Damage spreading and coupling in Markov chains

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In this paper, we relate the coupling of Markov chains, at the basis of perfect sampling methods, with damage spreading, which captures the chaotic nature of stochastic dynamics. For two-dimensional spin glasses and hard spheres we point out that the obstacle to the application of perfect-sampling schemes is posed by damage spreading rather than by the survey problem of the entire configuration space. We find dynamical damage-spreading transitions deeply inside the paramagnetic and liquid phases, and we show that critical values of the transition temperatures and densities depend on the coupling scheme. We discuss our findings in the light of a classic proof that for arbitrary Monte Carlo algorithms damage spreading can be avoided through non-Markovian coupling schemes.

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I. INTRODUCTION

Chaos manifests itself in Hamiltonian dynamical systems when any two nearby initial configurations drift apart with time. Chaos can also be defined for cellular automata and for Markov chain algorithms. In these dynamical systems, following Kauffman [1], the drifting-apart of configurations is termed "damage spreading". In contrast, for "regular" dynamics, two nearby initial configurations become identical after a finite time, and remain indistinguishable from then on. For Markov-chain Monte Carlo algorithms, the closely related case where the entire space of initial configurations becomes identical is termed "coupling". Once it has coupled, the Markov chain has lost all correlations with the initial configuration. The coupling of Markov chains has risen to great prominence when Propp and Wilson used it for a perfect sampling method for Markov chains named "Coupling From The Past" (CFTP)[2]. When applicable, this method overcomes the problem of estimating the correlation time of a Monte Carlo calculation. In the present article, we shall discuss the fruitful connection between damage spreading and coupling [3].

In systems with N elements (spins, hard spheres, etc), the configuration space generally grows exponentially with N, and CFTP thus faces two distinct challenges. First, it must *survey* the entire configuration space in order to prove coupling. Second, it must avoid damage spreading which would cause the coupling time to *explode*: it would become much larger than the correlation time as any two configurations have a very small probability for finding each other in a large space.

The surveying problem is avoided in systems with a special property called "partial order", as for example the ferromagnetic Ising model under heat-bath dynamics[2, 4]. For more general systems (without partial order, but with local update algorithms), such as spin glasses and hard spheres, a recent "patch" algorithm inspired by numerical block scaling ideas [3, 5] allows us to rigorously follow a superset of all initial conditions until it couples. This algorithm generates only modest overheads of memory and CPU time [3]. It was found that the coupling can be established after a time evolution very close to the coupling time.

The second problem, the explosion of the coupling time related to damage spreading, poses the veritable obstacle to the application of CFTP ideas. Damage spreading has been studied in many physical systems, in particular spin glasses [6]. In several spin glass models with heat-bath dynamics, it is now well established that a dynamical damage-spreading transition occurs at a critical temperature, $\beta_{\rm ds}$, located in the paramagnetic phase[7]: the dynamic is regular at temperatures higher than $1/\beta_{\rm ds}$ and chaotic at lower temperatures. Even for the two-dimensional $\pm J$ Ising spin glass, which has a thermodynamic phase transition at $T = 0$ [8–11], the transition to chaos takes place at finite temperature [7]. We study in this paper the damage spreading of spin glasses and hard spheres for different algorithms.

II. RANDOM WALKS IN HIGH DIMENSIONS

Before analyzing two-dimensional spin glasses and hard spheres, we illustrate coupling and damage spreading in a simple Markov chain algorithm that can be interpreted either as a random walk in an N-dimensional hypercubic lattice, as the dynamics of N distinguishable non-interacting particles in a one-dimensional lattice of length L, or as N non-interacting Potts spins with L states. For the random walk (see Fig. 1), each N-dimensional lattice site $i = \{i_0, \dots, i_{N-1}\}$ is described by integers $i_k \in \{0, \dots, L-1\}$ with periodic boundary conditions in the i_k . The particle can hop from site i to one of i's nearest neighbors in direction k, $j = i \pm \delta_k$, with $\delta_k = \{0, \dots, 1, 0, \dots\}$ (periodic boundary conditions are again understood). The probability for moving from i to

j is

$$p(i \to j) = \begin{cases} \frac{1}{3N} & \text{for } j = i \pm \delta_k \\ \frac{1}{3} & \text{for } j = i \\ 0 & \text{otherwise} \end{cases} . \qquad (1)$$

The simulation thus samples at each time step one dimension, k, among the N available ones (it moves in "x", or "y" or "z", etc). In dimension k, it then hops with probabilities 1/3 each to the left or to the right, or remains on the same site. Equation (1) also describes N distinguishable non-interacting particles on a one-dimensional lattice of length L, again with periodic boundary conditions: At time t, a randomly chosen particle k hops to the left or to the right, or it remains on the same site, each with probability 1/3, as above.

A two-configuration coupling is a random process $\tilde{p}(i \to j, i' \to j')$ for the joint evolution of two random walks such that integrating over one of them yields the original random walk of Eq. (1) for the other. After they meet, the two configurations evolve in the same way. The simplest choice for a coupling is the product ansatz,

$$\tilde{p}(i \to j, i' \to j') = \begin{cases} p(i \to j)p(i' \to j') & \text{if } i \neq i' \\ p(i \to j) & \text{if } i = i',\ j = j' \\ 0 & \text{otherwise} \end{cases} , \qquad (2)$$

where the two random walks evolve independently from each other if they are on different sites i and i', but stay together once they have met ($j = j'$ if $i = i'$). To implement this coupling for any number of configurations, one samples at each time step independent random moves at each site, so that particles on the same site experience the same randomness. In the above-mentioned representation of particles on the one-dimensional line, we consider the coupling of two N-particle systems, again described by Eq. (2), as the independent evolution, at time t, of the L^N possible configurations of the system. Naturally, the coupling time scales as L^N whereas the correlation time (in sweeps) behaves as L^2.

An alternative coupling consists in sampling, at time t, one dimension k common to all random walks. The two-configurations coupling scheme is then

$$\tilde{p}(i_k \to j_k, i'_k \to j'_k) = \begin{cases} p(i_k \to j_k)p(i'_k \to j'_k) & \text{if } i_k \neq i'_k \\ p(i_k \to j_k) & \text{if } i_k = i'_k, j_k = j'_k \\ 0 & \text{otherwise} \end{cases} \qquad (3)$$

so that two configurations i and j with $i_k = i'_k$ will preserve this common coordinate ($j_k = j'_k$). In the representation of N particles on a one-dimensional lattice, the same particle k is selected for each configuration, and for two different configurations, the particles labelled k stay together once they have met on the same site. The dynamics is then regular and the coupling time is $\tau_{\rm coup}/N \sim a \log N$ (see Fig. 2). The logarithmic behavior is explained by the fact that particles move independently from each other, the coupling time for the entire system is thus the maximum of the N coupling times for each particle.

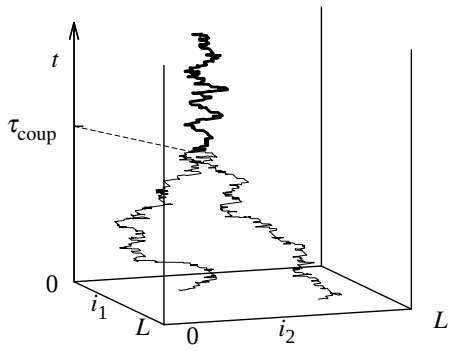

FIG. 1: Coupling of random walks in a periodic N-dimensional hypercubic lattice of length L. After the time $\tau_{\rm coup}$, the two random walks evolve identically. The chaotic coupling of Eq. (2) is shown. For the regular coupling of Eq. (3), the displacement at time t is in the same direction k, and it is a function of i_k only.

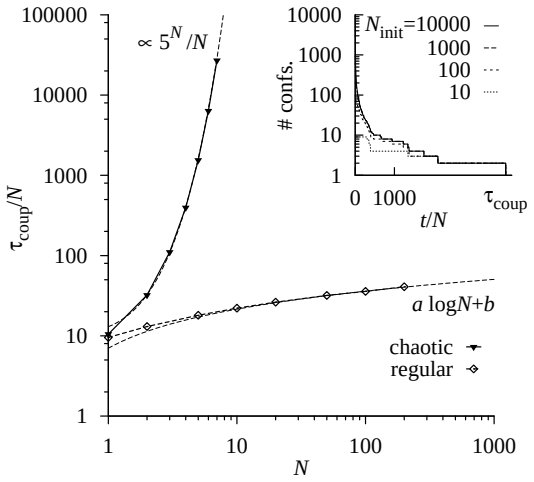

FIG. 2: Chaotic and regular couplings for the random walk in a N-dimensional hypercubic lattice of length $L = 5$ (see Eqs (2) and (3), respectively). The random process for a single random walk is defined by Eq. (1) in both cases. *Inset*: Number of configurations *vs.* time as a function of the number $N_{\rm init}$ of initial configurations, for $N = 6$, $L = 5$ for the chaotic coupling. The same realization of the coupling of Eq. (3) is used for all runs.

In conclusion, we see that the same N-dimensional random walk of Eq. (1), with a correlation time of order L^2, allows two very different coupling, chaotic and regular. In spin glasses and hard spheres, these regimes are realized for the same coupling at different temperatures.

III. SPIN GLASS

The random walk considered in Section II can also be considered as an L-state Potts model at infinite temperature evolving under heat-bath dynamics.

The product ansatz of Eq. (2) would correspond to the independent evolution of the spin configurations, and it is clearly chaotic. With the coupling of Eq. (3), in contrast, all spins evolve and couple independently at $\beta = 0$, and the global coupling time is again the maximum of the coupling times of the individual spins. The Monte Carlo dynamics is thus regular, and the diagram of Fig. 2 carries over to the general case with $L \geq 2$. At finite temperatures β, the energy of a spin configuration is given by

$$E = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j .$$

We first consider heat-bath dynamics, which consists in choosing one spin s_k and updating it with probabilities

$$\pi(s_k = \pm 1) = \frac{1}{1 + \exp(\mp 2 h_k \beta)}, \tag{4}$$

where the field on site k is given by $h_k = \sum_l J_{kl} s_l$. The coupling is defined by the use of the same random numbers for each configurations.

For the two-dimensional ferromagnetic Ising model (all $J_{ij} = 1, L = 2$), the dynamics remains regular at all temperatures. Below the Curie temperature, $\tau_{\rm coup}$ is very large, but so is the correlation time $\tau_{\rm corr}$, and the partial order implies that the complexity of $\tau_{\rm coup}/\tau_{\rm corr} \leq O(\log N)$ [2]. For the two-dimensional $\pm J$ Ising spin glass, the quenched random interactions satisfy $J_{ij} = J_{ji} = \pm 1$ with equal probability. Although this model is paramagnetic for all finite temperatures, Campbell and de Arcangelis[7] found a damage-spreading transition for the heat-bath algorithm at $\beta_{\rm ds} \simeq 0.59$. In previous work [3, 5], we succeeded in coupling large systems down to this temperature using the patch algorithm. We showed that the patch algorithm's upper bound on the coupling times agrees well with the lower bound obtained from a partial-coupling approach, where one checks coupling for a finite number $N_{\rm init}$ of random initial conditions rather than for the entire configuration space ($N_{\rm init} = 2^N$). As shown in the inset of Fig. 3, for one realization of the random process, the coupling time does not vary if $N_{\rm init} \gtrsim 10$, and the coupling time for $N_{\rm init} = 1000$ equals the coupling time for the entire configuration space.

In the main graph of Fig. 3, we show the coupling time $\tau_{\rm coup}/N$ as a function of N at constant temperature. A dynamical phase transition is again seen at the damage-spreading temperature $\beta_{\rm ds} = 0.58$. In the chaotic phase, $\tau_{\rm coup}/N$ grows exponentially with N, but only logarithmically in the regular phase. The dynamical phase transition in this model (without a spin glass phase at finite β), although not mathematically proven, appears firmly established. It is without influence on

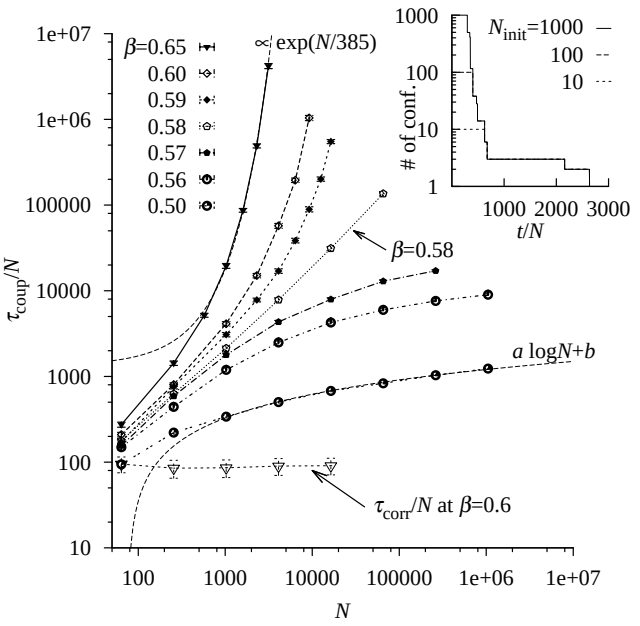

FIG. 3: Disorder-averaged coupling time for the heat-bath algorithm of the two-dimensional $\pm J$ Ising spin glass. Inset: Saturation phenomenon for $N = 64^2$ spins at $\beta = 0.56$.

single-particle properties. To illustrate this point, we verify that the correlation time $\tau_{\rm corr}/N$, computed with the autocorrelation function

$$q(t) = \frac{1}{N} \sum_{i=0}^{N} \langle s_i(0) s_i(t) \rangle , \tag{5}$$

remains constant in the chaotic phase and only $\tau_{\rm coup}/\tau_{\rm corr}$ diverges with $N \to \infty$.

After the heat-bath algorithm, we now discuss the Metropolis algorithm, where individual spins s_k are flipped with a probability depending on their local field. In the standard implementation, spin flips are accepted with a probability equal to 1 at infinite temperature. To allow coupling at any β we use

$$p(s_k \to -s_k) = \frac{2}{3} \min(1, \exp(-2\beta s_k h)). \tag{6}$$

At each step the same spin k is updated for all copies of the system. For this dynamics, several coupling schemes can be set up. If the same random number γ is used for each configuration, the coupling does not take place, as two opposite configurations will always stay opposite. We adapt the regular coupling of Eq. (3) and use two independent random numbers, γ_1 for "up" spins and γ_2 for "down" spins. The coupling time has then the same qualitative behavior as in Fig. 3, logarithmic at high temperatures and exponential at low temperatures, but with a critical temperature $\beta_{\rm ds} = 0.33$. The Metropolis algorithm, with this coupling scheme, has thus a higher dynamical critical temperature than the heat-bath algorithm, with which it shares all the qualitative features.

This confirms that the dynamic damage-spreading transition is algorithm dependent. One may also choose the random numbers in the Metropolis algorithm using γ for $s_k = 1$ and $1-\gamma$ for $s_k = -1$. This scheme correlates opposite spins better and the critical temperature is found to be $\beta_{\rm ds} = 0.52$. This results shows that, like for the random walk in Section II, the same Markov-chain allows for qualitatively different coupling.

IV. HARD SPHERES

After spin glasses, we now consider another key model in statistical physics, namely hard spheres. This model's Hamiltonian dynamics, realized in the event-driven molecular dynamics algorithm [4, 12], is chaotic for all densities and for all N [4, 13, 14]. In this section, we will present several Monte Carlo algorithms for hard spheres, which allow for coupling of the entire configuration space. Two of the algorithms remain regular below a finite critical packing fraction, $\eta_{\rm ds}$, in the limit $N \to \infty$. In the following discussion we are not concerned with algorithmic efficiency of the implementation, and only concentrate on the coupling properties.

A. Birth-and-death algorithm

In the grand-canonical birth-and-death Monte Carlo algorithm, particles are placed inside the box at random positions $\mathbf{x} = (x_k, y_k)$ at rate λ if no overlaps with previously placed disks are generated. The life time of each disk is sampled from an exponential distribution with rate 1. One realization of the algorithm is represented in the diagram of Fig. 4. The mean number $\langle N \rangle$ of particles in this system is controlled by the activity λ.

This model's state space is infinite, but the survey of all possible initial conditions is nevertheless feasible [5, 15]. For any realization of the algorithm, the possible configurations at time t are a subset of the finite set produced from a horizontal cut in the diagram of Fig. 4. The patch algorithm again yields sharp upper bounds for $\tau_{\rm coup}$ [5]. Surprisingly, this algorithm for hard disks remains regular below a finite density $\eta_{\rm ds}$ in the limit $N \to \infty$ [15, 16].

1. *Damage spreading for the birth-death algorithm*

We again study damage spreading in this model by applying the same Monte Carlo dynamics (same choice of $\mathbf{x}_i, t_i, \tau_i$) to $N_{\rm init}$ random hard-sphere initial conditions at time $t = 0$ with life times sampled from an exponential distribution. The data shown in Fig. 5 again indicate a dynamical phase transition between the regular regime at packing fractions $\eta < \eta_{\rm ds} \simeq 0.29$ and the chaotic regime above $\eta_{\rm ds}$. This density corresponds to the limiting density found with the patch algorithm [5].

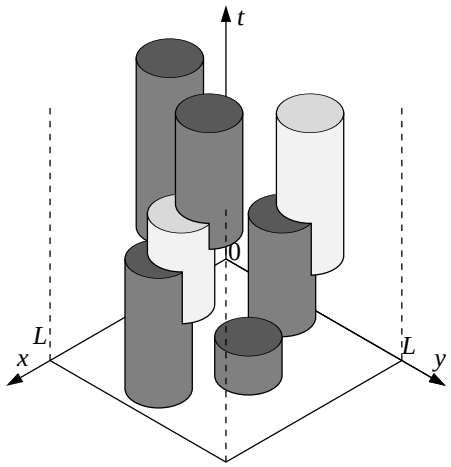

FIG. 4: Grand-canonical birth-and-death algorithm for hard disks. Disk i is placed at time t_i and at position $\mathbf{x}_i = (x_i, y_i)$ if no overlap is generated with previously placed disks. It disappears at time $t_i + \tau_i$. The configuration space of this system is infinite, yet the possible configurations at time t are a subset of the finite set produced from a horizontal cut in this diagram.

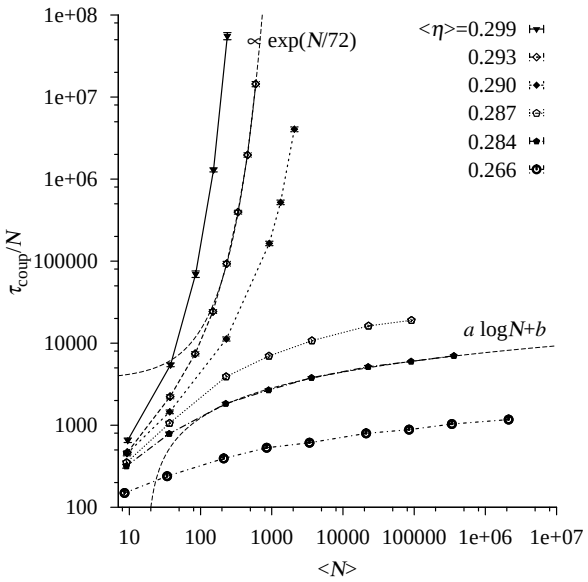

FIG. 5: Coupling time of the birth-and-death algorithm of Fig. 4 for two-dimensional hard spheres (estimated with $N_{\rm init} = 100$).

B. "Labelled displacement" algorithm

A canonical version of the birth-and-death algorithm is the "labelled displacement" algorithm where, at times $t = 0, 1, 2, \ldots$, a randomly chosen particle k is moved to a random position $\mathbf{x}_k$, if this move creates no overlaps. We see clear evidence of a dynamical phase transition at a critical density $\eta_{\rm ds} \simeq 0.13$ (see Fig. 6), which is smaller

than for the closely related birth-and-death algorithm.

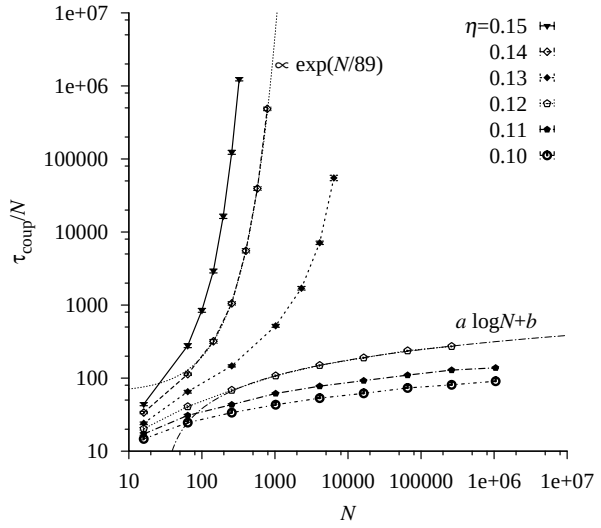

FIG. 6: Coupling time for the labelled displacement algorithm. The dynamical transition to chaos occurs at a lower density than for the birth-and-death algorithm of Fig. 5.

C. Spot algorithm

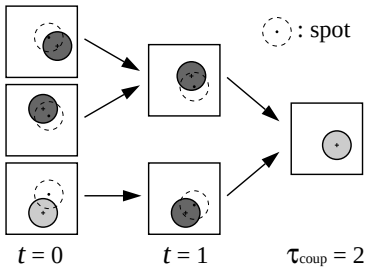

FIG. 7: Spot algorithm for hard spheres: The randomly chosen spot position defines the attempted move of a disk inside the spot. The spot radius satisfies $\sigma_{\rm spot} \leq \sigma$, and at most one disk is moved at time t. An example with $N = 1$ and $\sigma_{\rm spot} = \sigma$ is shown.

We finally study the coupling for a Markov-chain similar to the Metropolis algorithm: the spot algorithm. The Metropolis algorithm for N hard spheres consists in moving, at time t, a particle k by a random vector $\boldsymbol{\delta} = (\delta_x, \delta_y)$. As the configuration space is continuous, the coupling probability is zero if one uses a naive coupling scheme. The following spot algorithm is more successful (although we will show its coupling is chaotic at all densities): at time t, it places a spot, a disk-shaped region with radius $\sigma_{\rm spot} \leq \sigma$, at a random position $\mathbf{x}_s$. The spot contains at most one disk center, and the move consists in placing this disk at $\mathbf{x}_s$, if this creates no overlap with other particles (See Fig. 7). The spot algorithm satisfies detailed balance, and it generates the same moves as the Metropolis algorithm. Moreover, as illustrated in Fig. 7, it succeeds in coupling. However, as shown in Fig. 8, the coupling time of the spot algorithm is an exponential function of N for all densities: the coupling is always chaotic.

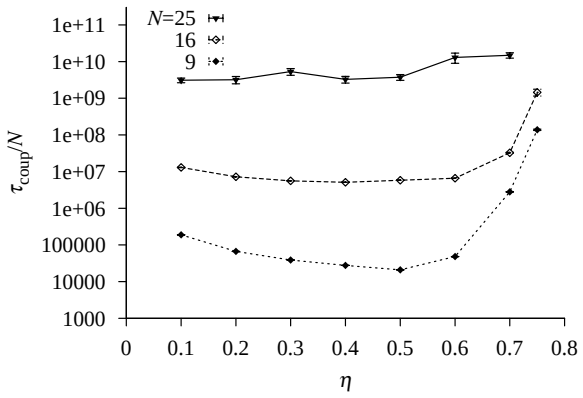

FIG. 8: Coupling time $\tau_{\rm corr}$ of the spot algorithm for N hard disks (estimated with $N_{\rm init} = 100$) as a function of packing fraction *eta*. For all η, the coupling time is exponential in N, and we conjecture the coupling to be chaotic. The inset shows the coupling times for the spot algorithm in one dimension as a function of N at constant η.

V. CONCLUSION

In conclusion, we have in this paper studied the relationship between the coupling of Markov chains, which is of critical importance for the subject of perfect sampling, and damage spreading, which exposes the chaotic nature of the Monte Carlo dynamics.

For the two-dimensional $\pm J$ Ising spin glass, which lacks an equilibrium phase transition at finite temperatures, we confirm the existence of a dynamical phase transition at $\beta_{\rm ds} \simeq 0.58$ [7] for the heat-bath algorithm. For lower temperatures the coupling time explodes. The Metropolis algorithm has the same damage spreading behavior but with higher critical temperatures: $\beta_{\rm ds} \simeq 0.33$ or $\beta_{\rm ds} \simeq 0.52$ for two simple coupling schemes. All damage-spreading transitions for this system are deeply inside the paramagnetic phase.

For the two-dimensional hard-sphere system, we analyzed three local Monte Carlo algorithms, the birth-and-death algorithm, inspired from Poisson point processes, its canonical version (the "labelled displacement" algorithm), and the spot algorithm, a straightforward adaptation of the Metropolis algorithm. The first algorithm shows a regular regime only for packing densities below $\eta_{\rm ds} \simeq 0.29$, the coupling time was then of the same order

of magnitude as the correlation time. The canonical version of the birth-and-death algorithm had a critical density of $\eta_{\rm ds} \simeq 0.13$. These transition densities are again deeply in the liquid phase.

Both for spin glasses and for hard spheres, the rigorous survey of the configuration space[3] remains feasible for all temperatures and densities. The application of perfect sampling methods to these challenging problems is thus not so much limited by the surveying problem, as the patch algorithm allows to track the evolution of the entire configuration space, but more by damage spreading, the underlying chaotic nature of the Monte Carlo dynamics.

In this context, it is of great interest that Griffeath [17] has constructed a coupling that always remains regular: It realizes the coupling at time t and at position X_t of two Markov chains that have started at time $t = 0$ at configurations X_0 and X_0' with the minimum of the probabilities to go from X_0 or from X_t' to X_t. Griffeath's coupling is non-Markovian and very difficult to construct in practice, but it may point the way to couplings that remain regular at lower temperatures and higher densities than the naive couplings we discussed in this paper.

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[1] S. Kauffman, J. Theor. Biol. **22**, 437 (1969).
[2] J. Propp and D. Wilson, Random Struct. Algorithms **9**, 223 (1996).
[3] C. Chanal and W. Krauth, Phys. Rev. Lett. **100**, 060601 (2008), 0707.4117.
[4] W. Krauth, Statistical mechanics: algorithms and computations (Oxford University Press, 2006).
[5] C. Chanal and W. Krauth, Phys. Rev. E **81**, 016705 (2010), 0910.1530.
[6] B. Derrida and G. Weisbuch, Europhys. Lett. **4**, 657 (1987).
[7] I. A. Campbell and L. de Arcangelis, Physica A **178**, 29 (1991).
[8] I. Morgenstern and K. Binder, Phys. Rev. Lett. **43**, 1615 (1979).
[9] W. L. McMillan, Phys. Rev. B **28**, 5216 (1983).
[10] R. R. P. Singh and S. Chakravarty, Phys. Rev. Lett. **57**, 245 (1986).
[11] R. N. Bhatt and A. P. Young, Phys. Rev. B **37**, 5606 (1988).
[12] B. J. Alder and T. E. Wainwright, J. Chem. Phys. **27**, 1208 (1957).
[13] Y. Sinai, Russ. Math. Surv. **25**, 137 (1970).
[14] N. Simányi, Invent. Math. **154**, 123 (2003).
[15] D. Wilson, Random Struct. Algorithms **16**, 85 (2000).
[16] W. Kendall and J. Moller, Adv. in Appl. Probab. **32**, 844 (2000).
[17] D. Griffeath, Probab. Theory Relat. Field **31**, 95 (1975).