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 2008 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 development 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: Towards a Petascale Computing Environment for Science and Engineering – multiyear acquisition of petascale system (by 2011) and mid-range systems as well as deployment of computational grids and advanced software systems to provide world-class HEC resources for academic research

OSD (HPCMP): Upgrade capabilities at multiple supercomputing centers

DOE/SC: Upgrade ORNL's Leadership Computing Facility (LCF) to 1 PF as a resource for scientific leadership; expand LCF resources at ANL through upgrade of BlueGene/P to 250+ TF for aging of materials and other computations; keep LBNL's NERSC-5 on path to 500 TF by 2010

NASA: Maintain a seamless environment for shared HEC capabilities, integrate user services with NASA missions; initiate acquisition of Columbia system follow-on at ARC; continue build-out of cluster system for Earth and space science research at GSFC

DOE/NNSA: Acquire innovative multicore, cell processor-based Roadrunner system

Applications

NSF: Modeling and simulation of complex systems across science and engineering; numerical algorithms and innovative software implementations that exploit and push the boundaries of cyberinfrastructure, computational science, and computing on the Teragrid; system software for applications that need to integrate computation and data acquisition while operating in heterogeneous and dynamically changing computing environments

NSF: Development and scaling of science and engineering applications whose access to petascale and grid systems would result in transformative advances in their respective scientific disciplines

OSD (HPCMP): New multiyear Computational Research and Engineering Acquisition Tools and Environments (CREATE) program to enhance development of highly scalable application codes

DOE/SC: Pioneer petascale applications; continue competitively selected FY 06 awards for SciDAC2 as well as partnerships with programs in genomics, nanoscale science, and fusion simulation; continue Institutes and Centers for Enabling Technology focusing on applied mathematics and computer science areas that support advanced scientific computation, modeling, simulation, and visualization (some application areas also supported by DOE/NNSA, NSF)

DOE/SC: Continue Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program – up to 80% of leadership systems and 10% of production systems allocated to external academic, industrial, and government research projects

NASA: From second round of National Leadership Computing System (NCLS) call for proposals, open part of Columbia system to external researchers pursuing demanding science and engineering challenges
NIST: Parallel and distributed application algorithms (e.g., large-scale multizone airflow analysis parallelization, with DARPA); fundamental mathematical tools and software infrastructure for HEC applications
DOE/NNSA: Develop and maintain weapons codes; deploy common capacity computing environment across labs
NOAA: Test Earth System Modeling Framework with modeling capabilities across the whole agency; evolve NOAA's R&D high-performance computing system into a "grid-like" environment
EPA: Develop algorithms and integrate state-of-the-art air quality models and tools for Remote Sensing Information Gateway distributed air-quality data modeling center (with NASA, NOAA)

Planning and Coordination Supporting Request
Computational science: Informing *Toward Better Understanding the Potential Impact of High-End Capability Computing on Science and Technology,* a National Academies study of the role of high-end computing in advancing cutting-edge research in major scientific fields – HEC agencies
Access to leadership-class computing: Coordination to make highest-capability HEC resources available to the broad research community with open calls for proposals, cycle sharing – DOE/NNSA, DOE/SC, NASA, NSF
System reviews, benchmarking: Collaborative efforts to evaluate HEC system performance – DARPA, DOE/NNSA, DOE/SC, EPA, NASA, NOAA, NSF, OSD
Acquisition procedures and analysis: Information sharing, streamlining of processes, and collaborative analysis of total cost of ownership – DOE/NNSA, DOE/SC, EPA, NASA, NOAA, NSF, OSD
Multiscale modeling in biomedical, biological, and behavioral systems: Interagency collaboration to advance modeling of complex living systems – NIH, NSF
Infrastructure for climate and weather modeling: Development of interoperable interfaces, software tools, and data standards – DOE/SC, EPA, NASA, NOAA, NSF (NCAR), OSD
Computational toxicology: Integration of HEC technologies with molecular biology to improve methods for risk assessment of chemicals – DOE/SC, EPA, NIH, OSD, FDA

Additional 2007 and 2008 Activities by Agency
NSF: Development of cyberinfrastructure software (e.g., for debugging, fault tolerance, performance tuning, middleware, data handling); operation and management support for Teragrid suppliers; data-rich science including bioinformatics, geoinformatics, and cognitive neuroscience
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 for international networks for biomedical data and software sharing (caBIG, BIRN); NIH Roadmap National Centers for Biomedical Computing (NCBCs); Cancer Imaging and Computational Centers; Modeling of Infectious Disease project (MIDAS, with NSF); P41 computational centers to develop tools and cyberinfrastructure; 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: Upgrade ORNL XT3 to 250 TF; install 100 TF BlueGene/P at ANL; expand SciDAC applications and infrastructure across DOE/SC and to include DOE/NNSA and NSF; support for computation- and data-intensive applications
NASA: Scale application codes for Columbia system; develop multitiered computing architecture
NIST: Virtual Measurement Laboratory – real-time tracker calibration, interfaces, representation, interaction analysis, selection, measurement, immersive visualization; high-accuracy computation of nanostructures, Object-Oriented Micromagnetics Modeling Framework; standards (interoperable MPI, sparse BLAS)
DOE/NNSA: Recompete Alliance Centers Program for Phase 2 with focus on predictive science; provide production-level computing environment
NOAA: Acceptance testing of new integrated R&D HEC system; integrated management and allocation of HEC resources; development, application, transition of advanced science and technology into operations
EPA: Port environmental applications to EPA Grid for faster, cost-effective risk assessments; assess related architecture, data management issues; scale, adapt environmental codes for exploratory data fusion techniques at differing temporal, spatial scales; integrate next-generation computing technology and mechanistic biology