



2012 Smoky Mountains Computational Sciences and Engineering Conference

September 5-7, 2012

Smoky Mountains

Computational Sciences and Engineering Conference

2012 Theme: Simulation Science for Complex Engineered Systems

Park Vista Hotel

Gatlinburg, Tennessee

<http://computing.ornl.gov/workshops/FallCreek12/>

Tuesday, September 4, 2012

- 6:30 p.m. Registration and networking session..... Park Vista Hotel
Welcome, announcements, conference overview..... Barney Maccabe, ORNL

Wednesday, September 5, 2012

- 7:30 a.m. Morning networking, session preparation, breakfast..... All
Conference goals / expected outcomes..... Barney Maccabe, ORNL
Session I: *Experience on Multi-petaflops Architectures* Jack Dongarra/Greg Peterson, UT
..... session chairs

Sequoia Bronis de Supinski, LLNL

Stampede Jay Boisseau, TACC, University of Texas

Break

TSUBAME 2.0 Satoshi Matsuoka, Tokyo Institute of Technology

Titan Buddy Bland, ORNL

Moderated panel session.....
..... Greg Peterson, Satoshi Matsuoka, Bronis de Supinski, Jay Boisseau, Buddy Bland

Working lunch: continue *Experience on Multi-petaflops Architectures* All

Individual breakout sessions: experience on multi-petaflops architectures

- 5:45 p.m. Poster session set up poster presenters only

- 6:00 p.m. Poster session: *Experience on Multi-petaflops Architectures, Accelerated Computational Science,*

Big Data Debbie McCoy, ORNL, session chair

Dinner.....

Complex Engineered Systems at Procter and Gamble Tom Lange, Procter & Gamble

- 9:00 p.m. End of day 1

Thursday, September 6, 2012

7:30 a.m.	Morning networking, session preparation, breakfast.....	All
	Session II: <i>Accelerated Computational Science and Big Data</i>	Jack Wells, ORNL, session chair
	<i>Seismology simulation and big data</i>	Jeroen Tromp, Princeton University
	<i>Drug discovery at the petascale and big data</i>	Jerome Baudry, University of Tennessee
	Break	
	<i>Data Impacts in the Consortium for Advanced Simulation of Light Water Reactors (CASL)</i>	
	Doug Kothe, ORNL
	<i>Past, present, and future of extreme data processing in the scientific data group</i>	
	Scott Klasky, ORNL
	Moderated panel session.....	Jack Wells, Jeroen Tromp, Jerome Baudry, Doug Kothe, Scott Klasky
	Working lunch: continue <i>Accelerated Computational Science and Big Data</i>	All
	Session III: <i>Data Analytics to Support Knowledge Discovery</i>	Arjun Shankar, ORNL
	Ramesh Menon, YarcData
	<i>Streaming applications</i>	Scott Schneider, InfoSphere, IBM
	Break	
	<i>GraphLab2: a distributed abstraction for large-scale machine learning</i>	Yucheng Low,
	University of Washington
	<i>Knowledge Discovery – Fabric: data systems architecture in support of broad, comprehensive and flexible data analysis functions in national healthcare space</i>	Edmon Begoli, ORNL
	Moderated panel session.....	Ramesh Menon, Yucheng Low, Scott Schneider, Edmon Begoli
5:30 p.m.	Break and poster session set up	All
	Poster session: <i>Data Analytics to Support Knowledge Discovery and Applications Requirements and Investments in Exascale</i>	Debbie McCoy, ORNL, session chair
8:30 p.m.	End of day 2	

Friday, September 7, 2012

7:30 a.m. Morning networking, session preparation, breakfast.....All

Session IV: ***Application Requirements and Investments in Exascale***.....

..... Robert Harrison, UT/ORNL Joint Institute for Computational Sciences, session chair

Industry strategy Peter Ungaro, President and CEO, Cray

Industry strategy David Turek, IBM

Break

Industry strategy Alan Gara, Intel

DOE requirements William Harrod, DOE

Moderated panel session...Robert Harrison, Peter Ungaro, David Turek, Alan Gara, William Harrod

Working lunch: continue ***Application Requirements and Investments in Exascale***All

Conference wrap-up

2013 Smoky Mountains Computational Sciences and Engineering Conference outlook

Adjourn

3:00 p.m. End of conference



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Posters

Wednesday, September 5

A Scalable Software Framework for Thermal Radiation Analysis, Kwai Wong, Joint Institute for Computational Sciences

Electron transfer and energy transfer in carbon materials, Jacek Jakowski, University of Tennessee

Interactive visual analysis for data-intensive applications, Bill Pike, Pacific Northwest National Laboratory

Mechanistic aspects of the nitrogen cycle: the action of copper-containing nitrite reductase, Yan Li, North Carolina State University

Quantifying the Impact of Single Bit Flips on Floating Point Arithmetic, James Elliott, North Carolina State University

SciDAC-3 Institute: SDAV, Scalable Data Management, Analysis and Visualization: SDAV technologies for the next generation fusion techniques, S. Klasky, M. Parashar, K. Schwan, N. Podhorszki and the SDAV Data Management Team

SciDAC-3 Institute: SDAV, Scalable Data Management, Analysis and Visualization: SDAV Support to Combustion Research with Visualization, Analysis, and Data Movements, N. Podhorszki, et al.

Toward High-throughput Virtual Docking with Multiple Receptor Conformations on High-Performance Computers, Sally Ellingson, University of Tennessee

3D supernova simulations using Chimera, Christopher Mauney, North Carolina State University

Posters

Thursday, September 6

Forward and Adjoint Simulations of Seismic Wave Propagation on Emerging Large-Scale GPU Architectures, Daniel Peter, Ebru Bozdag, and Jeroen Tromp; Princeton University

Integrated Regional Earth Systems Modeling (iRESM) - Framework for knowledge sharing and discovery for multi domain, coupled models, Kerstin Kleese-Van Dam, Pacific Northwest National Laboratory

Near real time and multi modal analysis for large scale experiments, Kerstin Kleese Van Dam, Pacific Northwest National Laboratory

Next Generation Data Analytics for Extreme Scale Scientific Data, George Ostrouchov, Wei-Chen Chen, Dave Pugmire, Norbert Podhorszki and Scott Klasky

PaRSEC, Wei Wu, University of Tennessee, Knoxville

Performance Counter Monitoring for the Blue Gene/Q Architecture, Heike McCraw, University of Tennessee

Petascale Informatics Applications Development on NICS Supercomputers, Bhanu Rekepalli, University of Tennessee

SciDAC-3 Partnership: EPSI, Center for Edge Plasma Simulations: On-the-fly data management for high performance multiscale fusion simulation on Titan, S. Klasky, M. Parashar, R. Moser, N. Podhorszki, S. Ku, C.S. Chang, J. Hesthaven, R. Tchoua, and the EPSI Team

Some big data challenges in observing, monitoring and modeling the earth system, Valentine Anatharaj, Oak Ridge National Laboratory

Towards Global Adjoint Tomography, Ebru Bozdag, Princeton University