Skip navigation

Home / SUG Meeting Minutes and Agendas / Statewide Users Group Meeting Agenda - December 3, 2015

Statewide Users Group Meeting Agenda - December 3, 2015

- Meeting Information

Wednesday, December 2nd

3:00 - 5:00 pm	Allocations Committee Meeting
6:00 - 7:30 pm	SUG Executive Meeting

Thursday, December 3rd

10:00 - 11:00 am	Software Committee Meeting Hardware Committee Meeting Face-to-Face with OSCHelp
11:00 - 11:45 am	Flash Talk Session 1
11:45 - 12:15 pm	Lunch
12:15 - 1:00 pm	OSC Organizational Update
1:00 - 1:40 pm	Keynote Address Suzy Tichenor Oak Ridge National Laboratory Director, Industrial Partnerships Program
1:40 - 2:20 pm	Keynote Address Dr. Daniel Lacks Case Western Reserve University Professor, Chemical Engineering

2:20 - 2:30 pm	Break
2:30 - 3:15 pm	Flash Talk Session 2
3:15 - 5:30 pm	Poster Session Social Networking
5:30 pm	Talk and Poster Winner Announcement

Keynote Addresses

Oak Ridge Leadership Computing Facility and Industry: Partnering for Success
Suzy Tichenor, Director of the Industrial Partnerships Program at Oak Ridge National Laboratory

In today's highly competitive world, companies are using modeling and simulation with high performance computing to gain important competitive advantages. Yet many firms have computational problems that exceed their internal computing capabilities. The Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory has an industrial partnerships program that helps companies access its Titan supercomputer, the nation's most powerful HPC system for open research. This talk will provide an overview of this program, and how companies are using Titan to make progress on their seemingly intractable computational challenges and advance in their use of large scale HPC systems.

Solvophobicity - what makes a surfactant effective when the solvent is not just water
Dr. Daniel Lacks, Professor of Chemical Engineering at Case Western Reserve University

We all know that surfactants partition to the surface of water, because one part of the surfactant molecule is "hydrophilic" and wants to be in the water, while the other part of the molecule is "hydrophobic" and wants to be out of the water. Perhaps the simplest example of a surfactant consists of a carboxylic acid, which is hydrophilic, connected to an alkane chain, which is hydrophobic. But what happens when the solvent is not just water, but a water-alcohol mixture? The alkane chain, which is hydrophobic, may not be "solvophobic" with this water-alcohol solvent. What molecular segments will be solvophobic, and can we determine the particular characteristics of the molecule that make it solvophobic? We describe in this talk our combined experimental-simulation investigation to address these questions.

Flash Talk Session 1

Iron abundance in the Sun
Sultana Nahar, The Ohio State University

Explaining double perovskite ordering phenomena through atomic resolution electron microscopy and simulation
Bryan Esser, The Ohio State University

Improving the Regional Arctic System Reanalysis with High-Performance Computing
Aaron Wilson, The Ohio State University

Gpu-Accelerated Molecular Dynamic Simulations of Active Nematics
Michael Varga, Kent State University

Virtual Weld Simulation in a High Performance Computing Environment
Elizabeth Kurth, Engineering Mechanics Corporation

Modeling liquid crystal plasma mirrors using PIC simulations
Ginevra Cochran, The Ohio State University

Flash Talk Session 2

Molecular Mechanisms of Hydrophobic Collapse
Sumit Sharma, Ohio University

How organization of clouds effects the climate
Thijs Heus, Cleveland State University

Lattice distortion and elastic properties of HfNbTaTiZr high entropy alloy
Changning Niu, The Ohio State University

Molecular bases for the selection of the chromophore of animal rhodopsins
Hoi Ling 'Calvin' Luk, Bowling Green State University

Evolutionary Models and the OSC
Bryan Carstens, The Ohio State University

Investigating the phase behavior of Lidocaine in 1-n-butyl-3-methylimidazolium based ionic liquids
Ryan Ley, Miami University

Poster Session

A DFT Study on CO Poisoning Effects on FeNC and CNx ORR catalysts
Qiang Zhang, The Ohio State University

RNPT: Monochromatic X-rays for cancer treatment

Sultana Nahar, The Ohio State University

Analytical and Clinical Validation of a Targeted RNA Sequencing-Based Method for Detection of Gene Fusions

Jharna Miya, The Ohio State University

CanDL: Cancer Driver Log

Esko Kautto, The Ohio State University

Atomistic modelling of Ti-Nb alloys

Chris Ehemann, The Ohio State University

The Draft Genome of Taraxacum kok-saghyz, an Alternative Natural Rubber Resource

Xiaofeng Zhuang, The Ohio State University

First-Principles-Based kinetic Monte Carlo simulation for thermal reduction of PdO(101) surface

Minkyu Kim, The Ohio State University

A Low-Scaling Quantum Chemistry Approach to the Simulation of Excited State Properties and Energy Transfer Processes in Sizable

Adrian Morrison, The Ohio State University

Distinct Conformational Dynamics of Human K-Ras and Oncogenic Mutants Studied by Long Molecular Dynamics Simulations

Yina Gu, The Ohio State University

Epigenetic and genomic landscape in cancer

Elizabeth Baskin, The Ohio State University

Noise Perturbation Improves Supervised Speech Separation

Jitong Chen, The Ohio State University

Molecular Dynamics of Small Molecule Penetrants in Microphase Separated Copolymers

Youngmi Seo, The Ohio State University

Deploying a next-generation informatics infrastructure for genomics research

Daniel Kinnamon, The Ohio State University

Computational Study of the Decarboxylation Reaction of Aminomalonic Acid

Daqing Gao, Central State University

Virtual Weld Simulation in a High Performance Computing Environment

Elizabeth Kurth, Engineering Mechanics Corporation

Design rules for rational control of polymer glass formation behavior and mechanical properties with small molecular additives

Jayachandra Hari Mangalara, University of Akron

Parallelization and Convergence of VASP DFT Code on OSC Machines
Nikolas Antolin, The Ohio State University

Ab initio study of point defects in Boron Arsenide (BAs)
Yaxian Wang, The Ohio State University

Modeling c+a dislocation behavior in Mg
Daniel Buey, The Ohio State University

Revisiting the TA+/TB- hypothesis: the importance of accounting for interfacial potentials
Travis P. Pollard, University of Cincinnati

Dislocation- Boundary Interaction in Titanium: Molecular Dynamics Study
Mohammad Shahriar Hooshmand, The Ohio State University

Investigating the phase behavior of Lidocaine in 1-n-butyl-3-methylimidazolium based ionic liquids
Ryan Ley, Miami University

Water Adsorption on Olivine(010) surface
Tingting Liu, The Ohio State University

Quantifying Ionic Aggregates during Mechanical Deformation of Ionomer Systems using Molecular Dynamics Simulations
Connor Barber, The Ohio State University

Navigation

‹ Statewide Users Group Meeting Agenda - Dec 4, 2014 | up | Statewide Users Group Meeting Agenda - June 4, 2015 ›

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