July 31–August 2, 2012 ♦ Reston, VA

Grand Challenge Goal:
Leverage the United States' leadership in advanced computing, modeling and simulation to deploy affordable, user-friendly, accessible platforms for broad use across America's energy sector.

Workshop Goals

- Refine the Secretary's vision of how advanced computing could change the U.S. energy future by enabling energy innovation.
- Attract and strengthen a team of end users (energy innovators), advanced computing technology developers, and supporters.
- Identify challenges and specific actions necessary to widen the use of advanced computing to enable better generation, delivery, storage, and use of energy.

Agenda

Tuesday, July 31 — Colloquiums

Time	Topic	Location
7:30 am	Registration and Coffee/Tea	Ballroom Foyer
8:30 am	Welcome, Introductions, and Colloquiums Overview *(Alex Larzelere, Department of Energy-NE)*	Grand Ballroom E-G
9:00 am	Colloquiums* (choose one): 1. Advanced Computing for Energy — Challenges, Successes and Opportunities 2. DOE Advanced Computing Resources for Energy Applications 3. Accessing Commercially Available Advanced Computing Resources and Expertise	 Grand Ballroom E-G Lake Fairfax Lake Anne
Noon	*Lunch (on your own)*	*Your choice*
1:30 pm	Colloquiums* (repeated): 1. Advanced Computing for Energy — Challenges, Successes and Opportunities 2. DOE Advanced Computing Resources for Energy Applications 3. Accessing Commercially Available Advanced Computing Resources and Expertise	 Grand Ballroom E-G Lake Fairfax Lake Anne
4:30 pm	Wrap Up Discussion, General Questions, and Actions *(Alex Larzelere, Department of Energy-NE)*	Grand Ballroom E-G
5:00 pm	*Adjourn*	

* Colloquium Presentations:

1. **Advanced Computing for Energy — Challenges, Successes and Opportunities**

(Moderator: Steve Hammond, National Renewable Energy Laboratory)

This colloquium features experts in the application of DOE Advanced Computing resources presenting a variety of projects, demonstrating that high performance computing can have significant impact on improving fundamental understanding, advancing technologies, and accelerating new products to market. The intent is to provide examples from a variety of energy topical areas in an effort to demonstrate a broad base of application. Attendees will be able to see a variety of applications and engage in conversation about software packages and computing resources that can be applied to their specific challenges. The overall goal is for attendees to become familiar with computing tools that are available and to stimulate interest in accessing tools and establishing partnerships with the Department.

- Electrons flow fast. Can power grid computation keep up? *(Henry Huang, Pacific Northwest National Laboratory)*
- Design, discovery, and detailed theory for photovoltaic materials using electronic structure methods *(Stephan Lany, National Renewable Energy Laboratory)*
- Direct Numerical Simulation of Turbulent Combustion: Fundamental Science towards Predictive Models *(Ramanan Sankaran, Oak Ridge National Laboratory)*
- Advanced Bioenergy, Biomass, and Biofuels: Molecular Level Design of Solutions Using Advanced Simulation and Modeling *(Mike Crowley, National Renewable Energy Laboratory)*
- Windplant Aerodynamics and Loads *(Fort Felker, National Renewable Energy Laboratory)*
- The Consortium for Advanced Simulation of Light Water Reactors: A DOE Energy Innovation Hub *(Doug Kothe, Oak Ridge National Laboratory)*

2. **DOE Advanced Computing Resources for Energy Applications**

(Moderator: Steven Lee, Department of Energy-SC)

This colloquium reaches out to energy innovators, especially those working in companies and DOE Applied Technology Programs, who are intrigued by the possibility of improving energy technologies through advanced computing (modeling, simulation, and analytics). This colloquium provides information on a wealth of software tools and computing resources that are available at the DOE national laboratories. The presenters will describe these resources, their design and purpose, the target platforms, and future plans.

- Overview of DOE Modeling, Simulation and Analytics for Energy Applications *(Steven Lee, Department of Energy-SC)*
- DOE Applied Mathematics Software for High Performance Computing *(Lori Diachin, Lawrence Livermore National Laboratory)*
- Scalable Data Management, Analysis, and Visualization Tools for Computational Science *(Arie Shoshani, Lawrence Berkeley National Laboratory)*
- Advanced Simulation and Analysis Software for Power Distribution Systems *(Rob Pratt, Pacific Northwest National Laboratory)*
- Advanced Software for Radiation Physics and Safety *(Tim Valentine, Oak Ridge National Laboratory)*
- DOE Advanced Computing Platforms and Programs *(Dan Hitchcock, Department of Energy-SC)*

3. **Accessing Commercially Available Advanced Computing Resources and Expertise**

(Moderator: Benjy Grover, Lawrence Livermore National Laboratory)

The intent of this colloquium is to provide the audience with an overview of software and platforms available in the commercial marketplace. Commercial software provides users with robust, easy to use, well-documented tools, with a range of options for consulting support to help end users get started quickly with design. The advent of cloud computing is meanwhile making access to computing power as easy as having internet access and a credit card. In this colloquium, providers of commercial tools will give a survey of their capabilities as they apply to energy innovation through modeling and simulation.

- Complexity, Reliability, and Competition: Energy Innovation through Engineering Simulation in the Cloud Computing Era *(Barbara Hutchings, ANSYS, Inc.)*
- Addressing Energy Challenges by Going Beyond Realistic Engineering Simulations *(Mahesh Kailasam, Dassault Systèmes)*
- Computational Methods In Energy Related Materials Science *(Nick Reynolds, Accelrys, Inc.)*
- The Cloud - Lowering Barriers to Computing, Software and Expertise *(Bob Graybill, Nimbis Services, Inc.)*
- Advanced Computing for Energy: Multi-Physics Analysis, Design Optimization, and Data Analytics *(Dave Corson and Shing Pan, Altair)*

Agenda

Wednesday, August 1 — Workshop (Day 1)

Time	Topic	Location
7:00 am	Registration and Coffee/Tea	Ballroom Foyer
8:00 am	Welcome, Introductions, and Workshop Overview *(Alex Larzelere, DOE-NE)*	Grand Ballroom E-G
8:30 am	DOE Assistant Secretaries Panel on DOE Applied Technology Programs – Advanced Computing for Energy – Promises and Challenges *(Moderator: Dana Christensen, National Renewable Energy Laboratory)* • Bringing Moore's Law to Clean Energy *(Dave Danielson, Department of Energy-EERE)* • Modeling and Simulation Challenges in Nuclear Energy *(Pete Lyons, Department of Energy-NE)* • National Risk Assessment Partnership (NRAP) Program for Risk Management *(Chuck McConnell, Department of Energy-FE)* • Computational Challenges for a Smarter Grid: An Optimization and Simulation Perspective *(Pat Hoffman, Department of Energy-OE)*	Grand Ballroom E-G
10:00 am	*Collaborative Discussions*	*Ballroom Foyer*
10:30 am	Panel on Energy Innovation through Advanced Computing: Success Stories *(Moderator: Steve Ashby, Pacific Northwest National Laboratory)* • Bringing High Performance Computing to Energy Problems *(Dave Turek, IBM)* • Advanced Computing at GE *(Gary Leonard, GE Research)* • Importance of Analysis in the Cummins Engine Development Process *(Wayne Eckerle, Cummins)* • Analysis Led Design *(Steve Gravante, Navistar)*	Grand Ballroom E-G
11:30 am	Panel on Energy Innovation through Advanced Computing: Potential and Challenges *(Moderator: Dona Crawford, Lawrence Livermore National Laboratory)* • Supercomputing applications for nuclear reactors – a Westinghouse perspective *(Sumit Ray, Westinghouse)* • Innovation Opportunities and Challenges for Advanced Computing in Smart Grid Operation *(David Sun, Alstom)* • Role of Computations and Mathematics in Delivering High Performance, Energy Efficient Buildings: Some Industry Perspectives *(Satish Narayanan, United Technologies Research Center)*	Grand Ballroom E-G
12:30 pm	*Working Lunch* Keynote Address: Changing our Energy Future Through Advanced Computing *(Secretary of Energy Steven Chu)*	*Regency Ballroom*
2:00 pm	Chair's Charge to the Workshop Participants: Challenges to Extending and Scaling Advanced Computing for Energy *(Alex Larzelere, DOE-NE)*	Regency Ballroom
2:15 pm	*Break*	*Ballroom Foyer*
2:30 pm	Breakout Sessions: 1. DOE Applied Programs – Grand Challenges *(Lead: Ray Stults, National Renewable Energy Laboratory)* 2. Current Users – Grand Challenges *(Lead: Moe Khaleel, Pacific Northwest National Laboratory)* 3. Potential Users – Grand Challenges *(Lead: John Grosh, Lawrence Livermore National Laboratory)*	Grand Ballroom E-G Lake Fairfax Lake Anne
	Adjourn at Breakout Session Lead's discretion	

Agenda

Thursday, August 2 — Workshop (Day 2)

Time	Topic	Location
7:30 am	Registration and Coffee/Tea	Ballroom Foyer
8:00 am	Breakout Sessions (continued): 1. DOE Applied Programs – Grand Challenges *(Lead: Ray Stults, National Renewable Energy Laboratory)* 2. Current Users – Grand Challenges *(Lead: Moe Khaleel, Pacific Northwest National Laboratory)* 3. Potential Users – Grand Challenges *(Lead: John Grosh, Lawrence Livermore National Laboratory)*	 Grand Ballroom E-G Lake Fairfax Lake Anne
9:45 am	*Break*	*Ballroom Foyer*
10:00 am	Breakout Group Initial Reports *(Breakout Session Leads)*	Grand Ballroom E-G
11:00 am	Breakout Sessions (continued) *Break for lunch on your own at breakout session lead's discretion*	Same as above
2:30 pm	*Break*	*Ballroom Foyer*
2:45 pm	Breakout Group Reports and Discussion *(Breakout Session Leads)*	Grand Ballroom E-G
4:30 pm	Workshop Conclusions and Next Steps *(Workshop Chairs: Steve Ashby, Dana Christensen, and Dona Crawford)*	Grand Ballroom E-G
5:00 pm	*Adjourn*	

Agenda

Friday, August 3 — Report Writers Only

Time	Topic	Location
8:00 am	Report Preparation Process *(Alex Larzelere)*	Lake Fairfax
8:30 am	Breakout Session 1 Recap *(Ray Stults)*	Lake Fairfax
8:50 am	Breakout Session 2 Recap *(Moe Khaleel)*	Lake Fairfax
9:10 am	Breakout Session 3 Recap *(John Grosh)*	Lake Fairfax
9:30 am	*Break*	*Lake Fairfax*
9:45 am	Discussion of Opening Report Section *(Alex Larzelere)*	Lake Fairfax
10:15 am	Discussion of Recommendations and Conclusions Section *(Alex Larzelere)*	Lake Fairfax
11:00 am	Report Design *(Lee Ann Dudney)*	Lake Fairfax
11:30 am	Action Items and Schedule	Lake Fairfax
Noon	*Adjourn*	