

## **Program of the Workshop on Large-Scale Computations in Statistical Physics<sup>1</sup>**

University of Southern Mississippi February 26–27, 1990

Chair, Workshop: Ras Pandey, Department of Physics and Astronomy, University of Southern Mississippi, Hattiesburg, MS39406-5046, USA.

*February 26, 1990*

Morning session, Chair: Grayson Rayborn

Welcome: Dr. G. David Huffman, Vice President for Academic Affairs

Keynote Address: Dr. Karen Yarbrough, Vice President for Research and Extended Services

Opening Lecture: K. Binder, University of Mainz

Computer simulation of phase transitions in adsorbed layers at surfaces

B. Swope, IBM Palo Alto Scientific Center

Million particle molecular dynamics simulations of nucleation of crystals in a supercooled atomic liquid

A. Ferrenberg, University of Georgia

High accuracy Monte Carlo study of 3D Ising critical behavior

Afternoon session, Chair: Kurt Binder

D. P. Landau, University of Georgia

Monte Carlo studies of dynamic critical behavior

P. A. Rikvold, Supercomputer Computations Research Institute, FSU

Nonequilibrium information from transfer-matrix calculations

C. Günther, P. A. Rikvold, and M. A. Novotny, Supercomputer Computations Research Institute, FSU

First-order transitions and tricritical points in a model for oxygen ordering in a  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

M. Herman, Tulane University

Solvent induced relaxation of excited state vibrational population of diatomics: A mixed quantum–classical simulation

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M. Sahimi, University of Southern California

Applications of large scale computations and statistical physics of disordered systems to transport and reaction in porous media

V. Privman, Clarkson University

New directions in finite size scaling theory

*February 27, 1990*

Morning session, Chair: David Landau

D. Stauffer, Jülich Supercomputer Center

Q2R cellular automata—An alternative Ising model algorithm?

R. Gerling, University of Erlangen

Classification of cellular automata

R. Pandey, University of Southern Mississippi

Computer simulation models for the immune response

P. B. Visscher, University of Alabama

Stress as an order parameter for the glass transition

H. Nakanishi, Purdue University

Scaling at the rod-to-flexible chain crossover in the stiff limit

Afternoon session, Chair: Dietrich Stauffer

R. Hall, Louisiana State University

Path integral studies of sodium cluster

Short presentations

High resolution Monte Carlo study of the 3D classical Heisenberg ferromagnet, P. Peczak and D. P. Landau, Center for Simulational Physics, University of Georgia

Phase diagram of the  $d=3$  Ising model with competing interactions, R. Heilmann, A. Ferrenberg, and D. P. Landau, Center for Simulational Physics, University of Georgia

Ising models with correlated disorder, J. Lee, Department of Physics and Astronomy, University of Southern Mississippi

Long- and short-range ion transport in heterogeneous polymers, K. Mauritz, Department of Polymer Science, University of Southern Mississippi

A general free volume-based theory for the diffusion of large molecules in amorphous polymers above  $T_g$ : Polymer-penetrant intersection, C. S. Coughlin, K. Mauritz, and R. F. Storey, Department of Polymer Science, University of Southern Mississippi

Maximum entropy reconstruction of equations of state—Hard core systems, L. R. Mead, Department of Physics and Astronomy, University of Southern Mississippi

Connectivity in a 2D lattice fluid, S. Gao and R. Pandey, Department of Physics and Astronomy, University of Southern Mississippi

The use of digital signal processors for nonlinear dynamics, T. Dunn, P. Stephenson, and R. Gibbs, Department of Physics, Louisiana Tech University

Computer support and facilities at the University of Southern Mississippi, D. Page and J. Waggle, Computing Center, University of Southern Mississippi

Concluding remarks: Grayson Rayborn, Chair, Department of Physics and Astronomy, University of Southern Mississippi