

2018 Annual Program Review Agenda

Sunday, July 15 – Thursday, July 19
Crystal Gateway Marriott Hotel, Arlington, VA

Updated Friday, August 10, 2018

Sunday, July 15

- 4:00 – 8:00pm **Registration** — *Grand Registration Desk*
- 5:30 – 6:00pm **New Fellow Orientation** — *Salon D*
- 6:00 – 7:00pm **New Fellow Dinner** — *Salon C*
- 7:00 – 9:00pm **Making Connections Reception & Game Night** — *Skyview*
All conference attendees who have arrived in D.C. are encouraged to attend.

Monday, July 16

- 7:00am – 6:00pm **Registration** — *Grand Registration Desk*
- 7:00 – 8:30am **Continental Breakfast** — *Salons H & J*
- 7:30 – 8:30am **Photo Session: Incoming Fellows (Portraits & Group Photo)** — *Madison*
- 8:30 – 8:45am **Krell Institute Welcome & Incoming Fellows Introduction** — *Salons A, B & C*
Robert Voigt — Vice President of Technical Programs, Krell Institute
- 8:45 – 9:00am **DOE Office of Science Welcome**
Barbara Helland — Associate Director, Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy
- 9:00 – 9:15am **DOE NNSA Welcome**
Mark C. Anderson — Director, Office of Advanced Simulation and Computing and Institutional R&D Programs, National Nuclear Security Administration, U.S. Department of Energy
- 9:15 – 10:00am **Keynote**
James Sethian — Professor of Mathematics and James Simons Chair in Mathematics, University of California, Berkeley; Director, Center for Advanced Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory
“The Center for Advanced Mathematics for Energy Research Applications”
- 10:00 – 10:20am **Break** — *Foyer, Salons A, B & C*

Session I — *Salons A, B & C*

Moderator: Christine Chalk, Office of Science, U.S. Department of Energy

- 10:20 – 10:40am **Alnur Ali** — Carnegie Mellon University
“Distributed Sparse Inverse Covariance Estimation from fMRI Data for Segmenting the Human Brain”
- 10:40 – 11:00am **Hilary Egan** — University of Colorado
“Ion Loss From Exoplanets”
- 11:00 – 11:20am **Gerald Wang** — Massachusetts Institute of Technology
“Engineering the Relationship Between Fluid Structure and Transport Under Nanoconfinement”
- 11:20 – 11:40am **Kyle Felker** — Princeton University
“Computational Efficiency of High-order Finite Volume Methods for Magnetohydrodynamics”

- 11:45am – 1:00pm **Luncheon & Civics Talk** — *Salons H & J*
Leland Cogliani — Senior Consultant, Lewis-Burke Associates LLC
- 1:15 – 1:25pm **Announcement of 2018 Frederick Howes Scholars** — *Salons A, B & C*
Jeffrey Hittinger — Director and Division Leader, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory; DOE CSGF Alumnus
- 1:25 – 2:10pm **Howes Scholar Presentation**
Seth Davidovits — Postdoctoral Research Fellow, Princeton University; DOE CSGF Alumnus
"Predicting and Utilizing Turbulence in Compressing Plasma"
- 2:10 – 2:25pm **Break** — *Foyer, Salons A, B & C*
- 2:10 – 5:00pm **DOE Laboratory Poster Session Set Up** — *Salons H, J & K*

Session II — *Salons A, B & C*
Moderator: Robinson Pino, Office of Science, U.S. Department of Energy

- 2:25 – 2:45pm **Julian Kates-Harbeck** — Harvard University
"Predicting Disruptions in Magnetic Confinement Fusion Reactors Via Deep Learning at the Largest Scale"
- 2:45 – 3:05pm **Hannah De Jong** — Stanford University
"Saturation Mutagenesis of MYH7 to Identify Hypertrophy-causing Variants"
- 3:05 – 3:25pm **Ryan McKinnon** — Massachusetts Institute of Technology
"Simulating Fluid-solid Interaction in Astrophysical Settings"
- 3:30 – 4:45pm **Practicum Session with DOE Laboratory Introductions** — *Salons A, B & C*
Intended for incoming fellows and those yet to complete a practicum. Each practicum coordinator will provide a brief introduction to their laboratory and speak to potential practicum experiences.
- 5:00 – 7:00pm **DOE Laboratory Poster Session** — *Salons H, J & K*
Welcome & Remarks
Dimitri Kusnezov — Chief Scientist and Senior Advisor to the Secretary, National Nuclear Security Administration, U.S. Department of Energy

Tuesday, July 17

- 7:00am – 6:00pm **Registration** — *Grand Registration Desk*
- 7:00 – 8:30am **Continental Breakfast** — *Salons H & J*
- 8:30 – 8:45am **CYSE Contest Award Presentation** — *Salons A, B & C*
Thomas R. O'Donnell — Senior Media Editor, Krell Institute

Session III — *Salons A, B & C*
Moderator: Thomas R. O'Donnell, Krell Institute

- 8:45 – 9:30am **Alumni Keynote**
Paul Sutter — Astrophysicist, The Ohio State University; Chief Scientist, COSI Science Center; DOE CSGF Alumnus
"Let's Talk About Talking About Science"
- 9:30 – 9:50am **Jay Stotsky** — University of Colorado
"Computational and Mathematical Studies of the Biomechanics of Biofilms"
- 9:50 – 10:10am **Joy Yang** — Massachusetts Institute of Technology
"Statistically Identifying Mechanisms of Phage-host Interactions in the Nahant Collection"
- 10:10 – 10:25am **Break** — *Foyer, Salons A, B & C*

Session IV — *Salons A, B & C*

Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy

- 10:25 – 10:45am **Mukarram Tahir** — Massachusetts Institute of Technology
"Molecular Design of Protein-mimetic Nanostructures"
- 10:45 – 11:05am **Aditi Krishnapriyan** — Stanford University
"Engineering Kinetics for Energy-Efficient Phase Change Materials: Application to Two-Dimensional MoS₂"
- 11:05 – 11:25am **Alex Kell** — Massachusetts Institute of Technology
"Invariant and Hierarchical Computation in Human Auditory Cortex"
- 11:25 – 11:45am **Thomas Thompson** — Harvard University
"The Earth isn't Flat: The Large Influence of Topography on Geodetic Fault Slip Imaging"
- 11:45am – 1:00pm **Luncheon** — *Salons H & J*

Session V — Salons A, B & C

Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy

- 1:15 – 1:35pm **Kathleen Weichman** — University of California, San Diego
"Ion Acceleration by Relativistic-intensity Lasers With Magnetized Electron Focusing"
- 1:35 – 1:55pm **Adam Sealfon** — Massachusetts Institute of Technology
"Population Stability: Regulating Size in the Presence of an Adversary"
- 1:55 – 2:15pm **Adam Riesselman** — Harvard University
"Predicting the Effect of Mutations With Generative Models of Evolutionary Sequences"
- 2:15 – 2:35pm **Thomas Anderson** — California Institute of Technology
"The Fast Hybrid Method for Wave Scattering: New Advances in Time-Domain Integral Equations"
- 2:35 – 2:50pm **Break** — *Foyer, Salons A, B & C*

Session VI — Salons A, B & C

Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy

- 2:50 – 3:10pm **Danielle Rager** — Carnegie Mellon University
"Relating Visual Working Memory Computations to Network Architecture in the Brain"
- 3:10 – 3:30pm **Jordan Hoffmann** — Harvard University
"How to Build a Bug"
- 3:30 – 5:00pm **Fellows' Poster Session Set-Up** — *Salons H, J & K*
- 4:00 – 4:30pm **Photo Session: Fellow/Alumni Portrait Retakes** — *Madison*
- 4:00 – 4:45pm **Fourth-Year/Outgoing Fellow Session & Portraits** — *Jefferson*
- 5:00 – 7:00pm **Fellows' Poster Session** — *Salons H, J & K*
Welcome & Remarks
Paul M. Dabbar — Under Secretary for Science, U.S. Department of Energy

Wednesday, July 18

- 7:00am – 5:00pm **Registration** — *Grand Registration Desk*
- 7:00 – 8:30am **Continental Breakfast** — *Salons D, E, F & G*
- 8:30 – 8:45am **Announcements** — *Salons A, B & C*
- 8:45 – 9:30am **Keynote** — *Salons A, B & C*
Katherine Lewis — Cognitive Simulation Project Leader, Lawrence Livermore National Laboratory

"Integrating Machine Learning with Simulations at Lawrence Livermore National Laboratory"

9:30 – 10:15am

Keynote — Salons A, B & C

Michael Heroux — Director of Software Technology, DOE Exascale Computing Project; Senior Scientist, Sandia National Laboratories; and Scientist in Residence, St. John's University, Minnesota
"Building the Exascale Software Stack: Challenges and Strategies"

10:15 – 10:30am

Break — Foyer, Salons A, B & C

HPC Workshop

Presented by DOE laboratory staff representing six facilities, the 2018 HPC Workshop will provide incoming through fourth-year fellows with hands-on training and access to Oak Ridge National Laboratory's Titan supercomputer. Fellows were surveyed and grouped into working teams prior to the program review. Non-fellows are welcome to attend the workshop as observers.

10:30 – 11:00am

Workshop Overview & Introduction to HPC Problems — Salons A, B & C

Organizers:

- Lawrence Berkeley National Laboratory/NERSC — **Jack Deslippe**
- Lawrence Livermore National Laboratory — **Jeffrey Hittinger**
- Oak Ridge National Laboratory — **Judith Hill**

Mentors:

- Argonne National Laboratory — **Hal Finkel**
- Oak Ridge National Laboratory — **Mark Berrill, Matthew Norman** and **Thomas Papatheodore**
- Lawrence Berkeley National Laboratory/NERSC — **Rahulkumar Gayatri** and **Charlene Yang**
- Lawrence Livermore National Laboratory — **Adam Kunen**
- Los Alamos National Laboratory — **Christoph Junghans**
- Sandia National Laboratories — **Michael Wolf**

11:00am – 12:00pm

Introduction to Broad HPC Concepts — Salons A, B & C

Intended for novice fellows. Session attendees have been preassigned.

11:00am – 12:00pm

Introduction to Performance & Scalability Tools — Salons H, J & K

Intended for intermediate and advanced fellows. Session attendees have been preassigned.

12:00 – 1:00pm

Luncheon — Salons D, E, F & G

1:00 – 6:00pm

Team-based Collaboration With DOE Laboratory Mentor Support — Salons H, J & K

The afternoon will include separate introductions to OpenMP3.5, MPI, CUDA and OpenACC, each followed by a working session focused on running and optimizing the corresponding version of BerkeleyGW code on Titan.

Thursday, July 19

7:00 – 8:00am

Continental Breakfast — Salons A, B & C

HPC Workshop

8:00am – 12:00pm

Team-based Collaboration With DOE Laboratory Mentor Support — Salons H, J & K

Continued collaboration and workshop closing session.

12:00 – 1:00pm

Luncheon — Salons A, B & C

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

