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D.P. Landau
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(Eds.)

Computer Simulation Studies in Condensed-Matter Physics XIV

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Preface

Over the last 30 years, Professor David P. Landau's trailblazing research achievements and influential leadership have helped establish computer simulation as a powerful and incisive mode of scientific investigation, now on a par in the physical sciences with experimental and theoretical research. This year, we were very pleased to organize a special one-day symposium honoring the 60th birthday of our distinguished colleague and friend. This event was held in conjunction with and immediately following the annual computer simulations workshop that Professor Landau founded 14 years ago. Many of the papers presented at this honorary symposium are integrated into this proceedings volume, and the accompanying photograph of participants serves to commemorate this very special event.

This volume contains both invited papers and contributed presentations on problems in both classical and quantum condensed matter physics. We hope that each reader will benefit from specialized results as well as profit from exposure to new algorithms, methods of analysis, and conceptual developments.

Athens, GA, USA
May 2001

S.P. Lewis
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Part VI Polymers and Complex Systems

1 Computer Simulation Studies in Condensed Matter Physics: An Introduction

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Computer simulation studies in condensed matter physics play an ever increasing role in many areas of investigation. The "status report" that is contained in this volume is the result of presentations and discussion that took place during the 14th Annual Workshop at the Center for Simulational Physics. The texts of both longer, invited presentations as well as a number of contributed papers are included. The reader will find that the scope of simulational/computational studies is broad and that substantial potential for cross-fertilization of methods between different sub-fields exists.

Part I contains five papers on recent work on non-equilibrium and dynamical behavior. In the first paper, Murakami et al. present molecular dynamics simulations of heat transport across a material connecting hot and cold reservoirs. They observe normal thermal conduction obeying Fourier's Law for three-dimensional systems, but not for systems of lower dimensionality. Next, Kaski et al. describe a novel interactive simulation environment with real-time visualization to explore dislocation dynamics and plasticity in a model two-dimensional, homogeneous crystal. They find that even a simple interaction model in their atomistic simulations captures many of the important behaviors that would be inaccessible to continuum models of materials. Results illustrating this point are presented for both single-dislocation systems as well as systems with interacting dislocations. Ito et al. review a non-equilibrium approach to investigating the equilibrium behavior of statistical mechanical models around phase transitions. This technique, which involves analyzing the relaxation process as the system approaches equilibrium, is illustrated for several model systems. Korniss et al. examine the dynamic phase diagram of a two-dimensional Ising ferromagnet driven by an oscillating external field. They present evidence based on finite-size scaling that no tri-critical point exists for this model in the thermodynamic limit, contrary to earlier claims. Mitchell et al. perform a series of density-functional theory calculations to parameterize a model potential for use in dynamic Monte Carlo simulations of bromine diffusion on Ag(100). Several test calculations assessing the validity of their model potential are described.

Part II contains papers on clusters, films, and interfaces. First, El-bayyari explores the low energy structures of gold microclusters via molecular dy-

namics simulations at constant temperature. Using an empirical many-body potential parameterized to bulk properties, he obtains a series of stable and metastable configurations for gold clusters containing 3–13 atoms. Patrykiejew et al. conduct Monte Carlo simulations to find stable and metastable structures for atomic adsorbate overlayers on a model fcc(100) surface. They consider several competitive types of domain patterning for adsorbate concentrations above 50%. Nurminen et al. present kinetic Monte Carlo simulations of a simple solid-on-solid model to address nucleation and growth of islands on a patterned substrate with nanoscale features. They find that the substrate patterning gives rise to spatial ordering of the islands. Smith and Haymet give a progress report on applying molecular dynamics to study the transport of solutes across the ice/water interface. Kholmurodov et al. simulate the impact of an energetic beam of aluminum clusters with an aluminum substrate using an optimized molecular dynamics code. They present a novel interpretation of the metal-on-metal spreading process based on the computed density and temperature distributions. To end this section, Kutana et al. investigate the shape and size of the blocking cone produced by shadowing effects in low energy ion-scattering experiments. Their simulations reveal a universal formula for the blocking cone size and show that the cone shape is appreciably asymmetric about the scattering axis.

Part III, which focuses on phase transitions, opens with a paper by Binder et al. that examines surface induced disordering in a bcc model binary alloy with nearest-and next-nearest neighbor interactions. They present very detailed results from a Monte Carlo simulation of a bcc alloy that disagree with theory. The simulations find different estimates for ν from the order parameter of the B2 phase and the order parameter of the DO_3 phase. Next, Janke and Kenna discuss a numerical analysis of phase transitions using the density of zeros of the partition function. They show how to distinguish between the order of the transition and apply their approach to several Potts and Ising models. Swendsen examines the spectrum of eigenvalues in the renormalization group approach to phase transitions. He shows that, for sufficiently large systems, if there are two eigenvalue exponents y_1 and y_2 there exists another eigenvalue equal to $y_1 + y_2$.

Part IV contains six papers on new methods and algorithms. Wang reviews Monte Carlo techniques that involve reweighting and then introduces the transition matrix Monte Carlo method. He shows that, in combination with new sampling algorithms, the transition matrix approach can be exceedingly efficient. In the second paper of this section Evertz et al. introduce a new cluster method for the Ising model. They use a new representation that contains both the bond variables of the high-temperature representation and those of the Fortuin-Kasteleyn clusters. This approach also sheds new light on the physical meaning of geometric properties of clusters. Park and Novotny then examine the relationship between Monte Carlo time and physical time using a quantum system coupled to a phonon heat bath. They apply this

dynamics to the square lattice Ising ferromagnet and obtain a quite different low-temperature prefactor than with Glauber dynamics. Okabe et al. first describe a new probability-changing cluster (PCC) algorithm that "tunes" the critical point automatically, and then apply it to the two-dimensional, site-diluted Ising model. They then use the Wang-Landau algorithm to study the three-dimensional q-state Potts model. They conclude that the choice of algorithm depends on the quantities of interest. Suzuki introduces a general scheme for using exponential product formulae to compute time-dependent quantities. He then proposes a new method for the numerical treatment of the Kohn-Sham hamiltonian. In the final paper of this section Adler et al. report on recent developments in the use of visualization techniques with a high-bandwidth internet connection for the analysis of atomic simulations. As an example they view spreading of an aluminum drop on a metal-oxide surface.

Part V of this volume focuses on quantum systems, including those examined via electronic-structure methods. First, Creutz reviews the difficulties associated with chiral symmetry in lattice gauge theories. He proposes a new route toward resolving these issues, based on a formulation that uses fermionic surface states in an extra space-time dimension. Next, Sandvik discusses the stochastic series expansion quantum Monte Carlo method for quantum lattice models. He reports on implementations of this method for the S=1/2 Heisenberg model, using a recently developed cluster updating scheme. Osborn describes applications of the meron-cluster algorithm to the attractive Hubbard model. He presents new results for the Kosterlitz-Thouless transition to the superconducting phase in this system. Matuttis and Ito have revisited the minus sign problem in standard auxiliary field formulations of the Hubbard model. Their results suggest that the minus problem may be substantially less severe than previously reported. Then, Amadon and White propose a new variational wavefunction for t-J ladder models, based on novel "distance" functions between basis states, which can serve as the starting point for Green's function Monte Carlo simulations. They report on applications of this variational approach to 2-leg ladder systems. Hennig et al. present ab-initio calculations of the ground-state phase diagram of the Ti-Zr-Ni quasi-crystal. They report on the energetic stability of quasi-crystal structures extracted from experimental diffraction data. Finally, Rogers and Rappe discuss their recently developed Riemannian differential-geometry approach for the derivation of the stress field in non-relativistic interacting quantum systems. They present an extension of this formalism within the framework of finite temperature density functional theory.

The last section (Part VI) in this status report contains papers on polymers and complex systems. Müller has studied binary polymer blends in a thin-film geometry within a coarse-grained lattice model formulation. He presents detailed Monte Carlo simulation results for the rich phase diagram and the critical behavior of this system. Zia and Astalos have applied statis-

tical physics methods to study the problem of population dynamics within the framework of the Penna-Desai bit string model. They report both Monte Carlo simulation and analytical results for the stochastic aspects and the long-time behavior of the model. Kutteh and Visscher discuss novel approaches for performing Stokesian dynamics simulations on systems of hydrodynamically interacting colloidal particles. They present results obtained with this method for acicular models of magnetic colloids. Dünweg et al. present a novel scheme for simulating polymer dynamics in solution by means of a molecular dynamics simulation/lattice Boltzmann hybrid scheme. They report results for the crossover from Zimm to Rouse dynamics, obtained with this approach. Buendia et al. report on a spring-network model for cross-linked polymer surfaces. They compare their simulations of the surface structure to atomic force microscopy experimental results for templated gel surfaces. Rapaport has studied flow phenomena in a vertically vibrated granular layer. For sawtooth-shaped substrate profiles, his simulations predict heretofore unobserved horizontal flows which could be used to separate large particles from small particles.

Part I

Nonequilibrium and Dynamical Behavior