Addendum to "Event-chain Monte Carlo algorithms for hard-sphere systems"

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Etienne P. Bernard*
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Werner Krauth†
Laboratoire de Physique Statistique, Ecole Normale Supérieure, UPMC, CNRS, 24 rue Lhomond, 75231 Paris Cedex 05, France

(Received 29 November 2011; revised manuscript received 14 May 2012; published 6 July 2012)

We extend the event-chain Monte Carlo algorithm from hard-sphere interactions to general potentials. This event-driven Monte Carlo algorithm is nonlocal and rejection free and allows for the breaking of detailed balance. The algorithm uses a discretized potential, but its running speed is asymptotically independent of the discretization. We apply the algorithm to two-dimensional soft spheres and discuss its possible implementation directly in the continuum limit.

DOI: 10.1103/PhysRevE.86.017701 PACS number(s): 05.10.Ln, 02.70.Ns, 02.70.Tt, 64.60.De

The event-chain algorithm [1], a nonlocal, rejection-free Markov chain algorithm for hard-sphere systems, has proved considerably faster than the local Monte Carlo algorithm. It has allowed us to show that two-dimensional melting in hard disks proceeds via a first-order liquid-hexatic transition [2].

In the present addendum to Ref. [1], we generalize the event-chain algorithm to the case of general potentials, extending the scope of the original method. As for event-driven molecular dynamics (MD), we discretize the potential (here on an energy scale δV), but unlike the MD algorithm [3,4], simulations at arbitrary small δV are feasible.

In the event-chain algorithm [1], a randomly chosen disk is moved in a straight line by a distance ℓ if this generates no overlap for all $\ell' \leqslant \ell$ or else until it hits another particle i'. The latter particle, i', then moves for the remainder of the distance ℓ or, again, until it hits yet another particle and so on (see Fig. 1). The event-chain move is microreversible, and it satisfies detailed balance if all the displacements are in the same direction. For hard disks, it is about 40 times faster than the local Monte Carlo algorithm [5], and it compares favorably with the MD method [6].

In the event-driven Monte Carlo algorithm, we consider a discretized potential $V(r)$, with discontinuities such that $V(r)$ and thus the total potential energy are multiples of a given energy step δV. From an initial configuration of energy E, a randomly chosen particle i is moved in a straight line until the total displacement, *at energy E only*, equals a fixed value ℓ or else until it "hits" another particle i'. A hit (event) occurs when further motion of particle i would increase the energy beyond E (see Fig. 2), and another particle, i', is moved instead. In a continuous system, the choice of i' is unique. The particle i' then moves for the remainder of the distance ℓ or, again, until it hits yet another particle and so on (see Fig. 2). In the absence of boundary effects, the move is guaranteed to terminate. It is again rejection free and microreversible. As in the event-chain algorithm for hard spheres, detailed balance may be broken, and the algorithm can be run with moves, say, in the $+x$ and $+y$ directions only.

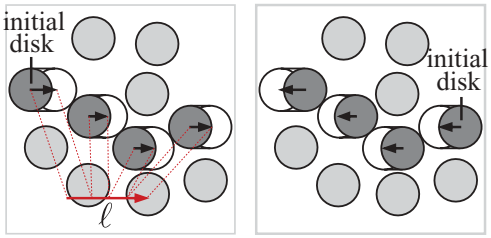

FIG. 1. (Color online) Event-chain algorithm for hard disks [1]. (left) Collective move, with the total displacement ℓ as a fixed parameter of the algorithm. The move is never rejected. (right) Return move, demonstrating microreversibility.

The event-driven Monte Carlo algorithm can be implemented by computing the intersection points of the potential discontinuities with the trajectory of particle i. One recovers $E(x)$ by adding up the signs in the sorted list of the intersections. This is illustrated in Fig. 2 for a simple potential. We note that the value of parameter ℓ is not crucial as long as the number n of particles displaced within one chain satisfies $1 \ll n \ll N$.

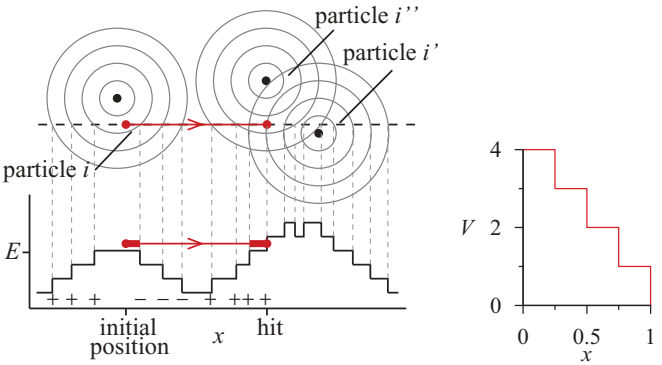

FIG. 2. (Color online) Event-driven Monte Carlo displacement. (left) Particle i moves from its initial configuration until its collision event with particle i' (concentric circles around particles represent the steps of the potential defined on the right). Only displacements at energy E are discounted from ℓ. (right) Discretized $1 - r$ potential used in this example.

*etienne.bernard@mit.edu
†werner.krauth@ens.fr

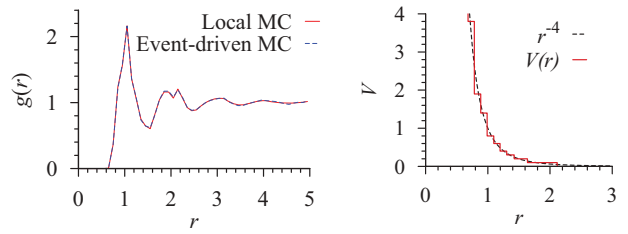

FIG. 3. (Color online) (left) Pair-correlation function $g(r)$ computed with the local and the event-driven Monte Carlo algorithms ($N = 64^2$, $N/V = 1$, $kT = 0.3$). Data agree, which shows the correctness of the algorithm. (right) Discretization of the r^{-4} potential used.

In Fig. 3, we consider particles interacting with the soft-sphere potential $V(r) = 1/r^4$. $V(r)$ is discretized with an energy step of $\delta V = 0.1$ at large distances and by multiples of δV at short distances. The algorithm described so far, which samples the constant-potential-energy ensemble is complemented with local Metropolis moves in order to sample the canonical ensemble. To demonstrate the correctness of the algorithm, we compare its pair-correlation function for a system with $N = 64^2$ particles with the output of a standard local Monte Carlo algorithm. With this simple implementation, we reach $\sim 2 \times 10^9$ displacements per hour on a 3 GHz workstation [7].

We now test the efficiency of the algorithm for a family of soft-sphere potentials: $V(r) = 1/r^4$, $1/r^8$, and $1/r^{16}$, discretized with an energy step of $\delta V = 0.1$, 0.1, and 0.08, respectively. We use the same protocol as in the hard-sphere case [1]: the time unit is a displacement of a particle, and we compare the autocorrelation functions of the bond-orientational order parameter Ψ obtained for the event-driven algorithm and an optimized local Monte Carlo algorithm [8]. We find a speedup of at least 5 for all potentials and parameters (see Fig. 4), similar to what was found for the hard-sphere system in the dense-liquid region [1]. Near the liquid-solid transition, we again notice speedups of $\sim$10 for systems of size $N = 32^2$ with $V(r) = 1/r^8$ and $1/r^{16}$ [9] (see Fig. 4), which are slightly lower than in the hard-sphere case ($\sim$15

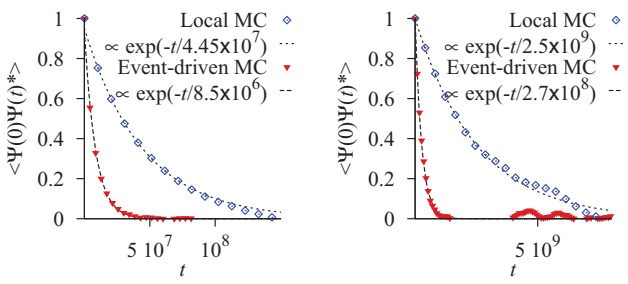

FIG. 4. (Color online) Autocorrelation function of Ψ of the event-driven and local Monte Carlo algorithms for $N = 32^2$ (cf. Ref. [1]). (left) $V(r) = 1/r^4$, $N/V = 1$, and $kT = 0.11$ (dense liquid). The speedup is $\sim$5. (right) $V(r) = 1/r^{16}$, $kT = 1$, and $N/V = 0.965$ (at the liquid-solid transition). The speedup is $\sim$10. Time is measured in displaced particles. The effective speedup is $\sim$1.5 times higher with our implementations.

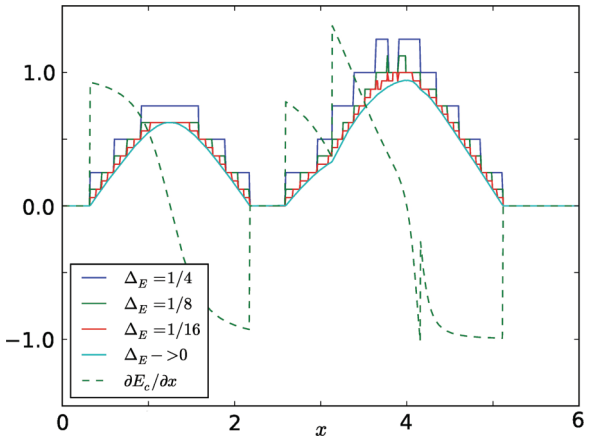

FIG. 5. (Color online) Energy $E(x)$ for the configuration of Fig. 2, for different discretizations of the $1 - r$ potential, and in the continuum limit. The derivative $\partial E_{\rm cont}/\partial x$ is piecewise monotonously decreasing.

for the $N = 32^2$ system). We expect the relative speed of the algorithm to increase further with system size. The effective speedup (in CPU time) is higher than the time measured in the number of collisions. Our implementation of the event-driven algorithm displaces each particle 1.5 times faster than the local Monte Carlo algorithm.

In the implementation suggested in Fig. 2, the number of steps between events scales $\propto 1/\delta V$, and the algorithm becomes very slow in the limit $\delta V \to 0$. Unlike for event-driven molecular dynamics [3], this difficulty can be overcome, and the speed of the algorithm remains constant for $\delta V \to 0$. The algorithm is straightforward for a convex potential as, for example, the continuum limit of the potential in Fig. 2:

$$V_{\rm cont}(r) = \begin{cases} 0 & \text{if } r > 1, \\ 1 - r & \text{otherwise,} \end{cases}$$

for which $E(x)$ is continuous and piecewise C^∞ while $\partial E/\partial x$ is piecewise monotonously decreasing (see Fig. 5). The root $E_{\rm cont}(x_{\rm root}) = E$ of the continuous potential is uniquely determined *via* a decision tree in subsequent C^∞ intervals of $E(x)$. (A more complicated decision tree exists for nonconvex potentials, so that the above root can always be computed exactly [10].) For finite δV, one must only identify the discontinuity steps of the potential in the interval $x_{\rm root} \pm \text{const}[\partial E/\partial x(x_{\rm root})]^{-1}$. We have implemented the algorithm for very large values of $1/\delta V$ (with $\ell \propto \delta V$) and achieved constant scaling of the algorithm [7].

The event-driven Monte Carlo algorithm can be implemented for arbitrarily small δV and does not slow down then (cf. Ref. [7], where $\delta V = 10^{-2}, \ldots, 10^{-6}$ are considered). The algorithm can furthermore be formulated in the $\delta V \to 0$ limit: To do so, it is necessary to sample the value of δV^{-1}, in between events, from a distribution with a very large mean. The collision process in Fig. 2, e.g., becomes probabilistic: For some values of δV, particle i' moves after the collision, whereas for others, it is particle i''. The probabilities for hitting i and i' depend on the positions of the two particles. The event (hit) in Fig. 2 is readily analyzed because only two particles are

involved [11]. In general, an event may depend on the positions of a larger number of particles and become quite intricate. We have not succeeded in establishing stochastic collision rules for arbitrary complex events.

In conclusion, in this addendum to Ref. [1], we have generalized the successful event-chain algorithm from hard spheres to general potentials and provided details on its implementation. This algorithm is an alternative to the local Monte Carlo algorithm [5]. We have demonstrated definite speedups for a family of discretized soft-sphere potentials and expect them to improve with system size. Moreover, arbitrarily small discretization steps can be handled efficiently, which is not the case in the event-driven MD [3,4,6].

Note added in proof. We note the existence of simultaneous work [12] on a related rejection-free algorithm for general potentials.

We thank M. N. Bannerman for helpful discussions.

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[7] See http://www.lps.ens.fr/∼krauth/index.php/Bernard_Krauth_b_2011 for a naive implementation of the algorithm, as well as an implementation with constant CPU time in the limit $\delta V \to 0$.
[8] Our local Monte Carlo algorithm displaces particles uniformly in a square of a given size δ; δ is optimized for speed of convergence (we then have ∼60–70% of rejections).
[9] For $V(r) = 1/r^4$, the correlation time at the transition is too large for us to obtain statistically relevant results.
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