Recent Developments in Computer Simulational Studies in Condensed Matter Physics

Tentative Program of the 2020 – 33rd Annual Workshop

Monday, February 17th

8:30 – 10:00 AM  Registration in Room 321C of the Physics Building
9:00 - 10:00 AM  Coffee, Tea and Pastries in 3rd floor CSP area
                  Informal discussion in Conference Room 322
10:00 – 10:05 AM  Alan Dorsey, Dean of Arts & Sciences
10:05 – 10:10 AM  Phillip Stancil, Department Head of Physics and Astronomy
10:10 – 10:15 AM  David P. Landau  Director, Center for Simulational Physics
                  Introductory Remarks
10:15 – 11:15 AM  Robin Selinger, Kent State University
                  “Parallel Finite Element Elastodynamics Studies of Programmable Shape-Morphing Materials”
11:30 – 11:45 AM  Kipton Barros, Los Alamos National Laboratory
                  “Machine learning an interatomic potential for aluminum”
12:00 PM          Lunch
2:00 – 3:00 PM    Hans Herrmann, ESPCI Paris
                  “Rotating Matter: The Bearing State”
3:15 – 3:30 PM    Efstratios Manousakis Florida State University
                  “Quantum Monte Carlo study of Weyl superconductivity”
                  Coffee break
4:00 – 4:15 PM    Stefan Boettcher, Emory University
                  “Ground State Properties of the Diluted Sherrington-Kirkpatrick Spin Glass”
4:30 – 4:45 PM    Markus Eisenbach, Oak Ridge National Laboratory
                  “High Performance First-Principles Computations of Phase Transitions in Alloys using Monte-Carlo Methods and Machine-Learning”
5:00 – 5:15 PM    Nima Karimitari, University of Georgia
                  “First-principles investigations of structure and vibrations of c(4x2) PF₃ on Cu(001)”
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9:00 – 10:00 AM  Coffee, Tea and Donuts in 3rd floor CSP area
Informal discussion in Conference Room 322

10:00 – 11:00 AM  Aniket Bhattacharya, University of Central Florida
“Scaling Theory of Driven Polymer Translocation through a Double Nanopore”

11:15 – 11:30 AM  Martin Weigel, Coventry University
“Critical behavior of the random-field Potts model”

11:45 – 12:00 PM  Alfred Farris (Oxford College of Emory University)
“Effects of Lattice Constraints in Coarse-Grained Protein Models: A Wang-Landau Study”

12:00 PM  Lunch

2:00 – 3:00 PM  Jerome Delhommelle, University of North Dakota
“Expanded Wang Landau simulations and Machine Learning: Towards a partition function-based prediction of properties”

3:15 – 3:30 PM  Matthew Wilson, University of Georgia
“Wang-Landau Simulations of Peptide Aggregation with Lattice Models”
Coffee break

4:00 – 4:15 PM  Per Rikvold (Florida State University)
“Visualization of two-phase flow in porous media”

4:30 – 4:45 PM  Stefan Schnabel, Universität Leipzig
“Fast simulation of a large polymer with untruncated interaction near the collapse”

5:00 – 5:15 PM  Douglas Barlow, Alderman Barlow Labs
“Monte Carlo Study of a Liquid-Liquid Phase Transition Using a Modified Gibbs Ensemble”
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*Tentative Program of the 2020 – 33rd Annual Workshop*

**Wednesday, February 19th**

9:00 – 10:00 AM  Coffee, Tea and Donuts in 3rd floor CSP area
Informal discussion in Conference Room 322

10:00– 11:00 AM  Erin Teich, University of Pennsylvania
“Local structure, dynamics, and glass formation in hard polyhedral systems”

11:15 – 11:30 AM  Joao Plascak, Universidade Federal de Minas Gerais
“Monte Carlo simulations of Fe-Al alloys in the disordered phase”

11:45 – 12:00 PM  Group Photo

12:00 PM  Lunch

2:00 – 3:00 PM  Jing Yang, Massachusetts Institute of Technology
“A multi-scale view of trabochemistry—connecting first-principles theory and experiments”

3:15 – 3:30 PM  Ying Wai Li, Los Alamos National Laboratory
“Machine-learning assisted studies of material properties”

4:00 – 5:00 PM  Tsuyoshi Okubo, University of Tokyo
“Tensor network study on extended Kitaev models”

5:15 – 5:45 PM  Posters

6:00 – 8:30 PM  Reception – Miller Learning Center North Tower
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_Tentative Program of the 2020 – 33rd Annual Workshop_

**Thursday, February 20th**

9:00 – 10:00 AM  
Coffee, Tea and Donuts in 3rd floor CSP area  
Informal discussion in Conference Room 322

10:00 – 11:00 AM  
_Beth Lindquist_, Los Alamos National Laboratory  
“Statistical Inference of Equilibrium Statistical Mechanical Models”

11:15 – 11:30 AM  
_Mona Asadinamin_, University of Georgia  
“Dynamical properties of lithium niobate: A DFPT study”

11:45 – 12:00 PM  
_Henrik Christiansen_, Universität Leipzig  
“Accelerating molecular dynamics simulations with population annealing”

12:00 PM  
Lunch

2:00 – 3:00 PM  
_Robin Cortes-Huerto_, Max-Planck-Institut fuer Polymerforschung  
“Free energies and non-equilibrium molecular dynamics in adaptive resolution simulations”

3:30 – 4:30 PM  
_Departmental Colloquium/Workshop Invited Talk_  
_Dennis Rapaport_, Bar-Ilan University  
“GPU molecular dynamics: Algorithms, performance and examples”

4:45 – 5:45 PM  
Posters
Recent Developments in Computer Simulational Studies in Condensed Matter Physics

Tentative Program of the 2020 – 33rd Annual Workshop

Friday, February 21st

8:30 – 9:00 AM  Coffee, Tea, and Donuts in 3rd floor new addition foyer
Informal discussion in Conference Room322

9:00 – 10:00 AM  Wolfhard Janke, Universität Leipzig
“Phase-ordering kinetics of the long-range Ising model”

10:15 – 11:15 AM  Luiz Pereira, Universidade Federal de Pernambuco
“Phononic thermal conductivity of 2D materials with molecular dynamics simulations”

11:30 – 11:45 AM  Nobuyasu Ito, RIKEN
“Phase diagram of a traffic simulation model”

12:00 PM  David Landau  Director, Center for Simulational Physics
Closing Remarks

Posters:  (Note . . . posters will be displayed all week and participants are encouraged to view them during coffee breaks)

Yifan Dai (University of Georgia)
“Bending-Stiffness Dependent Generic Structural Transitions of Helical Polymers”

Garrett Floyd (University of Georgia)
“Title”

Steven Hancock (University of Georgia)
"Monte Carlo Simulations of Insulator-Metal Transitions of Correlated-Type Materials"

Kedkanok Sitarachu (University of Georgia)
“Exact microcanonical statistical analysis of transition behavior in Ising chains and strips”
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**Posters (continued):**

**Mingyu Sun** (University of Georgia)
“Correcting Measurement Errors on a Quantum Computer”

**Shengming Zhang** (University of Georgia)
“Determining a hyperphase diagram of a model for polymers doubly grafted to an attractive homogeneous substrate”