THE CENTER FOR COMPUTATIONAL SCIENCES

Oak Ridge National Laboratory
2004 Fall Creek Falls Conference:
Delivering Computational Science for the Nation

http://www.ccs.ornl.gov/workshops/FallCreek04/

The Inn at Fall Creek Falls State Park

Central Daylight Savings Time

Sunday, October 17, 2004

6:00 p.m. Reception / Welcome – Governor's Suite ..... Thomas Zacharia
8:00 p.m. End of day one

Monday, October 18, 2004

7:30 a.m. **Breakfast**
8:30 a.m. Opening remarks and logistics ..... Thomas Zacharia
8:35 a.m. ***Discovery through high-end computing*** ..... Panel Lead: Malcolm Stocks
Panel Members – Malcolm Stocks, ORNL; Steve Jardin, PPPL; Peter Cummings, VU; Jackie Chen, SNL; T. P. Straatsma, PNNL (40 min. framing talk / 1 hour panel discussion)
10:15 a.m. **Break**
10:30 a.m. ***Innovative mathematical methods, algorithms, and software systems*** ..... Panel Lead: Steve Ashby
Panel Members – Steve Ashby, LLNL; Rusty Lusk, ANL; David Bernholdt, ORNL; Thom Dunning (40 min. framing talk / 1 hour panel discussion)
12:10 p.m. **Lunch**
Afternoon free time and recreation: your leisure for hiking, fishing, relaxing, etc.
5:00 p.m. **Reassemble & Refreshments**
5:30 p.m. Poster session previews ..... Authors
6:00 p.m. **Dinner**
7:00 p.m. **Poster session and social time** – Governor's Suite

Tuesday, October 19, 2004

7:30 a.m. **Breakfast**
8:30 a.m. Remarks and logistics ..... Thomas Zacharia
8:35 a.m. ***Design and evaluation of future computing architecture*** ..... Panel Lead: Bill Camp
Panel Members - Bill Camp, SNL; Jeff Vetter, ORNL; Scott Studham, ORNL; Bob Lucas, USC-ISI; David Koester, Mitre Corp. (40 min. framing talk / 1 hour panel discussion)
10:15 a.m. **Break**
10:30 a.m. ***Leadership-class computing resources*** ..... Panel Lead: Walt Brooks
Panel Members – Walt Brooks, NASA Ames; Sid Karin, UCSD; Leslie Southern, OSC; Buddy Bland, ORNL (40 min. framing talk / 1 hour panel discussion)
12:10 p.m. **Lunch**
1:00 p.m. ***HPC: Driving Economic Competitiveness*** ..... Suzy Tichenor, Council on Competitiveness
1:30 p.m. ***Applying Fundamental Models Reaction Engineering Problems*** ... Max Tirtowidjojo, Dow
2:00 p.m. **Break**
2:15 p.m. Views from Vendors
Technologies and Programs for HPC ..... David Barkai, Intel
2:45 p.m. ***High Bandwidth Computing with Cray*** ..... John Levesque, Cray
3:15 p.m. ..... Michael Henesey, IBM
3:45 p.m. ..... unconfirmed
4:15 p.m. Adjourn
4:30 p.m. Meeting of 2005 FCF Conference committees

Poster Session

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Monday, October 18, 2004

Governor's Suite

7:00 p.m.

Participants are encouraged to reassemble at 5:00 p.m. in the meeting room (Fall Creek II and III) for refreshments and to hear poster session previews by authors. Dinner is at 6:00 p.m. in the dining room. Poster session and social time will begin at 7:00 p.m. at the Governor's Suite.

Challenges in Computer Simulation of the Plasma-Surface Interactions for Fusion: Predrag Krstic, J. Hogan (ORNL), C. Reinhold (ORNL), R. Harrison (ORNL), B. Sumpter (ORNL), W. Shelton (ORNL), F. Meyer (ORNL), D. Stotler (PPPL), C. Skinner (PPPL), S. Stuart (Clemson U.), D. Ruzic (U. of ILL), E. Bylaska (PNNL), W. Jacob (IPP Garching), J. Roth (IPP Garching), R. Doerner (PISCES-B), and G. Federici (ITER)

Chemical EndStation (ChemES): The Future of High Performance Computational Chemistry: B.C. Hathorn (ORNL) and R.J. Harrison (ORNL)

The Coming Crisis in Computational Science: Doug Post

Computational Atomic and Molecular Physics and Transport Modeling of Fusion Plasmas: M. S. Pindzola, F. J. Robicheaux, S. D. Loch, J. Ludlow, U. Kleiman, D. R. Schultz, T. Minami, T-G. Lee, J. T. Hogan, D. C. Griffin, C. P. Ballance, T. Evans, N. R. Badnell, H. P. Summers, M. C. Witthoeft, M G O'Mullane, A. D. Whiteford, B. M. McLaughlin, P. G. Burke, K. A. Berrington, J. P. Colgan, C. J. Fontes, and D. P. Stotler

Computational Instrumentation for Nanoscience: T.C. Schulthess (ORNL), P.T. Cummings (VU & ORNL), G.M. Stocks (ORNL)

Decisive change in the understanding of high-temperature superconductivity through improved computing capability: T. A. Maier (ORNL), M. Jarrell (University of Cincinnati), T. C. Schulthess (ORNL), and J. B. White (ORNL)

FSP Project: Don Batchelor (ORNL), Steve Jardin (PPPL), Doug Post (LANL)

GYRO: A 5-D Gyrokinetic-Maxwell Solver: Mark Fahey (ORNL) and Jeff Candy (GA)

High-Fidelity Terascale Simulations of Turbulent Combustion - Fundamental Insights Towards Predictive Models: Jackie Chen (SNL)