Strategic Plan (FY 2006 – 2010)
Ch. 2: High Performance Computing

5yr Goal:
- To enable petascale science & engineering thro’ deployment & support of a world-class HPC environment comprising the most capable combination of HPC assets available to the academic community

Components:
- Acquisition, deployment, operation of science-driven HEC systems
- Development & maintenance of supporting software
  - New design tools, performance modeling tools, system software & fundamental algorithms
- Development and maintenance of portable, scalable applications software
HEC Program Elements

- **Acquisitions**
  - Track 1 - Petascale
  - Track 2 - Mid-range supercomputers

- **Operations**

- **HEC System Software**
  - Compilers, fault-tolerant OS, fault-survivability tools, system status monitoring, file-systems, PSEs, ...

- **HEC Petascale Application Development**
  - Scalable math libraries, scalable algorithms, data exploration tools, performance profiling and prediction, large application development

- **Coordinated with other agencies**
Recent High-end HPC Investments

Petascale Software Development (PetaApps, SDCI and STCI) 2006...

2007-2011-2016 Track 1 Petascale Acquisition (UIUC/NCSA)

TeraGrid Operations
TACC, NCSA, SDSC, PSC, ORNL, ANL, Indiana, Purdue, NCAR, LSU

TeraGrid Phase III (XD)

Track 2A: 2006-2011 TACC

Track 2B: 2007-2012 UTK

Track 2C: 2008-2013 PSC

Track 2D: 2009-2014 Multiple smaller resources

TACC - Texas Advanced Computing Center, Austin.
UTK - Univ. of Tennessee, Knoxville, Joint Institute of Computational Science.
NCSA - National Center for Supercomputer Applications, Univ. of Illinois, Urbana-Champaign.
SDSC - San Diego Supercomputer Center, Univ. of California, San Diego.
PSC - Pittsburgh Supercomputing Center
Greatly expanding capacity of the TeraGrid for digital exploration with reduced oversubscription and queue wait times.

- PSC-Phase 2 & UTK Phase 3
- UTK Phase 2
- UTK Phase 1 & Ranger upgrade
- TACC Ranger
- TG Aggregate 6-07

June 07
Early 08
Summer 08
2009
2010

180
684
925
> 1,500
> 2,800

TF/s Peak

0
750
1,500
2,250
3,000
Other Trends

- Growing power dissipation
- Complexity of system
- Complexity of programming
- Increase in uptake
- Declining investment
Blue Waters: the next-generation supercomputer

- climate science, particle physics, materials science, stellar evolution
- fluid dynamics, astrophysics and cosmology, condensed matter physics
- cell biology, nano-engineering, chemistry, plasma physics
- the influence of social networks on the spread of contagion

BLUE WATERS: 1 quadrillion calculations / 1 second
YOU: 1 quadrillion calculations = 31 million years
HPC is an increasingly important tool for understanding:

**Life**
- Satellite tobacco mosaic virus, P. Freddolino et al.
- Aldehyde dehydrogenase, T. Wymore and S. Brown

**Matter**
- I. Shipsey

**The Environment**
- K. Droegemeier et al.
- Community Climate System Model

**Society**
- John Q Public
  - S.-Y. Kim, M. Lodge, C. Taber
  - D. E. Atkins
Some Science We’ll Be Able To Do

**Pandemic Network Simulation and Analysis:** Models for simulating the spread of infectious diseases using graph-theoretic methods. The influence of social networks. In silico testing of mitigation strategies.

**Computational Proteomics:** Modeling proteins with ~1000 amino acids to examine protein-protein interactions and trans-membrane signaling. Inverse methods for macromolecular design.

**Environmental Decomposition of Complex Molecules:** Develop highly scalable, locally correlated, numerical quantum chemistry methods for molecules containing hundreds of heavy atoms. Study decomposition pathways of complex molecules in the environment.

**Ocean Modeling:** Study ice-ocean interactions using whole-globe coupled ice-ocean models.

**Cosmology:** Multi-scale cosmological modeling in support of research efforts in precision cosmology, including galaxy surveys, weak lensing, and the analysis of the cosmic microwave background.

**Computational Fluid Dynamics:** Study the evolution of transient, localized structures in inhomogeneous turbulence using adaptive mesh refinement (AMR).

**Mining the Internet Archive:** Studying the propagation of ideas and interactions.

**Analysis of Socio-Economic data:** Extraction of patterns and pattern evolution in multi-year socio-economic data collections.
Track 2d

- Track 2 = TeraGrid hardware funding line
- Track 2d = up to $20M in year 1 & constrained O&M
- Looking for innovation
- Up to four awards - two “production” and two “experimental” categories
  - A data-intensive, high-performance computing system
  - An experimental, high-performance computing system of innovative design
  - An experimental, high-performance grid test-bed for grid research (CS & applied)
  - A pool of loosely coupled grid-computing resources
- All “systems” to be made available to national community of users via the TeraGrid
Some examples of existing programs

NSF’s investments in HEC R&D are spread over several offices and divisions

- HECURA
- Science and Engineering Beyond Moore’s Law - proposed new effort, led by MPS
  Focuses on new paradigms for HW architecture, algorithms, & application software
  E.G. basic research on new types of logic devices: nanophotonics, spintronics, molecular computing, quantum computing
- STCI & SDCI
- Multicore Chip Design and Architecture (NSF and SRC)
  Innovative research on design, fabrication, architecture and programmability of homogeneous and heterogeneous multicore systems. - Includes hardware and software aspects
- PetaApps
  Funding for development of future simulation and analysis tools that can use petascale computing to advance the frontiers of scientific and engineering research.
- Application development in domain science and engineering programs. e.g. climate, nanoscale engineering, biosciences, chemistry, SBE
- National Center for Atmospheric Research
The next five years 2011 - 2016

- Over next year - develop a new five-year plan
- Looking for input on opportunities and priorities
  - From academia and industry
  - From consumers of leading-edge HPC and from researchers and developers of leading-edge HPC
- Anticipate greater emphasis on software development
- Over the current decade, NSF investments in HPC acquisition have been declining; future funding levels are uncertain
- NSF seeks to maintain a balanced cyberinfrastructure portfolio. Other CI areas include: data curation and data management, networking, middleware development, grid/cloud computing
- Exascale and beyond in computing and data are hard challenges
  - hope to expand partnerships with other agencies and foster international collaborations
- No investment similar to Track 2 is planned for 2010
Questions

- What are some of the research areas - hardware & software - which academia & industry would be interested in tackling together?
- What are the science grand challenges that would require the combination of international HPC resources to tackle?
- How does the cloud paradigm fit into the provisioning of high-performance computing resources?
Questions or Comments?