Editors' Suggestion

Irreversible Monte Carlo Algorithms for Hard Disk Glasses: From Event-Chain to Collective Swaps

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Equilibrium sampling of the configuration space in disordered systems requires algorithms that bypass the glassy slowing down of the physical dynamics. Irreversible Monte Carlo algorithms breaking detailed balance successfully accelerate sampling in some systems. We first implement an irreversible event-chain Monte Carlo algorithm in a model of continuously polydisperse hard disks. The effect of collective translational moves marginally affects the dynamics and results in a modest speedup that decreases with density. We then propose an irreversible algorithm performing collective particle swaps which outperforms all known Monte Carlo algorithms. We show that these collective swaps can also be used to prepare very dense jammed packings of disks.

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Sampling the Boltzmann distribution in dense fluids becomes a formidable computational problem as the glass transition is approached at large density or low temperature [1]. If conventional methods such as molecular dynamics or local Monte Carlo algorithms are used [2–4], the rapidly growing timescale characterizing the glassy dynamics also controls the sampling efficiency [5]. The microscopic mechanisms responsible for the dynamical slowing down continue to elude our understanding [6]. This represents a fascinating physics problem, but constitutes a major obstacle to the development of algorithms that can efficiently shortcut the slow dynamics to reach and study equilibrium states close to the glass transition. Glass formers are a challenging benchmark for systems exhibiting a complex and rugged energy landscape, even far beyond the realm of the physical world [7–10].

Recently, an efficient Monte Carlo algorithm was developed for size polydisperse fluids, where local Monte Carlo moves are performed in an enlarged configuration space composed of particle positions and diameters [11–13]. The sequential Swap of particle pairs respects detailed balance and ensures that the particle size distribution is conserved [11]. The resulting Swap Monte Carlo algorithm (hereafter called Swap) allows equilibration at very low temperatures, exploiting dynamic pathways unavailable to the local dynamics [13]. Swap paved the way for numerous physical studies [14–16] and computational developments [17,18]. Diameter dynamics can be implemented in molecular dynamics, both in thermal equilibrium [19] or in gradient descent [20,21]. For hard particles, this optimization strategy was exploited to produce jammed packings with large stability and novel physical properties [21–23].

The Swap algorithm samples the Boltzmann distribution owing to reversible evolution rules obeying detailed balance. In many areas of physics and applied mathematics, it was realized that giving up detailed balance—while preserving the target distribution—can be rewarded with sampling acceleration. Ironically, the seminal 1953 article [24] by Metropolis *et al.* presented an algorithm to sample the Boltzmann distribution for simple fluids whose elementary moves did not, strictly speaking, satisfy detailed balance. As long as the global balance condition is satisfied by the transition rates, the target distribution is correctly sampled, even if dynamic pathways again become unphysical.

In specific instances, it can be proved that irreversible algorithms carry out their sampling task faster than in equilibrium [25,26]. A successful implementation of these ideas for particle models is the event-chain Monte Carlo (ECMC) algorithm [27] that also operates in an enlarged configuration space where irreversible collective particle translations are performed. For hard disks near their hexatic ordering transition, ECMC offers a 2 orders of magnitude speedup that led to a better understanding of the phase diagram [28]. This approach was extended in various directions [29–36], but quantitative benchmark in dense disordered states is lacking.

Here we propose, implement, and benchmark irreversible Monte Carlo algorithms where collective and directed particle translations and diameter swaps are performed while maintaining global balance, see Fig. 1. We carefully test the respective and combined effects of these moves in continuously polydisperse models of hard disks displaying glassy dynamics in equilibrium, and that can be

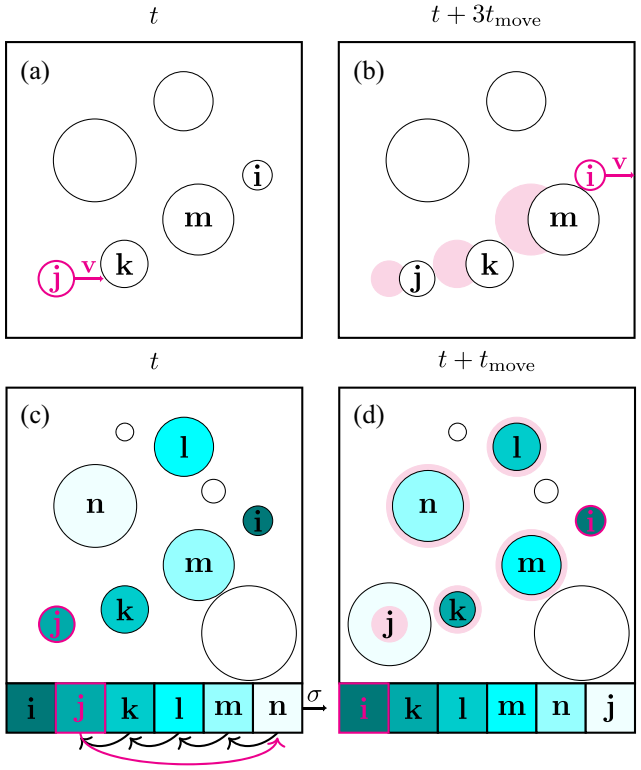

FIG. 1. (a),(b) Event-chain Monte Carlo algorithm: the lifted set of degrees of freedom, the active label j, and the speed direction $\mathbf{v}$ (magenta), produce a directed translational motion of a chain of three particles. (c),(d) Collective Swap algorithm: the active particle (in magenta) inflates while other particles deflate, resulting in a directed motion in diameter space (as seen at the bottom) and a collective swap of five particles.

compressed towards jamming [23]. We find that the directed translational moves used in ECMC marginally affect the dynamics, with a speedup that plummets with increasing density. By contrast, irreversible collective swaps (cSwap) produce an opposite trend offering a comfortable gain over Swap that improves with density. Combining both types of moves in a novel algorithm (cSwapECMC) provides an overall computational speedup reaching about 40 over the conventional Swap. In addition, cSwapECMC remains extremely efficient during nonequilibrium compressions, producing jammed packings comparable to gradient descent protocols preserving the particle size distribution.

We consider a two-dimensional mixture of $N = 1024$ hard disks in a periodic square box of linear size L with a fixed continuous polydispersity of about 25% (see Supplemental Material [37] for results on a different polydisperse model and different system sizes). Lengths are measured in units of the average diameter $\bar{\sigma}$, and the packing fraction is $\phi = N\pi\overline{\sigma^2}/(4L^2)$. We work in a density regime characterized by glassy dynamics, typically much beyond the one explored in [27] for monodisperse systems.

We run NVT Monte Carlo simulations [3]. To compare the efficiency of various algorithms, we need to carefully define a specific unit of time, t_{move}, adapted for each case. In Metropolis Monte Carlo (MMC) dynamics, a random particle is selected uniformly, and a random displacement is uniformly drawn from a square of length δ centered around the origin. We take $\delta = 0.115\bar{\sigma}$. The displacement is accepted if it creates no overlaps. One such attempt defines t_{move}. In Swap, we randomly alternate translational moves (as in MMC) with particle swaps with probability $p_{\text{swap}} = 0.2$. During t_{move}, two particles are randomly selected and their radii are exchanged if the swap does not create overlaps.

In both MMC and Swap, a configuration is specified by $\mathcal{C} = \{\mathbf{r}^N, \sigma^N\}$, encoding the N particle positions and diameters. For ECMC, the phase space is lifted by two additional degrees of freedom, corresponding to the label i of the active particle performing directed motion, and its direction of motion $\mathbf{v}$. During a time interval t_{move}, particle i travels along direction $\mathbf{v}$ until it collides with one of its neighbors, j. The activity label is then updated from i to j. After a time nt_{move}, with n an integer, a directed chain of n particles has moved in direction $\mathbf{v}$, see Fig. 1. To warrant ergodicity, both $\mathbf{v}$ and the activity label are uniformly resampled after the total directed displacements add up to a fixed total length ℓ (see Supplemental Material [37] for more details on the numerical implementation). Following the original choice [27,38], $\mathbf{v}$ is uniformly resampled from $\{\mathbf{e}_x, \mathbf{e}_y\}$. Of course, ECMC can be combined with Swap, which trivially leads to a new algorithm, SwapECMC.

We now show how to perform directed, irreversible, collective moves in diameter space to arrive at cSwap. We define a one-dimensional array containing the particle labels in order of increasing diameters and the operators $(\mathcal{L}, \mathcal{R})$ acting on the labels: $\mathcal{L}(i)$ returns the label of the particle immediately to the left of i (with a smaller radius); $\mathcal{R}(i)$ returns the label of the particle to the right (with a larger radius). During t_{move} we perform the following operations. A particle i is uniformly selected to become active and the state of the system is described by $\mathcal{C} = \{\mathbf{r}^N, \sigma^N, i\}$. We then determine the largest diameter $\sigma_j \in \sigma^N$ that particle i can adopt without generating an overlap. To preserve the particle size distribution, we now perform a cascade of swaps: $\sigma_i \leftarrow \sigma_j$ (maximal authorized expansion of i), followed by a series of incremental deflations $\sigma_j \leftarrow \sigma_{\mathcal{L}(j)}$, $\sigma_{\mathcal{L}(j)} \leftarrow \sigma_{\mathcal{L}^2(j)}, \ldots, \sigma_{\mathcal{L}^n(j)} \leftarrow \sigma_i$, with n such that $\mathcal{L}^n(j) = \mathcal{R}(i)$, thus completing the cascade. Finally, a lifting event occurs leading to $\mathcal{C}' = \{\mathbf{r}^N, \sigma'^N, \mathcal{L}(i)\}$, where σ'^N is reached after the collective swap. If i is the particle with the smallest diameter, $\mathcal{L}(i)$ is the particle with the largest diameter. To warrant ergodicity, we perform with probability $1/N$ a uniform resampling of the lifting label. Finally, ECMC can be combined with cSwap, leading to a fully irreversible algorithm, cSwapECMC. The invention and implementation of

irreversible and collective swap moves is our main algorithmic development. While cSwap is broadly applicable for any particle size distribution, its efficiency should be optimal for continuous distributions, or discrete ones with a large number of families. For bidisperse models, cSwap remains rejection-free and irreversible, but loses its collective character.

We must prove that the stationary state of the cSwap dynamics is the Boltzmann distribution, i.e., $\pi_{ss}(\{\mathbf{r}^N,\sigma^N,i\}) = \pi_{\mathrm{B}}(\mathbf{r}^N,\sigma^N)\nu(i)$, where $\pi_{\mathrm{B}} = [\int d\sigma'^N \pi_{\mathrm{B}}(\mathbf{r}^N,\sigma'^N)]^{-1} \equiv Z^{-1}$ is the Boltzmann distribution for a system of polydisperse hard disks for a fixed set of positions $\mathbf{r}^N$, and $\nu(i) = N^{-1}$ is the uniform distribution for lifting. Denoting by $p(\mathcal{C}\to\mathcal{C}')$ the transition probability from $\mathcal{C} = \{\mathbf{r}^N,\sigma^N,i\}$ to $\mathcal{C}' = \{\mathbf{r}^N,\sigma'^N,i'\}$, we must prove that the stationarity condition

$$\sum_{\mathcal{C}'} \pi_{ss}(\mathcal{C}')p(\mathcal{C}'\to\mathcal{C}) = \pi_{ss}(\mathcal{C}) \tag{1}$$

is satisfied by $\pi_{ss} = \pi_B/N$. The left-hand side is decomposed into label resampling and collective swaps:

$$p(\mathcal{C}'\to\mathcal{C}) = \frac{1}{N^2}\delta_{\sigma'^N,\sigma^N} + \left(1-\frac{1}{N}\right)\delta_{\mathcal{C}',\mathcal{C}^*}, \tag{2}$$

where $\mathcal{C}^*$ is the configuration reaching $\mathcal{C}$ after a cSwap move (we show below that $\mathcal{C}^*$ exists and is unique). Substituting (2) into (1), using the definition of π_{ss} and $\sum_{\mathcal{C}} = \sum_j \int d\sigma^N$, we get

$$\frac{1}{N}\pi_{\mathrm{B}}(\mathbf{r}^N,\sigma^N) + \left(1-\frac{1}{N}\right)\pi_{\mathrm{B}}(\mathbf{r}^N,\sigma^{*N}) = \pi_{\mathrm{B}}(\mathbf{r}^N,\sigma^N).$$

Since for hard disks, π_{B} is uniform over allowed configurations, stationarity is proven. Finally we construct the configuration $\mathcal{C}^* = \{\mathbf{r}^N,\sigma^{*N},i^*\}$ that will reach $\mathcal{C} = \{\mathbf{r}^N,\sigma^N,i\}$. We first transform $\sigma_{\mathcal{R}(i)} \leftarrow \sigma_{\mathcal{R}^2(i)}$ if the change does not generate any overlap. We then repeat this operation for $\mathcal{R}^2(i)$, $\mathcal{R}^3(i)$, etc. After n iterations, either the transformation $\sigma_{\mathcal{R}^n(i)} \leftarrow \sigma_{\mathcal{R}^{n+1}(i)}$ is no longer allowed, or the largest particle is reached. When n is reached, we set $i^* = \mathcal{R}^n(i)$ and transform $\sigma_{\mathcal{R}^n(i)} \leftarrow \sigma_{\mathcal{R}(i)}$. The resulting configuration defines σ^{*N}, as directly verified by performing a cSwap move on $\mathcal{C}^*$.

The above reasoning establishes the stationarity of the Boltzmann distribution. The general proof of ergodicity of the algorithm, as obtained for ECMC [44], is left for future work. As a test, we computed the stochastic matrix associated to the cSwap algorithm for a small system of $N = 4$ hard disks (see Ref. [37]) and analytically confirmed ergodicity in that case. For larger systems, we support our claim of ergodicity by extensive numerical tests of correct sampling using cSwap, as compiled in Supplemental Material [37].

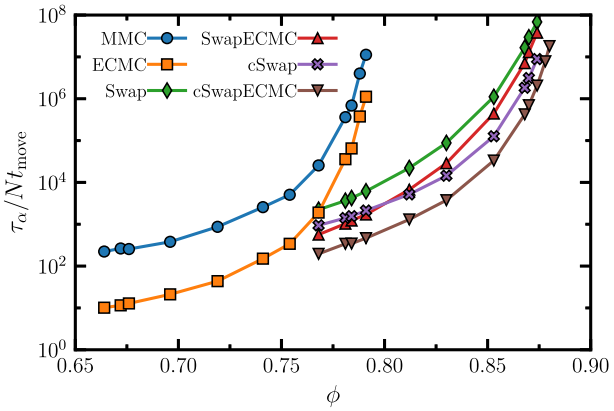

FIG. 2. Equilibrium relaxation time of six different Monte Carlo algorithms as a function of packing fraction. MMC and the faster ECMC fall out of equilibrium much before the four swap algorithms. The large speedup offered by Swap can be further improved using irreversible MC moves, cSwapECMC providing a further speedup of about 40 near $\phi = 0.88$.

We run simulations comparing MMC, ECMC, Swap, SwapECMC, cSwap, and cSwapECMC for increasing packing fractions. After careful equilibration, we measure a representative time correlation function for $2d$ glass formers, namely, the time autocorrelation of the global hexatic order $C_\psi(t)$, and define the structural relaxation time τ_α from $C_\psi(\tau_\alpha) = 1/e$ [37]. For each algorithm, we collect the evolution of the correlation time $\tau_\alpha(\phi)$ measured in units of Nt_{move} in Fig. 2. The most costly part of Monte Carlo moves is the overlap detection involving a sum over neighbors. Since one such sum is needed over the time t_{move} in each algorithm, the comparison in Fig. 2 accurately describes CPU times [37].

Each algorithm displays hallmarks of glassy dynamics, and we follow for about 5 decades the slowing down. The algorithms are split into two families, depending on the presence of swap moves. MMC and ECMC only contain translations and equilibration becomes difficult above $\phi \approx 0.79$. Yet, ECMC clearly outperforms MMC throughout the entire density range, but the edge of ECMC over MMC is lost as ϕ increases. This is demonstrated in Fig. 3(a), which shows that the ratio of their relaxation times decreases from ≈22 in the fluid, down to ≈10 near $\phi = 0.79$. This suggests that the irreversibility introduced by the directed chain moves does not help the system to discover new, faster pathways across the configuration space. This interpretation is confirmed by the snapshots in Figs. 3(b) and 3(c) showing particle displacements with respect to the system's center of mass from the same initial condition, using either MMC or ECMC. Despite the very different particle moves in both dynamics, the long time relaxation proceeds along a similar path. A similar conclusion was recently reached for systems submitted to transverse forces [45].

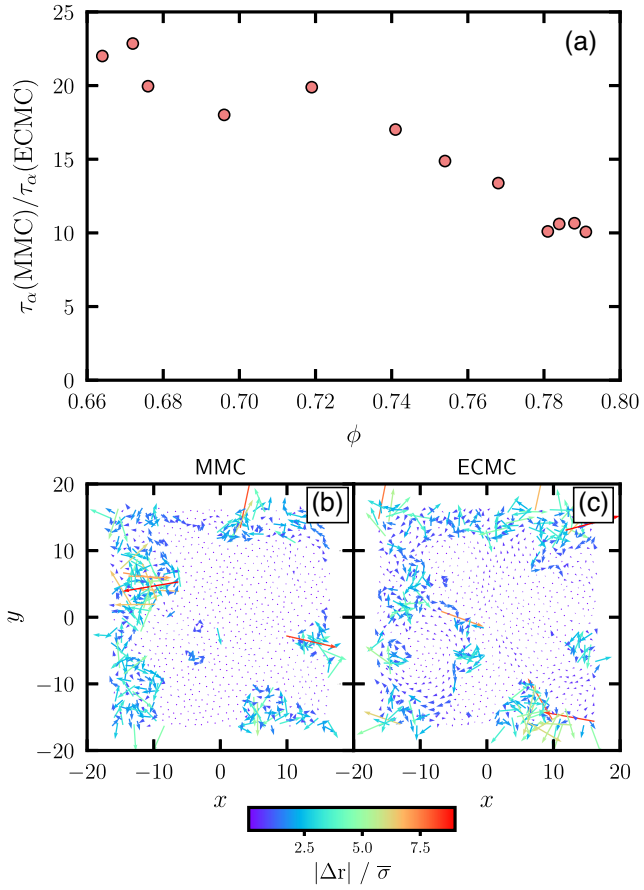

FIG. 3. (a) The speedup offered by ECMC over MC decreases with density. (b),(c) Comparison of the displacement field relative to the center of mass after a time comparable to the relaxation time starting from the same initial condition at $\phi = 0.79$ using MMC ($t = 4.6 \times 10^6 N t_{\mathrm{move}}$) or ECMC ($t = 2.2 \times 10^5 N t_{\mathrm{move}}$). Despite different dynamic rules, both algorithms follow similar dynamic pathways.

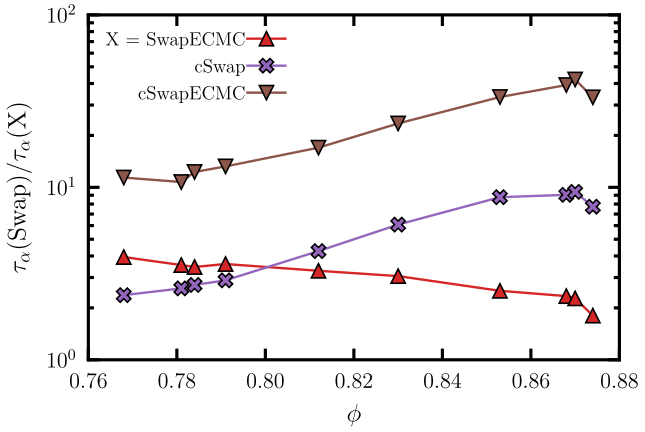

FIG. 4. Acceleration provided by three novel algorithms (SwapECMC, cSwap, cSwapECMC) with respect to conventional Swap Monte Carlo. In cSwapECMC, the combination of collective swaps and chain moves provides the fastest algorithm with a speed up increasing with ϕ and reaching 40.

By constrast, the four algorithms employing particle swaps sample the Boltzmann distribution much faster than MMC and ECMC and only become inefficient near $\phi \approx 0.88$, see Fig. 2. All algorithms thus display a dramatic speed up compared to MMC and ECMC. Using Swap as a reference, we again observe that the introduction of translational chains in SwapECMC provides a modest acceleration over conventional Swap of about 5 at $\phi = 0.77$, decreasing to about 2 at the largest density (see Fig. 4). Therefore, coupling Swap to ECMC is not very helpful. The situation is more favorable when collective swap moves are introduced, as the speedup offered by the irreversibility in cSwap now grows with density, as demonstrated in Fig. 4, to reach a factor about 10 near $\phi = 0.88$ over Swap. These results suggest that it is useful to combine cSwap and ECMC into cSwapECMC, where both translational and diameter moves are now collective and irreversible. Getting the best of both types of moves, cSwapECMC now offers a comfortable speed up over Swap that increases from 10 to about 40 at the largest packing fraction studied, clearly outperforming the Swap Monte Carlo algorithm.

An interesting avenue for our algorithms is the production of jammed disk packings, which are typically produced using specific nonequilibrium compression protocols [46,47]. Using conventional MMC for compressions, the jamming packing fraction ϕ_J can be reached using NPT Monte Carlo. The simplest protocol starts from an equilibrium hard disk configuration at ϕ_{init}, before suddenly turning the pressure to infinity [48]. At long times, the packing fraction saturates to a value ϕ_J, which is an increasing function of ϕ_{init} [49]. This is confirmed in Fig. 5, where the range $\phi_J \sim 0.855$–0.895 is covered. Very similar results are obtained using ECMC during compressions, see Fig. 5. Note that the preparation of equilibrium configurations for $\phi_{\mathrm{init}} > 0.79$ requires particles swaps [50], which are no longer used during compressions. Interestingly, introducing swaps during compressions from the same range of initial conditions leads to jamming densities that are considerably larger, $\phi_J \approx 0.904$–0.906 (Fig. 5). At the time of writing, such large packing fractions have only been obtained using gradient descent algorithms simultaneously optimizing diameters and positions to more efficiently pack the particles, followed by geometric triangulation methods [23]. That similar performances can be reached using cSwap suggests that these nonequilibrium algorithms in fact explore pathways similar to the ones allowed by swap moves. In addition, the very weak dependence of ϕ_J on ϕ_{init} rationalizes the surprising efficiency of augmented gradient-descent algorithms. A major advantage of cSwap is that the particle size distribution is strictly conserved, rather than annealed, during the compression.

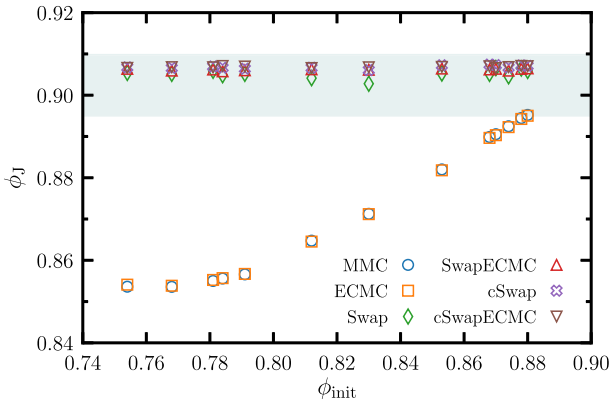

FIG. 5. Jamming packing fractions ϕ_J obtained after nonequilibrium compressions using different Monte Carlo algorithms, starting from fluid configurations equilibrated at $\phi_{\rm init}$. The four swap algorithms reach very large ϕ_J, nearly independently of $\phi_{\rm init}$. The light blue band covers the range of densities obtained using augmented gradient-descent techniques [23].

Using swap and event-chain Monte Carlo as stepping stones, we demonstrate that simple Monte Carlo algorithms with increasing efficiency can be devised, that provide a set of improved computational tools to more efficiently equilibrate deep glassy states, prepare more stable configurations, with lower configurational entropy, thus approaching closer the putative Kauzmann transition. In order to become new standards, the cSwap algorithm and its derivatives proposed here need to be pushed in several directions. A first encouraging result is the successful scaling of their performances with system size, see Ref. [37], in line with results for ECMC and Swap. A less obvious direction is the application to three dimensions, which is the subject of ongoing efforts, again with encouraging preliminary results. A third direction concerns the application to glass formers with soft potentials. Swap performances do not decrease with continuous potentials [13], and some extensions of ECMC to continuous potentials were successful [29,51]. Future work should develop extensions of cSwap for glass formers with continuous potentials to extend the range of applicability of irreversible Monte Carlo methods in the field of supercooled liquids. All these perspectives directly follow from our work; they should help the development of efficient, versatile, and simple to implement sampling methods for disordered systems with a complex free energy landscape.

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