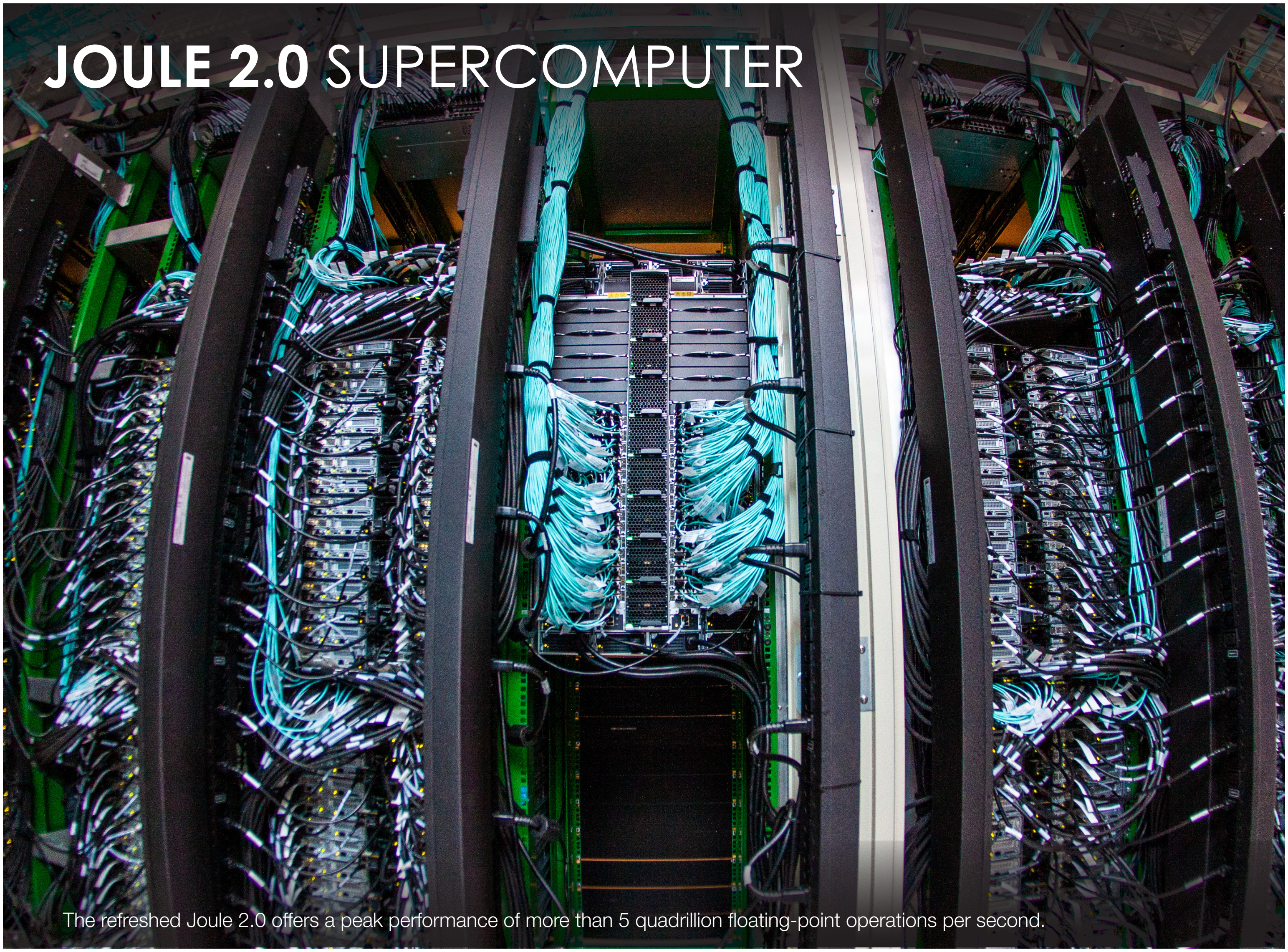
JOULE 2.0 SUPERCOMPUTER



The refreshed Joule 2.0 offers a peak performance of more than 5 quadrillion floating-point operations per second.

NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

INTRODUCTION

The National Energy Technology Laboratory (NETL) is home to Joule — among the world's fastest high-performance computers — along with advanced visualization centers serving the organization's research and development needs. The system underwent a $16.5 million refresh in fall 2018, providing an eight-fold increase in computational power. As of November 2018, Joule ranks 23rd in the nation and 52nd in the world among supercomputers.

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.

COMPUTATIONAL CAPABILITIES

Joule 2.0 is a 6.707 PFLOPS supercomputer that enables the numerical simulation of complex physical phenomena. The system includes:

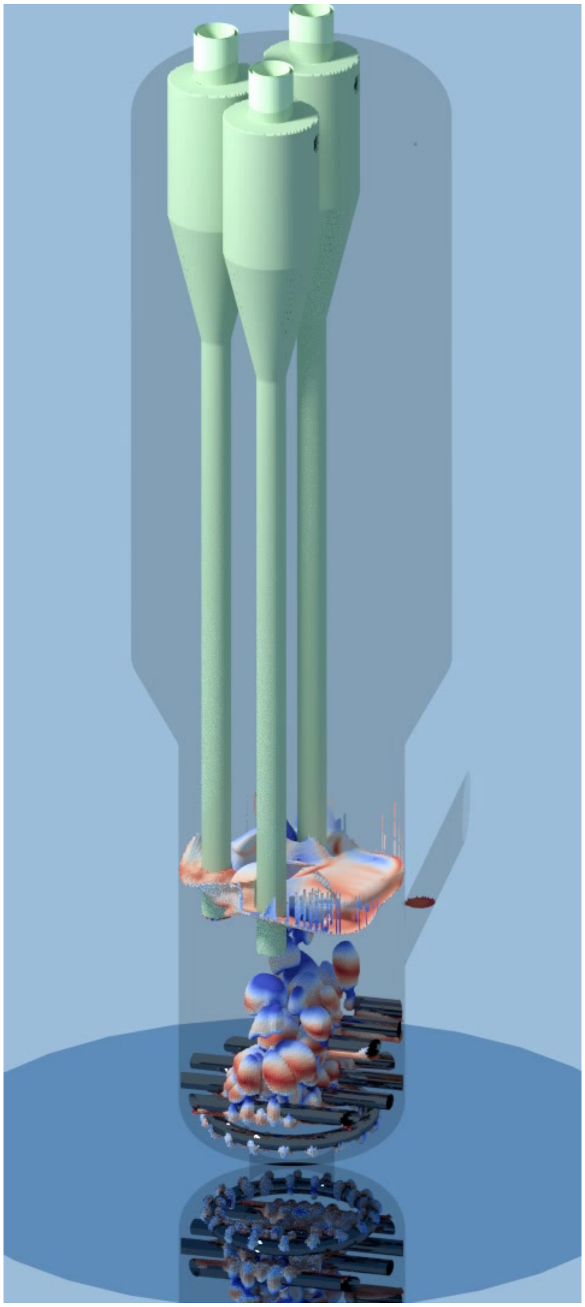
- 73,240 central processing unit (CPU) cores.
- 716,800 compute unified device architecture (CUDA) cores.
- 0.94 PFLOPS from graphics processing unit (GPU).

Joule 2.0 provides 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 allow 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 2.0 has enabled simulations on a scale that was previously not possible at NETL. For instance:

- Joule 2.0 is being used to develop optimal reactor designs based on computational fluid dynamics simulations. This approach 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.
- Joule 2.0 is expanding understanding of advanced combustion processes used in power generation cycles. Joule offers critical insight into innovative new approaches, such as pressure gain combustion and high-pressure oxy-combustion for supercritical CO2 power cycles, that helps researchers understand how to make these processes work more effectively to produce power.
- Joule 2.0 aids in the development of fuel cells via new models that help scientists and industry optimize the configuration and thereby increase power output and life span while reducing material costs and waste from production.
- Joule 2.0 enables configuration and process modeling for reactors and separations in the hunt for more efficient means to separate rare earth elements from coal, mine tailings and fly ash.
- Joule 2.0 expands possibilities for uncertainty quantification for all predictive simulations, which involves the timely completion of hundreds of simulations of complex models.
- Joule 2.0 is being used to develop and deploy 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 2.0 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 were 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 2.0 for simulating the Transport Integrated Gasification (TRIG) being developed by KBR, Southern and DOE. These simulations 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 2.0 has been used extensively to investigate new chemical structures that could provide enhanced carbon-capture capabilities. A class of ionic liquids shows 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 10 over the ionic liquid in bulk. This is an important 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 2.0. This allows for more complete mapping of cathode performance at various operating conditions and thereby yields a significant increase in the accuracy of model predictions for designing higher efficiency fuel cells.
- Joule 2.0 has enabled the calculation of gas chemical solubility in solvents – providing data that is not yet available in open literature – using calculations that could not be done before Joule was available.



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

A CRITICAL RESOURCE FOR NETL RESEARCHERS & COLLABORATORS

The Joule 2.0 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 2.0 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 used Joule 2.0 to process and analyze geophysical data from the Newberry Enhanced Geothermal System site while monitoring the stimulation of that well. The use of Joule significantly enhanced the team's capability to analyze data sets in support of an NETL project with DOE's Geothermal Technologies office.

JOULE – FULLY UTILIZED, HIGHLY EFFICIENT

Joule 2.0 is housed in an energy-efficient Modular Data Center. Joule routinely runs an average of 91-percent core utilization. For a supercomputer, this level represents full utilization — 100 percent 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 2.0 is extremely efficient in power utilization with a Power Utilization Effectiveness (PUE) of 1.01-1.06. 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 2-5 percent of the power consumed to cool the equipment, a feat achieved using 48 variable-speed fans to move ambient air augmented with evaporative media. Compared to conventional brick and mortar data centers that run PUEs of 1.4-2.0, Joule 2.0 is one of the world's most power efficient machines. The original Joule saved nearly $250,000 a year in electrical costs; the upgraded system is expected to save $400,000 a year.

Joule 2.0 impacts approximately 53 percent of all research publications produced by NETL and is necessary for a significant portion of NETL's research portfolio in support of FE goals. It is ingrained in the way that NETL does its work. When developing new approaches, materials or devices, researchers use this valuable tool to quickly evaluate options or variables and focus their efforts on more promising technologies. 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.

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