DISCOVERY IN ACTION

In the 1970s, Pacific Northwest National Laboratory's researchers worked in state-of-the-art computer facilities that included a digital computer system for data acquisition and process control system development. Today, PNNL is home to Constance, a fast, reliable supercomputer that is helping scientists do complex, advanced research in areas such as climate science and smart grid development.

COMPUTATIONAL SCIENCE

powers scientific discovery and innovation

This is the eighth of a 12-part series that features some of the scientific challenges PNNL has tackled over its 50-year history and highlights its vision for the future. PNNL is one of 10 national laboratories overseen by the U.S. Department of Energy's Office of Science and has been managed by Battelle since its inception in 1965. Through this enduring partnership—and by working closely with sponsors and collaborators—PNNL builds upon its legacy to advance science and solutions that improve the lives of Tri-Citians and people around the world. This edition focuses on how PNNL uses supercomputers, computational science and mathematics to build new scientific understanding that could help address significant national challenges in energy, the environment, national security and fundamental science.

PACIFIC NORTHWEST NATIONAL LABORATORY

Computers have come a long way in a few decades and, as a result, so has scientific understanding. The room-sized computers of the 1970s had only a fraction of the computing power of today's personal computers. Now, scientists are developing exascale computers that could perform about as many operations per second as 50 million laptops. Although the size and the power of the hardware has changed dramatically, the field of computing has always informed our approach to the biggest, most vexing challenges facing humankind.

"Whether we are trying to detect national security threats, manage the electricity grid or understand climate change, we are inundated with huge amounts of data—and we need to make that data actionable," said Doug Ray, associate laboratory director of fundamental and computational sciences at the Department of Energy's Pacific Northwest National Laboratory. "DOE has been a driving force in scientific computing since the Manhattan Project and operates some of the world's most powerful supercomputers."

For 50 years, PNNL has anticipated the need and helped define the field of working with big data. Its computing contributions have improved the safety of our skies; informed our view of the climate, including drought conditions right here in the Mid-Columbia; and made possible new chemistry for new types of fuels.

Powerful stuff

PNNL plays a leading role in making outstanding computing resources available to researchers around the world through EMSL, the Environmental Molecular Sciences Laboratory, a DOE national user facility. In November 2014, EMSL's Cascade was ranked the world's eighteenth most powerful supercomputer, but the vistas it opens to researchers are more important than its size. Cascade allows researchers to answer their biggest questions about molecular science and its applications to biologic and environmental science.

Super software

In 1986, PNNL was recognized by *R&D Magazine* for developing one of the year's top 100 innovations, the Computer Aided Genetic Engineering/Genetic Engineering Machine, or CAGE/GEM. This software toolkit can help researchers design genetic structures before performing expensive laboratory experiments. Licensed to a commercial partner, CAGE/GEM can isolate a genetic element in a DNA sequence and then graphically manipulate it to create new genetic constructs.

EMSL collaborators from PNNL and other institutions developed high-performance computational chemistry software that is used by thousands in the research community. NWChem, released as open-source software in 2010, allows researchers to tackle large, complex molecular-scale scientific problems in areas such as catalysis, materials, geochemistry, atmospheric chemistry and biochemistry.

In one project, a researcher from the University of Alabama is using EMSL's Cascade supercomputer and NWChem to study new catalyst materials for more controlled and efficient production of bioproducts. With help of the software and computing resources, he can better understand and predict certain reactions at the molecular level.

Model models

In 2006, PNNL was awarded a grant from SciDAC, or Scientific Discovery through Advanced Computing, to develop a computer model that can simulate biogeochemical processes on multiple scales. The sophisticated model combines various simulations representing different processes on a variety of scales ranging from microbial growth in pores to the migration of contaminants to rivers or wells. It could enable researchers to more accurately predict the movement and fate of groundwater contaminants to aid cleanup and protect human safety.

On the health front, PNNL supports a project led by the University of Wisconsin-Madison to build virtual models of the liver and the lung to better understand at the molecular level how humans respond to viral pathogens like Ebola, West Nile and influenza. The goal is to design and develop new drugs to thwart infection.

Picture this

In the 1990s, PNNL was helping define the field of visual analytics, which combines the way computers analyze data with the way people see and analyze information to enable new discoveries and insights from large amounts of information or complex data.

Over the years, PNNL has developed several software tools that help people analyze text, image, audio, video and numerical data to detect patterns, trends and relationships by presenting the information visually.

As a recognized leader, PNNL was chosen to lead the Department of Homeland Security's National Visualization and Analytics Center™, created to increase capabilities to discover and predict terrorist activities by collecting, combining and analyzing vast amounts of information.

Lightweight materials

As lighter materials with different melting points replace steel in vehicles, using welding to join parts of cars and trucks together becomes increasingly challenging. In a project led by Ford Motor Co., PNNL scientists are using computer modeling to help engineers understand how to weld different materials together. Xin Sun, who works on this project, is also using a DOE-developed model to understand the underlying mechanics of damage and fractures in transparent armor being developed for the U.S. military, used mainly for protective windshields and windows. Her work may lead to more resilient battlefield vehicles.

A tool for safer skies

A tool developed more than 10 years ago by PNNL researchers along with NASA and other collaborators can analyze large datasets collected by an aircraft's onboard instruments. It provides experts with information about flight patterns and operational conditions that they normally would not see. *The Morning Report* analyzes gigabytes of the day's flight information and presents data the next morning in graphic or tabular reports.

The Morning Report is a simple desktop application, but there are some serious mathematical and statistical algorithms working behind the scenes. The tool has been licensed to a flight recorder company, but it could also be used to monitor other complex systems, analyzing massive amounts of data and identifying typical patterns and atypical events.

Predicting future skies

PNNL set the standard for developing new ways to think about the future of our planet's climate. In one project, scientists are untangling complex factors that determine how long snowpack in mountains like Washington's Cascades lasts before melting into the water used to grow crops and water lawns. It takes some of the nation's top scientists and top computing resources to understand the complexities of a process that is central to our lives here in the Mid-Columbia.

Looking ahead

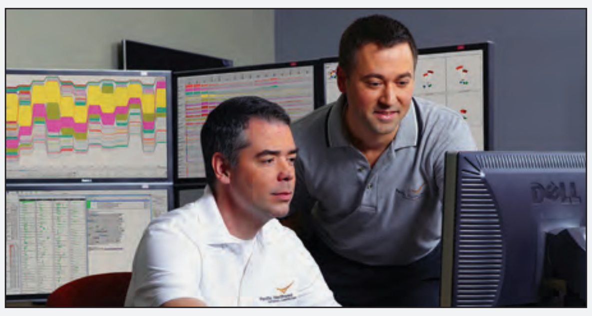
Researchers are striving to advance exascale computing, which may solve problems a thousand times bigger than what today's best computers can handle. Working at that scale requires supercomputers to perform different parts of calculations simultaneously, sometimes on different hardware, and then put the pieces back together.

In 2013, DOE awarded PNNL's Sriram Krishnamoorthy $2.5 million over five years through its Early Career Research Program to work on exascale computing challenges. Part of his effort will focus on understanding how parallel computing solves problems and making sure that different pieces of the full calculation are working as efficiently as possible.

"In support of DOE, PNNL will continue to develop hardware and software solutions that generate, analyze, store and share data for scientific research," Ray said. "Our expertise in high-performance computing, data science and computational mathematics is advancing scientific discovery and innovation."

Owned by the U.S. Department of Energy; operated by Battelle; and supported by academic, industrial and governmental collaborators, Pacific Northwest National Laboratory is celebrating 50 years of inspiring and enabling the world to live prosperously, safely and securely. Interdisciplinary teams at PNNL address many of America's most pressing issues in energy, the environment and national security through advances in basic and applied science. With an annual budget of about $1 billion and nearly 4,300 staff members, Battelle is the largest employer in the Tri-Cities.

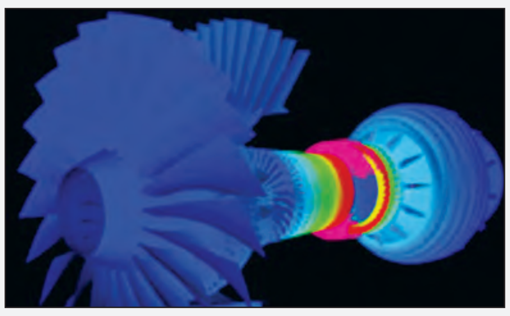
Learn more about PNNL at **www.pnnl.gov** and through stories to commemorate 50 years of scientific discovery contributed by employees, retirees and the community at **www.celebrate.pnnl.gov**.



IN-SPIRE™, a Windows-based software available for commercial license, provides tools for exploring text such as business documents, web data, accident reports, newswire feeds and message traffic. It conveys the gist of the documents through visual representations that cluster similar documents together and unveil common themes so analysts can explore relevant information.

The 3.4 petaflop Cascade supercomputer at EMSL, the Environmental Molecular Sciences Laboratory, is available to researchers around the world. The system's 23,000 Intel processors have 184,000 gigabytes of memory available—about four times as much memory per processor as other supercomputers.

PNNL's Katrina Waters conducts research that uses data from integrated gene and protein expression to reconstruct cell response networks. Her research may enable predictive modeling of disease and toxicity pathways.



In 2006, PNNL and Advanced Virtual Engine Test Cell Inc. set out to improve computer models that simulate turbine engine performance and could reduce manufacture time. This simulation of a full aircraft jet engine includes all major components. Color indicates pressure changes in the engine and temperature changes in the combustor.

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