High-End Computing

Infrastructure and Applications

Definition of HEC I&A PCA

The facilities and activities funded under the NITRD Program's HEC I&A PCA include R&D infrastructure and research and development to extend the state of the art in computing systems, science and engineering applications, and data management, keeping the U.S. at the forefront of 21st century science and engineering discoveries. HEC researchers develop, deploy, and apply the most advanced hardware, systems, and applications software to model and simulate objects and processes in biology, chemistry, environmental sciences, materials science, nanoscale science and technology, and physics; address complex and computationally intensive national security applications; and perform large-scale data fusion and knowledge engineering. For scientific researchers in every field, these advanced computing capabilities have become a prerequisite for discovery.

The R&D that produces these capabilities requires collaborations across Federal and academic institutions, industry, and the international research community. Interdisciplinary teams of scientists, engineers, and software specialists design and maintain the large, complex body of applications software. The largest and fastest computational platforms available are required because of the great range of space scales (from sub-atomic to supernova) and time scales (such as nanosecond to multi-century climate shifts) in the models and simulations. Modeling and simulation produce vast amounts of data that require leading-edge storage and visualization technologies.

Even with skilled teams and leading-edge technologies, however, today's HEC systems remain for the most part fragile and difficult to use. Specialized systems and applications software are needed to distribute calculations across hundreds or thousands of processors in a variety of massively parallel systems. Computational scientists are faced with a proliferation of architectures and variety of programming paradigms, resulting in a multitude of questions that must be addressed and tasks that must be performed in order to implement a modeling or simulation algorithm on any specific system architecture. But while this work progresses, advances in the size and speed of computing systems open up opportunities to increase the size, scale, complexity, and even nature of the modeling and simulation problems that can be addressed. The result is that a new cycle of systems and applications software R&D is required to enable scientists to take advantage of the increased computing power.

To maintain or accelerate the pace of scientific discovery, HEC I&A efforts are needed to develop breakthroughs in algorithm R&D, advances in systems software, improved programming environments, and computing infrastructure for development of the next-generation applications that will serve Federal agency missions. Focus areas include, but are not limited to, cyberinfrastructure tools to facilitate high-end computation, storage, and visualization of large data sets encountered in the biomedical sciences, climate modeling and weather forecasting, crisis management, computational aerosciences, Earth and space sciences, and a wide range of other human activities.

Broad Areas of HEC I&A Concern

- Algorithm R&D
- Data management and understanding

HEC I&A Agencies

			Participating Agency
NSF	NASA	NIST	DoD/HPCMPO
NIH	DOE/NNSA	EPA	
DOE/SC	NOAA		

HEC I&A PCA Budget Crosscut

FY 2004 Estimate	FY 2005 Request
$516.2 M	$505.7 M

- Programming environments
- Scientific applications
- Computational facilities

Technical Goals

- Understand the interaction between applications and architectures
- Provide mathematical and computational methods needed for critical mission agency applications
- Provide technology base for next-generation data management and visualization
- Enable new generations of mission agency computational applications
- Provide measures of progress
- Reduce time and cost in HEC procurements
- Reduce cost of ownership of HEC systems

Illustrative Technical Thrusts

- Scientific discovery through advanced computing
- Cyberinfrastructure
- Leadership computing
- System monitoring and evaluation
- Integrated end-to-end data management
- Visualization clusters
- Common procurement methodology

Benefits of HEC Applications to U.S. Science and Engineering

Application Area	Science Challenge	Potential at 100-1,000 Times Current HEC Capability
Astrophysics	Simulation of astrophysical environments such as stellar interiors and supernovae.	Yield understanding of the conditions leading to the origin of the heavy elements in the universe.
Nuclear Physics	Realistic simulations of the characteristics of the quark-gluon plasma.	By developing a quantitative understanding of the behavior of this new phase of nuclear matter, facilitate its experimental discovery in heavy ion collisions.
Catalyst Science/ Nanoscale Science and Technology	Calculations of homogeneous and heterogeneous catalyst models in solution.	Reduce energy costs and emissions associated with chemicals manufacturing and processing. Meet Federally mandated NOx levels in automotive emissions.
Nanoscale Science and Technology	Simulate and predict mechanical and magnetic properties of simple nanostructured materials.	Enable the discovery and design of new advanced materials for a wide variety of applications impacting many industries.
Simulation of Aerospace Vehicle in Flight	Simulate a full aerospace vehicle mission, such as a full aircraft in maneuver or an RLV in ascent or descent.	Reduce aerospace vehicle development time and improve performance, safety, and reliability.
Structural and Systems Biology	Simulations of enzyme catalysis, protein folding, and transport of ions through cell membranes.	Provide ability to discover, design, and test pharmaceuticals for specific targets and to design and produce hydrogen and other energy feedstock more efficiently.
Signal Transduction Pathways	Develop atomic-level computational models and simulations of complex biomolecules to explain and predict cell signal pathways and their disrupters.	Yield understanding of initiation of cancer and other diseases and treatments on a molecular level; prediction of changes in ability of microorganisms to influence natural biogeochemical cycles such as carbon cycling and global change.
Signal & Image Processing & Automatic Target Recognition	Replace electromagnetic scattering field tests of actual targets with numerical simulations of virtual targets.	Design more stealthy aircraft, ships, and ground systems and create the ability to rapidly model new targets, enabling more rapid adaptation of fielded weapon systems' ability to target new enemy weapon systems.
Climate Science	Resolve additional physical processes such as ocean eddies, land use patterns, and clouds in climate and weather prediction models.	Provide U.S. policymakers with leading-edge scientific data to support policy decisions. Improve understanding of climate change mechanisms and reduce uncertainty in the projections of climate change.
Solid Earth Science	Improved statistical forecasts of earthquake hazards (fault-rupture probabilities and ground motion).	Provide prioritized retrofit strategies. Reduced loss of life and property. Damage mitigation.
Magnetic Fusion Energy	Optimize balance between self-heating of plasma and heat leakage caused by electromagnetic turbulence.	Support U.S. decisions about future international fusion collaborations. Integrated simulations of burning plasma crucial for quantifying prospects for commercial fusion.
Combustion Science	Understand interactions between combustion and turbulent fluctuations in burning fluid.	Understand detonation dynamics (for example, engine knock) in combustion systems. Solve the "soot" problem in diesel engines.

Excerpt from a table in the "Federal Plan for High-End Computing" illustrating the critical role of HEC I&A in future scientific advances.