DOE CSGF | Department of Energy Computational Science Graduate Fellowship

2019 Annual Program Review Agenda

Sunday, July 14 – Thursday, July 18
Crystal Gateway Marriott Hotel, Arlington, VA

Updated Thursday, July 11, 2019

Sunday, July 14	
11:30am – 8:00pm	**Registration** — *Grand Registration Desk*
12:00 – 12:30pm	**New Fellow Orientation** — *Salons H & J*
12:30 – 1:30pm	**New Fellow Luncheon** — *Salons H & J*
2:00 – 5:00pm	**New Fellow Programming** — *Various*
7:00 – 9:00pm	**Making Connections Reception & Game Night** — *Salons H & J* *All conference attendees who have arrived in D.C. are encouraged to attend.*
Monday, July 15	
7:00am – 6:00pm	**Registration** — *Grand Registration Desk*
7:00 – 8:30am	**Continental Breakfast** — *Salons H & J*
8:30 – 8:45am	**DOE CSGF Welcome & Incoming Fellows Introduction** — *Salons A, B & C* **David Brown** — Director, Computational Research Division, Lawrence Berkeley National Laboratory
8:45 – 9:00am	**DOE Office of Science Welcome** **Steve Binkley** — Principal Deputy Director for Science Programs, Office of Science, U.S. Department of Energy
9:00 – 9:15am	**DOE NNSA Welcome** **Charles P. Verdon** — Deputy Administrator for Defense Programs, National Nuclear Security Administration, U.S. Department of Energy
9:15 – 10:00am	**Keynote** **Jarrod McClean** — Senior Research Scientist, Quantum Artificial Intelligence Lab, Google; DOE CSGF Alumnus *"Quantum Computation for Science"*
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	**Casey Berger** — University of North Carolina, Chapel Hill *"Complex Langevin in Nonrelativistic Rotating Bosonic Systems"*
10:40 – 11:00am	**Maximilian Bremer** — University of Texas *"Simulation of Shallow Water Flows Using HPX"*
11:00 – 11:20am	**Mario Ortega** — University of California, Berkeley *"A Rayleigh Quotient Fixed-Point Method for Alpha-Eigenvalue Problems"*
11:20 – 11:40am	**Helena Qi** — Massachusetts Institute of Technology *"Large-Scale Analysis of Electronic Effects in Protein Structure"*

11:45am – 1:00pm	**Luncheon** — *Salons H & J*
1:15 – 1:25pm	**Announcement of 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 – 1:55pm	**Howes Scholar Presentation - 2018 Awardee** **Sarah Middleton** — Computational Biologist, Functional Genomics, GlaxoSmithKline; DOE CSGF Alumna *"Single Cell Sequencing for Drug Discovery: Applications and Challenges"*
1:55 – 2:25pm	**Howes Scholar Presentation - 2019 Awardee** **Adam Riesselman** — Machine Learning – Lead Engineer, insitro; DOE CSGF Alumnus *"Reasoning About Biology With Data-Driven Approaches"*
2:25 – 2:55pm	**Howes Scholar Presentation - 2019 Awardee** **Chelsea Harris** — Research Associate, Michigan State University; DOE CSGF Alumna *"Toward Exascale Astrophysics of Magnetic Supernovae"*
2:55 – 3:15pm	**Break** — *Foyer, Salons A, B & C*
3:00 – 5:00pm	**DOE Laboratory Poster Session Set Up** — *Salons H, J & K*
3:15 – 4:15pm	**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 about potential practicum experiences.*
4:15 – 5:00pm	**Practicum Q&A Panel** *Current fellows will discuss their recent practicum experiences at laboratories across the country. Topics will include exploration of research topics, site selection, lab life, and what one can expect when embarking on this immersive opportunity afforded by the DOE CSGF.* ● **Matthew Carbone** — Columbia University (Brookhaven National Laboratory, 2018) ● **Harshil Kamdar** — Harvard University (National Renewable Energy Laboratory, 2018) ● **Morgan Kelley** — University of Texas (Argonne National Laboratory, 2018) ● **Quentarius Moore** — Texas A&M University (Sandia National Laboratories, New Mexico, 2018) ● **Kelly Moran** — Duke University (Los Alamos National Laboratory, 2017 and 2018)
5:00 – 7:00pm	**DOE Laboratory Poster Session** — *Salons H, J & K*

Tuesday, July 16

7:00am – 6:00pm	**Registration** — *Grand Registration Desk*
7:00 – 8:30am	**Continental Breakfast** — *Salons H & J*

Session II — *Salons A, B & C*
Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy

8:30 – 8:45am	**Announcements**
8:45 – 9:30am	**Keynote** **Wayne Joubert** — Computational Scientist, Oak Ridge Leadership Computing Facility, Oak Ridge National Laboratory *"Using Innovative Compute Hardware for Breakthrough Science: Computational Genomics at Exascale With the CoMet Application"*
9:30 – 9:50am	**Nicholas Boffi** — Harvard University *"Parallel Three-Dimensional Simulations of Quasi-Static Elastoplastic Solids"*
9:50 – 10:10am	**Hannah Klion** — University of California, Berkeley *"The Multi-D Effects of Jets on Neutron Star Merger Light Curves"*
10:10 – 10:25am	**Break** — *Foyer, Salons A, B & C*

Session III — *Salons A, B & C* **Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy**	
10:25 – 10:45am	**Emmet Cleary** — California Institute of Technology *"Bayesian Inversion of Climate Models"*
10:45 – 11:05am	**Richard Barnes** — University of California, Berkeley *"Algorithms for and Applications of Multi-Scale Geospatial Analysis"*
11:05 – 11:25am	**Alexander Williams** — Stanford University *"Examining Large-Scale Neural Data With Single-Trial Resolution"*
11:25 – 11:45am	**Zane Crawford** — Michigan State University *"A Novel Formulation of a Finite Element-Based Particle-in-Cell Method"*
11:45am – 1:00pm	**Luncheon & Civics Talk** — *Salons H & J* **Meyer Seligman** — Professional Staff Member, U.S. Senate Committee on Appropriations – Subcommittee on Energy and Water Development
Session IV — *Salons A, B & C* **Moderator: David Etim, National Nuclear Security Administration, U.S. Department of Energy**	
1:20 – 1:40pm	**Noah Mandell** — Princeton University *"Electromagnetic Gyrokinetic Turbulence Simulations in the Tokamak Edge With Discontinuous Galerkin Methods"*
1:40 – 2:00pm	**Ian Dunn** — Columbia University *"Exact Simulations of Electron-Phonon Dynamics: Direct and Iterative Projection Approaches for Removing Instabilities"*
2:00 – 2:20pm	**Carson Kent** — Stanford University *"Optimization in the Space of Measures: Machine Learning Using Optimal Transport"*
2:30 – 3:00pm	**Fourth-Year/Outgoing Fellow Session & Portraits** — *Jefferson*
3:00 – 5:00pm	**Fellows' Poster Session Set-Up** — *Salons H, J & K*
3:00 – 4:00pm	**Photo Session: Fellow & Alumni Portrait Retakes** — *Jackson*
4:00 – 5:00pm	**Photo Session: Incoming Fellows (Portraits & Group Photo)** — *Jackson*
5:00 – 7:00pm	**Fellows' Poster Session** — *Salons H, J & K*
Wednesday, July 17	
7:00am – 5:00pm	**Registration** — *Grand Registration Desk*
7:00 – 8:30am	**Continental Breakfast** — *Salons D, E, F & G*
Session V — *Salons A, B & C* **Moderator: Thomas R. O'Donnell, Krell Institute**	
8:30 – 8:45am	**CYSE Contest Award Presentation** **Thomas R. O'Donnell** — Science Media Editor, Krell Institute

8:45 – 9:45am

Alumni Q&A Panel: Early Career Insights
A group of recent alumni will speak about their experiences working in a variety of environments — including the pre- and post-graduation paths they took to arrive at where they are today.

- **Jaydeep Bardhan**, Moderator — Technologist in Residence, GlaxoSmithKline
- **Eileen Martin**, Panelist — Assistant Professor, Mathematics, Virginia Tech
- **Heather Mayes**, Panelist — Staff Scientist, National Renewable Energy Laboratory
- **Jarrod McClean**, Panelist — Senior Research Scientist, Quantum Artificial Intelligence Lab, Google
- **Andrew Stershic**, Panelist — Senior R&D Mechanical Engineer, Sandia National Laboratories, California

9:45 – 10:45am

Alumni Q&A Panel: Communication & Leadership
This group of alumni will share what they've learned in the process of building social media platforms, brands, companies and teams; and in writing and reviewing proposals for fellowships, funding, and computing allocations. One thing holds true for all of their experiences: Understanding your audience and communicating with clarity and purpose is key.

- **Paul Sutter**, Moderator — Astrophysicist, The Ohio State University
- **Judith Hill**, Panelist — Computational Scientist and Scientific Computing Group Leader, National Center for Computational Sciences, Oak Ridge National Laboratory
- **Amanda Randles**, Panelist — Assistant Professor, Biomedical Engineering, Duke University
- **Sarah Richardson**, Panelist — Chief Executive Officer, MicroByre
- **Samuel Skillman**, Panelist — Computational Scientist, Descartes Labs

10:45 – 11:00am

Break — *Foyer, Salons A, B & C*

11:00am – 12:00pm

HPC Workshop Preparation & NERSC Account Support — *Salons H, J & K*
Fellows and mentors will meet in their assigned groups, set up their workstations, and take final steps to ensure that all are set to run on NERSC's newest supercomputer, Cori.

12:00 – 1:00pm

Luncheon — *Salons D, E, F & G*

HPC Workshop — *Salons H, J & K*

The 2019 HPC Workshop will provide incoming through fourth-year fellows with hands-on training and access to NERSC's Cori supercomputer. Fellows will organize in teams, with each group assisted by a mentor. Non-fellows are welcome to attend the workshop as observers.

1:00 – 1:30pm

Workshop Overview & Introductions
Organizers:

- **Amanda Randles*** — Duke University
- **Jack Deslippe*** — Lawrence Berkeley National Laboratory/NERSC

Mentors:

- **Gerald Wang*** — Carnegie Mellon University
- **Erik Draeger** — DOE Exascale Computing Project
- **David Ozog*** — Intel
- **Brandon Cook** and **Stephen Leak** — Lawrence Berkeley National Laboratory/NERSC
- **Joshua Vermaas*** — National Renewable Energy Laboratory
- **Mark Berrill***, **Steven Hamilton*** and **Matthew Norman*** — Oak Ridge National Laboratory
- **Michael Wolf*** — Sandia National Laboratories, New Mexico
- **Matthew Reuter*** — Stony Brook University
- **David Rogers*** — University of South Florida
- **Eileen Martin*** — Virginia Tech

** DOE CSGF Alumni*

1:30 – 3:00pm

Introduction to MPI
Yanfei Guo — Assistant Computer Scientist, Argonne National Laboratory
"Parallel Programming With Message Passing Interface"

3:00 – 3:15pm

Break

3:15 – 5:15pm

MPI Hands-on Session
Yanfei Guo — Argonne National Laboratory
This collaborative session will use Conway's Game of Life as an example application.

5:15 – 5:30pm	**Break**
5:30 – 6:00pm	**Day 1 Conclusion**

Thursday, July 18

7:00 – 8:00am	**Continental Breakfast** — *Salons A, B & C*
	HPC Workshop — *Salons H, J & K*
8:00 – 8:15am	**Day 2 Overview**
8:15 – 9:30am	**Introduction to Intel VTune Amplifier and Intel Advisor** **Kevin O'Leary** — Senior Technical Consulting Engineer, Intel *An introductory section on performance profiling.*
9:30 – 9:45am	**Break & Hotel Check Out**
9:45 – 11:15am	**Intel Hands-on Session** **Kevin O'Leary** — Intel *Real-time analysis of programs using Intel® VTune™ Amplifier and Intel® Advisor.*
11:15am – 12:00pm	**DOE Exascale Computing Project (ECP)** **Erik W. Draeger** — Deputy Directory of Application Development, Exascale Computing Project *"DOE Exascale Computing Project (ECP) Objectives and Opportunities"*
12:00 – 12:30pm	**Workshop Conclusion & Comments**
12:30 – 1:30pm	**Luncheon** — *Salons A, B & C* *Buffet-style with grab-and-go options for those with afternoon departures.*