



# Recent Developments in Computer Simulational Studies in Condensed Matter Physics

## *Program of the 2006 19<sup>th</sup> Annual Workshop*

### Monday, February 20th

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| 8:30 – 10:00 AM  | Registration in Room 307B of the Physics Building  |
| 9:00 - 10:00 AM  | Coffee and donuts<br>Informal discussion in Conference Room 201  |
| 10:00 – 10:05 AM | <b>David P. Landau</b> (The University of Georgia)<br>Introductory Remarks   |
| 10:05 – 11:05 AM | <b>Mohamed Laradji</b> (The University of Memphis)<br>“Dissipative Particle Dynamics Studies of Self-Assembled Multicomponent Lipid Vesicles”            |
| 11:20 – 11:35 AM | <b>Keiko Aoki</b> (Institute of Computational Fluid Dynamics)<br>“Molecular Dynamics Simulation Methods for Anisotropic Systems”                         |
| 11:50 – 12:05 PM | <b>Bill Dennis</b> (University of Georgia)<br>“Simulating the interaction of high intensity ultrashort laser pulses with nanostructured optical devices” |
| 12:15 PM         | Lunch  |
| 2:00 – 3:00 PM   | <b>Simon Trebst</b> (University of California)<br>“Ensemble optimization techniques for the simulation of slowly equilibrating systems?”                 |
| 3:15 – 3:30 PM   | <b>Dennis Rapaport</b> (Bar-Ilan University)<br>“Visualizing Physical Phenomena”   |
|                  | Break  |
| 4:00 – 4:15 PM   | <b>Takashi Shimada</b> (University of Tokyo)<br>“Simulational Study of the Multiple States in Hippocampal Slices”  |
| 4:30 – 4:45 PM   | <b>Scott Thompson</b> (University of Georgia)<br>“A Theoretical Study of the (110) Surface of TiO <sub>2</sub> : Structural Analysis”                    |



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### Tuesday, February 21st

- 9:00 – 10:00 AM      Coffee and Bagels/Muffins  
Informal discussion in Conference Room 201
- 10:00 – 11:00 AM      **Kristen Fichthorn** (Pennsylvania State University)  
“Accelerated Molecular Dynamics of Thin-Film Epitaxy”
- 11:15 – 11:30 AM      **Lauren O’Malley** (Rensselaer Polytechnic Institute)  
“Velocity of Front Propagation in a Two Species Invasion Model  
with Preemptive Competition”
- 11:45 – 12:00 PM      **Farid Abraham** (UGA Graham Perdue Professor)  
“Shocking Porous Solids”
- Lunch
- 2:00 – 3:00 PM      **Markus Deserno** (MPI for Polymer Research)  
“Solvent-free Lipid-bilayer simulations: From Physics toward Biology”
- 3:15 – 3:30 PM      **Bismarck Vaz da Costa** (ICEX, Universidade Federal de Minas Gerais)  
“Vortex Fluctuation and Magnetic Friction”
- Break
- 4:00 – 4:15 PM      **Martino De Prato** (Max-Planck-Institute for Metallforschung)  
“The scaling function of the critical Casimir effect: a Monte Carlo study”
- 4:30 - 4:45 PM      **Atushi Kamimura** (University of Tokyo)  
“Rate Constant in far-from-equilibrium open systems”
- 5:00 – 5:15 PM      **Chenggang Zhou** (Oak Ridge National Lab and the University of Georgia)  
“Monte Carlo simulation of  $\text{Rb}_2\text{MnF}_4$  – a 2D Heisenberg model with dipolar  
interaction”



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## *Program of the 2006 19<sup>th</sup> Annual Workshop*

### Wednesday, February 22nd

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| 9:00 – 10:00 AM  | Coffee and donuts<br>Informal discussion in Conference Room 201  |
| 10:00 – 11:00 AM | <b>Nobuyasu Ito</b> (University of Tokyo)<br>“The Avogadro Challenge”  |
| 11:15 – 11:30 AM | <b>Steven Mitchell</b> (University of Georgia)<br>“Phase Separation in a Compressible 2D Ising Model”  |
| 11:45 – 12:00 PM | <b>Fumiko Ogushi</b> (University of Tokyo)<br>“Structure of Gas-Liquid Phase Interface”<br><br>Lunch   |
| 2:00 – 3:00 PM   | <b>Glenn Martyna</b> (IBM, Division of Physics Science)<br>“Using novel methods and parallel architectures to study materials and devices”                     |
| 3:15 – 3:30 PM   | <b>Joan Adler</b> (Technion Haifa)<br>“Visualizing Nanodiamond and Nanotubes”<br><br>Break   |
| 4:00 – 5:00 PM   | <b>Karsten Reuter</b> (Fritz-Haber-Institute)<br>“First-principles statistical mechanics for heterogeneous catalysis”  |
| 5:15 – 5:30 PM   | <b>Peter Grassberger</b><br>“Simulations of lattice animals and trees by means of a sequential Monte Carlo algorithm with importance sampling and re-sampling” |
| 6:00 – 7:30 PM   | <b>Reception</b> in the Student Learning Center on campus (see campus map)   |



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## *Program of the 2006 19<sup>th</sup> Annual Workshop*

### Thursday, February 23rd

- 9:00 – 10:00 AM      Coffee and bagels/muffins  
Informal discussion in Conference Room 201
- 10:00 – 11:00 AM      **Jorge Sofo** (Pennsylvania State University)  
“Mapping water dissociation at surfaces”
- 11:15 – 11:30 AM      **Naoki Yoshioka** (University of Tokyo)  
“Attraction-limited cluster-cluster aggregation of Ising dipolar particles”
- 11:45 – 12:00 AM      **Ibrahim Abou-Hamad** (Florida State University)  
“First-order Reversal Curve (FORC) Analysis of Kinetic Monte Carlo Simulations  
of First-and Second-Order Phase Transitions”
- Lunch
- 2:00 – 3:00 PM      **Marcus Martin** (Sandia National Laboratory)  
“Recent Advances in Configurational-bias Monte Carlo: Algorithms  
and Applications”
- 3:15 – 3:30 PM      **Manabu Machida** (Cornell University)  
“Simulational Study on the Linear Response for Huge Hamiltonians-  
Temperature Dependence of the ESR of a Nanomagnet”
- Break
- 4:00 – 5:00 PM      **Computational Astrophysics Talk**



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## *Program of the 2006 19<sup>th</sup> Annual Workshop*

### Friday, February 24th

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| 9:00 – 9:30 AM   | Coffee and muffins<br>Informal discussion in Conference Room 201  |
| 9:30 – 9:45 AM   | <b>Kurt Binder</b> (University of Mainz)<br>“Computer Simulation of Models for confined Two-Dimensional Colloidal Crystals: Evidence for the Lack of Positional Long range Order” |
| 10:00 – 11:00 AM | <b>Yong Duan</b> (University of California, Davis)<br>“Simulation of protein folding with atomistic models”   |
| 11:15 – 11:30 AM | <b>Emily Pritchett</b> (University of Georgia)<br>“Designing Controlled-Not Logic for Superconducting Quantum Computers”  |
| 11:45 – 12:00 AM | <b>Hans de Raedt</b> (University of Goningen)<br>“Computer Simulation of EPR-Bohm experiments”  |
| 12:15– 12:30 PM  | <b>David Landau</b> (The University of Georgia)<br>Closing Remarks  |