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HAL Id: jpa-00210932
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Submitted on 1 Jan 1989

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Short Communication

Test of parallel updating in Ising model simulation

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(Reçu le 28 novembre 1988, accepté le 13 janvier 1989)

Résumé.— Le cumulant d’ordre 2 et 4 de l’aimantation est calculé pour un modèle d’Ising avec une évolution simultanée de l’ensemble des spins, comme l’ont proposé Neumann et Derrida. Des simulations de Monte-Carlo montrent que cette méthode donne la valeur attendue pour la température critique dans le cas d’un réseau carré. Cependant, un écart faible mais significatif est observé entre les valeurs critiques des cumulants d’ordre 4 calculées pour une évolution simultanée ou une évolution séquentielle.

Abstract.— Simultaneous updating of Ising spins, following Neumann and Derrida, is tested on the second and fourth moments of the magnetization. Monte-Carlo simulations indicate that it gives a correct critical temperature for the square lattice Ising model, but a slight deviation for the critical value of the fourth cumulant.

Monte Carlo simulations of interacting spin systems [1] are traditionally carried out in such a way that the surrounding (interacting) environment of a particular spin is held fixed while the decision is made about whether or not to flip it; and the interacting neighbors are only treated after the spin is updated. This procedure is straightforward and easy to apply when traditional single-spin-flip simulations are carried out but introduce complications when one uses multispin coding or attempts to optimize an algorithm for a parallel or vector processing machine. In such cases one must separate the lattice into interpenetrating sublattices, chosen such that the

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spins on a given sublattice do not mutually interact; then one treats each sublattice in its entirety before considering other spins. This procedure makes the simulation relatively cumbersome, reducing as well the speed of the algorithm.

A great simplification was recently suggested by Neumann and Derrida [2] who carried out simultaneous flipping of all spins on the lattice using a fixed environment for each spin determined by the spin configuration which existed before any of the spins were flipped. This approach is in the tradition of simultaneous updating for cellular automata. (While a similar procedure is used in molecular dynamics it should be remembered that the update interval can be made arbitrarily small in molecular dynamics and hence the environment of a particular site becomes almost static during an update). They applied this approach to magnets and spin glasses and concluded that at least the first moments of various quantities were correctly reproduced. They warned, however, that certain distributions are no longer correct.

Since this approach not only simplifies vectorization but also runs faster than sequential updating, we believe that it is important to determine whether or not other equilibrium properties will be properly reproduced in models with short-range coupling. The simplest possible test is provided by the Ising square lattice for which a great deal is known about distribution functions of the order parameter $m$, etc. For example, above $T_c$ the mean square fluctuation $\langle m^2 \rangle = kT \chi / N$ is proportional to the susceptibility $\chi$; both diverge at the Curie point. At $T_c$, the order parameter $m$ decays with lattice size $L$ as $L^{-\beta/\nu}$; and the fourth order cumulant $U$ where [1].

\[ U = 1 - \langle m^4 \rangle / 3 \langle m^2 \rangle^2 \]

approaches [3] a fixed point value $U^* = 0.615 \pm 0.010$. In addition, characteristically the curves for $U$ versus $T$ for different $L$ cross at a temperature which approaches $T_c$ as $L$ becomes infinite.

We therefore simulated Ising square lattices with helical boundary conditions using a very simple and fully vectorized simultaneous updating computer program (no multispin coding, 6 million spin flip trials per second on a single processor of the Cray XMP using a symmetric Glauber transition probability) for temperatures near the critical temperature ($kT_c / J = 2.269$). (Although the finite $L$ results for helical boundary conditions are expected to be slightly different than when periodic boundary conditions are used, the results for $L \to \infty$ should be the same). At least 250,000 MCS/site were initially discarded to allow the system to reach equilibrium, and the following 750,000 MCS/site were then used to compute averages. Each data point was repeated using different initial configurations and different pseudo-random number sequences; in some cases also the random number generators were changed.

Overall averages, with error bars, were determined typically from five independent runs (except for the one comparison run with sequential updates).

Varying the temperature, in units of $J/k$, between 2.4 and 3, far above the critical
point, where finite-size effects are negligible, we found the fluctuations \( \langle m^2 \rangle \) of the magnetization to be only about half as large as those found by sequential updating. (We made two runs on a 1000*1000 lattice, see Tab. I). Thus the usual relation between \( \langle m^2 \rangle \) and the susceptibility is violated, compatible with the warnings of Neumann and Derrida. Right at \( T_c \), the decay of the squared order parameter with increasing lattice size at \( T_c \) is also given in table I. The data are well described by a power law with the expected exponent \( 2\beta/\nu = 0.25 \), but the prefactor is somewhat smaller than that obtained from sequential updating.

Table I.— (a) Fluctuation \( \langle m^2 \rangle L^2 \) versus temperature for 1000 ; (b) Fluctuation \( \langle m^2 \rangle L^{1/4} \) versus \( L \) at the Curie point. In both cases, the upper line gives parallel, the lower line sequential updating (in agreement with the exact results).

<table>
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<tr>
<th>( kT/J )</th>
<th>2.4</th>
<th>2.5</th>
<th>2.6</th>
<th>2.7</th>
<th>2.8</th>
<th>2.9</th>
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<td>27</td>
<td>13</td>
<td>11</td>
<td>10</td>
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<td>6</td>
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<tr>
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<td>47</td>
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<td>20</td>
<td>15</td>
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</table>

<table>
<thead>
<tr>
<th>( L )</th>
<th>10</th>
<th>20</th>
<th>40</th>
<th>80</th>
</tr>
</thead>
<tbody>
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<td>0.945(2)</td>
<td>0.936(10)</td>
<td>0.945(18)</td>
</tr>
<tr>
<td>seq.</td>
<td>1.115</td>
<td>1.127</td>
<td>1.122</td>
<td>1.122</td>
</tr>
</tbody>
</table>

With these deviations in \( \langle m^2 \rangle \) now determined, our question now is if these "errors" cancel out from the ratio \( \langle m^4 \rangle / \langle m^2 \rangle^2 \) entering the above cumulant. In figure 1 we plot the reduced fourth order cumulant \( U \) versus \( T \) for three different lattice sizes. We see that the curves all cross at a temperature which is within an error of less than 0.01 in \( kT/J \) the exact infinite-lattice critical temperature. In table II we show the values of \( U^* \) obtained at \( T_c \), including new data for \( L = 80 \). We see that \( U \) is essentially identical for all lattice sizes \( (U = 0.591 \pm 0.006 \text{ for } L = 80) \) but is clearly below the correct value of \( U^* = 0.615 \) found in table II by traditional sequential updating. (With minor modifications our program carried out sequential updating giving the correct value of \( U^* \) thus making programming errors an unlikely source of the discrepancy).

Table II.— Variation of fourth cumulant \( U^* \) versus \( L \) at the Curie point.

<table>
<thead>
<tr>
<th>( L )</th>
<th>10</th>
<th>20</th>
<th>40</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.588(1)</td>
<td>0.589(1)</td>
<td>0.586(3)</td>
<td>0.591(6)</td>
</tr>
<tr>
<td>seq.</td>
<td>0.619</td>
<td>0.618</td>
<td>0.616</td>
<td>0.615</td>
</tr>
</tbody>
</table>

The semi-universal quantity \( U \) is known [4] to depend strongly on the shape of the sample, even with sequential updates. With parallel updates this dependence is even
stronger: for 9*10 or 19*20 lattices, $U$ is only about half its above value, in agreement with a theoretical prediction of Derrida (Priv. Comm.). For these odd*even shapes our helical boundary conditions lead to two decoupled sublattices of even and odd sites, at even times, for which the statements of Neumann and Derrida apply.

Fig. 1.— Variation of cumulant $U$ with temperature (in units of $J/k$) for $L = 10$ (dots), 20($x$), and 40(+) The errors are of the order of the symbol sizes.

(F. Gutbrod, private communication, showed parallel updating to give wrong averages for the heat bath simulation of SU2 lattice gauge theory).

We thus conclude, consistent with Neumann and Derrida, that simultaneous updating, as applied to the Ising square lattice, introduces drastic errors in the susceptibility and subtle but noticeable errors into the ratio of the higher moments of the order parameter. This technique can thus not be used with impunity for treating arbitrary systems.

One of us (D.P.L.) wishes to thank the Humboldt Foundation for its support and Johannes Gutenberg-Universität Mainz for its hospitality during a portion of the time this work was carried out. This work was also supported in part by NSF grant # DMR-8715740. We wish to thank B. Derrida, E. Domany, G. LeCaer and D.W. Heermann for helpful discussions.

References