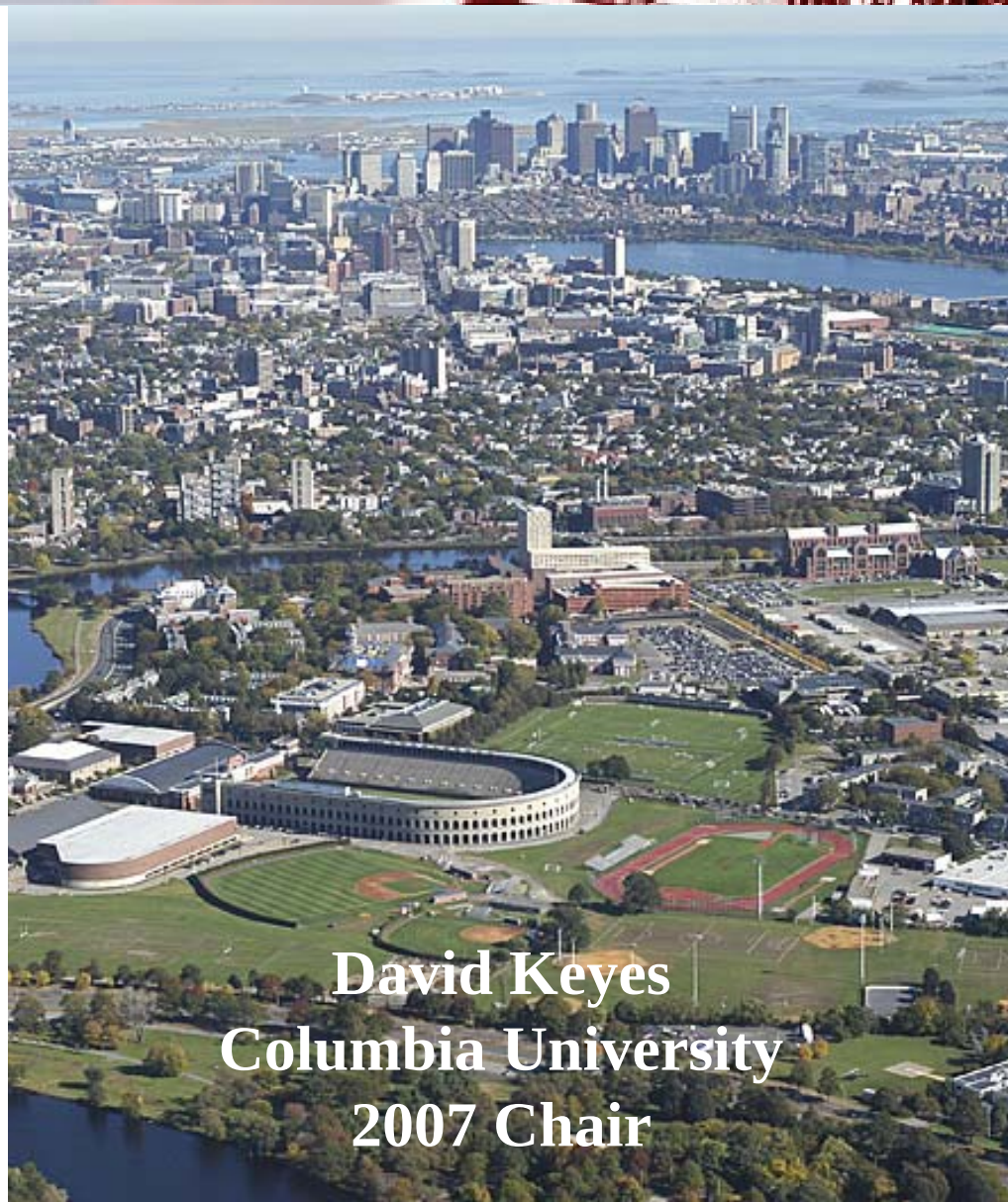
Scientific Discovery through Advanced Computing

SciDAC 2007

Boston, June 24-28

Office of Science
U.S. DEPARTMENT OF ENERGY

BOSTON POPS



David Keyes
Columbia University
2007 Chair


Welcome to
Boston!
www.scidac.org/Conference2007

Why I'm here today!

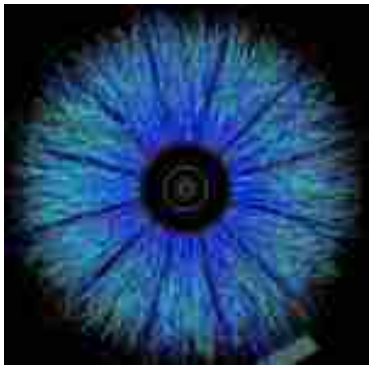
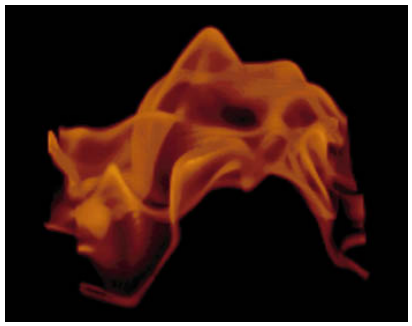
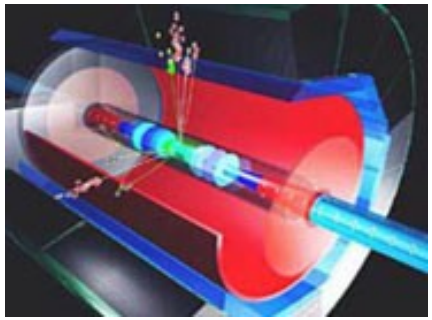
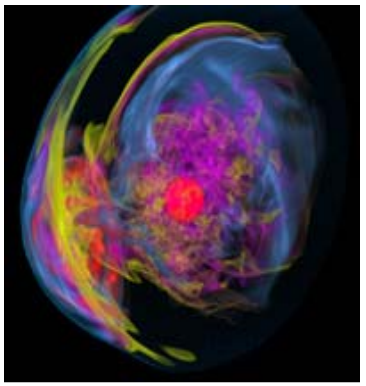
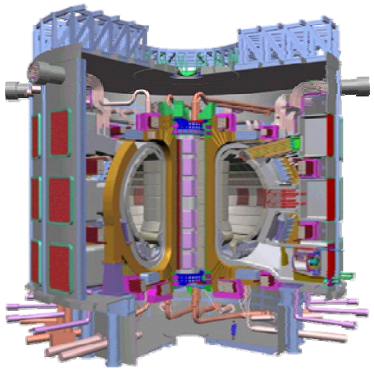
Dad, what you 'n' your friends are doing is more important for me 'n' my friends than attending our graduation!

Stuyvesant High School Robotics Team, 2006-2007

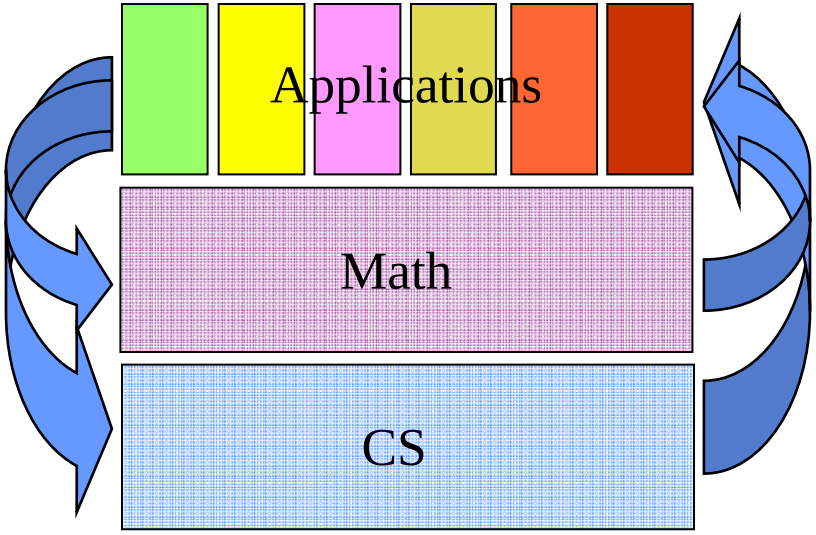
Are the world's problems primarily computational?

- No, but predictive simulation is critical to understanding them and prioritizing our responses
- We must ride the wave of hardware (peta-, exa-) to:
  - Help move to predictive capability from interpolatory
  - Couple together more interacting phenomena
  - Resolve a wider range of scales
- We must educate policy makers and the public about the limitations of simulations

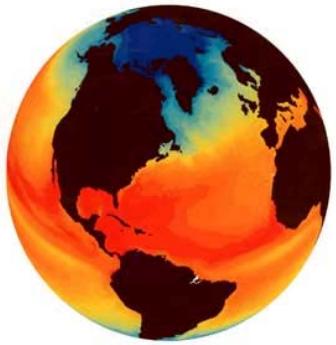
SciDAC: enabling technologies for multiple specialized applications

Many applications drive

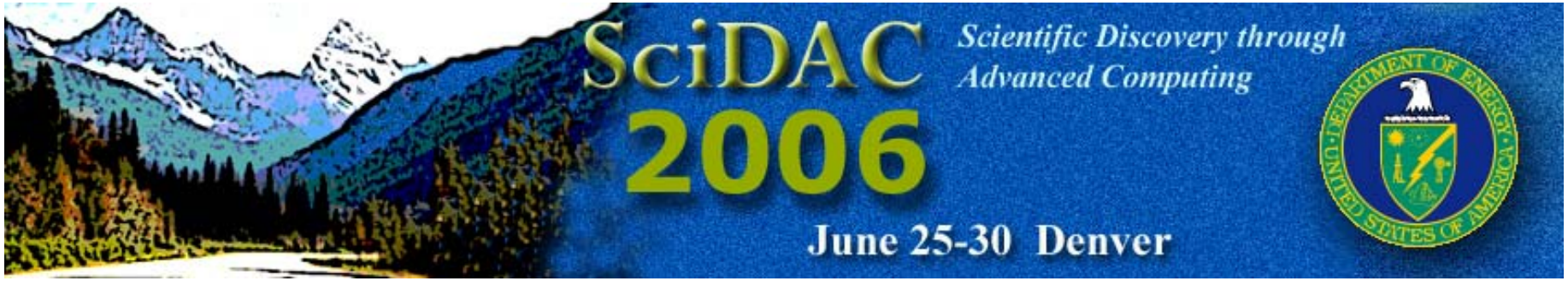


Enabling technologies respond



SciDAC 2007 follows a wonderful tradition…

- 4-day meeting – plenaries by day, posters by night
- Celebration of SciDAC-sponsored and other leading computational science research
- Fast-turnaround technical proceedings



Who are we this year?

- Over 300 for the conference, Monday-Thursday
- About 100 for the tutorial, Friday
- Representing
  - 55 universities
  - 20 laboratories
  - 14 industries (computer, consulting, publishing)
  - 5 agencies
  - 4 countries (Germany, Japan, Norway, USA)

The New England delegation

- **Boston University***
- **Brown**
- **Dartmouth**
- **Harvard***
- **MIT***
- **Tufts**
- **U Connecticut**
- **U Massachusetts**
- **U New Hampshire**
- **Worcester Polytechnic Institute**
- **Yale**

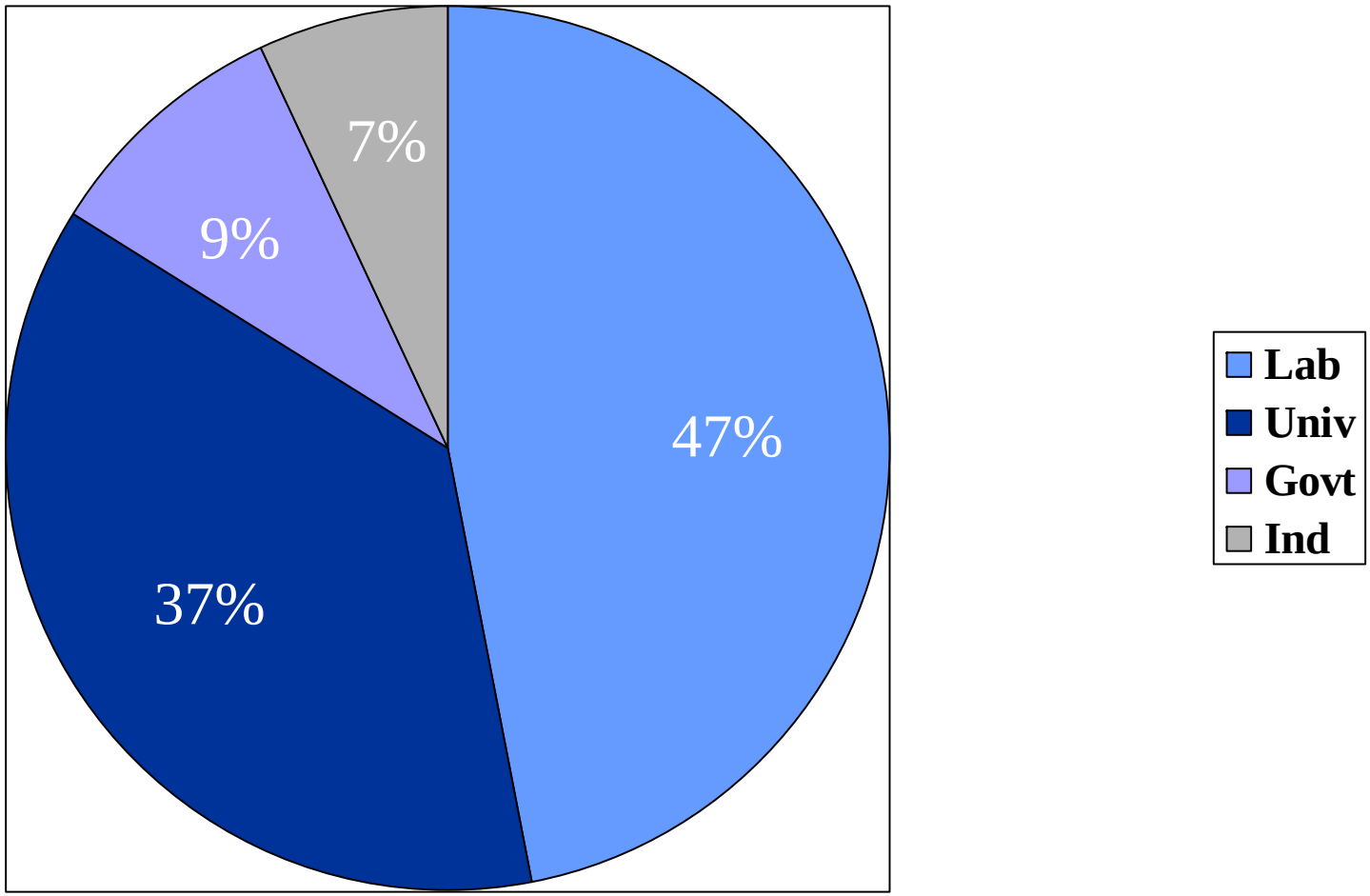
All of the Ivy League is represented except for the University of Pennsylvania

*** SciDAC partner institution**

Composition (conference only)

SciDAC is not just a lab program.

SciDAC 2007 is not just a PI meeting.



Features of SciDAC 2007

- **Theme: "linking the village"**
  - **applications**
  - **enabling applied mathematics**
  - **enabling computer science**
- **New SciDAC-2 application domains, being represented for the first time**
- **Unified by pursuit of the petascale**
  - **driven to tools designed for distributed, hierarchical memory**
  - **… getting *more* distributed and *more* hierarchical**

SciDAC 2007 features leads of other agencies with related programs

- **Tony Chan, Director, Mathematics & Physical Sciences, NSF**
- **Cray Henry, Director, High Performance Computing Modernization Program, DoD**
- **Toichi Sakata, Executive Director, RIKEN (*Rikagaku Kenkyusho*, Japan's Institute of Physical and Chemical Research)**

SciDAC 2007 features 36 other plenary talks and 72 invited posters

- **Plenary talks selected by the organizing committee to span SciDAC-funded areas,**
  - **consciously going outside SciDAC for many talks**
- **Posters are the heart of the meeting**
  - **as they were the core of the first three "roll up your sleeves" SciDAC annual meetings**
  - **36 technical posters each of Tuesday and Wednesday**
  - **… plus SciDAC Outreach Center "matrix"**
- **All 49 funded SciDAC projects announced in 2006 are represented by either a plenary or a poster!**

Thanks to the Organizing Committee!

- **Wes Bethel (LBNL)**
- **Rich Brower (BU)**
- **John Cary (TechX)**
- **Phil Colella (LBNL)**
- **Ian Foster (ANL)**
- **Giulia Galli (UCDavis)**
- **Peter Lichtner (LANL)**
- **Tony Mezzacappa ORNL)**
- **Habib Najm (SNL)**
- **John Negele (MIT)**
- **Rick Stevens (ANL)**
- **Bill Tang (PPPL)**
- **Pat Worley (ORNL)**
- **Dean Williams (LLNL)**
- **Kathy Yelick (Berkeley)**

Their work is not yet done: the proceedings looms!

SciDAC 2007 has a focus on developing the workforce

Peter Kekenes-Huskey,
Caltech, chemistry/biology

Tod Pascal,
Caltech, chemistry

Amber Sallerson,
UNC, applied math

Thanks,
Krell!

Michael Wolf,
UIUC, computer science

On pursuit of the petascale…

- **Rather than focusing only on scientific scope, applications talks are asked to bring out:**
  - **Performance issues (behavior of "node code")**
  - **Scaling issues (behavior as number of nodes approaches 10^5)**
  - **Work, bandwidth, or datasize complexity bottlenecks**
- **Rather than focusing only on building infrastructure for the long-term, enabling technologies talks are asked to bring out:**
  - **Support for particular petascale applications**
  - **Adapting to the petascale architectures**

"Not business as usual for the Office of Science" – Michael Strayer

Thursday's panels

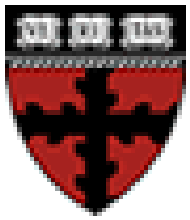
- **"Simulation and Modeling at the Exascale for Energy, Ecological Sustainability, and Global Security" (E3SGS) "town halls" and vendor projections**
- **Town Hall leads: *Jeff Nichols* (ORNL), *Horst Simon* (LBNL), *Rick Stevens* (ANL)**
- **Vendor participants: *Alan Edelman* (Star-P), *Randy Keiser* (DataDirect), *Jud Leonard* (SiCortex), *John Levesque* (Cray), *Jay Owen* (AMD), *James Sexton* (IBM)**
- **Community response and questions**

Thanks to our sponsors

- **SciDAC sponsors**
  - **U.S. DOE Office of Science**
  - **U.S. DOE National Nuclear Security Administration**
  - **U.S. National Science Foundation**
- **SciDAC 2007 conference sponsors:**

What's new this year?

- **Fifth-day tutorial on SciDAC-supported software**
  - **Aimed at new users**
- **Hosted at MIT on Friday, June 29, 2007 (John Negele, host)**
- **Led by members of the development teams**
- **Explicitly open to junior SciDAC participants Separate registration from the meeting, proper**
  - **Still possible to register yourself and your team members (lunch count taken Tuesday evening)**
- **Co-sponsored by the entire Boston-area SciDAC campuses and the SciDAC Outreach Center (David Skinner, lead)**



Tutorials available (Fri. at MIT)

- **Morning**
  - Tools for Geometry, Mesh, and Field Manipulation
  - Parallel I/O in Practice
  - Enabling Distributed Petascale Science
  - Data Parallel Software for Lattice QCD
  - Introducing VORPAL
- **Afternoon**
  - Adaptive Numerical Software for PDEs
  - Load-balancing and Partitioning using Zoltan
  - Scalable Solvers for PDE-based Simulations
  - Visualization and Analytics Technologies
  - High-performance Computing using CCA
- **All day**
  - Data Movement and Workflow Management

Special event: “Right-brain night”

- **A Monday night barrier-breaker, 7:30pm**
- **Science-inspired and other performance art**
- **Skits, verse, and music by and for SciDAC participants**
- **Including:**
  - **light verse about heavy subjects (QCD, turbulence, etc.)**
  - **skit about petascale climate science**
  - ***Brass Quadrature* and the *Grand Canonical Ensemble* premiering a new SciDAC anthem, “*Anthematica*”**

Why "Right-brain night"?

- **"When I'm not in my right mind, my left mind gets crowded" – *email tag of Phil Jones, LANL, bass trombone of "Brass Quadrature"***
- **"Geeks just wanna have fun"**
- **Being able to relate to each other in science-neutral areas, where we have a common culture (or common lack thereof ☺), helps us relate better in the science areas, where our cultures can be highly specialized and very different**
  - **See my talk "*Applications Scientists are from Mars, Enabling Technologists are from Venus*" (February 2007 PI Mtg, Atlanta)**