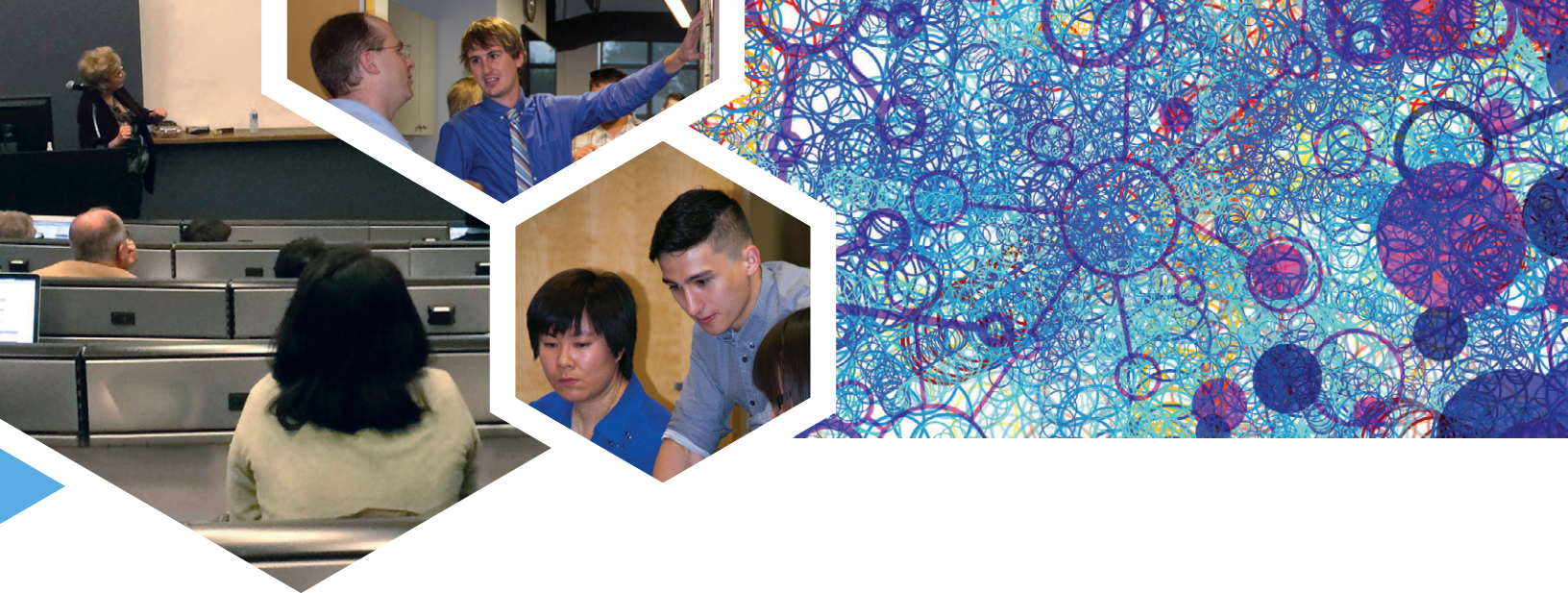




Statewide Users Group

Since the first meeting of the Statewide Users Group (SUG) in November 1986—almost a full year before the official 1987 establishment of the Ohio Supercomputer Center by the Ohio Board of Regents (now the Ohio Department of Higher Education)—Ohio research practitioner-advisors have been providing OSC’s leadership with sage program and policy advice. To that end, SUG established several standing committees to consider vital issues and meets as a whole twice a year to provide a forum for discussing current issues and trends and to present current developments in research.

The SUG Allocations Committee oversees a peer review grant process that allocates system resources to all academic users of the center. The Hardware and Operations Committee advises leadership on user needs and priorities for hardware configuration and acquisitions, as well as policy, procurement and operational issues. The Software and Activities Committee reviews software supported by the center for availability, clarity of documentation, quality of user interface, ease of use, logical development of the presentation, effectiveness, contribution to OSC resources and degree of restrictions. Eligible principal investigators of any OSC project are welcome to attend SUG general and committee meetings.

Guest speakers are a regular feature of SUG meetings. This past June, Jeff Graham, director of the Air Force Research Lab’s HPC facility at Wright-Patterson Air Force Base, spoke to SUG members on “AFRL DSRC: Not just a DoD Supercomputing Resource Center.” Graham was followed by Annika Peter, Ph.D., an assistant professor of physics at The Ohio State University, who presented “Exploring the Dark Side with Simulations.”

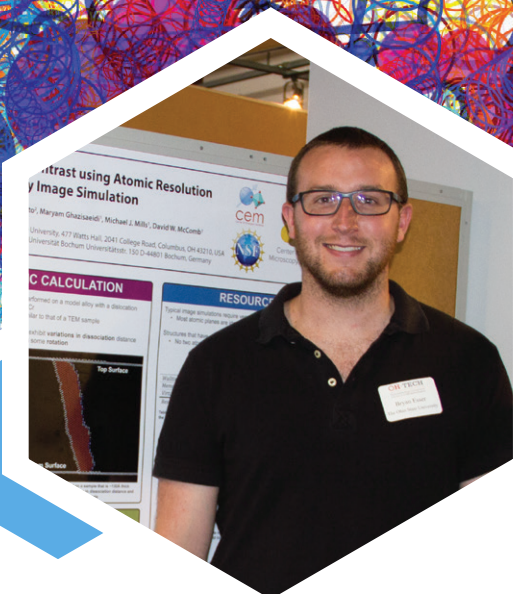
In December 2014, SUG heard from Evelyn M. Goldfield, Ph.D., program director for the chemistry division at

the National Science Foundation. As keynote speaker, Goldfield spoke on “NSF Support for High Performance Computing and Cyberinfrastructure.” Invited Speaker Ray Leto, president of a local engineering service provider, shared his perspectives with “TotalSim USA and the Ohio Supercomputer Center.” Earlier, at the June 2014 meeting, guest speaker Barry Dunietz, Ph.D., an assistant professor of chemistry and biochemistry at Kent State University, delivered a technical discussion titled “Two Tales on Computational Modeling of Charge Transfer Processes That Revise Understanding of Measured Spectra.”

Beginning with the December 2014 meeting, SUG has hosted flash talk and poster competitions. OSC added this particular feature to the meeting as a way of placing more focus on the research needs and outcomes of the center’s clients. The top entry in each category, as judged by a team of OSC staff, appears on the following pages.

SUG Executive Committee

Chair	Tom Beck, University of Cincinnati
Vice Chair	Hendrik Heinz, University of Akron (vacant as of August 2015)
Allocations Committee Chair	Christopher Hadad, The Ohio State University
Software Committee Chair	Rick Prairie, University of Cincinnati
Hardware Committee Chair	John Heimaster, The Ohio State University
Non-voting OSC Staff	David Hudak, Brian Guilfoos, Karen Tomko, Basil Gohar, Doug Johnson



June Poster Winner

Project Lead:

Bryan Esser,
The Ohio State University

Research Title:

Understanding dislocation core contrast using atomic resolution electron microscopy image simulation

Funding Source:

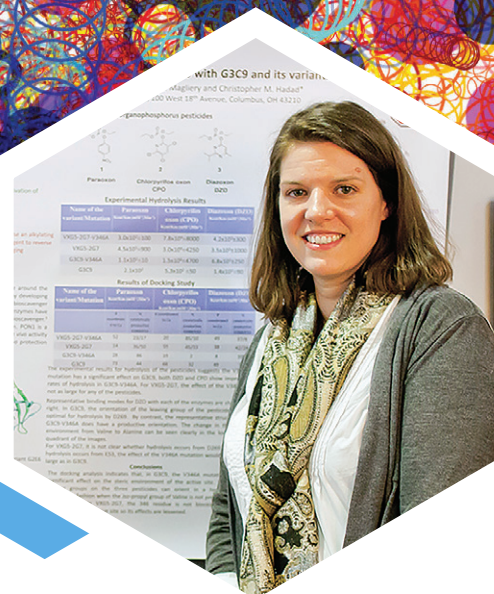
National Science Foundation

Bryan Esser, a graduate student majoring in materials science and engineering at The Ohio State University, took first place in the poster competition of the June 2015 meeting of OSC's Statewide Users Group. Esser also works as a graduate research associate at Ohio State's Center for Electron Microscopy and Analysis (CEMAS).

"Atomic resolution scanning transmission electron microscopy (STEM) is often used to analyze deformation mechanisms and properties," Esser explained. "Strong contrast has been observed around dislocation cores using medium-angle annular dark-field STEM, but not in high-angle conditions."

The research team to which Esser belongs conducted atomic-resolution image simulations at OSC using μ STEM, a software package for modeling the inelastic scattering of fast electrons. These simulations help to explain the nature of contrast variation as a function of scattering angles for thin-foil samples of these high-entropy alloys.

The research project is credited to Esser, as well as Timothy Smith, Maryam Ghazisaeidi, Ph.D., Michael Mills, Ph.D. and David McComb, Ph.D. (all of Ohio State), as well as Easo George, Ph.D., and Frederik Otto, Ph.D. (both of Ruhr University Bochum, Germany).



December Poster Winner

Project Lead:

Katharine Cahill,
The Ohio State University

Research Title:

Molecular docking study of organophosphorus pesticides with G3C9 and its variants

Funding Source:

National Institutes of Health

Katharine Cahill, a post-doctoral research associate specializing in organic chemistry and working in the Hadad Research Group at The Ohio State University, took first place in the poster competition of the December 2014 meeting of OSC's Statewide Users Group.

"Organophosphorus (OP) compounds are highly toxic chemicals capable of inhibiting the hydrolysis of the neurotransmitter acetylcholine by acetylcholinesterase," said Cahill. "Catalytic hydrolysis of OPs with enzymatic bio-scavengers, such as paraoxonase (PON1), is an active avenue of investigation towards the treatment of OP exposure."

G3C9 is a recombinant PON1 enzyme, which was developed for its improved solubility and has some effectiveness against OP pesticides. In this study, molecular docking simulations were performed at OSC on G3C9 and several of its variants. Docking analysis shows that, the V346A mutation significantly improves OP binding to the active site, compared to G3C9.

The research project was credited to Cahill, as well as her co-authors: Kiran Doddapaneni, Shameema Oottikkal, Thomas J. Magliery and Christopher Hadad, all of Ohio State.



June Flash Talk Winner

Project Lead:

Jason Brown,
The Ohio State University

Research Title:

A computational study of organophosphonate encapsulation in functionalized molecular baskets

Funding Source:

Defense Threat Reduction Agency,
National Institutes of Health

Jason Brown, a post-doctoral student specializing in organic chemistry and working in the Hadad Research Group at The Ohio State University, took first place in the flash talk competition of the June 2015 meeting of OSC's Statewide Users Group.

"Organophosphorus nerve agents (OPs) are a toxic class of compounds that have been used as pesticides and chemical warfare agents, and compounds for which there is a great need of effective therapeutics," Brown explained.

Gated molecular baskets conjugated to aliphatic amino acid functionalities have been examined for the binding and hydrolysis of the toxic nerve agent upon entering the bloodstream. Brown and the research group to which he belongs developed a computational protocol for the molecular baskets, including a Monte Carlo conformational search, molecular dynamics simulations and docking calculations, and ran the simulations on OSC systems.

In his talk, Brown acknowledged the contributions of Christopher Hadad, Ph.D., Jovica Badjic, Ph.D., Jeremy Beck, Ph.D., Ryan Yoder, Ph.D., Jeremy Erb, Ph.D., Paul Peterson, Ph.D., and Katharine Cahill, Ph.D. (all of Ohio State).



December Flash Talk Winner

Project Lead:

Matthew McMahon,
The Ohio State University

Research Title:

First PIC simulations modeling the interaction of ultra-intense lasers with sublayer with sub-micron, liquid crystal targets

Funding Source:

Defense Advanced Research Projects Agency

Matthew McMahon, a post-doctoral student specializing in physics and working as a graduate research associate with the High Energy Density Physics (HEDP) research group at The Ohio State University, took first place in the flash talk competition of the December 2014 meeting of OSC's Statewide Users Group.

"We recently introduced liquid crystal films as on-demand, variable thickness (50–5,000 nanometers), inexpensive targets for intense laser experiments," he said. "Here, we present the first particle-in-cell (PIC) simulations of short-pulse laser excitation of liquid crystal targets using the PIC code LSP, which is designed for large scale plasma simulations."

In order to accurately model the target evolution, McMahon and his research colleagues employed a low starting temperature and field ionization model. This was essential, as large starting temperatures lead to expansion of the target causing significant reduction of the target density before the laser pulse can interact. McMahon also described his group's investigation of the modification of laser pulses by very thin targets.

The project was credited to McMahon and his co-authors: Patrick Poole, Chris Willis, Ginevra Cochran, C. David Andereck and Douglass Schumacher, all of Ohio State.