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1995 J. Phys. A: Math. Gen. 28 L597

(http://iopscience.iop.org/0305-4470/28/23/001)

J. Phys. A: Math. Gen. 28 (1995) L597–L601. Printed in the UK

LETTER TO THE EDITOR

Cluster algorithm for hard spheres and related systems

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Received 13 September 1995

Abstract. In this paper, we present a cluster algorithm for the simulation of hard spheres and related systems. In this algorithm, a copy of the configuration is rotated with respect to a randomly chosen pivot point. The two systems are then superposed, and clusters of overlapping spheres in the joint system are isolated. Each of these clusters can be 'flipped' independently, a process which generates non-local moves in the original configuration. A generalization of this algorithm (which works perfectly well at small density) can be made to work successfully at densities around the solid–liquid transition point in the two-dimensional hard-sphere system.

Since the 1987 paper by Swendsen and Wang [1] (and the subsequent paper of Wolff [2]), the simulation of Ising or XY-type systems close to the critical point has been much simplified: just as for the physical system, conventional Monte Carlo algorithms (for a review cf [3]) suffer from critical slowing down, but the new algorithms overcome this problem and allow the calculation of *thermodynamic* quantities with great ease.

One of the long-standing problems in classical statistical physics is the hard-sphere liquid [4]. In two dimensions, the transition between the liquid and the solid order in the hard-sphere liquid has been the subject of unabating interest [5]. There are several competing theoretical scenarios for the transition, and Monte Carlo work has been going on for more than 30 years [6] (for a review cf [7]). However, the conventional local-move Monte Carlo simulations are greatly affected by the slowing down of the simulation around the transition. At present, the maximum size of the simulation box, which can be unequivocally thermalized, contains only of the order of 1000 particles [8]. Much larger simulations have been undertaken [9, 10] and sophisticated data analysis has been performed [10]. However, due to the fact that the probability distribution has not yet converged to its equilibrium value, these simulations are biased in a way which is very difficult to assess.

In this paper, we present a cluster algorithm, which is applicable to the hard sphere system in any dimension, and which is easily generalized to incorporate an additional potential. The main idea of the algorithm is to rotate a copy of the 'current' configuration, and to superpose this rotated copy with the original simulation box. Clusters are then isolated in the *joint* system. Each of the clusters is then flipped independently, i.e. the spheres belonging to a cluster are moved from the rotated copy into the original configuration and

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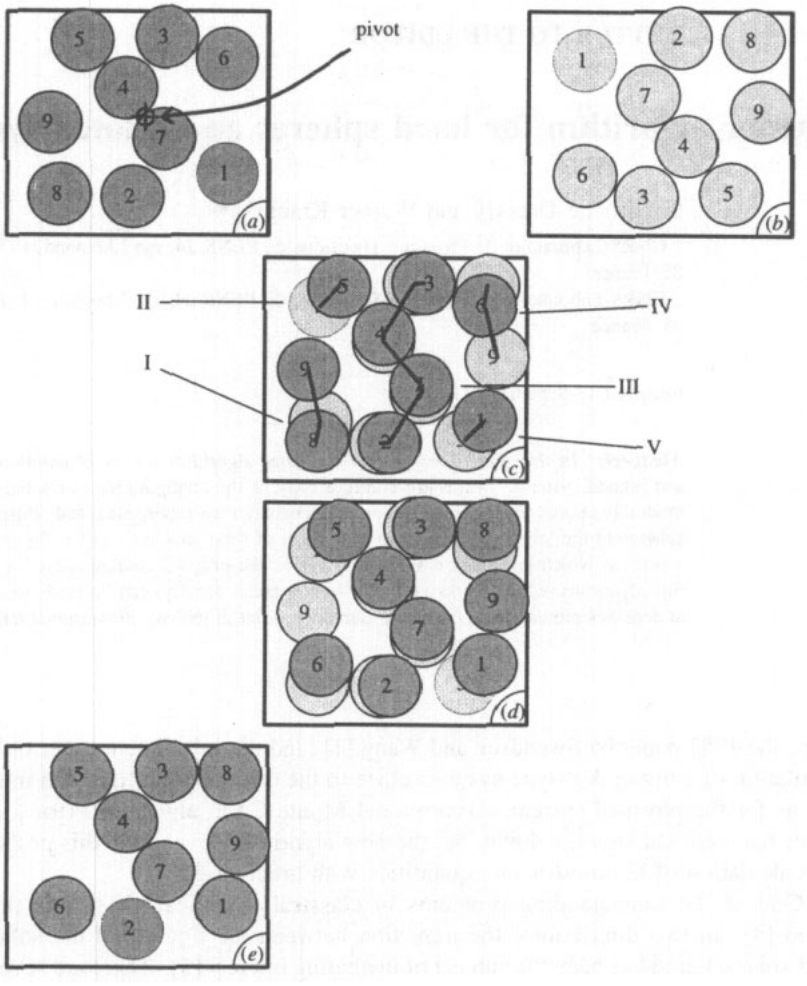

Figure 1. The algorithm presented in this paper performs non-local moves (*a*) → (*e*) by considering a randomly rotated copy (*b*) of the actual configuration (*a*). (*a*) and (*b*) are superposed (*c*), and clusters are isolated (*c*) and flipped (*d*) in the superposed configuration.

vice versa. For concreteness, consider figure 1, which illustrates the algorithm: the original configuration c_1 (figure 1(*a*)) is made up of N spheres of radius r in a box of size (L_x, L_y) (in the figure $N = 9$). In addition to the original configuration, we consider also a configuration c_2 (displayed in figure 1(*b*)), which is obtained from c_1 by a π-rotation: we generate c_2 by picking an arbitrary 'pivot' point $p = (p_x, p_y)$ with $0 < p_x < L_x, 0 < p_y < L_y$ (in the example, $p_x = 0.52\ L_x$, $p_y = 0.53\ L_y$). We then rotate c_1 around p of an angle π to obtain c_2†. The choice of the pivot is the essential Monte Carlo element of the algorithm.

The two configurations c_1 and c_2 are then superposed as shown in figure 1(*c*), where they form clusters of overlapping spheres‡. Two types of clusters are possible: 'even' clusters, made up of an equal number of spheres in c_1 and c_2, and 'odd' clusters, in which

† Periodic boundary conditions and the possible proximity of the cluster to the pivot have to be treated carefully.

‡ All the clusters in figure 1(*c*) can be determined in a total of $O(N)$ operations.

the numbers differ. In figure 1(*c*), for example, the cluster 'II' is even, while cluster 'I' is odd.

Generally, clusters appear in pairs (such as I and IV), with the possible exception of a single 'even' cluster which is symmetric around the pivot (III).

It is now easily seen that we may 'flip' the clusters, i.e. interchange between c_1 and c_2 the spheres belonging to a cluster. We are interested in performing a canonical simulation in which the individual numbers of spheres, both of c_1 and c_2, have to remain unchanged. We therefore choose to perform such flips for individual even clusters, or for pairs of odd clusters, such as I and IV. The result of one such cluster flip (of clusters I and IV) is shown in figure 1(*d*). Finally, we restrict our attention back to the updated configuration, c_1' in the original simulation box. By inspection of figure 1(*e*), which shows c_1', we see that picking p and flipping clusters I and IV has achieved a *non-local* Monte Carlo move: spheres 8 and 9 were moved from the lower left corner to the upper right one, and the sphere 6 from the upper right corner to the lower left one.

It should be evident that—given an arbitrary pivot point—the flip satisfies the detailed balance condition, and constitutes a viable Monte Carlo move. To see this one simply needs to consider the 'reverse' move (from figure 1(*e*) back to figure 1(*a*)), which has exactly the same probability of occurring as the original one.

Applying the same argument as above to an even cluster (such as V in figure 1(*c*)), we notice that small *even* clusters generate only *local* moves. Due to the limited benefits of worrying about (small) even clusters, we usually exclude them from our considerations. Many generalizations are possible: it is evident that the spheres can have different radii, etc; a potential can be taken into account in the usual way, by calculating the Boltzmann weights of the proposed flip and the reverse one; furthermore, the angle of the rotation around the pivot can be chosen at will. This only introduces some effects far from the pivot, which can be eliminated.

The simple algorithm which has just been described works perfectly well. At small density, the combined system of c_1 and c_2 breaks up into a large number of small clusters, which can be flipped independently. At higher density (i.e. above the percolation threshold of this combined system), there is a single percolating cluster (which it is useless to flip), and an *algebraically decaying* distribution of small clusters [11]. Just as in the Swendsen–Wang algorithm, there is a 'magical' point, the percolation threshold (which, for the Ising model, corresponds to the Curie temperature [12]). At this point, the behaviour of the algorithm is optimal. In our case, the 'magical point' is the percolation threshold of the system of *superposed* configurations, which unfortunately lacks physical interest. In two dimensions, we find this percolation threshold to be situated at a density of $\rho \sim 0.62$, definitely lower than the densities in which we are interested (as usual [8], the density is defined as the ratio of the number of spheres and the volume of the simulation box, $\rho = N/V$, normalized to $2/\sqrt{3}$ for the most compact state; in these units, the transition takes place around $\rho \approx 0.9$ [5, 10]). Around the percolation threshold, the algorithm decorrelates the whole system by flipping a few large clusters, as in the Wolff algorithm [2].

Close to the liquid–solid transition in the two-dimensional system, i.e. much above the percolation point, it is particularly difficult to find a sufficient number of small *odd* clusters, which generate the non-local moves. It is difficult to find odd clusters, but one rather often encounters configurations which *almost* constitute odd clusters, such as the ones presented in figure 2, which are kept from flipping by a few weak 'links'. We now present a stochastically correct trick which has allowed us to break up a large number of these weak links.

For fixed but arbitrary ϵ, we define an ϵ-cluster as a set of spheres which may have an

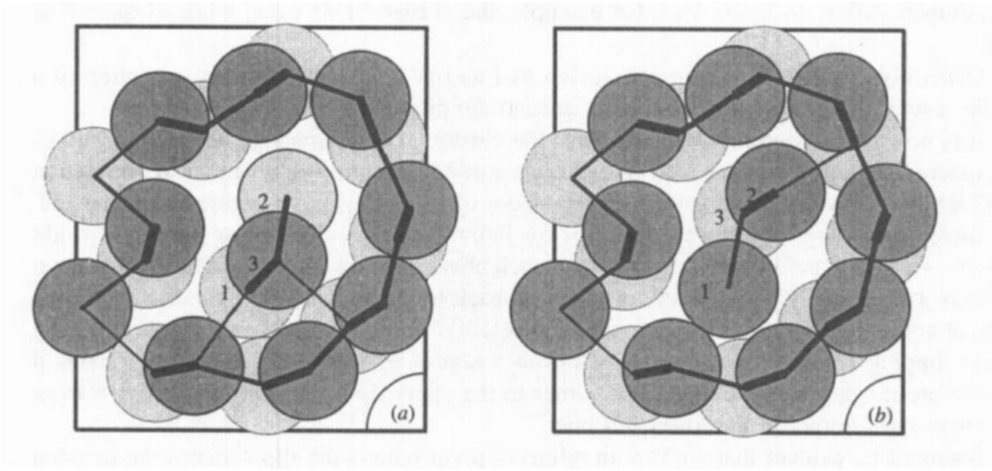

Figure 2. We present a trick which allows us to flip not only clusters (as in figure 1), but also ϵ-clusters.

arbitrary number of ϵ-links, i.e. links between a disc of the set and a disc of the boundary (in a different box), larger than $2 \times r - \epsilon$ (so that the overlap between the spheres is smaller than ϵ). In addition to having ϵ-links, the ϵ-cluster itself is held together by links which are not ϵ-links, i.e. which are shorter than $2 \times r - \epsilon$.

After isolating an ϵ-cluster, we 'freeze' the boundary, and perform a certain fixed number of n_{loc} *local* Monte Carlo moves exclusively of the spheres in the ϵ-cluster (without destroying it). Each time the number of ϵ-links falls to zero, we have obtained a true cluster, which we flip. It is easily shown that this exotic 'dynamic of ϵ-clusters' satisfies detailed balance, since we make sure that at each step both the initial and the final configuration are ϵ-clusters.

We have programmed the complete algorithm sketched in this paper. For small systems (up to 14 spheres), we performed extremely long runs both of a standard MC algorithm and of the present one. We find identical probability distributions, e.g. for the orientational order parameter [13] to a precision of 0.1%. Thus, there is very little room for doubt about the correctness of the present algorithm, and for programming errors in our actual implementation.

It is easily understood that, at high density, the main workload of the algorithm consists in the determination of the percolating cluster. Since we never actually 'flip' this cluster, most of the effort is thus spent in finding out what one does not want to do—a frustrating way of using CPU time. Only after discarding the percolating cluster do we have a chance of finding small odd clusters. A moment's thought suffices to understand that there is a faster way to find the small odd clusters. Consider the cluster IV in figure 1(*c*): it is evident that the non-local move can only be performed under the condition that, locally, it is possible to replace sphere 6 by two other spheres. Whether there is enough space at all in a given neighbourhood to replace n spheres by $n + 1$ can (for small $n = 0, 1, 2$) be decided by a *local* analysis which, in addition, is *independent* of the pivot (this remark is pertinent to clusters and ϵ-clusters). An improved algorithm of the kind presented in this paper thus first isolates the loci at which n spheres may be replaced by $n + 1$ (for small $n = 0, 1, 2$). Once this analysis is done, one chooses randomly pivots, and then does the—now trivial—cluster search, in regions which have survived the screening stage. Since the local analysis just

described can be reused a large number of times (and updated, once we have flipped a cluster, or ϵ-cluster), the cluster search is much simplified. The final algorithm is thus quite efficient in generating non-local moves.

Finally, let us stress that the method presented in this paper is very general, and may be applied to a large number of systems. The specific application to the hard-sphere liquid stands out as prototypical, and we hope that the algorithm will be helpful in elucidating the order of the transition, in the measure of correlation functions, etc. Work along these lines is in progress.

We acknowledge a very helpful discussion with D Marx.

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