

2015 Annual Program Review Agenda

Monday, July 27 – Thursday, July 30
Crystal Gateway Marriott Hotel, Arlington, VA

Updated Wednesday, August 5, 2015

Monday, July 27

- 11:30am – 6:00pm **Registration** — *Grand Registration Desk*
- 12:00 – 1:30pm **New Fellows Luncheon & Orientation** — *Salon H*
- 1:30 – 4:00pm **Introductory HPC Session** — *Salons A & B*
Required for incoming and first-year fellows. Others are also welcome.
- **Judith Hill** — Computational Scientist and Liaison Task Lead, Scientific Computing Group/National Center for Computational Sciences, Oak Ridge National Laboratory; DOE CSGF Alumna
 - **Jack Deslippe** — HPC Consultant, NERSC/Lawrence Berkeley National Laboratory; DOE CSGF Alumnus
 - **Hal Finkel** — Assistant Computational Scientist, Argonne Leadership Computing Facility, Argonne National Laboratory; DOE CSGF Alumnus
- 4:30 – 6:00pm **Making Fellow & Alumni Connections** — *Salons H & J*
All conference attendees who have arrived in D.C. are encouraged to attend.

Tuesday, July 28

- 7:30am – 6:00pm **Registration** — *Grand Registration Desk*
- 7:30 – 9:00am **Continental Breakfast** — *Salons H & J*
- 8:00 – 9:00am **Photo Session: Incoming Fellows (Head Shots & Group Photo)** — *Salon E*
- 9:00 – 9:15am **Welcome** — *Salons A, B & C*
Robert Voigt — Krell Institute
- 9:15 – 9:30am **Welcome** — *Salons A, B & C*
Steve Binkley — Associate Director of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy
- 9:30 – 9:45am **Welcome** — *Salons A, B & C*
Douglas P. Wade — Acting Director of Advanced Simulation and Computing, and Institutional Research and Development, Office of Defense Programs, National Nuclear Security Administration, U.S. Department of Energy
- 9:45 – 10:30am **Alumni Keynote** — *Salons A, B & C*
Sommer Gentry — Associate Professor of Mathematics, United States Naval Academy; DOE CSGF Alumna
“Optimization and Organs: Computational Methods for Rationing Transplantation”
- 10:30 – 10:45am **Break** — *Foyer, Salons A, B & C*
- 10:45 – 11:00am **Announcement of 2015 Frederick Howes Scholar** — *Salons A, B & C*
David Brown — Director, Computational Research Division, Lawrence Berkeley National Laboratory
- 11:00 – 11:45am **Howes Scholar Presentation** — *Salons A, B & C*
Devin Matthews — Postdoctoral Researcher, Science of High-Performance Computing Group/Institute for Computational Engineering and Science, University of Texas at Austin; DOE CSGF Alumnus

"Doing Computational Chemistry With Square Pegs and Round Holes"

11:45am – 12:45pm

Luncheon — *Salons H & J*

Session I — *Salons A, B & C*

Moderator: Michael Martin — Office of Science, U.S. Department of Energy

1:00 – 1:20pm

Heather Mayes — Northwestern University
"Harnessing HPC to Discover Reactions for Renewable Chemicals and Fuels"

1:20 – 1:40pm

Jarrod McClean — Harvard University
"Quantum Computers and Quantum Chemistry"

1:40 – 2:00pm

Christopher Ivey — Stanford University
"Geometric Volume of Fluid Methods for the Simulation of Two-phase Flow on Unstructured Meshes"

2:00 – 2:20pm

Sarah Loos — Carnegie Mellon University
"Verifying Distributed Car and Aircraft Systems With Logic and Refinement"

2:20 – 2:40pm

Break — *Foyer, Salons A, B & C*

Session II — *Salons A, B & C*

Moderator: Michael Martin — Office of Science, U.S. Department of Energy

2:40 – 3:00pm

Joshua Vermaas — University of Illinois at Urbana-Champaign
"Exploring Biomass Recalcitrance at the Petascale With Molecular Simulation"

3:00 – 3:20pm

Phoebe DeVries — Harvard University
"Geodetically Constrained Models of Viscoelastic Stress Transfer and Earthquake Triggering Along the North Anatolian Fault"

3:20 – 3:40pm

Jason Bender — University of Minnesota
"Nitrogen Dissociation in Hypersonic Flows: A Molecular Dynamics Investigation"

3:40 – 4:00pm

Omar Hafez — University of California, Davis
"Toward Automating Patient-specific Stress Analysis From Medical Imaging"

4:00 – 5:00pm

Break/Poster Set Up — *Salons H, J & K*

4:00 – 5:00pm

Fourth-Year/Outgoing Fellow Session — *Salon G*

5:00 – 7:00pm

Fellows' Poster Session — *Salons H, J & K*
Welcome & Remarks (5:05pm)
Franklin (Lynn) M. Orr — Under Secretary for Science and Energy, Office of Science, U.S. Department of Energy

Wednesday, July 29

7:30am – 5:00pm

Registration — *Grand Registration Desk*

7:30 – 9:00am

Continental Breakfast — *Salons H & J*

8:00 – 8:30am

Photo Session: Fellow/Alumni Retakes (Head Shots) — *Salon E*

8:30 – 9:00am

Photo Session: First-Year Fellows (Group Photo) — *Salon E*

9:00 – 9:15am

Announcements — *Salons A, B & C*
CYSE Contest Award Presentation
Bill Cannon — Science Media Manager, Krell Institute

9:15 – 10:00am

Invited Speaker — *Salons A, B & C*
Steve Esser — Research Staff Member, Cognitive Computing, IBM Almaden Research Center
"SyNAPSE and Cortical Processor"

10:00 – 10:15am **Break** — Foyer, Salons A, B & C

Session III — Salons A, B & C
Moderator: Carolyn Lauzon — Office of Science, U.S. Department of Energy

10:15 – 10:35am **Michael Rosario** — Duke University
“So Much Work, so Little Time: Maximizing Elastic Energy Within the Duration of Muscle Contraction”

10:35 – 10:55am **Hansi Singh** — University of Washington
“Salty, Saltier, and Saltiest: A Tale of Two Ocean Basins”

10:55 – 11:15am **Alexander Rattner** — Georgia Institute of Technology
“HPC Simulation of Phase-change Fluid Flows for Energy System Engineering”

11:15 – 11:35am **Curtis Lee** — Duke University
“A Cut Cell Embedded Boundary Method for Moving Boundary Problems With Ocean Applications”

11:35am – 12:50pm **Luncheon** — Salons H & J
Invited Speaker
Paul Doucette — Executive Director of Government Relations, Battelle

Session IV — Salons A, B & C
Moderator: Carolyn Lauzon — Office of Science, U.S. Department of Energy

1:00 – 1:20pm **Aurora Pribram-Jones** — University of California, Irvine
“An Efficient Formalism for Warm Dense Matter Electronic Structure”

1:20 – 1:40pm **Maxwell Hutchinson** — University of Chicago
“Experimental Validation of Direct Numerical Simulation of the Single-mode Rayleigh-Taylor Instability”

1:40 – 2:00pm **Matthew Zahr** — Stanford University
“High-order, Time-dependent PDE-constrained Optimization Using Discontinuous Galerkin Methods”

2:00 – 2:15pm **Break** — Foyer, Salons A, B & C

2:15 – 4:15pm **Supercomputing in a Nutshell (Track I Hands-On HPC Session)** — Salons F & G
*This hands-on session will introduce attendees to the world of supercomputing and will provide access to Titan, the second fastest supercomputer in the world (TOP500 November 2014 list). The workshop will cover the basics of supercomputing including how to access a system, the different components involved and their purpose, how to compile and run parallel code via the batch system, and general best practices. A brief introduction to OpenACC and practical examples for taking advantage of Titan's GPUs will also be included. **This session is designed for incoming and first-year fellows. Other non-fellow attendees are also welcome.***

- **Adam Simpson** — HPC User Support Specialist, Oak Ridge Leadership Computing Facility, Oak Ridge National Laboratory
- **Verónica G. Vergara Larrea** — HPC User Support Specialist, Oak Ridge Leadership Computing Facility, Oak Ridge National Laboratory

2:15 – 4:15pm **Optimize a Code for Many Core (Track II Hands-On HPC Session)** — Salons A, B & C
*This advanced, hands-on session is designed to teach participants concepts and strategies for optimizing applications on exascale-like HPC architectures. Attendees will learn to profile a short HPC code with Intel and Cray optimization tools to identify hotspots, bottlenecks and areas to parallelize. Participants will then get a chance to optimize the code, with an eye on preparing it to run well on the Intel Xeon Phi Cori system, due to arrive at the National Energy Research Scientific Computing Center (NERSC) in 2016. **NERSC access during this session will be limited to pre-authorized second-, third- and fourth-year fellows. Others are welcome as observers.***

- **Jack Deslippe** — HPC Consultant, NERSC/Lawrence Berkeley National Laboratory; DOE CSGF Alumnus
- **Rebecca Hartman-Baker** — HPC Consultant, NERSC/Lawrence Berkeley National Laboratory

3:00 – 4:30pm **Poster Set-Up** — Salons H, J & K

4:30 – 6:00pm

DOE Laboratory Poster Session — Salons H, J & K

Welcome & Remarks (4:35pm)

Dimitri Kusnezov — Chief Scientist, National Nuclear Security Administration, U.S. Department of Energy

Thursday, July 30

8:00 – 10:00am

Registration — Grand Registration Desk

8:00 – 9:30am

Continental Breakfast — Salons H & J

9:30 – 9:40am

Announcements — Salons A, B & C

Session V — Salons A, B & C

Moderator: Adam Boyd — National Nuclear Security Administration, U.S. Department of Energy

9:40 – 10:00am

Rogelio Cardona-Rivera — North Carolina State University

“Toward the Holodeck: Computational Models of Narrative and Their Relation to Human Cognition”

10:00 – 10:20am

Robert Parrish — Georgia Institute of Technology

“Partitioned Symmetry Adapted Perturbation Theory: A New Tool for Robust Analysis of Noncovalent Interactions”

10:20 – 10:40am

Andrew Stine — Northwestern University

“The Known Unknown: Computational Identification of Promising Enzymatic Reactions and Associated Genes”

10:40 – 11:00am

Chris Smillie — Massachusetts Institute of Technology

“A Strain Tracking Method Provides Insights Into Fecal Microbiota Transplantation”

11:00 – 11:30am

Break & Hotel Check Out — Foyer, Salons A, B & C

11:30am – 12:30pm

Luncheon — Salons H & J

Buffet-style with grab-and-go options for those with afternoon departures.

