Ohio Supercomputer Center

SUG

Statewide Users Group

Spring Conference
April 6, 2017

Ohio Supercomputer Center
An OH·TECH Consortium Member

Agenda

Thursday, April 6

8:15–9:00 am	SOCC Tour (invitation only)	Lobby and SOCC
9:00–10:00 am	Hardware Committee	BALE Conference Room
10:00–11:00 am	Breakout Sessions: How to Choose the Right File System for Your Work Overview of Profiling and Debugging Tools Using GPUs at OSC	 Polar Conference Room Csuri Conference Room BALE Conference Room
11:00–11:45 am	Keynote Address: Jonathan Bentz	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	Client Portal Overview	BALE Theater
3:15–4:45 pm	Poster Session, H'orderves, Networking	BALE Lobby
4:45 pm	**Poster and Flash Talk Winner Announcement**	**BALE Lobby**
4:45–5:30 pm	SOCC Tour (invitation only)	Lobby and SOCC

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

Flash Talks

1. Computational Investigation of Fruit Fly Aerodynamics in Forward Flight
   Chengyu Li | The Ohio State University
2. EpiTEome: Simultaneous Detection of Transposable Element Insertion Sites and their DNA Methylation Levels
   Josquin Daron | The Ohio State University
3. Measuring the Universe with WFIRST
   Xiao Fang | The Ohio State University
4. Theoretical Study of Molecular Determinants for ATP-Binding in Proteins - A High Level Quantum Chemical Analysis
   Xiche Hu | University of Toledo
5. Phonon Boltzmann Transport Equation Based Modeling of Time Domain Thermo-Reflectance Experiments
   Sandip Mazumder | The Ohio State University
6. Atomistic Understandings of Nanoporous Materials for Energy-Related Applications
   Chi-Ta Yang | The Ohio State University
7. Identification of Carnivory in Plants via Genomic Functional Annotation
   Gregory Wheeler | The Ohio State University
8. eComputational Modeling Reveals that Signaling Lipids Modulate the Orientation of K-Ras4A at the Membran
   Zhenlu Li | Case Western Reserve University
9. Modeling the Photodynamics of 11-cis Retinal Chromophore in Solution
   Madushanka Manathunga | Bowling Green State University
10. Prediction of Solubility of Non-Electrolyte Solutes using MOSCED Parameterized by SMD and SM8
    Jeremy Phifer | Miami University

Keynote Address | 11:00–11:45 am

Jonathan Bentz

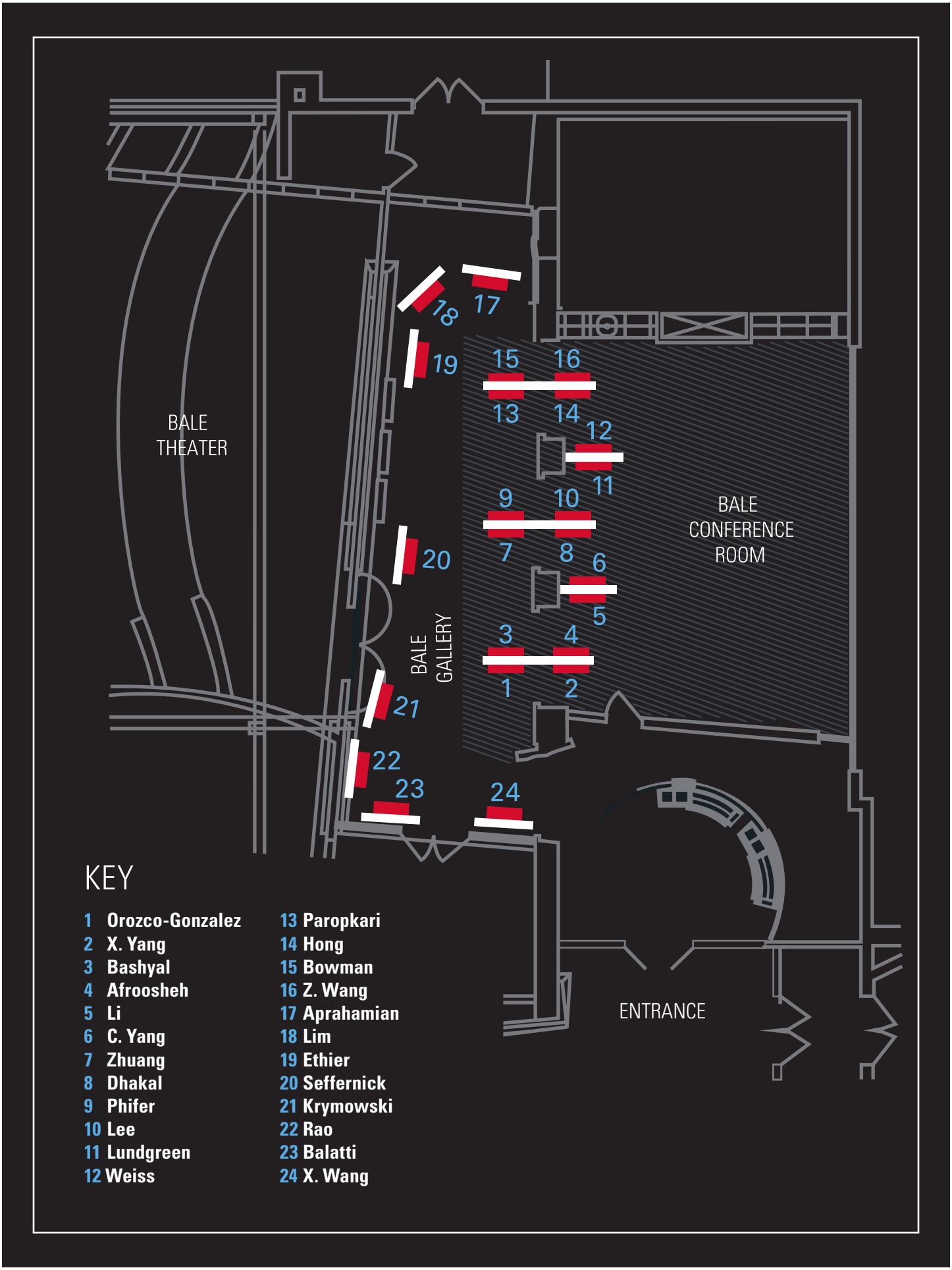
Solutions Architect

NVIDIA

Jonathan Bentz is a senior solutions architect with NVIDIA, focusing on higher education and research customers. In this role he works as a technical resource to support and enable the use of GPU computing. Jonathan has a background in computational chemistry and software engineering and frequently conducts hands-on programming sessions for CUDA, OpenACC and GPU-accelerated deep learning. In light of OSC's recent GPU adoption, Jonathan will discuss current advances in GPU hardware and software which directly impact accelerated applications in HPC and have been a catalyst in the rapid advancement of deep learning technologies.

Posters

1. QM/MM Geometry Optimization of Chromophore-Protein Complexes Using the ASEC Free Energy Gradient
   Yoelvis Orozco-Gonzalez | Bowling Green State University
2. Probing the Vibrational Phase Isotope Effect on the Photochemistry of Vision
   Xuchun Yang | Bowling Green State University
3. Role of Bond Ionicity in Correcting the Band Gap of ZnO Using DFT+U
   Keshab Bashyal | Bowling Green State University
4. Molecular Recognition Using Surface Raman Spectroscopy: DFT Study
   Sajjad Afroosheh | Bowling Green State University
5. eComputational Modeling Reveals that Signaling Lipids Modulate the Orientation of K-Ras4A at the Membrane
   Zhenlu Li | Case Western Reserve University
6. Atomistic Understandings of Nanoporous Materials for Energy-Related Applications
   Chi-Ta Yang | The Ohio State University
7. Construction and Application of the Draft Genome of Taraxacum kok-saghyz, an Alternative Natural Rubber Resource
   Xiaofeng Zhuang | The Ohio State University
8. Calculation of Infinite Dilution Activity Coefficient Using MOSCED: Expansion of the MOSCED Solvent Database to Amides, glycols a
   Pratik Dhakal | Miami University
9. Prediction of Solubility of Non-Electrolyte Solutes Using MOSCED Parameterized by SMD and SM8
   Jeremy Phifer | Miami University
10. The Analysis of Time-Harmonic Electromagnetic Interactions with Large-Scale Complex Platforms
    Chung Hyun Lee | The Ohio State University
11. Heat Transfer and Deposition in Gas Turbine Engines
    Ryan Lundgreen | The Ohio State University
12. Ab-Initio Study of Point Defects in Hexagonal Boron Nitride
    Elan Weiss | The Ohio State University
13. Stability of Salivary Microbiome
    Akshay Paropkari | The Ohio State University
14. CFD Simulations of Fate and Transport of Pesticide Droplets Discharged from Air-assisted Sprayers in Orchards
    Se-Woon Hong | The Ohio State University
15. Using Molecular Dynamics to Investigate Troponin C Evolution
    Jacob Bowman | The Ohio State University
16. A Speech Enhancement Alogrithm by Iterating Single- and Multi-Microphone Processing and its Application to Robust ASR
    Zhongqiu Wang | The Ohio State University
17. Incorporation of Mass Spectrometry Covalent Labeling Data into Rosetta Protein Structure Prediction
    Melanie Aprahamian | The Ohio State University
18. Atomistic Understandings of the Effects of Force Fields on their Predictions of CO2 Adsorption Properties in All-Silica Zeolites
    Jian Ren Lim | The Ohio State University
19. Analyzing the Structure and Entanglements in Absorbed Pairs of Hairy Nanoparticles Using Molecular Dynamics Simulations
    Jeffrey Ethier | The Ohio State University
20. Modeling Surface Induced Dissociation to Improve Protein-Protein Docking
    Justin Seffernick | The Ohio State University
21. Engineering 2D Materials with Functional Molecules
    Kevin Krymowski | The Ohio State University
22. First Principle Study of Twinning Formation in Ni3Al
    You Rao | The Ohio State University
23. tsRNA Profiling in Cancer
    Veronica Balatti | The Ohio State University
24. Big Data in Food Marketing: Prospects and Challenges
    Xiaojin Wang | The Ohio State University



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1 Orozco-Gonzalez
2 X. Yang
3 Bashyal
4 Afroosheh
5 Li
6 C. Yang
7 Zhuang
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9 Phifer
10 Lee
11 Lundgreen
12 Weiss
13 Paropkari
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15 Bowman
16 Z. Wang
17 Aprahamian
18 Lim
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20 Seffernick
21 Krymowski
22 Rao
23 Balatti
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