High End Computing (HEC) Infrastructure and Applications (I&A)

NITRD Agencies: NSF, OSD and DoD Service research organizations, NIH, DOE/SC, NASA, NIST, DOE/NNSA, NOAA, EPA

HEC I&A agencies coordinate Federal activities to provide advanced computing systems, applications software, data management, and HEC R&D infrastructure to meet agency mission needs and to keep the United States at the forefront of 21st-century science, engineering, and technology. HEC capabilities enable researchers in academia, Federal laboratories, and industry to model and simulate complex processes in biology, chemistry, climate and weather, environmental sciences, materials science, nanoscale science and technology, physics, and other areas to address Federal agency mission needs.

President's 2009 Request

Strategic Priorities Underlying This Request

Ongoing investment in Federal HEC facilities and advanced applications supports Federal agencies' science, engineering, and national security missions and helps sustain U.S. scientific leadership. Priorities include:

Leadership-class systems: Continue acquisition of highest-capability systems for cutting-edge scientific research and national security applications

Production-quality HEC resources: Invest in capacity platforms to expand Federal computing resources for critical agency needs and for the science and engineering communities

Advanced applications: Develop data- and compute-intensive applications for current and new HEC platforms

Highlights of Request

Acquisition of prototype leadership-class and production R&D systems

NSF: Continue multiyear acquisitions of the Track 1 petascale system and other midrange Track 2 systems to capitalize on the growing importance of cyberinfrastructure for advanced scientific discovery and education; Track-2 system (504 TF) at the Texas Advanced Computing Center becomes operational

OSD (HPCMP): Upgrade HEC platforms at multiple supercomputing centers

NIH: Selected acquisition of cluster and midrange compute-intensive systems

DOE/SC: Upgrade LCF system at ORNL to 1 PF (early FY 2009); expand ANL's LCF resources by upgrading BlueGene/P to 250-500 TF (late FY 2008); NERSC 104-TF XT4 in full production and integrated into a common high-performance file system

NASA: Continue annual investments in supercomputing systems to track Moore's Law (4X capacity every 3 years) and meet NASA's rapidly growing requirements for large-scale numerical modeling and simulation

DOE/NNSA: Acquire new production system to replace ASC Purple; continue operation of RoadRunner base system; deploy and operate TLCC07 capacity clusters; initiate operation of Sequoia Initial Delivery (ID) system

Applications

NSF: Multidisciplinary Cyber-enabled Discovery & Innovation (CDI) program, including petascale applications that focus on understanding complexity in natural, built, and social systems and increasingly data-intensive applications; software for applications that need to integrate computation and data acquisition in heterogeneous, dynamic computing environments

OSD (HPCMP): CREATE program to develop highly scalable application codes (aircraft, ships, antennae)

NIH: R&D for biomedical applications, such as the new NIH-wide Blueprint for Neuroscience Research activity

DOE/SC: Petascale multiphysics applications; integrated reviews of SciDAC2 projects; INCITE competition for access to LCF resources by outside researchers; mathematics for analysis of extremely large data sets; multiscale mathematics

NASA: Increase core computing capability and capacity, including visualization and storage

NIST: Mathematical modeling, computational simulation, and high-end visualization for measurement science applications

DOE/NNSA: Code validation and verification (V&V) and uncertainty quantification for predictive simulations

NOAA: Accelerate improvements in model-based computing of hurricane track and intensity forecast guidance

EPA: Applications in computational toxicology (aggregated resource repository, Virtual Liver model for predictions of dose-response), air quality (enhance code quality while maintaining modularity, portability)

HEC infrastructure

NSF: Develop numerical algorithms and innovative software implementations that push the boundaries of

cyberinfrastructure, computational science and engineering, and computing on the TeraGrid

OSD: Consolidate operations of supercomputing centers under single technical services contract; implement common cross-center services

NIH: Invest in grid computing infrastructure and tools for major R&D projects (e.g., BIRN, CaBIG, BISTI)

DOE/SC: Continue emphasis on unified approach to software, languages, and tools support to reduce barriers to effective use of complex HEC resources by application developers and users

NASA: Strategically grow, manage integrated HEC infrastructure; broaden HEC application and knowledge base

NIST: Development and analysis of fundamental mathematical algorithms and software; parallel and distributed algorithms; interoperable MPI; high-end visualization tools

DOE/NNSA: Deploy ASC common operating environment

NOAA: Explore ways to coordinate Federal HEC resources "on demand" (surge computing) for critical events

EPA: Continue building GEOSS systems for data, information exchange, including work with NASA and NOAA on real-time movement of large data sets through Remote Information Sensing Gateway

Planning and Coordination Supporting Request

Access to leadership-class computing: Coordination to make highest-capability HEC resources available to the broad research community – NSF, DOE/SC, NASA, NIST, DOE/NNSA, NOAA

System reviews, benchmarking: Collaborative efforts to evaluate HEC system performance – NSF, OSD, DOE/SC, NSA, NASA, DOE/NNSA, NOAA

Acquisition procedures and analysis: Information sharing, streamlining of processes, and collaborative analysis of total cost of ownership – NSF, OSD, DOE/SC, NASA, DOE/NNSA, NOAA, EPA

Multiscale modeling in biomedical, biological, and behavioral systems: Interagency collaboration to advance modeling of complex living systems (e.g., MIDAS Project) – NSF, NIH

Infrastructure for climate and weather modeling: Development of interoperable interfaces, software tools, and data standards – NSF (NCAR), OSD, DOE/SC, NASA, NOAA, EPA

Surge Computing: Discussing how to implement this capability – NOAA, NSF, OSD, DOE/SC

Computational toxicology: Integration of HEC technologies with molecular biology to improve methods for risk assessment of chemicals – OSD, NIH, DOE/SC, EPA, FDA

Additional 2008 and 2009 Activities by Agency

NSF: Expand TeraGrid to include new systems; develop cyberinfrastructure software (e.g., for debugging, fault tolerance, performance tuning, middleware, data handling); operational support for TeraGrid

OSD (HPCMP): Provide HEC services for DoD R&D and test communities (e.g., platforms, computational science software support); support six computational science institutes focused on DoD priority areas (air armament, health force protection, weather prediction, ground sensors, space situational awareness, rotorcraft)

NIH: Support international networks for biomedical data and software sharing (caBIG, BIRN); NIH Roadmap National Centers for Biomedical Computing (NCBCs); Cancer Imaging and Computational Centers; P41 computational centers; NLM information and analysis servers; bioinformatics resource centers for emerging and re-emerging infectious disease; proteomics and protein structure initiatives; systems biology centers

DOE/SC: Manage LCF facilities at ORNL and ANL; support computation-intensive and data-intensive applications; new generation of petascale tools; optimization and risk analysis in complex systems

NASA: Provide access to National Leadership Computing System (NCLS) to external researchers (through FY 2008); expand applications of visual supercomputing using hyperwalls and concurrent visualization; develop multitiered computing architecture

NIST: Virtual measurement systems, including uncertainty quantification, design of computational experiments, V&V, calibration; Virtual Measurement Laboratory

DOE/NNSA: Continue providing production-level systems and software environments to the weapons program and undergoing computing-related transformational activities under the Nuclear Weapons Complex Initiative

NOAA: Complete upgrade of new integrated R&D HEC system (2.1-fold increase over current system); integrate management, allocation of HEC resources; develop, transition advanced science/technologies into operations

EPA: Continue developing HEC applications for human health, ecology, pollution control, decision sciences; focus on large-scale data management and understanding, algorithm R&D