



Oak Ridge National Laboratory  
2005 Fall Creek Falls Conference  
**Computational Science at Scale**  
<http://www.ccs.ornl.gov/workshops/FallCreek05/>  
The Inn at Fall Creek Falls State Park  
Central Daylight Savings Time

**Sunday, October 16, 2005**

Arrival and dinner in dining room (please sign in)

- 6:00 p.m. Reception / Welcome {Fall Creek I} ..... Thomas Zacharia  
8:00 p.m. End of day one  
8:00 p.m. Meeting of 2006 Fall Creek Falls Conference Committee

**Monday, October 17, 2005**

- 7:30 a.m. **Breakfast buffet** (please sign in) ..... Dining Room  
8:30 a.m. Opening remarks ..... Fall Creek II and III  
*Diversity of Architectures for Scientific Discovery* ..... Thomas Zacharia

**Cray X1E Platform**

- 8:45 a.m. *GYRO on the Cray X1E: high performance on a five-dimensional code with extreme bandwidth requirements* ..... Jeff Candy, General Atomics  
8:55 a.m. *New Insights into High-Temperature Superconductivity from a Computational Solution of the 2D Hubbard Model* ..... Thomas Maier, ORNL  
9:05 a.m. *Plasma Turbulence Research on MPP platforms* ..... W. W. Lee, PPPL  
9:15 a.m. *Computational Design of the Low-Loss Accelerating Cavity for the International Linear Collider* ..... Rich Lee, Stanford  
9:25 a.m. *High-Fidelity Terascale Numerical Simulations of Turbulent Combustion* ..... Ramanan Sankaran, SNL  
9:35 a.m. *Unique Capabilities of the Cray X1E* ..... James Schwarzmeier, Cray  
9:45 a.m. *Using Global Addressing on X1 to develop efficient libraries* ..... John Levesque, Cray

**Inquisitor Panel:** Jerry Bernholc, NCSU; Jackie Chen, SNL; Jeff Nichols, ORNL; Mark Seager, LLNL

10:25 a.m. **Break**

**SGI Altix Platform**

- 10:35 a.m. *Impact of Columbia on NASA Science and Engineering Applications* ..... Rupak Biswas, NASA  
10:45 a.m. *Scaling Climate Applications on SGI Altix* ..... CJ Suchyta, SGI  
10:55 a.m. *SGI Altix Architecture* ..... Rhonda Dias, SGI  
11:05 a.m. *Altix Tools for Scaling Codes* ..... CJ Suchyta, SGI

**Inquisitor Panel:** Jerry Bernholc, NCSU; Jackie Chen, SNL; Jeff Nichols, ORNL; Mark Seager, LLNL

- 11:45 p.m. **Lunch** (please sign in) ..... Dining Room  
. Afternoon free time and recreation at your leisure for hiking, fishing, relaxing

- 4:45 p.m. Poster session set up ..... Fall Creek I  
4:45 p.m. Reassemble ..... Fall Creek II and III

**Vendor Views**

- 5:00 p.m. *Productive Supercomputing with Cray Inc.* ..... John Levesque, Cray  
5:10 p.m. *IBM Update* ..... George Chiu, IBM  
5:20 p.m. *Building Blocks for Petascale Computing* ..... David Barkai, Intel  
5:30 p.m. *SGI Technology Update* ..... Sid Mair, SGI  
5:40 p.m. **Private Buffet Dinner** ..... Fall Creek II and III  
7:00 p.m. Poster session and refreshments ..... Fall Creek I  
8:30 p.m. End of day two

**Poster Session**

Monday, October 17, 2005

7:00 p.m.

Fall Creek I

***Achievements in ISIC/SAPP Collaborations for Electromagnetic Modeling of Accelerators***

Rich Lee, et al., Stanford

***Automatic Mapping of MATLAB Code to Parallel FPGAs on the SGI Altix***

Rhonda Dias, SGI

***Computational tools for chemical data assimilation***

Adrian Sandu, Virginia Tech

***Design and Implementation of Parallel Graph Algorithms on the Cray MTA-2***

Kamesh Madduri, Georgia Institute of Technology

***High-Performance Networking for Large-Scale Scientific Applications***

Q. Wu and N. Rao, Oak Ridge National Laboratory

***Large Eddy Simulation of Turbulence-Chemistry Interactions in Reacting Flows***

J. Oefelein and R. Barlow; Sandia National Laboratories

***Performance of Fusion RF Computation (AORSA) on High Performance Computers***

Lee Berry, et al., Oak Ridge National Laboratory

***Some Current Challenges in Computational Ecology***

Dali Wang, University of Tennessee, Knoxville

***Terascale Direct Numerical Simulations of Turbulent Combustion***

J. Chen, E. Hawkes, and R. Sankaran; Sandia National Laboratories

***Trace Based Performance Analysis***

Vaddadi Chandu, Georgia Institute of Technology

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**Tuesday, October 18, 2005**

- 7:30 a.m. **Buffet Breakfast** (please sign in)..... Dining Room
- 8:30 a.m. **Remarks and announcements** ..... Fall Creek II and III

**Cray XT3 Platform**

- 8:45 a.m. ***The Red Storm Architecture and Sandia's Initial Application Experience*** ..... Jim Tompkins, SNL
- 8:55 a.m. ***Computational Study of Models for Colossal Magnetoresistive Manganites*** ..... Gonzalo Alvarez, ORNL
- 9:05 a.m. ***Using Global Addressing on X1 to develop highly optimized Libraries*** ..... Adrian Tate, Cray
- 9:15 a.m. ***A MPP Capable of Scaling to Petaflop*** ..... John Levesque, Cray
- 9:25 a.m. ***The Performance Analysis Infrastructure for the Cray XT3*** ..... Luiz DeRose, Cray

**Inquisitor Panel:** Rupak Biswas, NASA; Jackie Chen, SNL; Al Geist, ORNL; Mark Seager, LLNL

10:05 a.m. **Break**

**IBM BlueGene Platform**

- 10:15 a.m. ***Tantalum Resolidification on BlueGene with DDCMD*** ..... Fred Streitz, LLNL
- 10:25 a.m. ***Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L*** ..... Bob Germain, IBM
- 10:35 a.m. .... Fred Streitz, LLNL
- 10:45 a.m. ***Blue Gene/L Architecture*** ..... George Chiu, IBM
- 10:55 a.m. ***Blue Gene/L Programming Environment*** ..... Manish Gupta, IBM

**Inquisitor Panel:** Rupak Biswas, NASA; Jackie Chen, SNL; Al Geist, ORNL; Mark Seager, LLNL

- 11:30 a.m. **Closing remarks and adjourn**
- Lunch available in dining room (please sign in)**