



# Office of Advanced Scientific Computing Research

2007 Applied Mathematics Research Program Annual PI Meeting

May 22 – 24, 2007

## POSTER SESSION

**Tuesday, May 22, 2007**

No.	Title	Authors
1	Predicting the Electronic Properties of 3D, Million Atom Nanostructures	A. Canning, O. Marques, C. Voemel, L-W Wang , Lawrence Berkeley National Laboratory ; S. Tomov, J. Langou and J. Dongarra, University of Tennessee; Knoxville
2	Density matrix methods as eigensolver replacements in density functional theory	Richard Muller, Rich Lehoucq, Sandia National Laboratories
3	Inverse Problem in Seismic Imaging	Maria Cameron, LBNL, Sergey Fomel (UT Austin), Jamie Sethian, LBNL
4	Spectral Methods for the Analysis of Stochastic Dynamical Systems	Bert Debuschere, Sandia National Laboratories, Livermore, CA; Habib Najm, Sandia National Laboratories, Livermore, CA; Dongjin Kim, Georgetown University, Washington, DC; Olivier Le Maitre, Universite d'Evry Val d'Essonne, Evry, France
5	A network-particle computational method for dense suspensions	Alexander Panchenko, Department of Mathematics, Washington State University; Alexander Tartakovsky, PNNL)
6	New Results from "VEGA" Vulnerability of Electric Grids Analyzer	Javier Salmeron, Kevin Wood, Naval Postgraduate School
7	A multiscale coupling of continuum elasto-viscoplasticity and discrete dislocation dynamic	Firas Akasheh, Washington State University; Hussein M. Zbib, Washington State University
8	Multiscale Models of Morphogenesis	Mark Alber, University of Notre Dame
9	Multilevel Upscaling in Multiscale Modeling and Parameter Estimation	David Moulton (co-PI), Los Alamos National Laboratory, Los Alamos, NM; Daniel Tartakovsky (co-PI), LANL/UCSD; Scott MacLachlan, Delft University of Technology, The Netherlands; Ethan Coon, Columbia University, New York, NY
10	Coarse-graining and microscopic reconstruction in simulations of stochastic systems	Petr Plechac, Oak Ridge National Laboratory
11	Convergence Analysis for Takizuka & Abel and Nanbu's Collision Models	CM Wang, University of California, Los Angeles; Tungyou Lin, University of California, Los Angeles; Russel Cafilisch, University of California, Los Angeles; Bruce Cohen, Lawrence Livermore National Laboratory; Andris Dimits, Lawrence Livermore National Laboratory
12	Fast Marching Methods for the continuous Traveling Salesman Problem	June Andrews, Department of Mathematics, University of California Berkeley; James Sethian,
13	Statistical Mechanics and Complex Dynamics in Rapidly Rotating Bounded Flows	Chjan Lim, Rensselaer Polytechnic Institute



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No.	Title	Authors
14	Towards 1,000,000 Atom First Principles Electronic Structure Simulation Code	William A. Shelton, Oak Ridge National Laboratory
15	A Linear Scaling 3-Dimensional Fragment Method for Petascale Nanoscience Simulations	Zhengji Zhao, Lin-Wang Wang, Juan Meza, Computational Research Division, Lawrence Berkeley National Laboratory
16	Analytic Jacobians in the Solution of Nonlinear PDEs	Paul D Hovland, Argonne National Laboratory; Boyana Norris, Argonne National Laboratory
17	Parallel Optimization Using TAO	Jorge More, ANL/MCS Division; Todd Munson, ANL/MCS Division; Jason Sarich, ANL/MCS Division
18	A polynomial-time interior-point method for conic optimization, with inexact barrier evaluations	Simon P. Schurr, University of Waterloo; Dianne P. O'Leary, Andre L. Tits, University of Maryland
19	Convergence of a Constraint-Reduced Variant of Mehrotra's Predictor-Corrector Algorithm	Luke Winternitz, Stacey Nicholls, Andre L. Tits, Dianne P. O'Leary, University of Maryland
20	Convex Duality and Entropy-Based Moment Equations: Characterizing Degenerate Densities	Cory D. Hauck, Los Alamos National Laboratory; Andre L. Tits, C. David Levermore, University of Maryland
21	A Fitness Landscape Analysis of the Capacitated Vehicle Routing Problem	Jean-Paul Watson, SNL
22	Recent Advances in High Order methods for Simulation of Richtmyer-Meshkov Instability	David Gottlieb and Wai-Sun Don Brown University



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No.	Title	Authors
1	An Eigensolver with Lowrank Updates for Spin-Fermion Models	E. D'Azevedo*, P. Nukala, G. Alvarez, Computer Science and Mathematics Division, Oak Ridge National Laboratory
2	A simple, fast, high-order Helmholtz solver	Leonid Kunyansky, University of Arizona
3	Robust and Scalable Factorization-based Preconditioners Suitable for Petascale Simulations	Ming Gu, University of California at Berkeley; Xiaoye Sherry Li, Lawrence Berkeley National Lab; Panayot S. Vassilevski, Lawrence Livermore National Lab <sup>o</sup>
4	Adaptive Multimethod Linear Solvers for Nonlinear PDEs	Lois Curfman McInnes, Argonne National Laboratory; Boyana Norris, Argonne National Laboratory; Sanjukta Bhowmick, Argonne National Laboratory and Columbia University; Dinesh Kaushik, Argonne National Laboratory; Padma Raghavan, Penn State University
5	AMS: A Scalable Maxwell Solver	Tanio Kolev, Panayot Vassilevski, LLNL
6	3D Boundary Integral Analysis by a Fast Spectral Method	S. Nintcheu Fata, L. J. Gray, T. Kaplan, ORNL
7	Multiscale numerical methods for flows in heterogeneous porous media using limited global information	Yalchin Efendiev, Texas A&M, Tom Hou (Caltech), Victor Ginting (Colorado State)
8	Low Mach Number Modeling of Type Ia Supernovae	Ann S. Almgren, John B. Bell, Mike Zingale, * LBNL
9	A Stable Finite Difference Method for the Elastic Wave Equation on Complex Domains with Free Surface Boundary Conditions	Daniel Appelo, LLNL; Anders Petersson, LLNL; Bjorn Sjogreen, LLNL
10	Characterization of Implicit LES Methods	A. J. Aspden, LBNL; J. B. Bell, LBNL
11	Comparison of Flux-Corrected-Transport and High Resolution Godunov Methods on Overlapping Grids	J. W. Banks, Sandia National Laboratory; J. N. Shadid, Sandia National Laboratory
12	Domain Adaptive High Order Accurate Algorithms for PDEs in Moving Geometry	Bill Henshaw, Kyle Chand, LLNL
13	A Cartesian AMR framework for detonation- and shock-driven fluid-structure interaction sim	Ralf Deiterding, ORNL



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14	High-Resolution Discretization of the Gyrokinetic Vlasov-Poisson Equation on Mapped Grids	M. Dorr, Lawrence Livermore National Laboratory; J. Hittinger, Lawrence Livermore National Laboratory; P. Colella, Lawrence Berkeley National Laboratory; D. Martin, Lawrence Berkeley National Laboratory
15	Lagrangian Simulations of Combustion	Ahmed F Ghoniem, Massachusetts Institute of Technology; Fabrice Schegel, Massachusetts Institute of Technology; Daehyun Wee, Massachusetts Institute of Technology
16	Implicit Interface Finite Element Method for Elliptic Interface Problems	Jae-Seok Huh, Student, Department of Mathematics, UC Berkeley; James A. Sethian, Professor of Mathematics, UC Berkeley
17	The Analysis of Particle Migration in Dilute Suspensions Using a TC-BEM	Marc Ingber (U of New Mexico), Alan Graham (LANL), Shihai Feng (LANL), Lisa Mondy (SNL)
18	Mimetic Discretizations	Konstantin Lipnikov, Los Alamos National Laboratory; Mikhail Shashkov, Los Alamos National Laboratory
19	Computational Nanophotonics and NEKCEM	Misun Min, Argonne National Laboratory; Paul Fischer, Mathematics and Computer Science Division
20	Solving PDEs on Irregular Domains with Moving Interfaces	Ying Shan, Lawrence Berkeley National Laboratory; J.A. Sethian, Lawrence Berkeley National Laboratory
21	A subgrid-Scale Turbulence Model for Simulating Compressible Flows	Paul R. Woodward, University of Minnesota
22	Implementing an Interior Point Method for Linear Programs on a CPU-GPU System	Jin Hyuk Jung, Dianne O'Leary, University of Maryland