbb{P}[\tau^N > (m - 1)T_{\text{poll}}]
\]
\[
= (1 - p)^{(k-1)mT_{\text{poll}}} p(1 - p)^{(m-1)T_{\text{poll}} + t - 1} (1 - p)^{(N-k)(m-1)T_{\text{poll}}}
\]
\[
= p(1 - p)^{N(m-1)T_{\text{poll}} + (k-1)T_{\text{poll}} + t - 1}
\]
\[
= \mathbb{P}[\tau^1 = N(m - 1)T_{\text{poll}} + (k - 1)T_{\text{poll}} + t].
\]
This concludes the proof of Lemma 4.7.

Now we turn to the proof of Proposition 4.6.

Proof. [Proof of Proposition 4.6] We first prove (i). For $j \in \{1, 2, \ldots, N\}$, let $\tau^j$ be a random variable representing the first exit time from $S$ of the $j$th replica in the parallel step of ParRep, if the replica were allowed to keep evolving indefinitely. Then by (A2), $\tau^1, \ldots, \tau^N$ are independent and all have the same distribution as $\tau^\nu$, so by Theorem 4.3, $\tau^1, \ldots, \tau^N$ are i.i.d. geometric random variables with parameter $p$. Now by Lemma 4.7, $T_{\text{acc}}$ is a geometric random variable with parameter $p$.

Now we turn to (ii) and (iii). Observe that $K = k$ if and only if $X_{\text{acc}} = X_{k}$. and there exists $m \in \mathbb{N}$ such that $\tau^1 > mT_{\text{poll}}, \ldots, \tau^{k-1} > mT_{\text{poll}}, (m - 1)T_{\text{poll}} < \tau^k < mT_{\text{poll}}$, and $\tau^{k+1} > (m - 1)T_{\text{poll}}, \ldots, \tau^N > (m - 1)T_{\text{poll}}$. From Theorem 4.3 and (A2) we see that $X_{\text{acc}}^k$ is independent of $\tau^1, \ldots, \tau^N$, so we conclude that $X_{\text{acc}}$ is independent of $K$. From this and (A2) it follows that $X_{\text{acc}} \sim X^\nu_{\text{acc}}$. To see that $X_{\text{acc}}$ is independent of $T_{\text{acc}}$, let $\sigma(K, \tau^K)$ be the sigma algebra generated by $K$ and $\tau^K$. Note that knowing the value of $K$ and $\tau^K$ is enough to deduce the value of $T_{\text{acc}}$; that is, $T_{\text{acc}}$ is $\sigma(K, \tau^K)$-measurable. Also note that by the above and Theorem 4.3 $X_{\text{acc}} = X^\nu_{\text{acc}}$ is independent of $\sigma(K, \tau^K)$. To see that $T_{\text{acc}}$ and $X_{\text{acc}}$ are independent, use the preceding to compute for suitable test functions $f, g$:
\[
\mathbb{E}[f(T_{\text{acc}})g(X_{\text{acc}})] = \mathbb{E}[\mathbb{E}[f(T_{\text{acc}})g(X_{\text{acc}}) | \sigma(K, \tau^K)]]
\]
\[
= \mathbb{E}[f(T_{\text{acc}})\mathbb{E}[g(X_{\text{acc}}) | \sigma(K, \tau^K)]]
\]
\[
= \mathbb{E}[f(T_{\text{acc}})] \mathbb{E}[g(X_{\text{acc}})].
\]
This concludes the proof of Proposition 4.6.

5 Numerical Examples

5.1 Random Walk

Consider a random walk on $\mathbb{Z}$ with transition probabilities $p(i, j)$ defined as follows:
\[
p(i, j) = \begin{cases} 
3/4, & i < 0 \text{ and } j = i + 1, \\
1/4, & i < 0 \text{ and } j = i - 1, \\
1/3, & i = 0 \text{ and } |j| \leq 1, \\
1/4, & i > 0 \text{ and } j = i + 1, \\
3/4, & i > 0 \text{ and } j = i - 1, \\
0, & \text{otherwise.} 
\end{cases}
\]

We use ParRep to simulate the first exit time, $\tau^\nu$, of the random walk from $S = [-5, 5]$, starting from the QSD $\nu$ in $S$. At each point except 0, transitions towards 0 are more likely than transitions towards the boundaries $-5$ or 5.

We perform this simulation by using the dephasing and parallel steps of ParRep: under Assumption 4.4 (A2) the accelerated time $T_{\text{acc}}$ should have the same law as $\tau^\nu$. The parameter of the geometric law of $\tau^\nu$ can be analytically computed in this simple case. We perform $10^6$ ParRep simulations to obtain statistics on the
distribution of $T_{acc}$ and the gain in wall clock time. We find that using $T_{corr} = T_{phase} = 25$ gives accurate results (Figure 2). To measure the gain in wall clock efficiency using ParRep, we introduce the parallel time $T_{par}$, defined using the notation of Algorithm 3.1 as $T_{par} = MT_{poll}$, where $M$ is defined by $\tau^K \in [ (M - 1)T_{poll} + 1, MT_{poll} ]$. Thus, the “wall clock time” of the parallel step is $C T_{par}$, $C$ being the computational cost of a single time step for one replica. Note the significant parallel time speedup in ParRep compared with the direct sampling time (Figure 3). The speedup is approximately linear in $N$. 

$\begin{align*}
8 \times 10^{-3} \\
7.5 \\
7 \\
6.5 \\
6 \\
5.5 \\
5 \\
4.5 \\
4 \\
3.5 \\
3 \\
2.5 \\
2 \\
1.5 \\
1 \\
0.5 \\
0 \\
0 & 1000 2000 3000 4000 5000 6000 7000 8000 \\
0 & 1 \\
2 & 3 \\
4 & 5 \\
6 & 7 \\
8 & x 10^{-4} \\
\end{align*}$

Figure 2: Probability mass function of $T_{acc}$ estimated by $10^6$ ParRep simulations with $N = 10$ replicas and $T_{phase} = T_{corr} = 25$ vs. exact distribution of $\tau^\nu$ (smooth curve).

5.2 Discretized Diffusions

Consider an overdamped Langevin equation in $\mathbb{R}^d$ (obtained from (1) in the zero-mass or the infinite damping limit),

$$dX_t = -\nabla V(X_t) dt + \sqrt{2/\beta - 1} dW_t. \tag{7}$$

The associated Euler-Maruyama discretization is

$$X_{n+1} = X_n - \nabla V(X_n) \Delta t + \sqrt{2/\beta - 1} \Delta t \xi_n \tag{8}$$

where $\xi_n \sim N(0, I)$ are $d$-dimensional i.i.d. random variables. It is well-known that $(X_n)_{n \geq 0}$ is then an approximation of $(X_n \Delta t)_{n \geq 0}$.

5.2.1 Existence and uniqueness of the QSD

Let us first check that under a regularity assumption on $V$, the QSD of the Markov chain $(X_n)_{n \geq 0}$ associated to a bounded domain $S \subset \mathbb{R}^d$ is uniquely defined. Inspired by a 1D example in [6], we have:

**Proposition 5.1.** Assume $S \subset \mathbb{R}^d$ is bounded and $\nabla V$ is bounded on $S$. Then (8) satisfies Assumption 4.1, and thus the QSD $\nu$ in $S$ is uniquely defined.

**Proof.** We first show that at all starting points, there is a positive probability of persisting in $S$. Computing

$$P(X^*_1 \in S) = \mathbb{E} [1_S(X^*_1)] = \int_{\mathbb{R}^d} 1_S(y)(2\pi)^{-d/2} \exp \left\{ - \frac{|y - x + \nabla V(x) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} dy \geq |S| \min_{y \in S} \left\{ (2\pi)^{-d/2} \exp \left\{ - \frac{|y - x + \nabla V(x) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} \right\} > 0. \tag{9}$$
Figure 3: Cumulative distribution function of parallel time required for ParRep sampling with $T_{\text{poll}} = 10$ and, from top: $N = 100, 25, 10$. The bottom curve is the (analytic) cumulative distribution function of $\tau^*$ (corresponding to $N = 1$).

Next, we compute

$$
\mathbb{E} \left[ f(X^*_T) \mathbf{1}_{(\tau^* > 1)} \right] = \int_S f(z)(2\pi)^{-d/2} \exp \left\{ -\frac{|z - x + \nabla V(x) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} dz \\
= \int_S f(z)(2\pi)^{-d/2} \exp \left\{ -\frac{|z - y + \nabla V(y) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} \\
\times \exp \left\{ -\frac{|z - x + \nabla V(x) \Delta t|^2 - |z - y + \nabla V(y) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} dz \\
\geq C \int_S f(z)(2\pi)^{-d/2} \exp \left\{ -\frac{|z - y + \nabla V(y) \Delta t|^2}{4\beta^{-1} \Delta t} \right\} dz \\
= C \mathbb{E} \left[ f(X^*_T) \mathbf{1}_{(\tau^* > 1)} \right]
$$

(10)

where

$$
C = \min_{x,y,z \in S} \exp \left\{ -\frac{|z - x + \nabla V(x) \Delta t|^2 - |z - y + \nabla V(y) \Delta t|^2}{4\beta^{-1} \Delta t} \right\}.
$$

Since $S$ is bounded and terms in the brackets are bounded, $C > 0$. In Assumption 4.1 we can then take $k = 1$ and $\delta = C$. Theorem 4.2 then ensures that the QSD is uniquely defined, and this concludes the proof.

5.2.2 Numerical example

As an example, we consider the 1D problem

$$
dX_t = -2\pi \sin(\pi X_t)dt + \sqrt{2}dW_t, \quad X_0 = \frac{1}{2},
$$

(11)

and look for the first time of exit from $(-1,1)$. We discretize with $\Delta t = 10^{-2}$, and we use $N = 1000$ replicas. The dephasing and decorrelation times are $T_{\text{corr}} = T_{\text{phase}} = 1$, corresponding to 100 time steps.
Figure 4: Exit time distributions for the Euler-Maruyama discretization of (11) with 95% Clopper-Pearson confidence intervals (dashed lines). Confidence interval width increases at larger $t$, as there are fewer samples, and lower bounds are absent once the values become negative. There is excellent agreement between the serial, unaccelerated simulation data ($T = \tau^K \Delta t$), and our ParRep algorithm ($T = T_{acc}^{\text{corrected}}$). The naive data ($T = T_{acc}^{\text{naive}}$) gives a significant deviation.

Consider a naive implementation of the continuous time ParRep algorithm in [12, 13] to the discretized process. In that algorithm, the accelerated time is (in units of physical time instead of time steps)

$$T_{acc}^{\text{naive}} = N\tau^K \Delta t,$$

with $\tau^K$ the same as in Algorithm 3.1 above. This gives rise to the staircasing of the distribution: $T_{acc}^{\text{naive}}$ is by construction a multiple of $N\Delta t = 10$. See Figure 4. This staggering worsens as the number of replicas increases. In our ParRep algorithm we use the accelerated time formula (again in units of physical time)

$$T_{acc}^{\text{corrected}} = T_{acc} \Delta t,$$

where $T_{acc}$ is defined as in Algorithm 3.1 above. Notice from Figure 4 we have excellent agreement between the serial data and the ParRep data. We comment further on this in the next section.

5.2.3 Error introduced by a naive implementation of ParRep

In light of the discretization example, one may ask what kind of errors were introduced in previous numerical studies which used ParRep with (12). Taking $T_{\text{poll}} = 1$ for simplicity, we calculate

$$\mathbb{E} \left[ \left| T_{acc}^{\text{corrected}} - T_{acc}^{\text{naive}} \right| \right] = \mathbb{E} \left[ \left| (N(\tau^K - 1) + K)\Delta t - N\tau^K \Delta t \right| \right] = \Delta t \mathbb{E} \left[ |N - K| \right] = \Delta t \sum_{k=1}^{N} (N - k) \mathbb{P}(K = k).$$

Using calculations analogous to those used to study $T_{acc}$, it can be shown that

$$\mathbb{P}(K = k) = \frac{(1 - p)^{k-1} p}{1 - (1 - p)^N}.$$

Therefore the error in the number of time steps per parallel step is

$$\text{Absolute Error} = \frac{N\Delta t}{1 - (1 - p)^N} - \frac{\Delta t}{p}, \quad \text{Relative Error} = \frac{pN}{1 - (1 - p)^N} - 1.$$

Consider the relative error, writing it as

$$pN \left[ \frac{1}{1 - r^N} - \frac{1}{(1 - r)^N} \right],$$

where $r = 1 - p$. 

We claim the quantity in the brackets,

\[ f(r, N) = \frac{1}{1 - rN} - \frac{1}{(1 - r)N} = \frac{r^N - Nr + N - 1}{N(r^{N+1} - Nr^N - Nr^N + N^2)}, \tag{14} \]

is bounded from above by one. Indeed, for any \(0 < r < 1\), we immediately see that \(f(r, N)\) is zero at \(N = 1\) and one as \(N \to \infty\). Let us now reason by contradiction and assume that \(\sup_{r \in (0,1), N > 0} f(r, N) > 1\). Since \(f\) is continuous in \(N > 0\) and \(0 < r < 1\), there is then a point \((r, N)\) such that \(f(r, N) = 1\), which also rewrites

\[ g_N(r) = 0 \]

where \(g_N(r) = Nr^{N+1} - (N + 1)r^N + 1\).

Note that \(g_N(0) = 1\) and \(g_N(1) = 0\) for all values of \(N\). Computing the derivative with respect to \(r\), we observe

\[ g'_N(r) = -N(N + 1)(1 - r)r^{N-1} < 0. \]

Therefore, \(g_N(r)\) is decreasing, from one at \(r = 0\) to zero at \(r = 1\), in the interval \((0, 1)\). Hence, \(g_N(r) = 0\) has no admissible solution, and \(f\) is bounded from above by one.

Consequently, we are assured

\[ \text{Absolute Error} \leq N\Delta t, \quad \text{Relative Error} \leq pN. \tag{15} \]

Thus, so long as \(pN \ll 1\), the relative error using the naive accelerated time will be modest, especially for very metastable regions where \(p \ll 1\). So long as \(N\Delta t \ll 1\), the absolute error will also be small.

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