CScADS Workshop on **Libraries and Algorithms for Petascale Applications**

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with funding from the
DOE Office of Science through the
Scientific Discovery through Advanced Computing (SciDAC)

DOE SciDAC Program

- Portfolio of coordinated research efforts directed at exploiting the emerging capabilities of terascale and petascale computing
- These research projects respond to
  - the extraordinary difficulties of realizing sustained peak performance for scientific applications that require terascale and petascale capabilities to accomplish their research goals
  - the need for developing collaborative software environments where distributed resources and expertise are combined to address complex questions that no single institution can manage alone

DOE SciDAC-2 Mission

- Develop comprehensive scientific computing software infrastructure to enable petascale science
- Develop new generation of data management and knowledge discovery tools for large data sets

DOE SciDAC-2 Program Investments

- Enabling technologies
  - Computer science
  - Applied math
  - Visualization and data mgmt.
- Science application areas
  - Physics
  - Climate
  - Groundwater
  - Fusion energy
  - Life sciences
  - Materials and chemistry

Participants
– 17 labs
– 55 universities
– 3 companies

Center for Scalable Application Development Software

- The Center was created to facilitate the scalability of applications to the petascale and beyond while fostering the development of new tools by the computer science community through support of common software infrastructures and standards.

Center for Scalable Application Development Software

- Partners
  - Rice University
    - Kennedy (late), Mellor-Crummey, Cooper
  - Argonne National Laboratory
    - Beckman, Lusk, Gropp
  - University of California - Berkeley
    - Yelick
  - University of Tennessee
    - Dongarra
  - University of Wisconsin - Madison
    - Miller

Center for Scalable Application Development Software

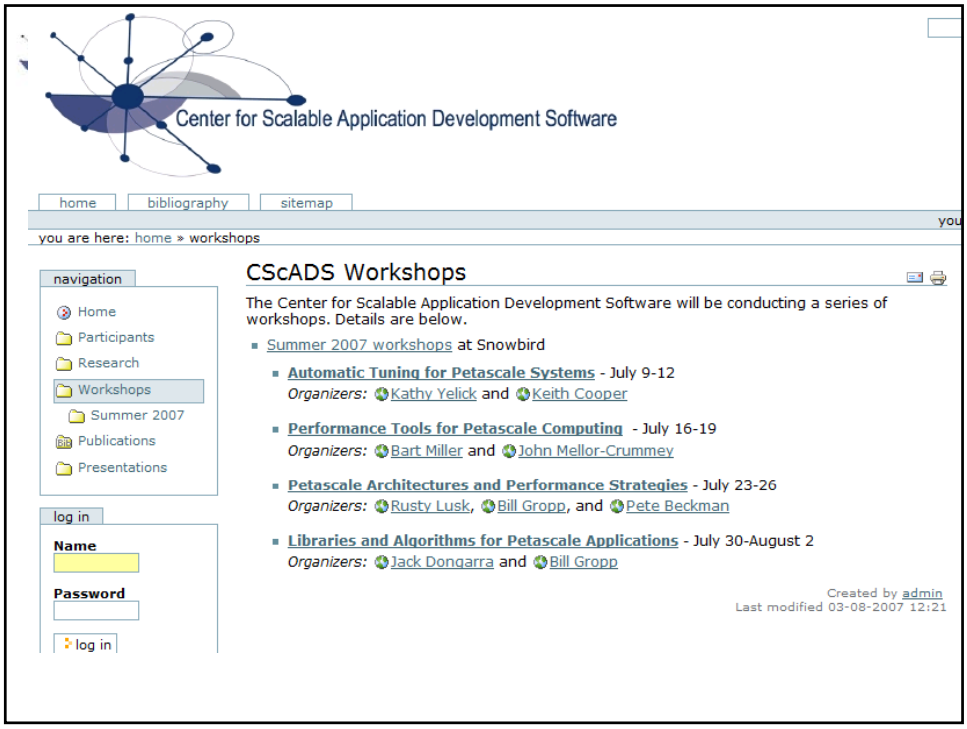
Software tools that help automate the process of scaling applications in three different dimensions

- scaling from simple high-productivity languages on a laptop to efficient applications on high-end, single-processor workstations
- scaling from small numbers of processors to full processor ensembles consisting of thousands of processors with minimal loss of efficiency
- scaling from a single abstract program representation to tuned implementations for many different high-end machines and heterogeneous processors with minimal programming effort

Center for Scalable Application Development Software

Scope of Activities

- Community outreach and vision building
- Research and development
- Open source software infrastructure



Workshop Charge

- Identify important open problems and challenges for performance tools for petascale systems
- Brainstorm on promising approaches to open problems
- Identify infrastructure needs to address key challenges
- Assess available infrastructure
- Identify opportunities for synergy
  - opportunities to
    - consolidate and harden existing infrastructures
    - reuse existing components developed by others
    - refactor and extend existing components to apply them to new challenges
- Collaborate on design of sharable components
- Identify targets of opportunity for further investment of resources
  - strategic investment targets for the DOE Office of Science?

Workshop Goal

- The goal is to identify challenges for library and algorithm developers from the needs of the SciDAC applications, and to foster collaboration between the communities.
- Specific topics to include the effective use of multicore processors (both algorithms and libraries) and the use of automatic tuning in libraries, but would not be restricted to those topics.

Workshop Structure

- 2.5 days: invited presentations
- Monday
  - Applications
- Tuesday and Wednesday morning
  - Software and Libraries
- Thursday morning
  - Working groups meeting
- Thursday afternoon
  - Working groups prepare summary and presentation

Meals

- The workshop will cover meals for participants.
- Breakfasts will be provided to workshop participants.
- Lunch and dinner for participants will be on your own at the dining establishment of your choice; participants will be reimbursed a flat "per diem" rate to offset the cost of these meals.
- Monday and Wednesday there will be a banquets.

Few Changes Because of Airline Cancellations

- Monday
  - All talks moved up (except Edo's)
  - Marc Baboulin's talk moved from Tuesday to Monday at 3:40
- Tuesday
  - Jim Amundson's talk at 8:30
  - Demmel, Li, Sorensen, Heroux talks' moved down a slot

Revised Agenda

Monday	June 30th	Applications
8:00 – 8:30	Continental Breakfast	Meeting Room: Cliff Lodge
8:30 – 9:00	Welcome and Introduction	Jack Dongarra, UTK and ORNL and Bill Gropp ANL
8:30 – 9:10	Steve Jardin, Princeton Plasma Physics Laboratory	Algorithmic Needs for Fusion Magnetohydrodynamics (MHD) and Other Predominantly Hyperbolic Systems of Equations
9:10 – 9:50	Rich Lee, SLAC	Finite-Element Electromagnetic Simulations for Particle Accelerators at Petascale
9:50 – 10:20	Break	
10:20 – 11:00	Serguei Ovchinnikov, Tech-X Corporation	Some Scalability Issues in VORPAL and PETSc Applications
11:00 – 11:40	Johan Carlsson, Tech-X Corporation	Concurrent Divide-and-Conquer Library with Petascale Electromagnetics Applications
11:40 – 12:20	Ron Shepard, ANL	Some Algorithms in Quantum Chemistry
12:20 – 2:00	Lunch	On your own (Covered by per diem)
2:00 – 2:40	Ichitaro Yamazaki, UC Davis	Algorithmic Challenges in Quantum Monte-Carlo (QMC) Simulation of Strongly-Correlated Materials
2:40 – 3:20	Kenneth Roche, ORNL	UNEDF Project: Comments on Some Perceived Software Issues and Opportunities for Collaboration
3:20 – 3:40	Break	
3:40 – 4:20	Marc Baboulin, U of Tennessee & Cerfacs	Very Large Least Squares for Parameter Estimation: Algorithm and Application
4:20 – 5:00	Edo Apra, ORNL	Software needs for Quantum Chemistry Software
6:00	Dinner – Banquet	

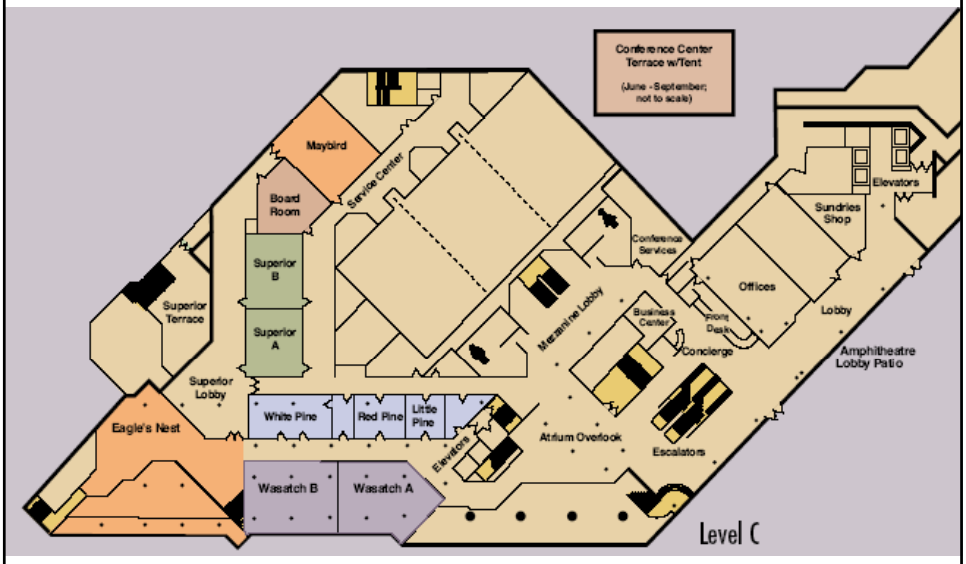
Tuesday	July 31st	Software and Libraries
8:00 – 8:30	Continental Breakfast	
8:30 – 9:15	Jim Amundson, FNAL	Computational Challenges in State-Of-The-Art Accelerator Beam Dynamics.
9:15 – 10:00	Jim Demmel, UC Berkeley	The Future of High Performance Linear Algebra Libraries
10:00 – 10:30	Break	
10:30 – 11:15	Sherry Li, LBNL	Development of Sparse Direct Solvers and Eigensolvers in TOPS
11:15 – 12:00	Dan Sorensen, Rice U	Invariant Subspace Computation in Scientific Computing
12:00 – 1:30	Lunch	On your own (Covered by per diem)
1:30 – 2:15	Mike Heroux, SNL	An Overview of Trilinos: Packages for Parallel Formulation and Solution of Scientific and Engineering Problems
2:15 – 3:00	Sanjukta Bhowmick, Columbia U	Machine Learning Techniques for Linear Solver Selection
3:00 – 3:30	Break	
3:30 – 4:15	Karen Devine, SNL	Dynamic Load Balancing and Partitioning using the Zoltan Toolkit
4:15 – 5:00	Alfredo Buttari, U of Tennessee	Parallel Tiled Algorithms for Multicore Architecture
6:00	Dinner	On your own (Covered by per diem)
7:30 -	General Discussion and Optional Hands-on Session	

No Change Wednesday and Thursday

Wednesday	August 1st	Software and Libraries
8:00 – 8:30	Continental Breakfast	
8:30 – 9:15	Julien Langou, U of Colorado, Denver	Latency-Avoiding and Fault-Tolerant Algorithms for Dense Linear Algebra and Petascale Architectures
9:15 – 10:00	Stan Tomov, U of Tennessee	Computer Science/Math Challenges Related to Nano-Technology Applications
10:00 – 10:30	Break	
10:30 – 11:15	Hong Zhang, ANL	PETSc and its On-going Research and Development
11:15 – 12:00	Lori Diachin, LLNL	Interoperable Meshing Tools for Advanced Petascale Simulations
12:00 – 1:30	Lunch	On your own (Covered by per diem)
1:30 – 6:00	Enjoy the Snowbird area (Hiking maps provided)	
6:00	Dinner - Banquet	

Thursday	August 2nd	Summary and Priories for DOE: Challenges for Libraries and Algorithms
8:00 – 8:30	Continental Breakfast	
8:30 – 10:00	Bill Gropp and Jack Dongarra	
10:00 – 10:30	Break	
10:30 – 12:00	Community Building and Engaging Applications	
12:00 – 1:30	Lunch	On your own (Covered by per diem)
1:30 – 6:00	Wrap up session	

Cliff Lodge Registration (Level C)



We can use this room at night

- Should we take donations and make a run to the package store?

Reception/Banquet (Level B)