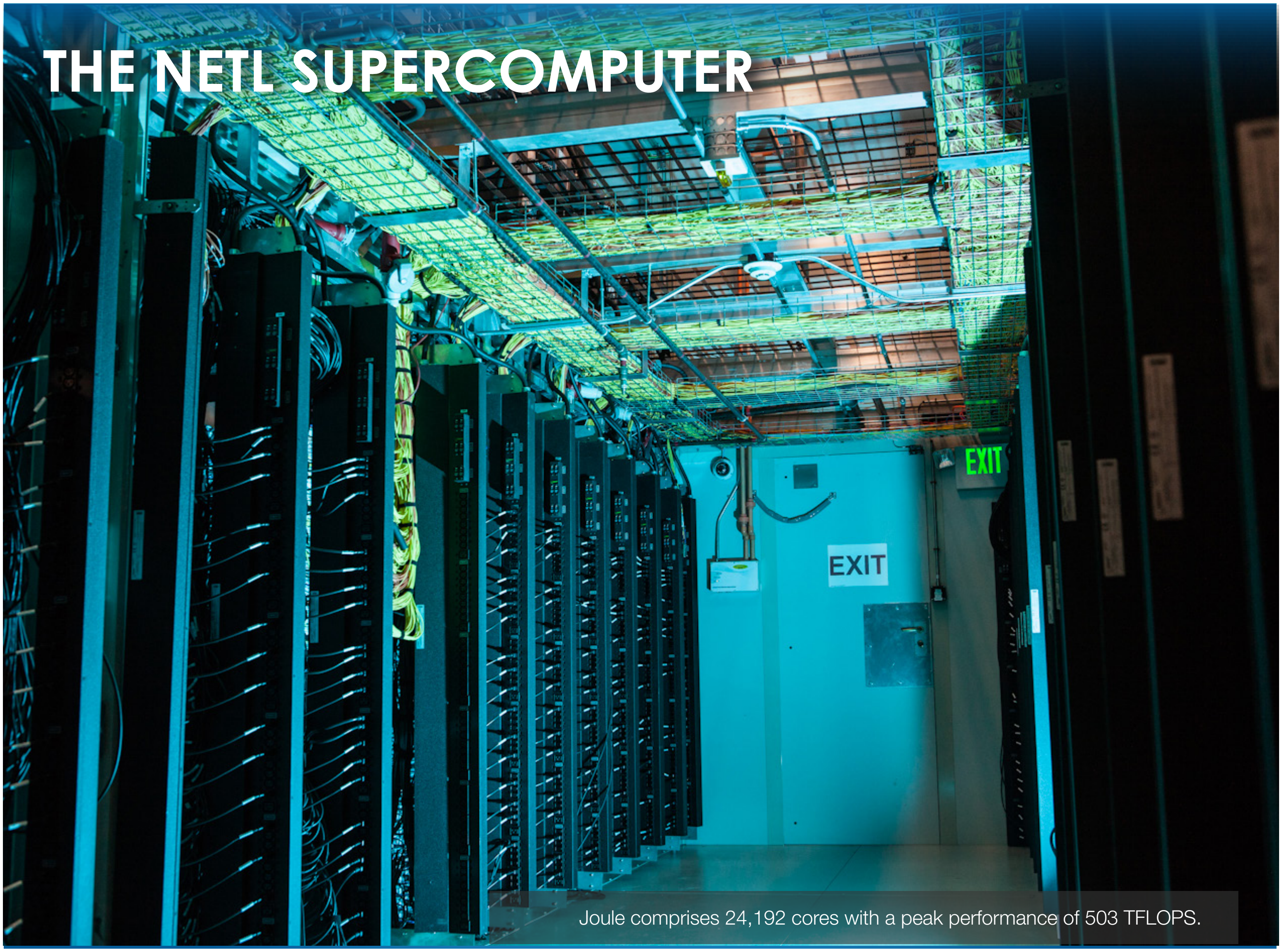
THE NETL SUPERCOMPUTER



Joule comprises 24,192 cores with a peak performance of 503 TFLOPS.

NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

INTRODUCTION

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

Supercomputing provides the foundation of NETL's research efforts on behalf of the Department of Energy, and NETL maintains supercomputing capabilities to effectively support its research to meet DOE's Fossil Energy goals. Supercomputing allows NETL researchers to simulate phenomena that are difficult or impossible to otherwise measure and observe. Faster supercomputers enable more accurate simulations, generating greater confidence in using simulation results for decision making. This simulation-based engineering approach helps NETL to reduce the cost and time of technology development at every stage: speeding up the discovery of new materials, increasing the reliability and performance of novel devices, and reducing the risk inherent in scaling up processes. Ultimately, supercomputing gives NETL and its industry partners an innovation advantage, enabling the development of globally competitive technologies and a sustainable, affordable energy portfolio for the nation.

R&D190, August 2018

COMPUTATIONAL CAPABILITIES

Joule is a 503 TFlops (trillion floating-point operations per second) supercomputer that enables the numerical simulation of complex physical phenomena. 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. Facilities associated with Joule allows enhanced visualization, data analysis, as well as data storage capabilities that enable researchers to discover new materials, optimize designs, and predict operational characteristics.

IMPACTS ON RESEARCH INTO A BROAD SPECTRUM OF FOSSIL ENERGY TECHNOLOGIES

Joule has enabled simulations on a scale that was previously not possible at NETL. A few examples are given in the following paragraphs.

- Joule is being used for developing and deploying the simulation tools of the Carbon Capture Simulation Initiative (CCSI), a multi-lab/university simulation research initiative for accelerating carbon capture technologies for power plants and industrial sources, such as cement plants, chemical plants, refineries, paper mills and manufacturing facilities. A CCSI model of a carbon capture device, for example, runs on Joule, to support a collaborative project with ADA-ES Inc., to accelerate their solid sorbent-based carbon capture process.

- Joule is being used to probe the viability of new high entropy metal alloys that hold great promise for high-temperature applications such as high-efficiency gas turbines. The computational capability of Joule allowed far more metal compositions to be investigated than was previously possible and significantly increased the understanding of these novel materials and the speed at which they can be brought to market.

- The NETL Gasification program is supported by researchers using Joule for simulating the Transport Integrated Gasification (TRIG) being developed by KBR, Southern and DOE. These simulations in particular help researchers to understand the performance of the gasifier when Mississippi lignite is used as the fuel. This capability allows researchers to conduct simulations that are difficult or impossible to probe experimentally (e.g., coal jet penetration into a high pressure gasifier).

- Joule has been used extensively to investigate new chemical structures that could provide enhanced carbon-capture capabilities. A class of ionic liquids show promise for these applications, but their high viscosity and low gas diffusivity limit their utility in bulk applications. Joule simulation results show that ionic liquids confined to porous substances such as silica slit pores or carbon nanotubes can exhibit much higher effective gas diffusivity and enhance carbon dioxide capture effectiveness by a factor of ten over the ionic liquid in bulk. This is the next step in the march toward economically viable carbon capture.

- Fuel cell models of critical cathode reactions have been accelerated from hours to seconds using Joule. 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.

- Joule 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 Joule was available.

- Joule is being used to conduct computational fluid dynamics simulations of reactors at Idaho Waste Treatment Unit in support of an NETL project with DOE's Environmental Management office.

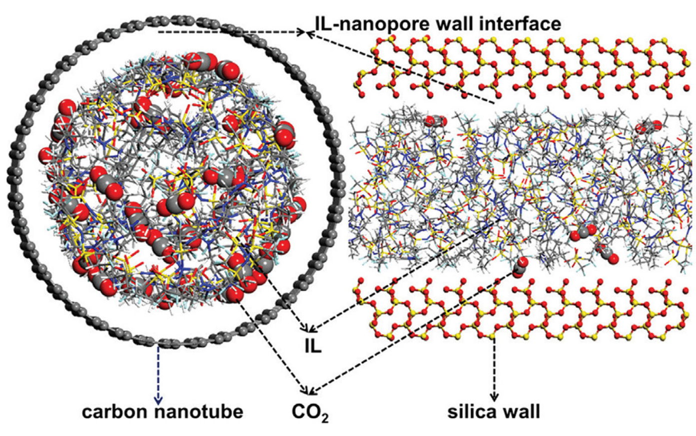


Figure 1. CO_2 absorption into ionic liquid confined inside carbon nanotubes (left) and silica slit pores (right) obtained from classical molecular dynamics and Monte Carlo simulations.

A CRITICAL RESOURCE FOR NETL RESEARCHERS & COLLABORATORS

The Joule facilities support effective collaboration among researchers at 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.

Joule is also a regional resource for research and education. In the region, students and professors from West Virginia University, University of Pittsburgh, Carnegie Mellon University and Oregon State University work seamlessly with NETL researchers in a virtual environment enhancing collaboration and making the sharing of results and insights instantaneous. For example, a research team at Oregon State University has used Joule to process and analyze geophysical data from the Newberry Enhanced Geothermal System site for the monitoring of the stimulation of that well. The use of Joule significantly enhanced the team's capability to analyze datasets in support of an NETL project with DOE's Geothermal Technologies office.

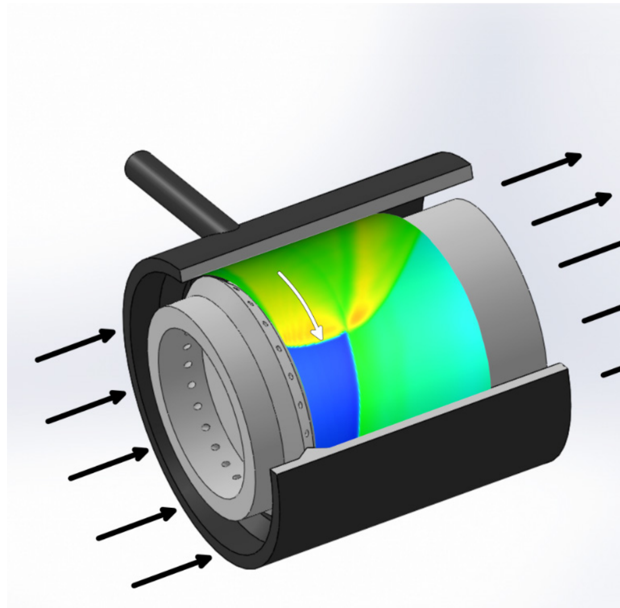


Figure 2. The Rotating Detonation Engine provides a method of transforming the combustion that occurs with prime movers such as gas turbine engines to one that uses detonation.

JOULE – FULLY UTILIZED, HIGHLY EFFICIENT

Joule is housed in an energy efficient Modular Data Center with a prefabricated power supply. Joule routinely runs an average of 91% core utilization. For a supercomputer, this level represents full utilization—100% is not achievable as there are always jobs of different sizes waiting for enough cores to launch and parasitic loads associated with writing files to memory where CPU time is not being used for computational purposes.

Joule is extremely efficient in power utilization with a Power Utilization Effectiveness (PUE) of 1.02–1.06 (PUE is the ratio of power consumed by the resource for computations and cooling divided by power consumed for just computational equipment). That means it only takes 2–6% of the power consumed to cool the equipment. Compared to conventional brick and mortar data centers that run PUEs of 1.4–2.0, Joule is one of the world's most power efficient machines. Joule provided 637% more computational power over the previously existing NETL computational clusters while consuming 11.5% less energy.

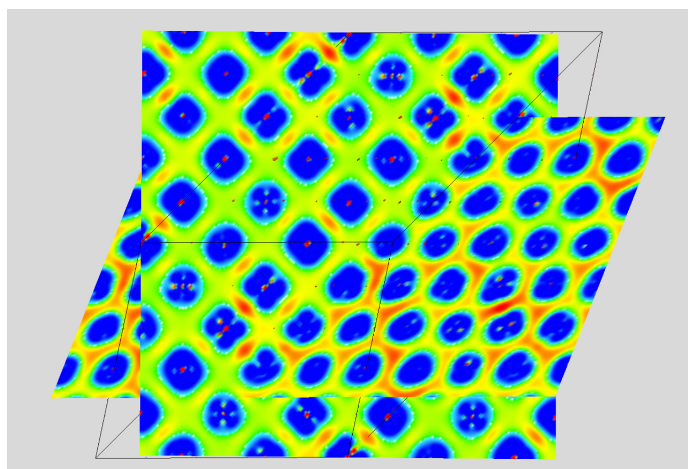


Figure 3. Electron difference charge density distributions in {1 1 1} and {1 0 0} planes in quinary CoCrFeMnNi high entropy alloy, a class of materials that can withstand severe environments.

EMERGING AREAS OF SUPERCOMPUTER USAGE

Joule is expected to be refreshed in 2017, providing a considerable increase in its computational power. The following are some examples of areas where additional computational power will accelerate the research:

- A new effort is underway at NETL to develop optimal reactor designs based on computational fluid dynamics simulations. This approach, if successful, will revolutionize how gasifiers and others chemical reactors are designed, enabling the design of low-cost, high-efficiency reactors that can be reliably replicated rather than (unreliably) scaled-up. The approach entails the use of a large number of multiphase computational fluid dynamics simulations, each simulation being computationally intensive.

- New hurricane models in the development of Fuels Cells to help scientists and industry optimize the configuration and thereby increase power output and lifespan while reducing material costs and waste from production.

- Configuration and process modeling for the reactors and separations in the hunt for more efficient means to separate rare earth elements from coal, mine tailings, and fly ash.

Another emerging area at NETL is the use of uncertainty quantification for all predictive simulations. This requires that hundreds of simulations of complex models to be completed in a timely manner, which necessitates the use of a supercomputer. As this capability matures at NETL, the need for even greater computing capability becomes critical.

Joule is necessary for a significant portion of NETL's research portfolio in support of FE goals. It has become ingrained in the way that NETL does its work. When developing new approaches, materials, or devices, researchers use this valuable tool to quickly cull options or variables that will not work and focus their efforts on more promising ones. In addition, Joule allows research to be conducted that experimentation alone cannot achieve. Without guidance from those simulations, experimental investigations will be far more time consuming and costly, or perhaps not feasible at all.

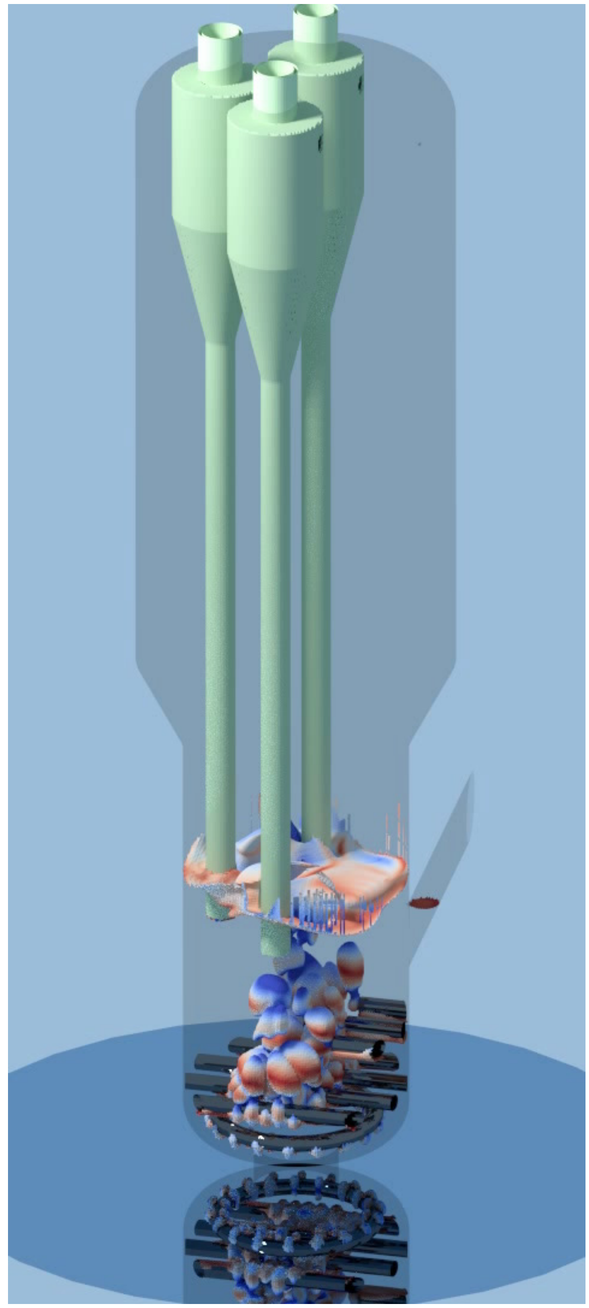


Figure 4. Bubbling pattern in a reactor at a nuclear waste treatment plant predicted by a simulation that is helping to optimize the reactor operation.

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