

Computer Simulation Studies in Condensed Matter Physics: An Introduction

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Computer simulation studies in condensed matter physics now play a fundamental role in many areas of investigation. The “status report” which is contained in this volume is the result of presentations and discussion that occurred during the 19th Annual Workshop at the Center for Simulation 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 simulation/computational studies is broad and that substantial potential for cross-fertilization of methods between different sub-fields is evident.

The volume opens with four papers on materials properties. First, Fichthorn and Miron address the challenges associated with simulating rare events, where many time scales may be relevant. They use the hyperdynamics approach to accelerate dynamical simulation of such systems in a manner that correctly samples the equilibrium state of the fast processes while evolving the trajectories at a time scale relevant for the slow processes. This is achieved by on-the-fly consolidation of broad basins of high-frequency localized states into coarser states that incorporate the equilibrium properties of the smoothed-away minima. The authors demonstrate the technique on a realistic model system of the diffusion of Co clusters on the Cu (001) surface. Dennis and Liebig study the intensity dependence of the reflectance of three types of dielectric interference filters. They simulate the reflectance of both low- and high-intensity pulses using the finite-difference time-domain method and incorporating nonlinear optical behaviors in the field equations. The three systems are compared to assess the robustness of their reflective properties against nonlinear effects at extremely high intensities. Abraham extends his earlier work on crack instability in brittle fracture by applying a recently discovered scaling law to a model solid with a crack constrained to unidirectional travel. He finds that suppression of crack instabilities leads to constant steady-state crack speeds equivalent to crack speeds in a linear solid with elastic modulus equal to the effective elastic modulus of his model solid. To conclude this Part, Thompson and Lewis use density functional theory to conduct a detailed study of the

surface structure of TiO_2 (110), making contact with a recent high-precision experiment. They find that bond angles converge relatively slowly with respect to model approximations, whereas bond lengths converge rapidly. Their results suggest changing the way surface structures for covalently bonded solids are reported, emphasizing bond lengths and angles, and not absolute positions.

In Part II, new models, methods, and perspectives are highlighted. In the first invited presentation Trebst et al. discuss the use of extended ensemble Monte Carlo methods to study equilibrium behavior in many-particle systems. They show how one possible method of optimization may be achieved by biasing the random walk by the inverse square root of the diffusivity. This approach is applied to a dense fluid, and they also show how to optimize parallel tempering simulations. Next, Ito describes the “Avogadro challenge” in which new computer technology in the form of Petaflop computing will enable us to approach simulation of macroscopic properties using microscopic models. The emphasis is on transport phenomena and both numerical estimates for properties as well as structures, e.g. vortices and bubbles, that result from such simulations are presented. Adler et al. then describe the visualization of nanostructures of carbon using AViz, a visualization package developed by the Computational Physics group at the Technion. The thrust of the discussion is on the challenges of using visualization to differentiate similar, competing structures. In the next paper Aoki describes methods for properly simulating anisotropic systems with periodic boundary conditions. A factor is introduced into the appropriate Lagrangian with the consequence that the normal pressure and the surface tension are given correctly. Sample data are shown for a system of soft spherocylinders. To conclude this part, De Raedt et al. introduce a model that is strictly causal and local. Although there are no principles of quantum mechanics involved, the model can correctly reproduce the single-spin expectation values and two-spin correlation functions in an Einstein-Podolsky-Rosen-Bohm experiment.

Part III contains four papers that examine non-equilibrium and dynamic behavior. O’Malley et al. have applied a dynamical Monte Carlo simulation approach to study a two-dimensional two-species lattice model describing the spread of an invading advantaged gene, allele or species into a disadvantaged resident population. Their results for the invasion front characteristics exhibit important qualitative differences from continuum-limit mean-field behavior. The differences are attributed to the absence of lattice discreteness and noise in the continuum-limit mean-field approximation. Next, Ogushi, Yukawa and Ito have performed molecular dynamics simulations for the dynamics and thermal structure of the gas-liquid interface in a three-dimensional Lennard-Jones system. They study the short- and long-time dynamical behavior of the density and temperature profiles which arise when a temperature gradient, imposed on an initial equilibrium state of the system, forces the nucleation of a gas-liquid interface. Their results demonstrate the existence of a temperature gap between the two emerging phases, indicative of an enhanced heat flow resistance across the interface. Kamimura, Yukawa and Ito have investigated the

chemical reaction dynamics in far-from-equilibrium open systems within the framework of a stochastic model for a network of mutually catalytic replication reactions, controlled by an externally imposed energy flow. Their reaction-rate results show Arrhenius or non-Arrhenius behavior, respectively, under either low- or high-energy flow conditions. The authors suggest a possible alternative mechanism for biological systems to attain higher energy states in far-from-equilibrium situations. To close this part Hamad, Robb and Rikvold describe a comparative study of the dynamics of first- and second-order phase transitions by means of first-order reversal curve (FORC) analyses, applied to kinetic Monte Carlo simulation results for electrochemical deposition models. In the first-order case, their FORC results are indicative of a competition between the applied time-dependent electrochemical potential and the tendency towards phase ordering. In the second order case, by contrast, their results are characteristic of relaxational behavior towards a single equilibrium state.

Magnetic systems are featured in Part IV, beginning with Costa et al. who combine Monte Carlo and molecular dynamics simulations to study the microphysics of friction induced by magnetic forces for a model of a magnetic reading head moving across a magnetic film. They find that heat dissipation in this model system correlates to the appearance of magnetic vortices. Next, Machida, Iitaka, and Miyashita present a new technique for calculating linear response functions for quantum spin Hamiltonians on a large Hilbert space. It is based on a Chebyshev expansion of thermal and time-evolution operators that circumvents the need for high-dimensional diagonalization to obtain spin-spin correlation functions. Applied to a molecular nanomagnet, this technique gives results in close agreement with experiment. To conclude this section, Yoshioka et al. simulate cluster-cluster aggregation for a model system composed of Ising dipolar particles using molecular dynamics. They find that this system exhibits the behavior of attraction-limited cluster aggregation of dipolar particles. Various aspects of the dynamical properties of this model system are presented.

The last Part of this volume contains four papers on biological and soft condensed matter. Opening this Part is Shimada who reports on neuronal network simulations, aimed at elucidating the multiple internal states of neurons, and the transitions between such states that can be induced by cellular current injection, as recently observed in hippocampal slices from the brains of rats. The simulations demonstrate how multistable states can be induced in a network consisting of connected neurons that do not exhibit multistability in isolation. The comparison of different network topologies shows that shorter-range clustered network connectivity is required for the emergence of well-controlled network activity involving transitions between these states. Then, Laradji and Kumar have studied the dynamics of self-assembled multi-component lipid membranes using dissipative particle dynamics simulations. The effects on the dynamics of domain interface and surface tension, as well as lipid volume fraction, and trans-bilayer lipid distribution asymmetry, are investigated. Symmetric bilayers are found to exhibit a rich repertoire of dy-

namical behaviors, involving the coalescence and budding of local domain structures. Transbilayer asymmetry strongly affects both the curvature of the membranes and their dynamics. Next, Deserno gives a broad overview of solvent-free lipid bilayer simulations, their impact on our current understanding of the physics of these systems, and their relevance to biology. He outlines how the “solvent-free” modeling approach allows one to circumvent the explicit inclusion of the solvent by means of appropriately constructed effective pair potentials acting directly between the lipid monomers. A wide range of physically and biologically relevant properties can then be investigated, ranging from the bilayer self-assembly to their structure, equilibrium phase diagram and dynamics. Lastly, Ricci et al. report on Monte Carlo studies of the effects of boundaries on spatially confined two-dimensional colloidal crystals, based on a point particle model with inverse power law interaction potentials. They demonstrate that “flat” confining walls, will destroy positional long-range order in confined geometries, while locally enhancing orientational long-range order. Certain corrugated boundaries can restore positional long-range order, thereby illustrating the strong boundary sensitivity of such systems even for very distant boundaries.

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