the ENERGY lab

R&D FACTS

Strategic Growth Area

The NETL SuperComputer

Introduction

The National Energy Technology Laboratory (NETL) is home to the NETL SuperComputer (NETLSC)—one of the world's largest high-performance computers—along with advanced visualization centers serving the organization's research and development needs.

A unique and collaborative tool tailored for science and engineering calculations in support of Fossil Energy (FE) research, the NETLSC advances FE and NETL missions by applying complex model simulations for advanced energy technology development; simulations like these will help overcome technical barriers in development quickly, reliably, and cost-efficiently. The NETLSC design balances computational requirements, efficiency, usability, and collaboration techniques to deliver a premier system to the Lab and its partners.

Computational Capabilities

NETLSC is a 503 TFlops (trillion floating-point operations per second) high-performance computer (HPC) that enables the numerical simulation of complex physical phenomena that are difficult or impossible to measure, such as coal jet penetration into a gasifier.

This system provides the capabilities for running modeling tools at various scales ranging from molecules, to devices, to entire power plants and natural fuel reservoirs. NETLSC includes facilities for enhanced visualization, data analysis, as well as data storage capabilities that enable researchers to discover new materials, optimize designs, and predict operational characteristics.

Pictured are the computational nodes inside of modular datacenter.

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RESEARCH PARTNERS

SGI

Visualization Centers: Improving Collaborative Efforts

The NETLSC facilities suppor t ef fective collaboration among researchers and will improve interaction across NETL. In addition to secure desktop access for users, visualization centers—dedicated space for collaboration and simulation work—are installed at each of the three NETL research sites: Morgantown, Pittsburgh, and Albany.

Datacenter Efficiency and Usage

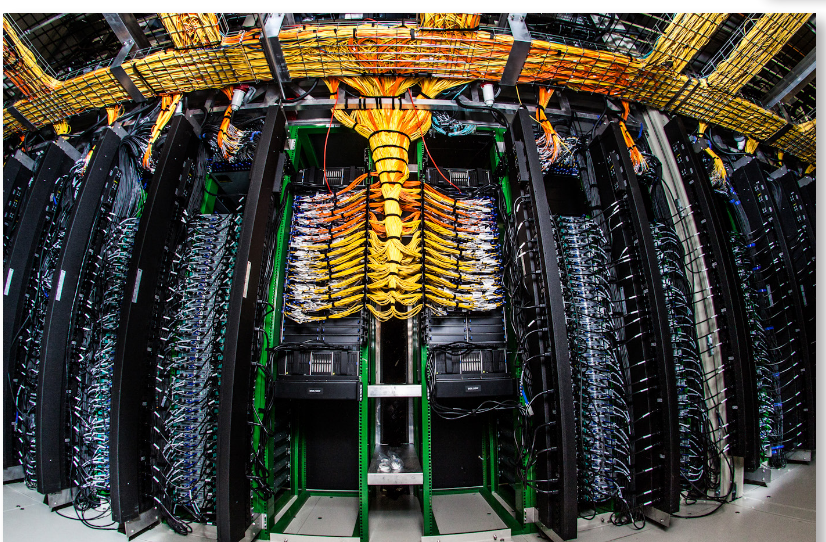
The NETLSC is recognized by Top 500 as one of the top 100 supercomputers in the world. In addition, it is one of the most energy efficient in the world, using only 5.7 percent of inputted power for cooling versus 50-100% usage for traditional data centers. In order to achieve this level of efficiency, all of the computational, visualization, network hardware, and primary storage servers are installed in a high-efficiency modular data center (MDC). Unlike traditional datacenters which use chilled air for cooling, the MDC only uses ambient air for most of its cooling needs supplemented with a small amount of water for evaporative cooling on extremely hot days.

Since its commissioning, the usage of the NETLSC has continually increased from mid-70 percent to a consistent average utilization of about 95 percent. This is a result of working with the user community to manage time allocations and alter queue structures to more fully take advantage of the system, including set asides for high-value license allocations, leadership queues, and changing the way jobs are structured so there are always jobs waiting in the queue to start when running jobs complete.

The NETLSC was funded under ARRA (American Reinvestment and Recovery Act) and represents a vast improvement over the previously existing NETL computational clusters—the system is completely networked and therefore provides the ability to run large jobs that small, individual clusters simply cannot. In addition, the NETLSC provides 637% more computational power over the previously existing clusters while consuming 11.5% less energy.

The NETLSC is currently scheduled for an update in FY16 (HPCs have an expected life cycle of approximately three years after which standard warranties run out, replacement parts are not readily available, and maintenance costs rapidly escalate after three years). Since ARRA funds are expended, the replacement, or refresh, will be funded through normal DOE channels. The refresh will be placed in the same MDC that houses the current version of the NETLSC and, because technology has advanced, will only require 2/3 of the space and energy consumption of the current equipment. The annual cost to sustain NETL's super computing capabilities is estimated at $5-$6 million.

An external shot of the modular datacenter shows the filters for the free-cooling air technology. Using this technology the SBEUC is able to operate with a Power Utilization Effectiveness (PUE) of 1.06—for every kilowatt of power used for computation only 60 additional watts are required for cooling.



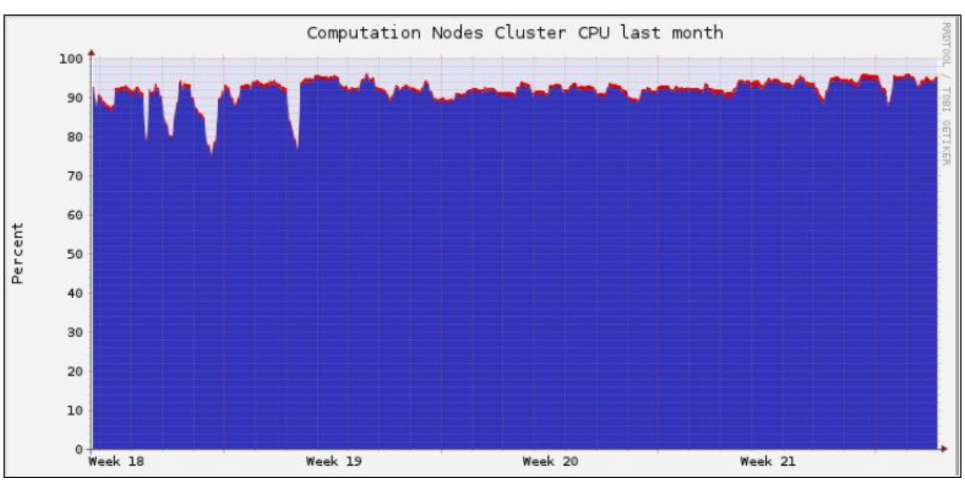
This image shows two of three Mellanox Infiniband 648-port switches, which are arranged in a Fat-Tree topology allowing for 40Gb/s non-blocking bandwidth between 1,512 computational nodes.

Thanks to advances in technology, the computational power of the next generation equipment will be much greater. It is estimated the new system will provide 5 PETA-Flops (quadrillion Flops) of computational power, or approximately 10X the computational power of the current version. This advance in computational capability is a normal course of evolution—the software that is used by national laboratories and industry advances on pace with new hardware and requires HPC users to obtain the higher capacity systems as the old ones are replaced. The benefit is that, as in this case, the new units are more efficient and provide an enhanced capability that the older systems are not able to provide.

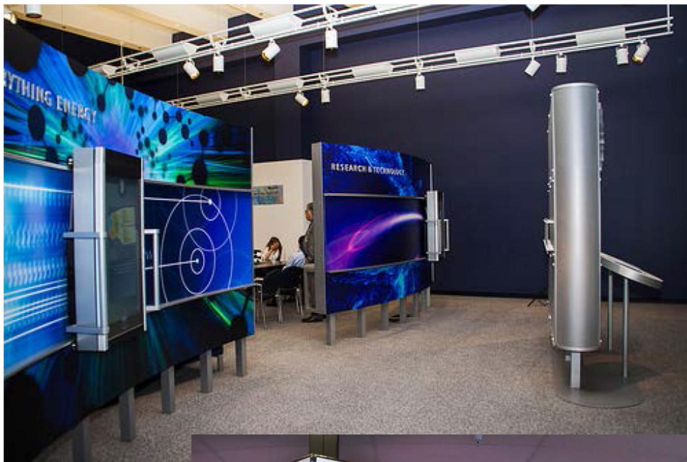
Benefits to R&D – More Work, Faster Results, Increased Accuracy

The NETLSC has provided a tremendous boost to the quantity and pace of computer-based research and development at NETL. As an example, fuel cell models of critical cathode reactions have been accelerated from hours to seconds using the NETLSC. This allows for more complete mapping of cathode performance at various operating conditions and thereby yielding a significant increase in accuracy of model predictions for designing higher efficiency fuel cells. Another example is the use of the NETLSC for simulation of industrial-scale circulating fluidized bed gasification for comparison and validation with industry data. Use of the supercomputer has enabled very large-scale, complex simulations over a broad range of gasifier operating conditions. Comparison of these results with industry measurement is underway to validate the model for use in predicting gasifier behavior to aid designers and operators. At a more fundamental level, the NETLSC has facilitated research projects with direct impact on various technologies ranging from catalyst development for syngas and natural gas conversion; to catalytic systems for CO_2 utilization processes; to development of optimized solid sorbents for CO_2 capture; to identification of novel ionic liquid and hybrid nanostructured membranes for CO_2 gas separation; to novel nanostructured composite materials for energy conversion and new gas sensor materials. The supercomputing capabilities at NETL now enable the analysis of more complex atomic, molecular and crystalline systems. The use of highly accurate but computationally very demanding first principles calculations allows screening of a large number of crystalline structure, as in the case of solid sorbent developments, and of testing a large number of binding configurations in complex nanoporous materials. In one recent exciting extension of energy research, NETL supercomputing capabilities have been essential to explain the binding, reactivity and the charge transfer that take place upon adsorption of acetone on the nanohybrid titanium dioxide-carbon nanotube system, which can be then used in an inexpensive "breathalyzer" to test for and monitor diabetes. The NETLSC has also greatly accelerated progress on the development of high-performance alloys for extreme environment applications. The facility allows the simultaneous simulation of literally hundreds of alloy configurations to evaluate their performance at condition, greatly accelerating the pace of research. This work includes the study of various nickel/iron/chromium/aluminum alloys for hydrogen separation and for advanced refractory metal alloys. The NETLSC has enabled the calculation of gas chemical solubility in solvents—providing data that is not yet available in the open literature—using calculations that could not be done before the NETLSC was available. The NETLSC is providing resources to aid in design and scale-up of sorbentbased CO_2 capture technology to industrial-scale application. Many simulations can now be run simultaneously for model validation at laboratory scales. In addition, very large scale simulations can now be run for predicting performance of solid-sorbent CO_2 capture systems based on these validated models.

The user base for the system is constantly expanding, sup-porting a growing group of fossil energy researchers, both in-house and external to NETL. In addition, the size and number of simulations is constantly increasing to continue the advance of simulation-based research and development.



A picture of utilization during a typical month—showing an average of 94.7% utilization.



NETL Visualization Center.