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SPEEDING-UP SIMULATIONS OF INTERACTING SYSTEMS NEAR CRITICAL POINTS BY THE MULTIGRID MONTE CARLO METHOD

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Abstract: With multigrid coarse-to-fine transformations, loss of computer performance due to very slow long-wavelength relaxations can be eliminated. For systems with short-range interactions, effective interactions can however be modified according to renormalization-group considerations. With coarse-to-fine grid transformations alone, deviations indicate whether fine-to-coarse transformations are also necessary.

1. Introduction

Computer simulations have become very effective for many problems which cannot be treated by analytic methods. However, in complex systems, very slow relaxations at long wavelength restrict the application of vector and parallel computers. For the numerical solution of partial differential equations, the multigrid method [1] has demonstrated how it is possible to speed up slow long-wavelength relaxations by many orders of magnitude. A condition for the solution of such systems by this method is their selfsimilarity, i.e. the couplings between grid points remain unchanged in the mapping procedure from fine-to-coarse grids. For equilibrium systems with short-range interactions, renormalization-group theory [2] shows that effective interactions have to be recalculated at each fine-to-coarse mapping except at fixed points corresponding to critical points.

2. Multigrid theory

Multigrid procedures [1] usally start with fine grids, iterate, transform to coarser grids, iterate again and return to the fine grid. This algorithm can be extended to several levels. For a short-range interaction, the interaction has to be renormalized as demonstrated for the Ising model at $T > T_c$ in [3]. The mapping from fine-to-coarse grids specifies the "melting" of blockspins on the fine grid. In our simulations, large blockspins with renormalized interactions were used at the outset and were allowed to melt only during successive iterations. The entropy was kept constant in each melting step.

3. Results

Figure 1 shows thermodynamic quantities for the two-dimensional Ising model normalized to exact values [4-6] computed with the multigrid Monte Carlo method. Deviations from

1 close to the critical point indicate that if the information of additional multigrid levels is used, blockspin melting at constant entropy is by itself unsatisfactory. Therefore, fine-to-coarse mappings are also needed, in which renormalized interactions can be estimated as demonstrated in [3].

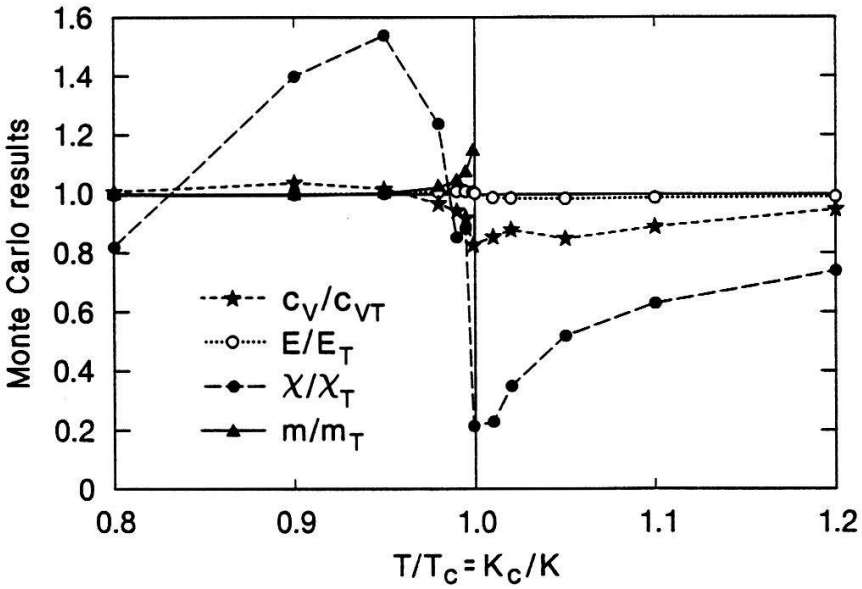

Figure 1: Plot of specific heat c_V, energy E, susceptibility χ and order parameter m normalized to their exact theoretical values [4-6] for two-dimensional Ising models with 1024×1024 and 4096×4096 spins.

4. Conclusions

Renormalization-group multigrid Monte Carlo calculations are very useful to improve the performance of numerically intensive calculations. Interactions have to be renormalized if the fine-to-coarse decimation step cannot be treated via a mapping to a percolation problem [7]. Fine-to-coarse mappings have to be combined with coarse-to-fine mappings for adequate blockspin melting.

5. References

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