

PNNL Institutional Computing

MISSION

Pacific Northwest National Laboratory (PNNL) Institutional Computing (PIC) provides an ongoing laboratory-level investment focused on Laboratory needs and DOE missions. The PIC program is part of PNNL's overall computing strategy that nurtures a culture of computational science by offering PNNL scientists and engineers cost-effective computing services that will help advance scientific discovery and have impact on PNNL mission areas.

The PIC program is designed to:

▶ **Increase the effectiveness of programmatic and initiative-funded computing investments**

Historically, projects made their own arrangements for computing. This worked, but budget constraints led to relatively small systems often without provision for backup. When projects cease, computing equipment is orphaned with no budget available to support ongoing maintenance.

▶ **Capture, preserve, protect, and share research data**

Typically, PNNL computer systems have not provided for long-term data archiving, and data are not easily available to research collaborators. PIC provides ongoing data archival and retrieval services.

▶ **Contribute to U.S. Department of Energy and PNNL sustainability goals**

PIC is housed in PNNL's award-winning **Computational Sciences Facility (CSF)**. Completed in late 2009, the CSF has a total of 12,500 square feet of raised-floor space and takes advantage of geothermal cooling technology. Over time, PIC potentially replaces 30 or more small clusters housed in various PNNL facilities with consequent savings in space, power, and cooling.

▶ **Increase productivity of Science and Technology (S&T) software developers and the quality and security of developed code**

PIC provides a common cluster environment and Subject Matter Experts (SMEs) who are available to users for consulting on a variety of topics, ranging from getting started on PIC to implementing parallel input/output (I/O) to high-speed data transmission over networks.



PNNL's Computational Sciences Facility (CSF)



PNNL's Science & Technology Major Initiatives will benefit from the PIC

S&T Major Initiatives associated with PNNL's Leadership Positions benefit from PIC as Laboratory Directed Research and Development (LDRD) projects will be granted access to PIC computing resources. LDRD projects with special needs will have access to systems including testbeds to support alternative architecture, alternative operating systems, and latest-generation technologies such as accelerators.

Projects funded with programmatic dollars will meet their computing needs more effectively by contributing compatible hardware to PIC and benefiting from PIC's established infrastructure (ongoing maintenance support; high-speed interconnect; storage; backup; archive; and pre-arranged software like compilers, libraries, and debuggers). Contributing projects will have guaranteed access to CPU hours and data storage on the PIC system proportional to their investment and also will be able to access free hours via the idle queue. In addition, projects can acquire special-purpose testbeds if that is appropriate.

In contrast with user facilities measured by system utilization, PIC will not oversubscribe its job queues. This means LDRD and project users should never have to wait unduly to have jobs launch. The provision of an idle queue will help keep PIC busy with workload that can be pre-empted should high-priority jobs have a need.

Any PNNL user with high performance computing needs can request access to PIC on a limited-access basis. With prior approval, PNNL users can have access to large-scale configurations of PIC for Proof of Concept testing.

GOVERNANCE

The PIC Director is responsible for day-to-day operations, guided by an Advisory Board with members drawn from all of PNNL's directorates. The Director is responsible for managing allocation of PIC resources, including budget, staff, and CPU hours and data storage distribution.

The Director recommends appropriate investments to refresh PIC technology and prepares an annual budget request in conjunction with the Advisory Board subject to approval by PNNL's Executive Committee. PIC users and projects seeking PIC support will deal directly with the Director.

PIC users can make arrangements to access PIC large configurations for scalability testing and large-scale experiments.

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TECHNOLOGY

PIC supports large-scale general-purpose clusters with high-speed interconnects and special-purpose testbeds. Mass storage and archival systems are fully integrated with PIC to facilitate easy access and sharing of data. PIC also supports server instances to host persistent services such as databases, web servers, and application frameworks.

PIC resources generally will be located in PNNL's research network and can accommodate access by external scientific collaborators. Compute nodes and storage can be moved to other PNNL networks as needed. Similarly, testbeds will be provided to meet specific LDRD or project needs.

Technology refresh will occur on an annual basis in consultation with users via PNNL's established Greenbook process developed by EMSL, the Environmental Molecular Science Laboratory, a national scientific user facility sponsored by the DOE Office of Science.

<http://pic.pnnl.gov>

ABOUT PNNL

Pacific Northwest National Laboratory, a U.S. Department of Energy Office of Science laboratory, solves complex problems in energy, the environment, and national security by advancing the understanding of science. PNNL employs nearly 5,000 staff members, conducts annual business in excess of \$1 billion, and has been managed by Ohio-based Battelle since the Lab's inception in 1965.



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