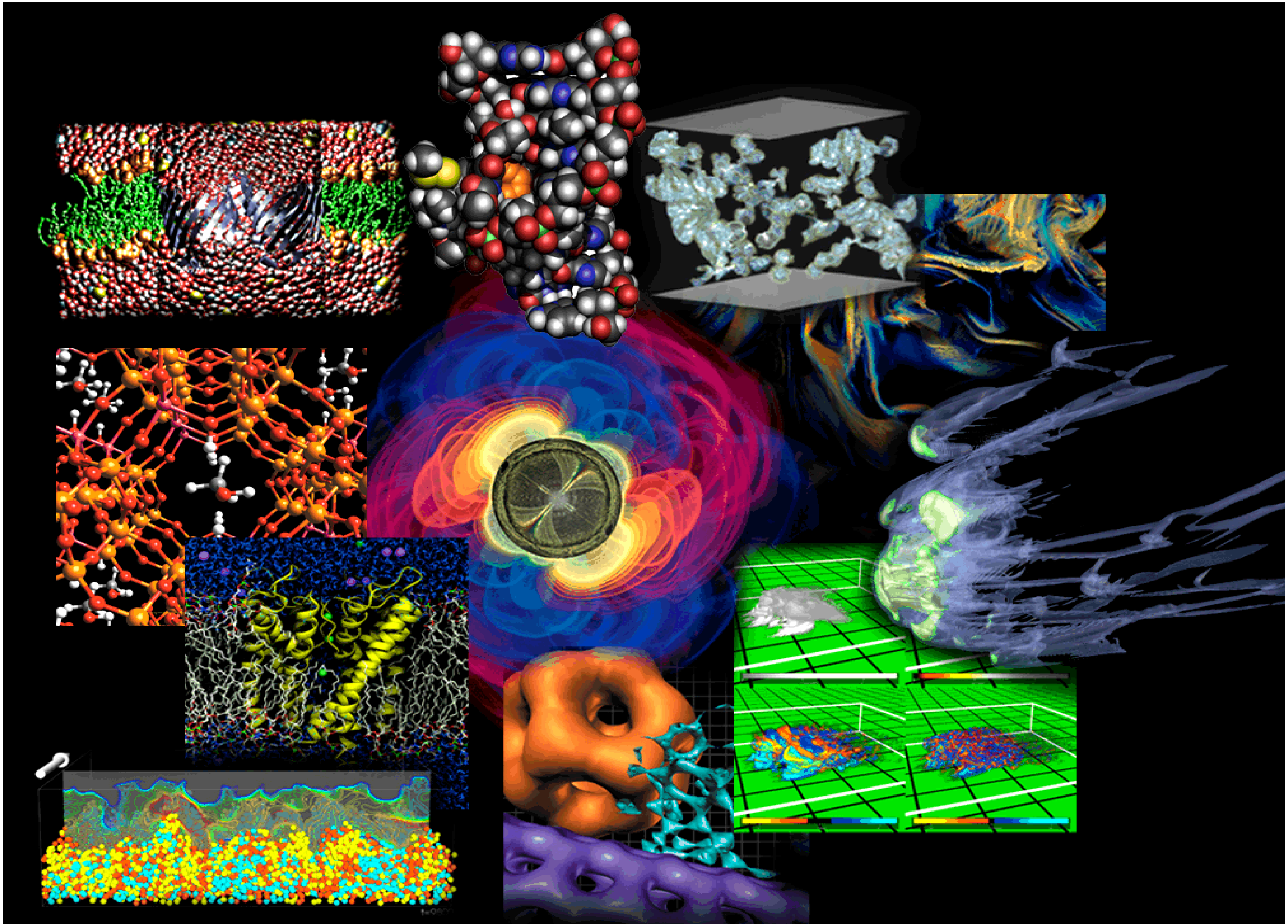

Source: NCSA

Future of Computational Science

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January 27, 2005

George Mason University

Outline of Talk

- **Prior Computational Science Recommendations**
  - Lax Panel (1982!)
  - High-End Computing Revitalization Task Force
  - Council on Competitiveness
  - Others
- **Draft Report on Computational Science by President's Information Technology Advisory Committee (PITAC)**
- **Interactive discussion regarding GMU experiences and input to PITAC study**

Networking and Information Technology Research and Development Program

- **Networking and Information Technology R&D Program (NITRD) helps focus interagency IT R&D:**
  - Identify common research needs
  - Plan multi-agency research programs
  - Coordinate and collaborate on research announcements and funding
  - Review research results and adjust accordingly
- **Includes R&D programs of twelve participating agencies totaling $2B**
- **Evolved from the Federal High Performance Computing and Communications Initiative (HPCC), Computing Information and Communications Program (CIC), and Next Generation Internet Program (NGI)**
- **Assessed by the President's Information Technology Advisory Committee (PITAC)**

PITAC Draft Definition of Computational Science

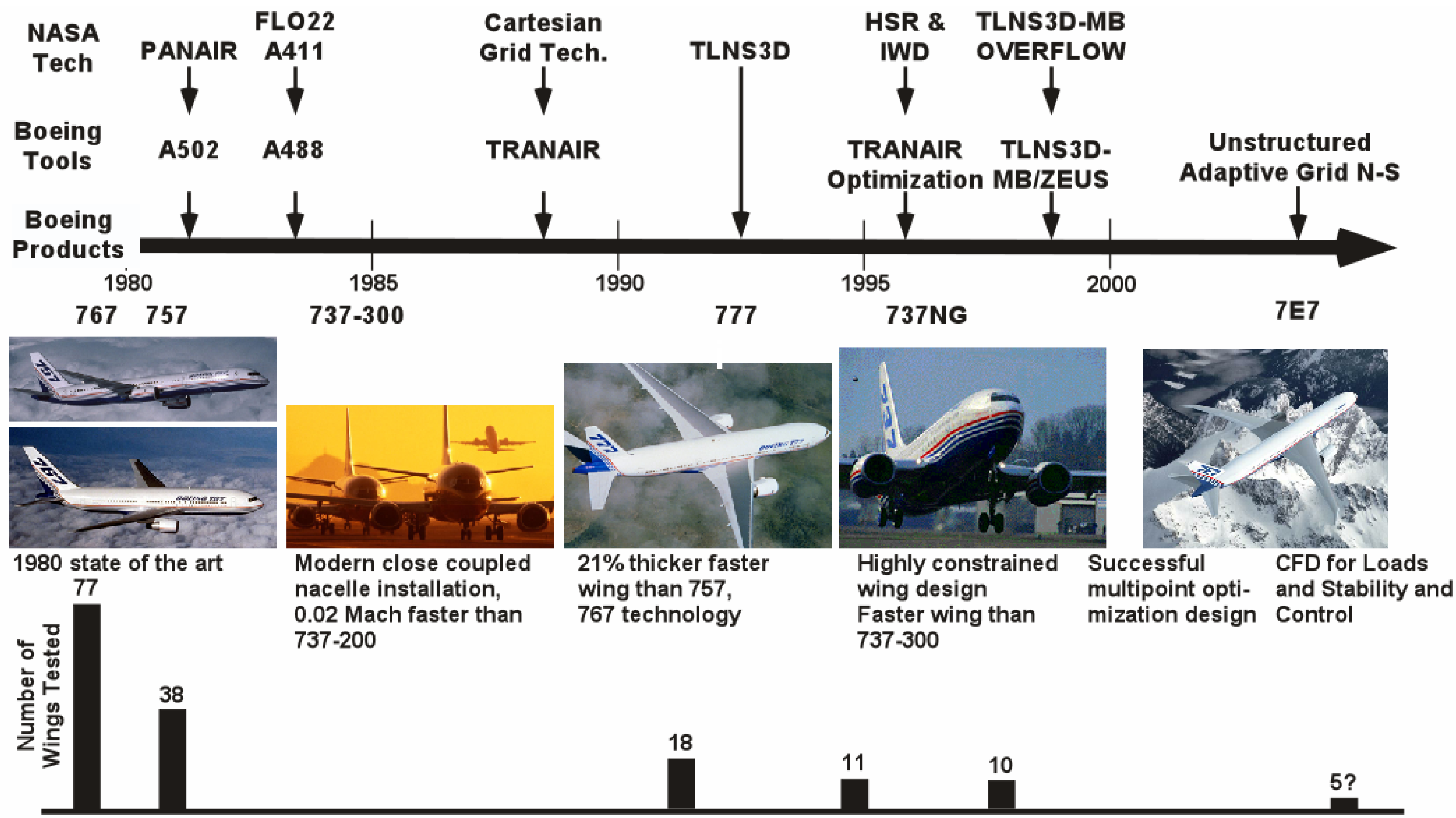
Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems. Computational science fuses three distinct elements:

- numerical algorithms and modeling and simulation software developed to solve science (e.g., biological physical, and social), engineering, and *humanities* problems;
- advanced system hardware, software, networking, and data management components developed through computer and information science to solve computationally demanding problems;
- the computing infrastructure that supports both science and engineering problem solving and developmental computer and information science.

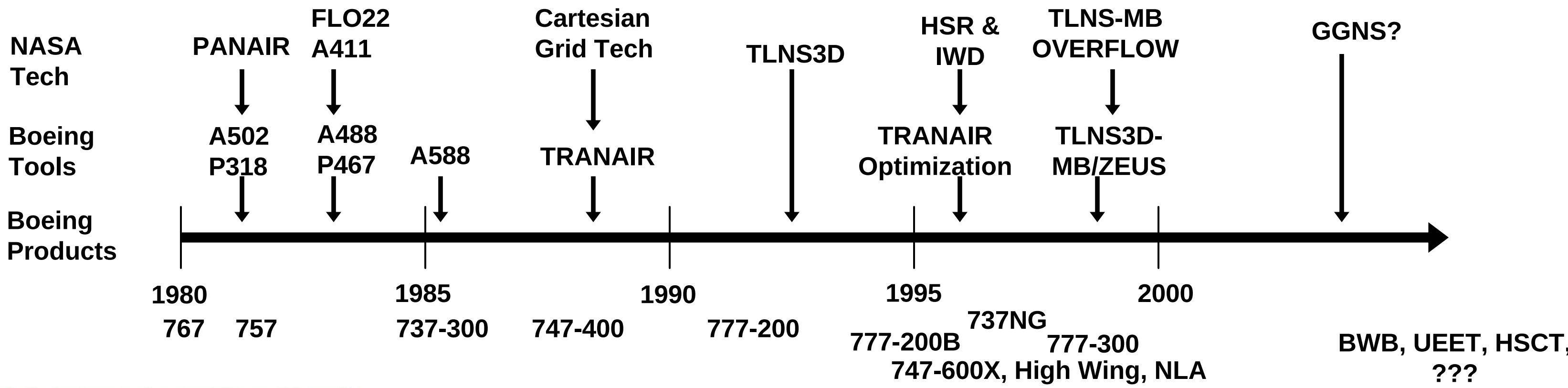
Context for Request that PITAC Examine Computational Science

- **Historical Government role in fostering CS**
- **Importance of CS to agency missions**
- **Contribution of CS to economic prosperity**
- **Sense that "all is not well"**
  - Ageing population of computational scientists
  - Difficulty of using current computational environments
  - Limited progress on recognized CS problems
  - Concern that CS will not achieve potential
  - Debates about Federal investment strategy (e.g. software maintenance)
- **HECRTF debated many of these issues**
  - see http://www.itrd.gov/hecrtf-outreach/

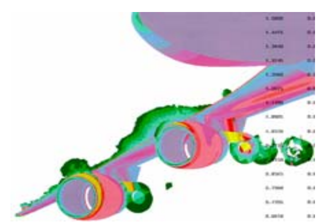
Impact of CFD on Wind Tunnel Testing for Configuration Lines Development



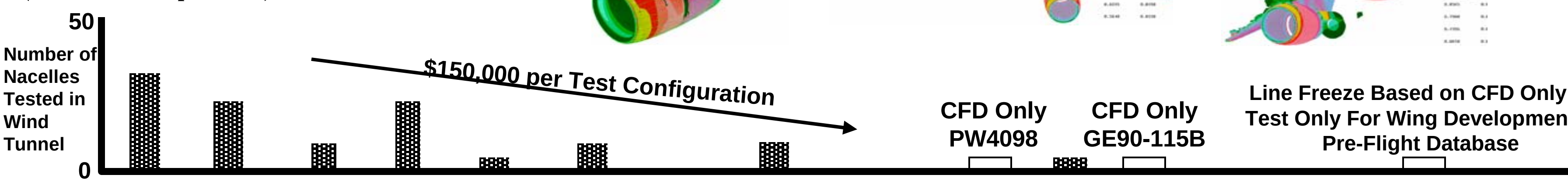
Impact of CFD on Wind Tunnel Testing for Propulsion Integration



Integrated Wing/Body/Nacelle/Strut Installation Aerodynamic Design Using CFD Including Powered Jet Effects



Isolated Nacelle Aerodynamic Design Using Euler Codes
Installed Testing to Develop & Validate Design
(Powered & Unpowered)



Report of the Panel on Large Scale Computing in Science and Engineering (Lax Panel)

The Panel recommends that a long-term National program on Large Scale Computing should be initiated immediately, with the participation of the appropriate Federal agencies, the universities, and industry. The goals of this National Program should be:

- Increased access for the scientific and engineering research community through high bandwidth networks to adequate and regularly updated supercomputing facilities and experimental computers
- Increased research in computational mathematics, software, and algorithms necessary to the effective and efficient use of supercomputer systems
- Training of personnel in scientific and engineering computing
- Research and development basic to the design and implementation of new supercomputer systems of substantially increased capability and capacity beyond that likely to arise from commercial sources

http://www.pnl.gov/scales/docs/lax_report_1982.doc

High End Computing Revitalization Task Force

Improvement needed in Time to Solution of Problems*

- Models and algorithms
- Languages, system software and development/run-time environments
- Formulation and coding
  - Verification, validation, and optimization
  - Run-time assistance
  - Visualization, analysis, and synthesis to extract meaning from results
- Computer systems
  - Better balanced architectures
  - Better alignment with applications
  - Performance modeling tools including benchmarks

Computational scientists shouldn't have to be expert in computer science and low-level coding to get their work done!

* **See DARPA HPCS program**

High End Computing Revitalization Task Force (cont.)

- **Market forces limit ability of computer industry to respond to HEC needs**
- **Need better ways to develop and maintain software for computational science**
- **Need better educational and career paths for computational scientists**
  - Make computational science a true third leg for R&D
- **Need broader availability of computing systems for computational science**
  - Capacity systems for broad applications
  - Leadership systems to advance state-of-the-art

Council on Competitiveness/IDC Survey of Business

- High-Performance Computing Is Essential to Business Survival
- Companies Are Realizing a Range of Financial and Business Benefits from Using HPC
- Companies Are Failing to Use HPC as Aggressively as Possible
- Business and Technical Barriers Are Inhibiting the Use of Supercomputing
- Companies Don’t Have the HPC Tools They Want and Need
- Most Companies Do Not Rely on Remote Access to HPC
- Dramatically More Powerful and Easier-to-Use-Computers Would Deliver Strategic, Competitive Benefits
- Dramatically More Powerful and Easier-to-Use-Computers Could Add Billions to the Bottom Line

http://www.compete.org/pdf/HPC_Users_Survey.pdf

Draft PITAC Computational Science Report: Research Areas and Priorities

Findings

- **Today's computational science ecosystem is unbalanced, with a software base that is inadequate to support and track evolving hardware and application needs.**
- **The creation and long-term maintenance of software that is key to computational science requires the support of the Federal government. This software includes operating systems, libraries, compilers, software development and data analysis tools, application codes and databases.**

http://www.itrd.gov/pitac/meetings/2005/20050112/20050112_reed.pdf

Draft PITAC Computational Science Report: Research Areas and Priorities

- **Finding: Computational science has no clear roadmap outlining decadal priorities for investment, with a clear assessment of those priorities derived from a survey of the problems and challenges.**
- **Recommendation: Create a multi-decade computational science roadmap that identifies the most important problems (e.g., algorithms, applications, architecture, infrastructure, and software) and prioritizes investment areas, funding levels, and recommended schedules to guide government (both individual agency and interagency), academic and industry investment.**
- **Agencies strategies for computational science should be shaped in response to the decadal roadmap. The result should be strategic plans that recognize and address roadmap priorities and funding requirements.**

Draft PITAC Computational Science Report: Short Term vs. Long Term

Findings

- **Short-term investment and limited strategic planning have led to excessive focus on incremental research rather than on long-term sustained research with lasting impact that can solve important problems.**
- **Developing leading-edge computational science applications is a complex process involving teams of people that often must be sustained for a decade or more to yield the full fruits of investment.**
- **A sustained infrastructure is needed that provides access to leading-edge capabilities for computational science. This will require long-term investments and strategic procurements coupled with evolving scientific roadmaps.**
- **Data intensive computational science, based on ubiquitous sensors and high resolution detectors, is an emerging opportunity to couple observation-driven computation and analysis, particularly in response to transient phenomena.**

Draft PITAC Computational Science Report: Short Term vs. Long Term

Recommendations

- Sustain investment in long-term computational science research and infrastructure development.
- Encourage diversification of funding agency research portfolios to create a more balanced mixture of long-term and high-risk projects on the one hand and shorter-term, lower-risk activities on the other.
- Increase investment and focus on sensor- and data-intensive computational science in recognition of the explosive growth of experimental data, itself a consequence of increased computing capability.
- Create a next-generation software, architecture, and algorithms program whose goal is to build advanced prototypes of novel computing systems.

Draft PITAC Computational Science Report: Computational Science Training

Findings:

- **Interdisciplinary education in computational science and computing technologies is inadequate, reflecting the traditional disciplinary boundaries in higher education.**
  - Interdisciplinary computational science research and education would also benefit from inclusion of the social sciences and humanities, particularly as complex scientific and engineering problems touch public policy.
  - Only systemic change to university organizational structures will yield the needed outcomes.
- **The limited number of senior leaders in computational science willing to assume national roles has constrained community advocacy and agency leadership.**

Draft PITAC Computational Science Report: Computational Science Training

Recommendations:

- **Real world, complex problems require collaborative research.**
  - Challenge universities to substantially change their structures to value and reward interdisciplinary and collaborative research and education.
  - Set aside funds to support the demonstration of new educational models that are multidisciplinary.
  - Offer experiential and collaborative learning environments at the graduate and undergraduate level and tie these environments to ongoing research and development efforts (which may be supported through centers and institutes).
  - Learning experiences should place students in real-world situations, including internships and field experiences.
- **Fund curriculum development in computational science, targeting best practices, models and structures.**

Draft PITAC Computational Science Report: Computational Science Training

Recommendations:

- **Establish a leadership development program for computational sciences that targets younger researchers and exposes them to the processes and challenges associated with project management, community planning and government relations.**
- **Examine the current rules for government service, which often impose substantial financial and personal hardships on those who serve. Seek interpretations that are more flexible and engaging for dual career families.**

Draft PITAC Computational Science Report: Keeping Pace with Change

Findings:

- There is a disconnection between commercial practice and the computing infrastructure needs of government and academia. Commercial needs are (in several cases) no longer driving technology acceleration.
- 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.
- 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 and simulation using sensor data from diverse sources.

Draft PITAC Computational Science Report: Keeping Pace with Change

Recommendations

- **Invest in alternative architectures that are better matched to the needs of computational science, notably systems with better memory architectures (higher bandwidth, latency hiding), lower performance variability and improved I/O systems.**

- **Require deposit of scientific data and research software as a component of funding review. Develop one or more national repositories of data and research software for community use.**

Interactive Discussion

- Do you agree/disagree with these findings and recommendations?
- Which are the most important?
- Is PITAC missing something?
- What advice can you give PITAC based on experience in building and maintaining the GMU School of Computational Sciences?

Thank you