4.0 Computational Resources at NERSC

The resources furnished by the NERSC High-Performance Computing Facility are the focal point of high-performance production computing for the DOE Office of Science scientific programs. These resources include an assortment of hardware, a large ensemble of installed software, network connectivity to sites that use the facility, and user support services.

Hardware

The NERSC HPCF now provides all of its computational resources via massively parallel processing (MPP) systems, including cluster systems, and specialized compute servers for visualization and mathematical software.

NERSC supports a diverse workload, but one which tends increasingly towards capability computing, which can require a large fraction of an entire computing resource

Massively Parallel Supercomputers

Distributed-memory Massively Parallel Processor (MPP) systems are now common in scientific computing. For suitable problems, these systems are capable of very high computational performance, and of addressing capability computing problems that require very large numbers of numerical calculations and very large amounts of memory. NERSC has one large MPP system in production, and is actively preparing to evolve along with the MPP and cluster systems available in the open market.

The IBM SP (seaborg.nersc.gov) is one of the larger unclassified systems in existence. First installed in September 2001 and doubled in size in 2003, it is now composed of 380 compute nodes (6080 processors), with over 7 TB of memory and 44 TB of disk. This system has a peak performance of 1.5 Gflops per processor, for a theoretical peak of over 9.1 Tflops. Another system is being investigated that, when put into production, is expected to deliver over 2.8 Tflops and contain over 1.2 TB of memory.

Clusters

In the area of cluster computing, NERSC supports Parallel Distributed Systems Facility (PDSF), a networked distributed computing environment used to meet

the detector-simulation and data analysis requirements of large-scale High Energy Physics (HEP) and Nuclear Science (NS) investigations. PDSF is composed of some 344 compute nodes with dual Pentium III or AMD 2100/2600 processors.

Knowledge gained from NERSC's past cluster work is being used in studying possible future systems.

High-Performance Storage Systems

HPSS is a modern, flexible, performance-oriented mass storage system, designed and developed by a consortium of government and commercial entities. It is used at NERSC for data storage, archives, and system backups. The current configuration consists of two libraries, totalling over 8.8 PB of tape capacity, served by 8 STK tape robots, 50 TB of disk cache, and multiple data-movers and meta-data servers. The theoretical throughput is 3.2 GB/sec.

Servers

NERSC operates servers that provide direct and indirect services to staff and users. The two most visible are a 12 processor SGI Onyx 3400 (escher.nersc.gov) for visualization processing; and, a 4 node, 8 processor Linux system of AMD Athlon processors (newton.nersc.gov) for symbolic mathematics computing. A new SGI Altix system is being configured, which will replace the current visualization serverin the next few months. A CVS repository server is also maintained to support software collaboration among groups of NERSC users.

NERSC also operates servers that are less directly visible, but nonetheless essential for the secure but accessible utilization of NERSC's resources. These systems support security applications (monitoring and intrusion detection), addressing and authentication services (LDAP), e-mail, account support databases (NIM), and web-based documentation and information services.

Grid Computing

The Grid promotes a standard large-scale science environment that spans many different projects and provides the needed infrastructure, data transfer and storage resources, and computing services in a relatively uniform and

supportable way. All NERSC production computing and storage systems are now Grid-enabled, and can be accessed by client software based on the Globus Toolkit. These capabilities are in daily use, especially in PDSF, where job submission and data transfers are routinely accomplished by Grid client-ware, and in HPSS, where Grid-based data transfer capabilities exist.

Software

The software infrastructure is what a user truly interacts with, and it determines to a large extent the usability and security of any particular system. This complex includes distributed computing tools, operating systems, networking and access software, compilers and debuggers, performance tools, software libraries, job control and queuing systems, and third-party applications that are of importance to many users in the community.

System Software

The operating system and supporting software layers must be a robust software suite or the underlying hardware will not be well utilized. The operating system must allow users to manage files, run interactive and batch jobs, import and export data, compile and develop programs effectively, and support significant third-party applications. Network access software is a component of this, and its components also protect against unauthorized access and compromise of proprietary information. NERSC supports several operating systems on MPP and server systems, and interacts with vendors on their maintenance and development.

Standard programming languages and debugging and performance tools are essential components of any high-performance computing resource. The following languages are supported, some by multiple compilers, as part of a fully integrated, interoperable environment for compilation and debugging: Fortran 77/9x, C, C++, Java, assembler, and various shell and scripting languages. Tools to monitor and diagnose performance problems are also provided.

Basic Scientific Libraries and Environments

In addition, communication libraries, such as MPI, are available and are augmented by tools to make their use amenable to debugging and performance

tuning. Various I/O libraries such as netCDF, HDF, etc., support code portability and data exchange.

Finally, graphics and visualization libraries are provided on MPP and server systems for post-processing and transformation of numerical output into static and dynamic graphics of many types.

Scientific Application Codes and Systems
NERSC supports a wide variety of third-party software applications from the independent software vendor community: for example, computational chemistry programs such as Gaussian, NWChem, Amber, and Molpro; mathematical applications such as Mathematica, Maple, and Matlab; and visualization applications such as AVS and Ensight. NERSC provides ongoing licensing and support of commercial applications, and staff liaisons to their vendors.

Human Resources
NERSC provides effective, high-quality client support to assist users in accomplishing their scientific work. This support includes provision of servers, tools, information systems, consulting services, and training. NERSC staffers continuously develop their skills in new areas, such as Gridware, to keep up with emerging trends.

User Support Services
The NERSC service architecture aims to ensure a response to client problems within four working hours, and resolution of 95% of problems within two working days. In addition to basic Help Desk services, NERSC offers some direct scientific support to the DOE scientific community in their computational and data management efforts. Such support includes technical advice in system usage; scientific advice on algorithmic, programming, and application problems; and support for the development of new applications, tools, and utilities. NERSC also provides training and instruction in the use of technical resources, and maintains on-line documentation for all NERSC systems.

NERSC also provides support and tools for user account initialization, monitoring, management, and security for staff and users and

their allocations. Much of this is provided by state-of-the-art tools and databases with continuously advancing capabilities.