

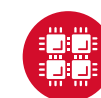


Ohio Supercomputer Center

SUG

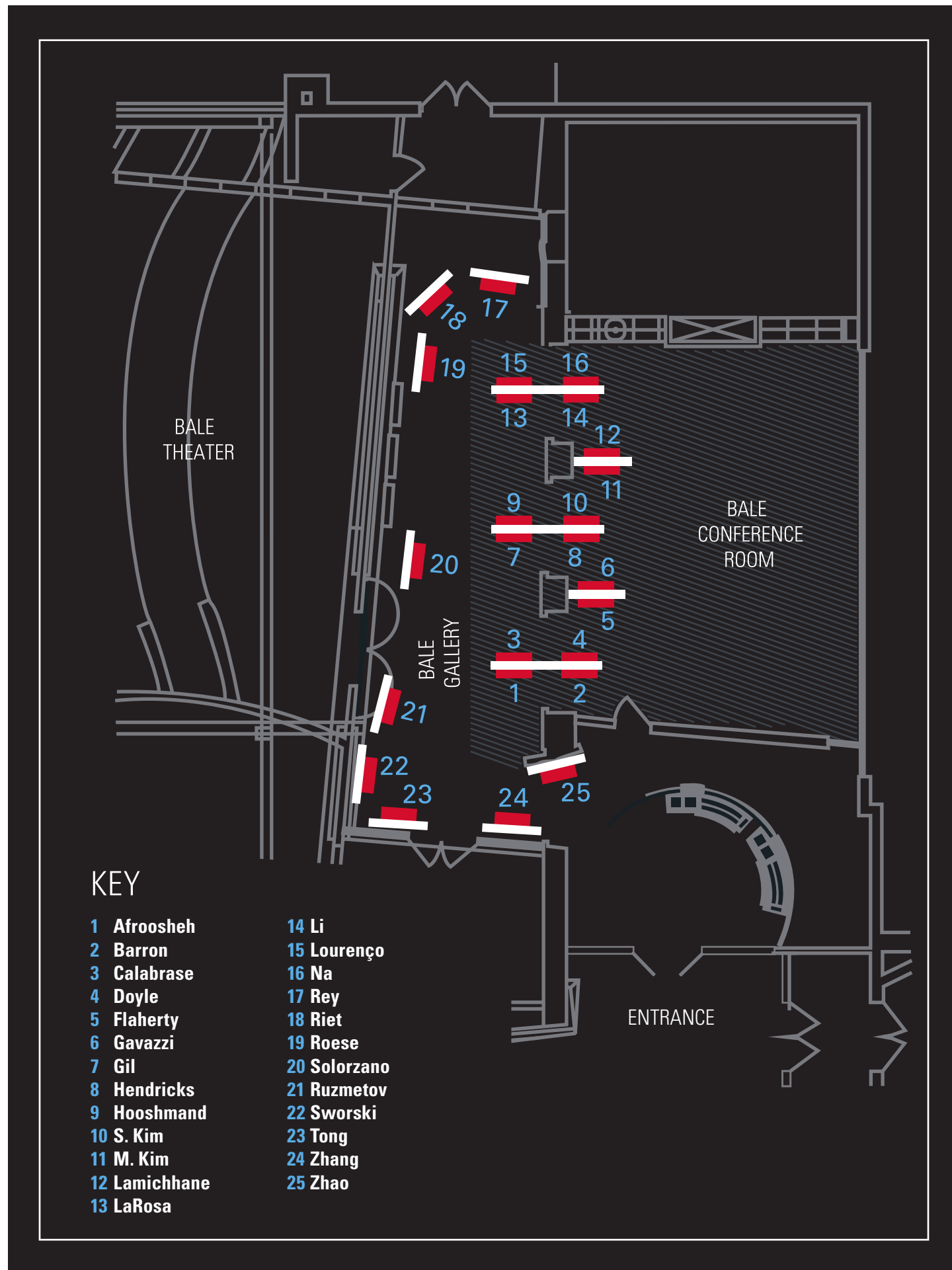
Statewide Users Group

Autumn Conference
September 28, 2017



Ohio Supercomputer Center

An OH·TECH Consortium Member



Agenda

Thursday, September 28		
8:15–9:00 am	SOCC Tour (invitation only)	Lobby and SOCC
9:00–10:00 am	Hardware Committee Software Committee	BALE Conference Room Room 214
10:00–11:00 am	Breakout Sessions: OnDemand and App Development Big Data Interface Lab: Visualiation & Virtual Environments	BALE Conference Room Polar Conference Room Room 208
11:00–11:45 am	Keynote Address: Bryan C. Carstens	BALE Theater
11:45 am–12:00 pm	Lunch Pick-up	BALE Lobby
12:00–12:55 pm	OSC Presentation (food welcome)	BALE Theater
1:05–1:50 pm	Flash Talk Session 1	BALE Theater
2:00–2:50 pm	Flash Talk Session 2	BALE Theater
3:00–3:15 pm	Break	
3:15–4:45 pm	Poster Session, Hors d’Oeuvres, Networking	BALE Lobby
4:45 pm	Poster and Flash Talk Winner Announcement	BALE Lobby

At 5:30pm there will be a social hour (not sponsored by OSC) at the Smokehouse Brewing Company.

Flash Talks

1. Bioinformatics: From Reference Genomes to Individuals using Existing Datasets
R. Keith Slotkin | The Ohio State University

2. Functional Group Effect on Electrolyte Liquid Structure
Andrew Eisenhart | University of Cincinnati

3. Speech segmentation with a neural net model of working memory
Cory Shain | Ohio State University

4. Incorporation of Mass Spectrometry Covalent Labeling Experimental Data into Rosetta Scoring Function
Melanie Aprahamian | The Ohio State University

5. Journal Information Extractor –SW Model
Yuxi Cheng | The Ohio State University

6. Cochannel Speech Separation in Reverberant Conditions
Masood Delfarah | The Ohio State University

7. Reverse engineering of the human genome: predicting protein-DNA interactions across multiple cell types
Yichao Li | Ohio University
8. Morphology Effects on Diffusion of Selective Penetrants in Diblock Copolymers from Molecular Dynamics Simulations
Kuan-Hsuan Shen | The Ohio State University

9. Effects of Copolymer Sequence on Adsorption and Dynamics Near Nanoparticle Surfaces in Simulated Polymer Nanocomposites
Alex Trazkovich | The Ohio State University

10. Modeling Surface Induced Dissociation to Improve Protein-Protein Docking
Justin Seffernick | The Ohio State University

11. Reducing irradiation of normal tissue with alternative X-rays sources and nanoparticles: Monte Carlo simulations
Maximillian Westphal | The Ohio State University

12. Automatic Rhodopsin Modeling for High-Throughput Computational Photobiology
Xuchun Yang | Bowling Green State University

Keynote Address

Bryan C. Carstens

Associate Professor,
Vice Chair

Department of Evolution,
Ecology and Organismal Biology
at The Ohio State University

A Chicago native, Bryan Carstens earned a bachelor’s degree in English and another in Zoology/Animal Biology from Michigan State University in 1998. He earned a master’s degree in Zoology from Michigan State University in 2001 and a doctorate in Genetics from the University of Idaho in 2004.

Currently, Carstens and his research team at The Ohio State University use computational approaches to understand how biological diversity is generated. By investigating evolutionary processes, his goal is to generate realistic models of the historical demography and quantify the probability of these models given collected genomic data.

Posters

1. Modeling Surface Enhanced Raman Spectroscopy with Implicit and Explicit Solvents
Sajjad Afroosheh | Bowling Green State University

2. Reconciling Linear Measurements of Fractal Cloud Structures
Nick Barron | Cleveland State University

3. What Determines the Shape of a Cloud?
William Calabrase | Cleveland State University

4. Examination of the mulitpole decomposition of electrostatic potential in the single-ion solvation process
Carrie Doyle | University of Cincinnati

5. Characterizing the turbulent Structure of the Atmospheric Boundary Layer Using Large Eddy Simulations
Justin Flaherty |Cleveland State University

6. Thermodynamic and kinetic representations of cooperative allosteric binding in calmodulin
Daniel Gavazzi | Kent State University

7. The Solvophobic Effect
Dan Gil |Case Western Reserve University

8. Searching for Supersymmetry at the Large Hadron Collider
Khalida Hendricks | The Ohio State University

9. Oxygen Diffusion around (10-12) Twin Boundary in Ti
Mohammad Shahriar Hooshmand | The Ohio State University

10. Predicting Disordered Regions of Proteins
Stephanie Kim | The Ohio State University

11. First-Principles Kinetic Monte Carlo Simulation of CO Oxidation on PdO(101)
Minkyu Kim | Ohio State University

12. Computational Study of Lattice Dynamics of Defects in ZnO
Aneer Lamichhane | Bowling Green State University

13. Dislocation-phase boundary interactions in Ni and fcc Co
Carlyn LaRosa | The Ohio State University
14. Reverse engineering of the human genome: predicting protein-DNA interactions across multiple cell types
Yichao Li | Ohio University

15. Local environment structure and dynamics of CO₂ in the related ionic liquids
Tuanan Lourenço | Fluminense Federal University

16. Finite Element based Particle-in-Cell Simulations of Micromachined Plasma Beam Devices
Dong-Yeop Na | The Ohio State University

17. Using Artificial Neural Networks to model evaporation and CO₂ fluxes in a coastal reef.
Camilo Rey | The Ohio State University

18. MD Simulation of Diffusion in MgO
Adriaan Riet | Case Western Reserve University

19. Parameterizing MOSCED with Electronic Structure Calculations to Predict Vapor-Liquid Equilibrium
Sydnee Roesse | Miami University

20. Point defects and the electronic structure of the antiferromagnetic phases of CrN
Tomas Rojas Solorzano |Ohio University

21. Binding thermodynamics and kinetics of an Intrinsically Disordered Protein
Talent Ruzmetov | Kent State University

22. How High Does the Lower Atmosphere Go?
Vladimir Sworski | Cleveland State University

23. Development of innovative ventilation systems of manure-belt layer houses for improved indoor environment
Xinjie Tong | The Ohio State University

24. CO and Phosphate Poisoning Effects on FeN/C and CNx: A First-principles Study
Qiang Zhang | The Ohio State University

25. Large-scale Computation for Plasma Opacities
Lianshui Zhao | The Ohio State University