

BES Computing and Data Requirements in the Exascale Age
November 3-5, 2015
Rockville MD

Monday, November 2 Evening meeting at 7pm in the Lincoln Room for chairs and breakout leads to discuss the next day's activities.

Tuesday, November 3

7:30 – 8:30 Registration, Refreshments

8:30 – 8:40 Welcome & Introductions - Michael Banda, Tom Devereaux, Theresa Windus

8:40 – 9:20 View from Basic Energy Sciences - Harriet Kung, Associate Director, BES

9:20 – 9:50 Genesis of this Meeting, Barb Helland, ASCR

9:50 – 10:20 Transformative Opportunities to Enable the Transformative Opportunities
John Sarrao, Los Alamos National Laboratory

10:20 – 10:40 Break

10:40 – 11:10 BES Facilities: Data Production, Analysis, & Storage, Craig Tull, Lawrence Berkeley National Laboratory

11:10 – 11:50 Requirements Gathering for ASCR Facilities
Katherine Riley, Argonne National Laboratory

11:50 – 12:10 Charge to Working Groups – Michael Banda, Tom Devereaux, Theresa Windus

12:10 – 1:00 Working Lunch

1:00 Breakout Sessions: Science Drivers

Quantum Materials, Core Challenges in Heavy-Element Chemistry, Exotic States, Emergence

- Aurora Clark, Washington State University, and Andy Millis, Columbia University

Catalysis, Photosynthesis, Light Harvesting, Combustion

- Laura Gagliardi, University of Minnesota, and Thanos Panagiotopoulos, Princeton University

Materials & Chemical Discovery

- Ilja Siepmann, University of Minnesota
- Chris Wolverton, Northwestern University

Computing & Data Challenges @ BES Facilities

- Thomas Proffen, Oak Ridge National Laboratory

- 2:30 – 2:50 Break
- 4:00 Break
- 4:15 Preliminary Reports Breakout Leads, 15 minutes each
- 5:30 Q&A: Harriet Kung, Associate Director, BES and Steve Binkley, Associate Director, ASCR
- 6:15 Dinner on your own

Wednesday, November 4

- 8:00 Refreshments
- 8:30 Computational materials science: a multi-disciplinary enterprise, Thomas Schulthess, Director, Swiss National Supercomputing Centre, ETH Zurich
- 9:10 Summary by Chairs, Outline of Report
Michael Banda, Tom Devereaux, Theresa Windus
- 9:30 Break
- 10:00 Breakouts – Continuation of 1:00 PM Tuesday Sessions; Outline Sections, Start Writing
- Quantum Materials, Core Challenges in Heavy-Element Chemistry, Exotic States, Emergence
- Aurora Clark, Washington State University, and Andy Millis, Columbia University
- Catalysis, Photosynthesis, Light Harvesting, Combustion
- Laura Gagliardi, University of Minnesota, and Thanos Panagiotopoulos, Princeton University
- Materials & Chemical Discovery
- Ilja Siepmann, University of Minnesota
 - Chris Wolverton, Northwestern University
- Computing & Data Challenges @ BES Facilities
- Thomas Proffen, Oak Ridge National Laboratory
- 12:00 Working Lunch

1:00 Breakout Sessions: Computing Landscape

Next Generation Programming

- Jackie Chen, Sandia National Laboratories, and Anouar Benali, Argonne National Laboratory

Advances in Quantum Algorithms

- Mark Gordon, Iowa State University, and Paul Kent, Oak Ridge National Laboratory

Math & Computer Science

- Jamie Sethian, University of California, Berkeley, and Lori Diachin, Lawrence Livermore National Laboratory

Data Management, Analytics, Visualization & Preservation

- Craig Tull, Lawrence Berkeley National Laboratory, and Kerstin Kleese van Dam, Brookhaven National Laboratory

Soft Matter, Biochemistry, Bioinspired Materials: Included here are

Multiscale Methods & Algorithms and Classical Molecular Dynamics

- Priya Vashishta, University of Southern California, and Mark Stevens, Sandia National Laboratories

2:30 – 2:50 Break

4:00 Break

4:20 Reports on Wednesday Breakouts, Breakout Leads, 15 minutes each

5:20 Summary and Thanks from Chairs

5:45 End for Most Participants

Thursday, November 5

8:30 Cochairs, Leads, Writers meet to continue working on report

12:00 End of Meeting