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 banquet.

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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
We can use this room at night

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