

*Proceedings*

---

**HPCMP Users Group Conference**

**2006**

# HPCMP USERS GROUP CONFERENCE 2006

## TABLE OF CONTENTS

<b>Editor's Preface</b> _____	<b>xi</b>
<b>1. COMPUTATIONAL STRUCTURAL MECHANICS (CSM)</b>	
Numerical Simulations of Explosive Blast Pressures during Wall Breaching _____ <i>Stephen Akers, Jay Ehrgott, and Denis Rickman</i>	3
Fracture of Kinetic Energy Rods Subject to Oblique Impact _____ <i>Robert Anderson</i>	9
Statistical Fatigue and Residual Strength Analysis of New/Aging Aircraft Structure _____ <i>Scott Fawaz and Börje Andersson</i>	13
<b>2. COMPUTATIONAL FLUID DYNAMICS (CFD)</b>	
High-Fidelity Simulations for Maneuvering Unmanned Combat Air Vehicle Configurations _____ <i>Raymond Gordnier, Scott Sherer, and Miguel Visbal</i>	23
Computational Science and Engineering Advances Understanding of Complex Unsteady Flows in High Performance Fans and Compressors _____ <i>Steve Gorrell, Fu-Lin Tsung, Jixian Yao, and Rhonda Vickery</i>	31
Quasi-Steady Vortex Tracking in Rotorcraft CFD on the Cray X1 _____ <i>YikLoon Lee</i>	39
Applied Computational Fluid Dynamics in Support of Aircraft/Store Compatibility and Weapons Integration _____ <i>Joseph Keen</i>	45
High Resolution Simulation of Full Aircraft Control at Flight Reynolds Numbers _____ <i>Scott Morton, James Forsythe, David McDaniel, Stefan Goertz, Russell Cummings, Stefan Siegel, Kenneth Wurtzler, and Kyle Squires</i>	52
Blade-Vortex Interaction Airloads Prediction Using Multidisciplinary Coupling _____ <i>Joon Lim, Mark Potsdam, Roger Strawn, Ben Sim, and Tor Nygaard</i>	59
Time-Accurate Numerical Prediction of Free Flight Aerodynamics of Projectiles _____ <i>Jubaraj Sahu</i>	66
Accuracy and Performance Testing of Three-Dimensional Unsaturated Flow Finite Element Groundwater Programs on the Cray XT3 Using Analytical Solutions _____ <i>Fred Tracy</i>	73
LES and DES of High Reynolds Number, Supersonic Base Flows with Control of the Near Wake _____ <i>J. Sivasubramanian and H.F. Fasel</i>	80

### 3. CFD COUPLED TO CHEMISTRY, MAGNETIC FIELDS, AND STRUCTURES (CFD, CSM, & CCM)

Development of Plasma-Based Flow Control Techniques for Scramjet Flow Paths _____	91
<i>Datta Gaitonde and Martin Lindsey</i>	
Quantifying Behind Armor Debris Fragments from CTH Using the Interdisciplinary Computing Environment _____	98
<i>Jerry Clarke and Eric Mark</i>	
Model and Code Development in Support of the Portfolio for Multiphase Flow Technology _____	102
<i>Eugene Hertel and James Stewart</i>	
Effects of Projectile and Cover Material Strength and Projectile Shape on the Impact Initiation of Composition B _____	106
<i>W. Lawrence and J. Starkenberg</i>	
Combustion Chamber Fluid Dynamics and Hypergolic Gel Propellant Chemistry Simulations for Selectable Thrust Rocket Engines _____	110
<i>Michael Nusca and Michael McQuaid</i>	
Numerical Simulation of the Combustion of Aluminum Shock-Dispersed-Fuel Charges ____	119
<i>Allen Kuhl, Boris Khasainov, John Bell, and Vince Beckner</i>	
Chemical Oxygen-Iodine Laser Technology Development Using 3-D Navier-Stokes Simulation _____	124
<i>Timothy Madden</i>	

### 4. SHIP HYDRODYNAMICS AND DESIGN

Hydrodynamics Prediction of High Speed Sea Lift (HSSL) Ships _____	135
<i>Joseph Gorski, Ronald Miller, Pablo Carrica, Mani Kandasamy, Tao Xing, and Fred Stern</i>	
The Increasing Use of Visualization in Ship Hydrodynamics _____	141
<i>Joseph Gorski, Michael Ebert, Susan Brewton, Peter Chang, Ronald Miller, Joseph Slomski, William Smith, and Wesley Wilson</i>	
Unsteady Naval Hydrodynamic Computations Using Lagrangian Vorticity Methods ____	148
<i>Stephen Huyer</i>	
Direct Phase-Resolved Simulations of Large-Scale Nonlinear Ocean Wave-Fields _____	157
<i>Guangyu Wu, Yuming Liu, and Dick K.P. Yue</i>	
Progress Towards Modeling Ship/Aircraft Dynamic Interface _____	163
<i>Susan Polsky</i>	
Modeling Breaking Ship Waves for Design and Analysis of Naval Vessels _____	169
<i>Gabriel Weymouth, Kelli Hendrickson, Douglas Dommermuth, Dick K.P. Yue, Paul Adams, and Randall Hand</i>	

## 5. COMPUTATIONAL CHEMISTRY AND MATERIALS SCIENCE (CCM) AND COMPUTATIONAL BIOLOGY

Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys _____	177
<i>Mark Asta, Dallas Trinkle, and Christopher Woodward</i>	
Multiscale Simulations of Quantum Structures _____	182
<i>J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Ranjan, S. Wang, and L. Yu</i>	
Density-Fitting Method in Symmetry-Adapted Perturbation Theory Based on Kohn-Sham Description of Monomers _____	189
<i>Rafał Podeszwa, Robert Bukowski, and Krzysztof Szalewicz</i>	
Calculations of Light-Absorption Driven Molecular Rotors _____	193
<i>Jaroslav Vacek, Jana Chocholoušová, Lukáš Kobr, John Miller, and Josef Michl</i>	
Massively Parallel Simulations on Light-Induced Charge Transfer in Molecules _____	197
<i>Mark Pederson, Tunna Baruah, B.J. Powell, and Wendell Anderson</i>	
New Ferroelectrics for Naval SONAR and Modeling of Nanoscale Ferroelectric Nonvolatile Memory Materials _____	205
<i>Alexie Kolpak, Ilya Grinberg, Shawn Brown, and Andrew M. Rappe</i>	
Modeling Subsurface Phenomena for Tetrahedral Meshes _____	212
<i>Barry White and Owen Eslinger</i>	
Nonlinear Response of Strongly Correlated Materials to Large Electric Fields _____	218
<i>J.K. Freericks, V. Turkowski, and V. Zlatić</i>	

## 6. COMPUTATIONAL ELECTROMAGNETICS AND ACOUSTICS (CEA)

Intrusion Detection System Modeling _____	229
<i>Keesook Han and Joseph Giordano</i>	
Seismic Propagation from Activity in Tunnels _____	236
<i>Stephen Ketcham, Jason McKenna, Roy Greenfield, and Thomas Anderson</i>	
Swathbuckler: Real-Time Wide Swath Synthetic Aperture Radar Image Formation Using Embedded HPC _____	244
<i>Richard Linderman, Joshua Corner, and Scot Tucker</i>	
Virtual Prototyping of Directed Energy Weapons _____	252
<i>Matthew Bettencourt, David Amdahl, Lester Bowers, Keith Cartwright, Andrew Greenwood, Timothy Fleming, Michael Haworth, Nathaniel Lockwood, Peter Mardahl, Robert Peterkin, Jr., John Luginsland, and Jack Watrous</i>	
Virtual Prototyping of Directed Energy Weapons on Thousands of Processors _____	259
<i>Matthew Bettencourt, Lester Bowers, Keith Cartwright, Andrew Greenwood, Timothy Fleming, Michael Haworth, Nathaniel Lockwood, and Peter Mardahl</i>	

## **7. CLIMATE/WEATHER/OCEAN MODELING AND SIMULATION (CWO)**

Multi-Scale Predictability of High-Impact Weather in the Battlespace Environment _____	267
<i>James Doyle, Carolyn Reynolds, Justin McLay, Joao Teixeira, and Craig Bishop</i>	
Global Ocean Prediction Using HYCOM _____	271
<i>E. Joseph Metzger, Harley Hurlburt, Alan Wallcraft, Eric Chassignet, James Cummings, and Ole Martin Smedstad</i>	
Fine-Resolution Global Sea-Ice/Ocean Modeling and Data Assimilation _____	275
<i>Julie McClean, Detelina Ivanova, James Carton, Benjamin Giese, Elizabeth Hunke, and Mathew Maltrud</i>	
CWO Data Mining _____	280
<i>Mahnas Mohammadi-Aragh, Derek Irby, Robert Moorhead, and Rick Schumeyer</i>	
Successes and Future of the Joint Weather Research and Forecasting Model Distributed Center Project _____	283
<i>F. Anthony Eckel, Steven Rugg, and Stephen Klotz</i>	
Characterization of Stratospheric Clear Air Turbulence for Air Force Platforms _____	288
<i>Alex Mahalov, Mohamed Moustouai, and Basil Nichols</i>	
Characterization of High Altitude Turbulence for Air Force Platforms _____	296
<i>Frank Ruggiero, Joseph Werne, Alex Mahalov, and Basil Nichols</i>	

## **8. ELECTRONICS, NETWORKING, AND SYSTEMS/C4I (ENS) AND SIGNAL/IMAGE PROCESSING (SIP)**

Nonlinear Equalization for RF Receivers _____	303
<i>Brandon Kam, Benjamin Miller, Joel Goodman, and Gil Raz</i>	
Sourcery VSIPL++ HPEC Benchmark Performance _____	308
<i>Jules Bergmann and Don McCoy</i>	
VSIPL++ Acceleration Using Commodity Graphics Processors _____	315
<i>Dan Campbell</i>	
Real-Time 3-D Ladar Imaging _____	321
<i>Peter Cho, Hyrum Anderson, Robert Hatch, and Prem Ramaswami</i>	
Parallelization and Automation of a Blind Deconvolution Algorithm _____	327
<i>Charles Matson and Kathy Borelli</i>	

## **9. INTEGRATED MODELING AND TEST ENVIRONMENTS (IMT)**

High Performance Computational Environment for Real-Time Hardware-in-the-Loop Simulation _____	333
<i>Carlos Godoy</i>	
Distributed Tests: An ARMY Perspective _____	337
<i>Kenneth LeSueur, Ken Yetzer, Mike Stokes, Ashok Krishnamurthy, and Alan Chalker</i>	

## 10. COMPUTATIONAL INFRASTRUCTURE AND SOFTWARE AND HARDWARE PERFORMANCE

Early Experiences on the NRL Cray XD1 _____	347
<i>Jeanie Osburn, Wendell Anderson, Marco Lanzagorta, and Robert Rosenberg</i>	
High Performance Evolutionary Computing _____	354
<i>Edwin Núñez, Edwin Banks, Paul Agarwal, Marshall McBride, and Ron Liedel</i>	
Targeting CCM-, CEA-, and CSM-Based Computing to Specific Architectures Based upon HPCMP Systems Assessment _____	360
<i>Paul Bennett, Sam Cable, Mahin Mahmoodi, and Thomas Oppé</i>	
Performance Modeling of Emerging HPC Architectures _____	367
<i>Nikhil Bhatia, Sadaf Alam, and Jeffrey Vetter</i>	
Optimization of LAMMPS _____	374
<i>James Fischer, Vincent Natoli, and David Richie</i>	
Loop-Level Profiling and Analysis of DoD Applications Using TAU _____	378
<i>Shirley Moore, David Cronk, Sameer Shende, and Allen Malony</i>	
Fluent VTK Extractor _____	384
<i>Raymond Maple, Ryan Osterday, and Rhonda Vickery</i>	
CaseMan: A Case Management Tool for CFD Applications _____	389
<i>Alan Shih, Corey Shum, Mark Dillavou, Ralph Noack, Bharat Soni, and Greg Power</i>	
Prototype Visualization Tools for Multi-Experiment Performance Analysis _____	394
<i>Roberto Araiza, Jaime Nava, Alan Taylor, Patricia Teller, David Cronk, and Shirley Moore</i>	
Building and Running Application Codes on the ARL Linux Network Cluster (JVN) _____	399
<i>George Petit</i>	
The Development of a Utility of Assessing the Performance Impact of Shared/Distributed File Systems and Database Interactions in High-Performance Simulations _____	404
<i>Andrew Watkins and Richard Schumeyer</i>	
Information Management Support for Interactive High-Performance Computing Frameworks _____	410
<i>George Ramseyer, Virginia Ross, and Richard Linderman</i>	
An Interactive Web-Based HPC Reservation System _____	417
<i>Randy Schauer and Steven Thompson</i>	
ezHPC Security Architecture _____	422
<i>George Moncrief, Trent Townsend, and Scotty Swillie</i>	

## 11. MATLAB, OCTAVE AND PYTHON

Octave and Python: High-Level Scripting Languages Productivity and Performance Evaluation _____	429
<i>Juan Carlos Chaves, John Nehrbass, Brian Guilfoos, Judy Gardiner, Stanley Ahalt, Ashok Krishnamurthy, Jose Unpingco, Alan Chalker, Andy Warnock, and Siddharth Samsi</i>	
Enhancements to MatlabMPI: Easier Compilation, Collective Communication, and Profiling _____	435
<i>Judy Gardiner, John Nehrbass, Juan Carlos Chaves, Brian Guilfoos, Stanley Ahalt, Ashok Krishnamurthy, Jose Unpingco, Alan Chalker, and Siddharth Samsi</i>	
Interfacing PC-Based MATLAB Directly to HPC Resources _____	440
<i>John Nehrbass, Sidharth Samsi, Juan Carlos Chaves, Jose Unpingco, Brian Guilfoos, Stanley Ahalt, Ashok Krishnamurthy, Alan Chalker, and Judy Gardiner</i>	
Applications in Parallel MATLAB _____	445
<i>Brian Guilfoos, Judy Gardiner, Juan Carlos Chaves, John Nehrbass, Stanley Ahalt, Ashok Krishnamurthy, Jose Unpingco, Alan Chalker, Laura Humphrey, and Siddarth Samsi</i>	
<b>UGC 2006 ABSTRACTS AUTHOR LIST _____</b>	<b>449</b>
<b>AUTHOR INDEX _____</b>	<b>455</b>