

SciDAC-3 Principal Investigator Meeting
Monday, September 10, 2012
Agenda

Hilton Washington, DC/Rockville Executive Meeting Center
1750 Rockville Pike
Rockville, MD 20852
Phone: 301-468-1100

7:00am – 8:15am	Continental Breakfast Registration		Plaza Foyer Ballroom Foyer
8:15am – 8:45am	Opening Remarks Steven Lee, DOE/ASCR & Esmond Ng, Lawrence Berkeley National Laboratory		Plaza I and II
8:45am – 10:15am	SciDAC Institute Overviews Chair: Steven Lee, DOE/ASCR		Plaza I and II
	8:45am – 8:50am	SciDAC Institute Introductions Steven Lee, DOE/ASCR	Plaza I and II
	8:50am – 9:35am	<i>The Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) Project</i> Lori Diachin, Lawrence Livermore National Laboratory	Plaza I and II
	9:35am – 10:05am	<i>Quantification of Uncertainty in Extreme Scale Computations (QUEST)</i> Habib Najm, Sandia National Laboratories	Plaza I and II
	10:05am – 10:15am	Q & A	Plaza I and II
10:15am – 10:45am	Break		Plaza Foyer
10:45am – 12:15pm	SciDAC BES Application Partnership Project Overviews Chair: James Davenport, DOE/BES		Plaza I and II
	10:45am – 10:50am	BES Project Introductions James Davenport, DOE/BES	Plaza I and II
	10:50am – 11:15am	<i>Scalable Computational Tools for Discovery and Design – Excited State Phenomena in Energy Materials</i> James Chelikowsky, University of Texas-Austin	Plaza I and II
	11:15am – 11:40am	<i>Large-Scale Dynamics Simulations of Superconductors: New Fundamental Scientific Insights, Computational Challenge, and Broad Impact</i> Andreas Glatz, Argonne National Laboratory	Plaza I and II
	11:40am – 12:05pm	<i>Simulating the Generation, Evolution and Fate of Electronic Excitations in Molecular and Nanoscale Materials with First Principles Methods</i> Martin Head-Gordon, University of California-Berkeley	Plaza I and II
	12:05pm – 12:15pm	Q & A	Plaza I and II

12:15pm – 1:45pm	Working Lunch (see seating assignment)		TBD
1:45pm – 3:15pm	SciDAC BER Application Partnership Project Overviews Chair: Dorothy Koch, DOE/BER		Plaza I and II
	1:45pm – 1:50pm	BER Project Introductions Dorothy Koch, DOE/BER	Plaza I and II
	1:50pm – 2:15pm	<i>Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System</i> William Collins, Lawrence Berkeley National Laboratory	Plaza I and II
	2:15pm – 2:40pm	<i>Prediction of Ice and Climate Evolution at Extreme Scales (PISCEES)</i> Stephen Price, Los Alamos National Laboratory	Plaza I and II
	2:40pm – 3:05pm	<i>Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)</i> Forrest Hoffman, Oak Ridge National Laboratory	Plaza I and II
	3:05pm – 3:15pm	Q & A	Plaza I and II
3:15pm – 3:45pm	Break		Plaza Foyer
3:45pm – 4:30pm	Institute Poster Introductions Chairs: Youssef Marzouk, MIT & Stefan Wild, Argonne National Laboratory		Plaza I and II
4:30pm – 6:00pm	Poster Session		Roosevelt/Madison
6:00pm	Dinner Break		On Your Own
6:00pm – 9:00pm	Project Meetings (optional)		TBD

SciDAC-3 Principal Investigator Meeting
Tuesday, September 11, 2012
Agenda

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7:00am – 8:30am	Continental Breakfast Registration		Plaza Foyer Ballroom Foyer
8:30am – 8:45am	General Announcements		Plaza I and II
8:45am – 10:20am	SciDAC Institute Overviews Chairs: Lucy Nowell, DOE/ASCR & Ceren Susut-Bennett, DOE/ASCR		Plaza I and II
	8:45am – 8:50am	SciDAC Institute Introduction Lucy Nowell, DOE/ASCR	Plaza I and II
	8:50am – 9:35am	<i>The Scalable Data-management, Analysis, and Visualization (SDAV) institute</i> Arie Shoshani, Lawrence Berkeley National Laboratory	Plaza I and II
	9:35am – 9:40am	SciDAC Institute Introduction Ceren Susut-Bennett, DOE/ASCR	Plaza I and II
	9:40am – 10:10am	<i>The SciDAC-3 Institute for Sustained Performance, Energy, and Resilience</i> Robert Lucas, Information Sciences Institute	Plaza I and II
	10:10am – 10:20am	Q & A	Plaza I and II
10:20am – 10:50am	Break		Plaza Foyer
10:50am – 12:20pm	SciDAC NP Application Partnership Project Overviews Chair: Ted Barnes, DOE/NP		Plaza I and II
	10:50am – 10:55am	NP Project Introductions Ted Barnes, DOE/NP	Plaza I and II
	10:55am – 11:20am	<i>Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics</i> Frithjof Karsch, Brookhaven National Laboratory	Plaza I and II
	11:20am – 11:45am	<i>Nuclear Computational Low Energy Initiative</i> Joseph Carlson, Los Alamos National Laboratory	Plaza I and II
	11:45am – 12:10pm	<i>Connecting Lattice QCD and Nonrelativistic Effective Theory: A Multi-Scale Approach to Nuclear Physics</i> Wick Haxton, University of California-Berkeley & Thomas Luu, Lawrence Livermore National Laboratory	Plaza I and II
	12:10pm – 12:20pm	Q & A	Plaza I and II

12:20pm – 1:45pm	Working Lunch (see seating assignment)		TBD
1:45pm – 2:50pm	SciDAC FES Application Partnership Project Overviews Chair: John Mandrekas, DOE/FES		Plaza I and II
	1:45pm – 1:50pm	FES Project Introductions John Mandrekas, DOE/FES	Plaza I and II
	1:50pm – 2:15pm	<i>Overview of the Fusion Edge Physics Simulation Project (EPSI)</i> Choong-Seock Chang, Princeton Plasma Physics Laboratory	Plaza I and II
	2:15pm – 2:40pm	<i>Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing</i> Brian Wirth, University of Tennessee-Knoxville	Plaza I and II
	2:40pm – 2:50pm	Q & A	Plaza I and II
2:50pm – 3:20pm	Break		Plaza Foyer
3:20pm – 4:05pm	SciDAC Application Partnership Poster Introductions Chairs: Wes Bethel, Lawrence Berkeley National Laboratory & Karen Devine, Sandia National Laboratories		Plaza I and II
4:05pm – 5:35pm	Poster Session		Roosevelt/Madison
6:00pm	Dinner Break		On Your Own
6:00pm – 9:00pm	Project Meetings (optional)		TBD

SciDAC-3 Principal Investigator Meeting
Wednesday, September 12, 2012
Agenda

Hilton Washington, DC/Rockville Executive Meeting Center
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7:00am – 8:30am	Continental Breakfast Registration		Plaza Foyer Ballroom Foyer
8:30am – 10:25am	SciDAC BES Application Partnership Project Overviews Chair: Mark Pederson, DOE/BES		Plaza I and II
	8:30am – 8:35am	BES Project Introductions Mark Pederson, DOE/BES	Plaza I and II
	8:35am – 9:00am	<i>Charge Transfer and Charge Transport in Photoactivated Systems: Developing Electron-Correlated Methods for Excited State Structure and Dynamics in the NWChem Software Suite</i> Christopher Cramer, University of Minnesota	Plaza I and II
	9:00am – 9:25am	<i>Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments</i> Roberto Car, Princeton University	Plaza I and II
	9:25am – 9:50am	<i>Discontinuous Methods for Accurate, Massively Parallel Quantum Molecular Dynamics: Lithium Ion Interface Dynamics from First Principles</i> John Pask, Lawrence Livermore National Laboratory	Plaza I and II
	9:50am – 10:15am	<i>Predictive Computing for Condensed Matter</i> Lucas Wagner, University of Illinois at Urbana-Champaign	Plaza I and II
	10:15am – 10:25am	Q & A	Plaza I and II
10:25am – 10:55am	Break		Plaza Foyer
10:55am – 12:25pm	SciDAC HEP Application Partnership Project Overviews Chair: Lali Chatterjee, DOE/HEP		Plaza I and II
	10:55am – 11:00am	HEP Project Introductions Lali Chatterjee, DOE/HEP	Plaza I and II
	11:00am – 11:25am	<i>Community Petascale Project for Accelerator Science and Simulation (COMPASS)</i> Panagiotis Spentzouris, Fermi National Accelerator Laboratory	Plaza I and II

	11:25am – 11:50am	<i>Searching for Physics Beyond the Standard Model: Strongly-Coupled Field Theories at the Intensity and Energy Frontiers</i> Paul Mackenzie, Fermi National Accelerator Laboratory	Plaza I and II
	11:50am – 12:15pm	<i>Computing at the Cosmic Frontier</i> Salman Habib, Argonne National Laboratory	Plaza I and II
	12:15pm – 12:25pm	Q & A	Plaza I and II
12:25pm – 1:00pm	Wrap-Up Steven Lee, DOE/ASCR & Esmond Ng, Lawrence Berkeley National Laboratory		Plaza I and II
1:00pm	Meeting Adjourned		