

SciApps - 10

Challenges and Opportunities for Scientific Applications: learning to sustain the Petaflop with eyes on the Exaflop horizon.

This Workshop will bring together an interdisciplinary team of computational scientists to share experience, knowledge, and best practices on the implementation of a wide range of scientifically demanding and computationally paced applications on leading-edge high-performance scientific computer systems. Our goal for this workshop is to offer a cross discipline venue to facilitate interactions among current and potential leadership class computing users, explore opportunities to strengthen application development and obtain insight into near term and medium term application requirements and scientific mission goals. Access to DOE's Leadership Class Computing facilities is open to any academic, government, or industry research organization via the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program (<http://DOEleadershipcomputing.org> and <http://www.sc.doe.gov/ascr/incite/>).

When: August 3 – 6, 2010

Where: Oak Ridge National Laboratory, Building 5100 (JICS) Room 128

Agenda

August 3 2010		
8:00	Welcome and Purpose	Ricky Kendall and Doug Kothe
8:30	DOE Leadership Computing Overview	Barbara Helland
9:00	NSF Computing Overview	
9:30	The INCITE Program	Julia White
10:00	Break	
10:15	Architecture Overview	Steve Poole
	Computational Science Software Ecosystem	
11:15	Programming Models	
11:45	Operating Systems	
12:15	Libraries	
12:45	Lunch	Guest Speaker
14:00	Requirements Gathering, Validation, and Synthesis	Hai Ah Nam
15:00	What Software Engineering Practices Computational Scientists should know and use	Wayne Joubert
16:00	Break	
16:15	The Joule Exercise: Importance and Impact	Rebecca Hartman-Baker
17:00	Tour of the OLCF	Buddy Bland
17:30	Adjourn for the day	
18:30	Dinner (TBD)	

August 4 2010		
8:00	Case Study: S3D	Ramanan Sankaran
8:30	Requirements and science goals for sustained petascale Combustion Science	
9:15	Future requirements and science goals for Combustion Science	
10:00	Break	
10:15	Case Study: Denovo	
10:45	Requirements and science goals for sustained petascale Nuclear Energy	John Turner
11:30	Future requirements and science goals for Nuclear Energy	Doug Kothe
12:15	Lunch	
1:30	Case Study: Chimera/Genesis	Bronson Messer
2:00	Requirements and science goals for sustained petascale Astrophysics	
2:45	Future requirements and science goals for Astrophysics	
3:30	Break	
3:45	Case Study: TBD	
4:15	Requirements and science goals for sustained petascale National Security	
5:00	Future requirements and science goals for National Security	
5:45	Adjourn	

August 5 2010		
8:00	Case Study: WL-LSMS and DCA++	Markus Eisenbach
8:30	Requirements and science goals for sustained petascale Materials and Nanoscience	
9:15	Future requirements and science goals for Materials and Nanoscience	
10:00	Break	
10:15	Case Study: NWChem	
10:45	Requirements and science goals for sustained petascale Chemistry	Theresa Windus
11:30	Future requirements and science goals for Chemistry	Robert Harrison
12:15	Lunch	
1:30	Case Study: CCSM	Ilene Carpenter
2:00	Requirements and science goals for sustained petascale Climate Science	
2:45	Future requirements and science goals for Climate Science	Jim Hack
3:30	Break	
3:45	Case Study: Gromacs	

4:15	Requirements and science goals for sustained petascale Biophysics
5:00	Future requirements and science goals for Biophysics
5:45	Adjourn

August 6 2010

8:00	Case Study: MADNESS	
8:30	Requirements and science goals for sustained petascale for the MADNESS framework	
9:15	Future requirements and science goals for the MADNESS framework	Robert Harrison
10:00	Break	
10:15	Case Study: NUCOR	Hai Ah Nam
10:45	Requirements and science goals for sustained petascale	
11:30	Future requirements and science goals for	
12:15	Lunch	Aorsa: Richard Barrett
1:30	Case Study:GTC	
2:00	Requirements and science goals for sustained petascale Fusion Simulation	
2:45	Future requirements and science goals for Fusion Simulation	
3:30	Break	
3:45	Workshop Roundtable Discussion	Doug Kothe
4:45	Wrap up	Ricky Kendall
5:00	Adjourn	