Computational Science Subcommittee: Preliminary Observations

President's Information Technology Advisory Committee

Subcommittee on Computational Science

Daniel A. Reed, Chair

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SC04 Town Hall Meeting

November 10, 2004

About the President's Information Technology Advisory Committee (PITAC)

- PITAC members are appointed by the President to provide independent expert advice on maintaining America's preeminence in advanced information technology.
- Chartered by Congress under the High-Performance Computing Act of 1991 (P. L. 102-194) and the Next Generation Internet Act of 1998 (P. L. 105-305). It is formally renewed through Presidential Executive Orders.
- Federally chartered advisory committee operating under the Federal Advisory Committee Act (FACA) (Public Law 92-463) and other Federal laws governing such activities.
- Reports to the President through the Office of Science and Technology Policy, Executive Office of the President.

Subcommittee on Computational Science

- ***Daniel A. Reed***, Ph.D., ***Chair***, Chancellor's Eminent Professor, Vice-Chancellor for Information Technology and CIO, and Director, Renaissance Computing Institute, University of North Carolina at Chapel Hill
- ***Ruzena Bajcsy,*** Ph.D., Director, Center for Information Technology Research in the Interest of Society (CITRIS), University of California, Berkeley
- ***Manuel A. Fernandez***, Managing Director with SI Ventures
- ***José-Marie Griffiths***, Ph.D., Dean, School of Information and Library Sciences, University of North Carolina at Chapel Hill
- ***Randall D. Mott***, Senior Vice President and Chief Information Officer, Dell Computer

Subcommittee's Charge (1/3)

June 9, 2004 letter from Dr. John H. Marburger, III, Science Adviser to the President

1. How well is the Federal Government targeting the right research areas to support and enhance the value of computational science? Are agencies' current priorities appropriate?
2. How well is current Federal funding for computational science appropriately balanced between short term, low risk research and longer term, higher risk research? Within these research arenas, which areas have the greatest promise of contributing to breakthroughs in scientific research and inquiry?

Subcommittee's Charge (2/3)

3. How well is current Federal funding balanced between fundamental advances in the underlying techniques of computational science versus the application of computational science to scientific and engineering domains? Which areas have the greatest promise of contributing to breakthroughs in scientific research and inquiry?
4. How well are computational science training and research integrated with the scientific disciplines that are heavily dependent upon them to enhance scientific discovery? How should the integration of research and training among computer science, mathematical science, and the biological and physical sciences best be achieved to assure the effective use of computational science methods and tools?

Subcommittee's Charge (3/3)

5. How effectively do Federal agencies coordinate their support for computational science and its applications in order to maintain a balanced and comprehensive research and training portfolio?
6. How well have Federal investments in computational science kept up with changes in the underlying computing environments and the ways in which research is conducted? Examples of these changes might include changes in computer architecture, the advent of distributed computing, the linking of data with simulation, and remote access to experimental facilities.
7. What barriers hinder realizing the highest potential of computational science and how might these be eliminated or mitigated?

Subcommittee Work Plan

- June 9: Charge from the White House
- June 17: PITAC meeting (Arlington, Virginia)
- September 16: Information gathering meeting (Chicago)
- October 19: Information gathering meeting (Arlington, Virginia)
- November 4: PITAC meeting (Arlington, Virginia)
- *November 10: Birds of a Feather (BOF) at Supercomputing 2004*
- November-December: Report drafting and input solicitation
- January 2005: PITAC meeting - major review of the draft report
- February - March 2005: Editing
- March 2005: Review and approval of final draft report

Preliminary Observations

Computational Science: Essential to Scientific Discovery (1/2):

- Computing has become the third component of scientific discovery, complementing theory and experiment.
- Computing is so integral to the scientific process that its limitations now constrain scientific discovery.
- The explosive growth in the resolution of sensors and scientific instruments has led to unprecedented volumes of experimental data. Computational science now broadly includes modeling, simulation, and scenario assessment using sensor data from diverse sources.

Preliminary Observations

Computational Science is Essential to Scientific Discovery (2/2):

- Complex multidisciplinary problems, from public policy through national security to scientific discovery and economic competitiveness, have emerged as new drivers of computational science, complementing the historical focus on single disciplines.
- Developing leading edge computational science applications is a complex process involving teams of people that must be sustained for a decade or more to yield the full fruits of investment.

Preliminary Observations

Current State of Computational Science:

- There is a disconnect between commercial practice and the computing infrastructure needs of government and academia. Commercial needs are (in several cases) no longer driving technology acceleration.

- Short-term investment and limited strategic planning have led to excessive focus on incremental research rather than on the long-term research with lasting impact that can solve critical problems.

Preliminary Observations

Paths to Progress (1/3):

- Computational science would benefit from a roadmap outlining decadal priorities for investment, with a clear assessment of those priorities derived from a survey of the problems and challenges. Agencies could then respond to these with a strategic plan in recognition of those priorities and funding requirements.

Preliminary Observations

Paths to Progress (2/3):

- Solutions must be "right sized" for the problems
  - temporally, recognizing the time to solution
  - socially and fiscally, recognizing complexity and sustainability

- Diverse solutions are needed for different structural issues
  - community organization/coordination for increased leverage
  - structural infrastructure investment
    - creating baselines for community research and development
  - coordination across agencies and missions for R&D transfer

Preliminary Observations

Paths to Progress (3/3):

- Strategic execution, based on systemic assessment of programs and components within a long-term, strategic plan, is needed within and across agencies to create a vibrant, holistic research environment and infrastructure. Individual programs and solicitations must be viewed and managed within the context of strategic and tactical goals.

- Sustained investment in computational science infrastructure, defined broadly to include people, software, data, and systems, is needed to fully realize the promise of computational science.

Preliminary Observations

Paths to Progress - People (1/2):

- The limited number of senior leaders in computational science has constrained community advocacy and agency leadership.
- Interdisciplinary education in computational science and computing technologies is inadequate, reflecting the traditional disciplinary boundaries in higher education. Only systemic change to university organizational structures will yield the needed outcomes.

Preliminary Observations

Paths to Progress - People (2/2):

- There are few, if any, rewards for interagency coordination and collaboration on science, technology, and infrastructure development pipelines. The result has been loss of critical opportunities to sustain and develop critical capabilities, and transfer them to the commercial sector.

Preliminary Observations

Paths to Progress - Software:

- Easy to use, accessible, scalable software that interoperates with existing user environments is not adequately available.

- Community verification and validation of computational science results, via access to the software and data, are needed to accelerate scientific discovery.

Preliminary Observations

Paths to Progress - Hardware:

- National computing resources, high end computers, are not readily accessible/available to both small and large agencies and industry. Even when such systems are available, they are not sufficiently easy to use.

- A sustainable infrastructure is needed that provides access to leading edge capabilities for computational science. This requires long term investments.

Report Schedule

- *November 10*
  - *Birds of a Feather (BOF) at Supercomputing 2004*
- November-December
  - report drafting and input solicitation
- January 2005
  - PITAC meeting with major review of draft report
- February - March 2005
  - editing
- March 2005
  - approval of final draft report at PITAC meeting

Questions For Today

1. What are the important problems in computational science that should be addressed that are not being addressed today? What opportunities and visions might be pursued if additional resources were available? What major breakthroughs in science could then be realized?

2. Is the portfolio of Federal funding programs for computational science appropriately balanced between short term, lower risk research and longer term, higher risk research? If not, what adjustments would be desirable?

Questions For Today

3. How can computational science research be better integrated into the scientific disciplines that are heavily dependent on it to enhance scientific research and inquiry?

4. Consider the ways in which Federal agencies coordinate IT research, development, prototyping, and procurement in support of science and engineering research. How could this coordination be improved?

Community Input: Groundrules

- Today: three minutes of oral comments
  - we want to hear from as many people as possible

- After today
  - up to five pages of written material, sent to
    - **pitac-comments@nitrd.gov**