



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Tuesday, May 22, 2007

- 8:00 – 9:30** **NIF/TSF tours (Optional for early arrivers)**
- 9:30 – 9:40** **Welcome and Logistics – Armadillo Auditorium**
Dona Crawford, Lawrence Livermore National Laboratory
Walt Polansky, U.S. Department of Energy
Lori Diachin, Lawrence Livermore National Laboratory
- 9:40 – 11:00** **Plenary Talks (2 talks, 40 minutes each) – Armadillo Auditorium**
- *Optimization Research in 2007: Incremental, Transformational, or Recycled? (Page 1)*
Prof. Margaret Wright, New York University
 - *Adaptive Control of Multiscale Modeling Error, with Applications to Large-Scale Molecular Systems (Page 1)*
Prof. Tinsley Oden, University of Texas at Austin
- 11:00 – 11:15** **BREAK**
- 11:15 – 12:45** **Parallel Sessions**
- **Numerical Methods – Armadillo Auditorium**
Session Chair: Dr. Milo R. Dorr, Lawrence Livermore National Laboratory
 - *Mimetic discretizations and what they can do for you (Page 22)*
Dr. Pavel Bochev, Sandia National Laboratories
 - *Adaptive finite volume method for distributed non-smooth parameter identification (Page 23)*
Prof. Eldad Haber, Emory University, *Early Career Principal Investigator*
 - *Advances in Tracking Interfaces: Semiconductors, InkJets, Seismic Imaging and Transport (Page 24)*
Dr. Jamie Sethian, Lawrence Berkeley National Laboratory
 - **Numerical Methods – Black Diamond Room**
Session Chair: Prof. Bill Kalies, Florida Atlantic University
 - *High-Order Methods for Petascale Science (Page 26)*
Dr. Paul Fischer, Argonne National Laboratory
 - *Simulation Environments for Electromagnetic Scattering (Page 26)*
Prof. Leslie Greengard, New York University, Courant Institute
 - *Solving Multi-Material and Multi-Physics Problems on Overlapping Grids (Page 26)*
Dr. William Henshaw, Lawrence Livermore National Laboratory
- 12:45 – 1:45** **WORKING LUNCH**
Terascale Simulation Facility Tour Video – Armadillo Room



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Tuesday, May 22, 2007

1:45 – 3:45

Parallel Sessions

• **Multiscale – Armadillo Auditorium**

Session Chair: Dr. John Shadid, Sandia National Laboratories

- *Atomistic-Continuum Adaptivity and Phase Transformation for the Quasicontinuum Approximation (Page 12)*
Prof. Mitchell Luskin, University of Minnesota
- *Analysis of Atomistic-to-Continuum (AtC) Coupling Methods (Page 12)*
Dr. Richard Lehoucq, Sandia National Laboratories
- *Wavelet-based Spatiotemporal Multiscale in Diffusion Problems with Chemically Reactive Boundary (Page 20)*
Dr. Sreekanth Pannala, Oak Ridge National Laboratory
- *Multiscale energy constraints in rotating and stratified flows (Page 14)*
Dr. Susan Kurien, Los Alamos National Laboratory

• **Optimization – Black Diamond Room**

Session Chair: Dr. Jorge Moré, Argonne National Laboratory

- *What's New in Mixed-Integer Nonlinear Optimization (Page 34)*
Dr. Sven Leyffer, Argonne National Laboratory
- *Optimization: Preconditioners, PDE Constraints and Equilibrium (Page 34)*
Prof. Jorge Nocedal, Northwestern University
- *Speeding the Training of Support Vector Machines and Solution of Quadratic Programs (Page 35)*
Prof. Dianne O'Leary, University of Maryland
- *Inverse problems for systems constrained by reaction diffusion equations (Page 35)*
Prof George Biros, University of Pennsylvania, *Early Career Principal Investigator*

3:45 – 4:25

Plenary Talk – Armadillo Auditorium

Predictive Capability in Computational Science and Engineering (Page 2)
Dr. William Oberkampf, Sandia National Laboratories

4:30– 6:00

Poster session - Multiscale, Optimization emphasis

6:30 – 8:30

Working Dinner – Wentz Vineyards

Keynote Speaker – Dr. Joe Grcar, Lawrence Berkeley National Laboratory



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Wednesday, May 23, 2007

8:00 – 8:30 **Continental Breakfast**

8:30 – 8:40 **Opening Remarks**

8:40- 10:00 **Plenary Talks – Armadillo Auditorium**

- *Numerical modeling of low Mach number flows (Page 3)*
Dr. John Bell, Lawrence Berkeley National Laboratory
- *Recent Developments in Systems Solvers (Page 4)*
Prof. Tom Manteuffel, University of Colorado

10:00-10:15 **BREAK**

10:15 – 12:15 **Parallel Sessions**

- **Numerical Methods – Armadillo Auditorium**
Session Chair: Prof. Marsha Berger, New York University
 - *A Local Corrections Algorithm for Solving Poisson's Equation in Three Dimensions (Page 27)*
Dr. Phillip Colella, Lawrence Berkeley National Laboratory
 - *Numerical Methods of Electromagnetics for Complex Inhomogenous Systems (Page 28)*
Prof. Wei Cai, University of North Carolina at Charlotte
 - *Systematic Deceleration of Fast Modes in Multi-Scale Systems (Page 28)*
Prof. Ilya Timofeyev, University of Texas at Houston. *Early Career Principal Investigator*
 - *Mimetic Methods for Partial Differential Equations (Page 29)*
Dr. Mikhail Shashkov, Los Alamos National Laboratory
- **Linear/Nonlinear Solvers – Black Diamond Room**
Session Chair: Dr. Esmond Ng, Lawrence Berkeley National Laboratory
 - *Multiresolution analysis and low separation rank methods for scientific simulations (Page 10)*
Dr. George Fann, Oak Ridge National Laboratory
 - *Fast Iterative Solution of Models of Incompressible Flow (Page 7)*
Prof. Howard C. Elman, University of Maryland
 - *Inexact Krylov Subspace Methods for PDEs and Control Problems (Page 9)*
Prof. Daniel Szyld, Temple University
 - *A Newton-Krylov solver for fully implicit 3D extended MHD (Page 9)*
Dr. Luis Chacon, Los Alamos National Laboratory



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Wednesday, May 23, 2007

- 12:15 – 1:15** **WORKING LUNCH:** Terascale Simulation Facility Tour Video – Armadillo Room
- 1:15 – 1:30** **GROUP PHOTO:** Terascale Simulation Facility
- 1:30 – 2:45** **Panel on Future Architectures – Armadillo Auditorium**
Panel Moderator: Dr. Steve Louis, Lawrence Livermore National Laboratory
Panelists:
- Dr. William Gropp, Argonne National Laboratory
 - Dr. Matthew Leininger, Sandia National Laboratory/Lawrence Livermore National Laboratory
 - Dr. Stephen Poole, Oak Ridge National Laboratory
 - Dr. John Shalf, Lawrence Berkeley National Laboratory
- 2:45 – 3:45** **Plenary Talks (2 talks, 30 minutes each) – Armadillo Auditorium**
- *Architecture Trends and Implications for Algorithms (Page 4)*
Dr. William Gropp, Argonne National Laboratory
 - *Understanding the Science in Data: Challenges at the Petascale*
Dr. Chandrika Kamath, Lawrence Livermore National Laboratory
- 3:45 – 4:00** **BREAK**
- 4:00 – 5:30** **Poster session - Numerical Methods, Solvers emphasis**
- 6:00 pm** **Dinner on your own**



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Thursday, May 24, 2007

8:00 – 8:30 **Continental Breakfast**

8:30 – 10:30 **Parallel Sessions**

- **Multiscale – Armadillo Auditorium**

Session Chair: Dr. Andris Dimitz, Lawrence Livermore National Laboratory

- *Dimensional reduction for multiscale problems (Page 15)*
Prof. Alexandre Chorin, Lawrence Berkeley National Laboratory
- *Mortar multiscale methods for flow in porous media (Page 17)*
Prof. Ivan Yotov, University of Pittsburgh
- *Algorithms and Software for Multiscale Simulation of Chemically Reacting Systems (Page 17)*
Prof. Linda Petzold, University of California at Santa Barbara
- *Multiscale Approach to Self-Organization of Microtubules and Actin Filaments (Page 16)*
Dr. Dmitry Karpeev, Argonne National Laboratory

- **Optimization/Solvers – Black Diamond Room**

Session Chair: Prof. Andre Tits, University of Maryland

- *New Heuristic Techniques for General Mixed-Integer Programs (Page 36)*
Dr. Cynthia Phillips, Sandia National Laboratories
- *Orbital Branching (Page 38)*
Prof. Jeff Linderth, Lehigh University, *Early Career Principal Investigator*
- *Algebraic Multigrid with Applications (Page 6)*
Dr. Robert Falgout, Lawrence Livermore National Laboratory
- *Parallel segregated Schur complement methods for fluid density functional theories (Page 10)*
Dr. Michael Heroux, Sandia National Laboratories

10:30 – 10:45 **BREAK**



Office of Advanced Scientific Computing Research
2007 Applied Mathematics Research Program Annual PI Meeting
May 22 – 24, 2007

AGENDA

Thursday, May 24, 2007

10:45 – 12:45

Parallel Sessions

- **Multiscale – Armadillo Auditorium**

Session Chair: Prof. Mark Alber, University of Notre Dame

- *Multiscale Numerical Methods for Plasma Kinetics (Page 17)*
Prof. Russell Caflisch, University of California at Los Angeles
- *Multi Spatial and Time Scale Coupling in Rotating and Stratified Flows (Page 19)*
Dr. Leslie Smith, University of Wisconsin
- *Multiscale modeling of spatially distributed biological systems (Page 13)*
Prof. Dion Vlachos, University of Delaware
- *Multiscale Strategies for Critical Phenomena in Heterogeneous Materials (Page 15)*
Dr. Kim Ferris, Pacific Northwest National Laboratory

- **Numerical Methods – Black Diamond Room**

Session Chair: Prof. Paul Woodward, University of Minnesota

- *Adaptive Hybrid Mesh Optimization and Refinement (Page 30)*
Dr. Ahmed Khamayseh, Oak Ridge National Laboratory
- *Models and Computational Algorithms for Multiphase Magnetohydrodynamics (Page 30)*
Dr. Roman Samulyak, Brookhaven National Laboratory
- *Efficient Nonlinear/Non-Gaussian Hydrological Estimation in Composite Media (Page 31)*
Prof. Juan Restrepo, University of Arizona
- *Lagrangian Simulations of Combustion (Page 32)*
Prof. Ahmed Ghoniem, Massachusetts Institute of Technology

12:45 – 1:45

WORKING LUNCH: Terascale Simulation Facility Tour Video – Armadillo Room

1:45 – 3:00

Open Forum Discussion – Armadillo Auditorium

Opportunities and Challenges for Applied Math

Led by David Brown and Walt Polansky

3:00 pm

Adjourn

3:15 – 5:00

NIF tours (Optional for those not leaving right away) – Building 581