



Recent Developments in Computer Simulational Studies in Condensed Matter Physics

Tentative Program of the 2009 – 22nd Annual Workshop

Monday, February 23rd

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| 8:30 – 10:00 AM | Registration in Room 321C of the Physics Building |
| 9:00 - 10:00 AM | Coffee and Donuts or Muffins in 3 rd floor new addition foyer
Informal discussion in Conference Room 322 |
| 10:00 – 10:05 AM | Bill Dennis (The University of Georgia - Head, Dept. of Physics & Astronomy) |
| 10:05 – 10:10 AM | David P. Landau (The University of Georgia)
Introductory Remarks |
| 10:25 – 11:25 AM | Francesca Tavazza (NIST)
“Atomistic Study of Tensile Deformation and Breaking Mechanisms
in Gold Nanowires” |
| 11:40 – 11:55 PM | Jindrich Kolorenc (North Carolina State)
“Electronic Structure of Solid FeO at High Pressures by Quantum
Monte Carlo Methods” |
| 12:00 PM | Lunch |
| 2:00 – 3:00 PM | Clare McCabe (Vanderbilt University)
“Molecular Modeling of Nanostructured Systems” |
| 3:15 – 3:30 PM | Nobuyasu Ito (University of Tokyo)
“MD simulation of thermal flow with liquid and gas phases” |
| | Break |
| 4:00 – 4:15 PM | Tristan Bereau (Carnegie Mellon University)
“Generic coarse-grained model for protein folding and aggregation” |
| 4:30 – 4:45 PM | Lucas Mol (Universidade Federal de Minas Gerais)
“Planar to paramagnetic phase transition in ferromagnetic thin films” |
| 5:00 – 5:15 PM | Lev Shchur (Landau Institute for Theoretical Physics)
“Criticality in the DLA Cluster Growth” |



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Tuesday, February 24th

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| 9:00 – 10:00 AM | Coffee and Donuts or Muffins in 3 rd floor new addition foyer
Informal discussion in Conference Room 322 |
| 10:00 – 11:00AM | Valentino Cooper (Oak Ridge National Laboratory)
“First principles simulations of sparsely packed solids” |
| 11:15 – 11:30 AM | Xiaojia Tang (University of Georgia)
“System Biology of Biological Clock for Neurospora Crassa” |
| 11:45 – 12:00 PM | Wolfhard Janke (University of Leipzig)
“Fractals Meet Fractals: Self-Avoiding Random Walks on Percolation Clusters” |
| 12 Noon | Lunch |
| 2:00 – 3:00 PM | Naoki Kawashima (University of Tokyo)
“Directed-loop quantum Monte Carlo simulation of bosonic systems” |
| 3:15 – 3:30 PM | Aniket Bhattacharya (University of Central Florida)
“On Universal Aspects of Forced Polymer Translocation Through a Nano-Pore” |
| 3:30 – 4:00 PM | Break |
| 4:00 – 4:15 PM | Anastasios Malakis (University of Athens, Greece)
“Strong Violation of Critical Phenomena Universality: Wang-Landau Study
Of 2D Blume-Capel Model Under Bond Randomness” |
| 4:30 – 4:45 PM | Shigenori Matsumoto University of Tokyo)
“Critical Behavior of the Square Lattice Blume-Capel model
with an Alternating Anisotropy and Next Nearest Neighbour Interaction” |



Recent Developments in Computer Simulational Studies in Condensed Matter Physics

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Wednesday, February 25th

- 9:00 – 9:30 AM Coffee and Donuts or Muffins in 3rd floor new addition foyer
Informal discussion in Conference Room 322
- 9:30 – 10:30 AM **Andrey Milchev** (Bulgarian Academy of Sciences)
“Pulling an Absorbed Polymer Chain off a Solid Surface”
- 10:45 – 11:00 AM **Gerd Schroeder-Turk** (University of Erlangen-Nuernberg)
“Hard Sphere Fluids Confined in Model Porous Media-Morphology
Vs Thermodynamic Properties”
- 11:15 – 11:30 AM **Mark Novotny** (Mississippi State University)
“Computational Efficiency of Rejection Free and Monte Carlo with Absorbing
Markov Chains Algorithms for Interacting Particles Systems”
- 11:45 – 12:00 PM **Tomoaki Nogawa** (University of Tokyo)
“Polydispersity effect on the solid-fluid transition in hard sphere system”
- Lunch
- 2:00 – 3:00 PM **David Sholl** (Georgia Tech)
“Simulation of Hydrogen Diffusion in Metals and Metal Hydrides”
- 3:15 – 3:30 PM **Per Arne Rikvold** (Florida State University)
“Degree Correlations in a Dynamically Generated Model Food Web”
- Break
- 4:00 – 5:00 PM **William Swope** (IBM Almaden Research)
“Protein Folding Simulations on the IBM BlueGene Supercomputer”
- 6:00 – 7:30 PM **Reception** in the North Tower of the Student Learning Center on campus



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Thursday, February 26th

- 9:00 – 9:30 AM Coffee and Donuts or Muffins in 3rd floor new addition foyer
Informal discussion in Conference Room 322
- 9:30 – 10:30 AM **Martin Weigel** (University of Mainz)
“Generalized-ensemble simulations and cluster algorithms”
- 10:45 – 11:00 AM **Efstathios Manousakis** (Florida State University)
“Frustration and Novel Order in Quantum Antiferromagnets
Driven by Hund’s Rule Coupling”
- 11:15 – 11:30 AM **Andrei Galiutdinov** (University of Georgia)
“Implementing GHZ States with Josephson Phase Qubits”
- 11:45 – 12:00 AM **Keola Wierschem** (Florida State University)
“Simulation of 2D Melting of Lennard-Jones Solid”
- Lunch
- 2:00 – 3:00 PM **Michal Bajdich** (North Carolina State)
“Pairing in cold atoms and other applications in quantum Monte Carlo”
- 3:15 – 3:30 PM **Michael Geller** (University of Georgia)
“Quantum Logic with Weakly Coupled Qubits”
- Break
- 4:00 – 5:00 PM Joint Workshop/Departmental Colloquium in Room 202
Wolfgang Christian (Davidson College)
“Building a Computational-Physics-Education Digital Library”



Recent Developments in Computer Simulation Studies in Condensed Matter Physics

Tentative Program of the 2009 – 22nd Annual Workshop

Friday, February 27th

- 8:30 – 9:00 AM** Coffee and Donuts or Muffins in 3rd floor new addition foyer
Informal discussion in Conference Room322
- 9:00 – 10:00 AM **Michael Bachmann** (University of Leipzig)
“Conformational Mechanics of Molecular Structure Formation Processes”
- 10:15 – 10:30 AM **Joan Adler** (Technion)
“Experiment (NEXAFS) versus simulation (DOS) for Carbon Allotropes
and Mixtures”
- 10:45 – 11:00AM **Daniel Seaton** (University of Georgia)
“A Wang-Landau study of the phase transitions in a flexible homopolymer”
- 11:15 – 11:30AM **Bob Swendsen** (Carnegie Mellon University)
“Optimized Convergence for Multiple Histogram Analysis”
- 11:30 – 11:45 **David Landau** (University of Georgia)
Closing Remarks