REPORT TO THE PRESIDENT

Computational Science: Ensuring America's Competitiveness

President's Information Technology Advisory Committee

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Executive Summary

Nearly half a century ago, the Soviet Union's successful launch of Sputnik – the world's first satellite – shook the political and intellectual foundations of the United States, galvanizing the Federal government to open a new era in research and education in the sciences, engineering, and technology. Today, U.S. leadership in science, engineering, and technology is again being challenged. But this time the challenge is far more diffuse, complex, and long-term than one bold technological achievement by a single U.S. competitor. In the 21st century global economy, burgeoning science and engineering capabilities of countries around the world – spurred by U.S.-pioneered computing and networking technologies – are increasingly testing the Nation's preeminence in advanced scientific research and development (R&D) and in science- and engineering-based industries.

Though the information technology-powered revolution is accelerating, this country has not yet awakened to the central role played by computational science and high-end computing in advanced scientific, social science, biomedical, and engineering research; defense and national security; and industrial innovation. Together with theory and experimentation, computational science now constitutes the "third pillar" of scientific inquiry, enabling researchers to build and test models of complex phenomena – such as multi-century climate shifts, multidimensional flight stresses on aircraft, and stellar explosions – that cannot be replicated in the laboratory, and to manage huge volumes of data rapidly and economically. Computational science's models and visualizations – of, for example, the microbiological basis of disease or the dynamics of a hurricane – are generating fresh knowledge that crosses traditional disciplinary boundaries. In industry, computational science provides a competitive edge by transforming business and engineering practices.

While it is itself a discipline, computational science serves to advance all of science. The most scientifically important and economically promising research frontiers in the 21st century will be conquered by those most skilled with advanced computing technologies and computational science applications. But despite the fundamental contributions of computational science to discovery, security, and competitiveness, inadequate and outmoded structures within the Federal government and the academy today do not effectively support this critical multidisciplinary field.

Principal Finding

Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation. Advances in computing and connectivity make it possible to develop computational models and capture and analyze unprecedented amounts of experimental and observational data to address problems previously deemed intractable or beyond imagination. Yet, despite the great opportunities and needs, universities and the Federal government have not effectively recognized the strategic significance of computational science in either their organizational structures or their research and educational planning. These inadequacies compromise U.S. scientific leadership, economic competitiveness, and national security.

Principal Recommendation

Universities and the Federal government's R&D agencies must make coordinated, fundamental, structural changes that affirm the integral role of computational science in addressing the 21st century's most important problems, which are predominantly multidisciplinary, multi-agency, multi-sector, and collaborative. To initiate the required transformation, the Federal government, in partnership with academia and industry, must also create and execute a multi-decade roadmap directing coordinated advances in computational science and its applications in science and engineering disciplines.

Traditional disciplinary boundaries within academia and Federal R&D agencies severely inhibit the development of effective research and education in computational science. The paucity of incentives for longer-term multidisciplinary, multi-agency, or multi-sector efforts stifles structural innovation.

To confront these issues, universities must significantly change their organizational structures to promote and reward collaborative research that invigorates and advances multidisciplinary science. They must also implement new multidisciplinary structures and organizations that provide rigorous, multifaceted educational preparation for the growing ranks of computational scientists the Nation will need to remain at the forefront of scientific discovery.

Federal R&D agencies face similar structural issues. To address them, the National Science and Technology Council (NSTC) must commission the National Academies to launch fast-track studies that recommend changes and innovations – tied to strategic planning and collaboration – in the Federal R&D agencies' roles and portfolios to support revolutionary advances in computational science. Federal R&D agencies must be actively involved in this process, and individual agencies must implement changes and innovations in their organizational structures to accelerate the advancement of computational science.

Scientific needs stimulate exploration and creation of new computational techniques and, in turn, these techniques enable exploration of new scientific domains. The continued health of this dynamic computational science "ecosystem" demands long-term planning, participation, and collaboration by Federal R&D agencies and computational scientists in academia and industry. Instead, today's Federal investments remain short-term in scope, with limited strategic planning and little cooperation across disciplines or Federal R&D agencies.

For these reasons, the NSTC must commission the National Academies to convene one or more task forces to develop and maintain a multi-decade roadmap for computational science and the fields that require it, with a goal of assuring continuing U.S. leadership in science, engineering, the social sciences, and the humanities.

Because the Nation's research infrastructure has not kept pace with changing technologies, today's computational science ecosystem is unbalanced, with a software base that is inadequate to keep pace with and support evolving hardware and application needs. By starving research in enabling software and applications, the imbalance forces researchers to build atop inadequate and crumbling foundations rather than on a modern, high-quality software base. The result is greatly diminished productivity for both researchers and computing systems.

In concert with the roadmap, the Federal government must establish national software sustainability centers whose charge is to harden, document, support, and maintain vital computational science software whose useful lifetime may be measured in decades. Software areas and specific software artifacts must be chosen in consultation with academia and industry. Software vendors must be included in collaborative partnerships to develop and sustain the software infrastructure needed for research.

The explosive growth in the number and resolution of sensors and scientific instruments has engendered unprecedented volumes of data, presenting historic opportunities for major scientific breakthroughs in the 21st century. Given the strategic significance of this scientific trove, the Federal government must provide long-term support for computational science community data repositories. These must include defined frameworks, metadata structures, algorithms, data sets, applications, and review and validation infrastructure. The Government must require funded researchers to deposit their data and research software in these repositories or with access providers that respect any necessary or appropriate security and/or privacy requirements.

The PITAC is also concerned about the Nation's overall computational capability and capacity. Today, high-end computing resources are not readily accessible and available to researchers with the most demanding computing requirements. High capital costs and the lack of computational science expertise preclude access to these resources. Moreover, available high-end computing resources are heavily oversubscribed.

The Government must provide long-term funding for national high-end computing centers at levels sufficient to ensure the regularly scheduled deployment and operation of the fastest and most capable high-end computing systems that address the most demanding computational problems. In addition, capacity centers are required to address the broader base of users. The Federal government must coordinate high-end computing infrastructure across R&D agencies in concert with the roadmapping activity.

The PITAC believes that supporting the U.S. computational science ecosystem is a national imperative for research and education in the 21st century. Like any complex ecosystem, the whole flourishes only when all its components thrive. Only sustained, coordinated investment in software, hardware, data, networking, and people, based on strategic planning, will enable the United States to realize the promise of computational science to revolutionize scientific discovery, increase economic competitiveness, and enhance national security.

The Federal government must implement coordinated, long-term computational science programs that include funding for interconnecting the software sustainability centers, national data and software repositories, and national high-end leadership centers with the researchers who use those resources, forming a balanced, coherent system that also includes regional and local resources. Such funding methods are customary practice in research communities that use scientific instruments such as light sources and telescopes, and increasingly in data-centered communities such as those that use biological databases.

Leading-edge computational science is possible only when supported by long-term, balanced R&D investments in software, hardware, data,