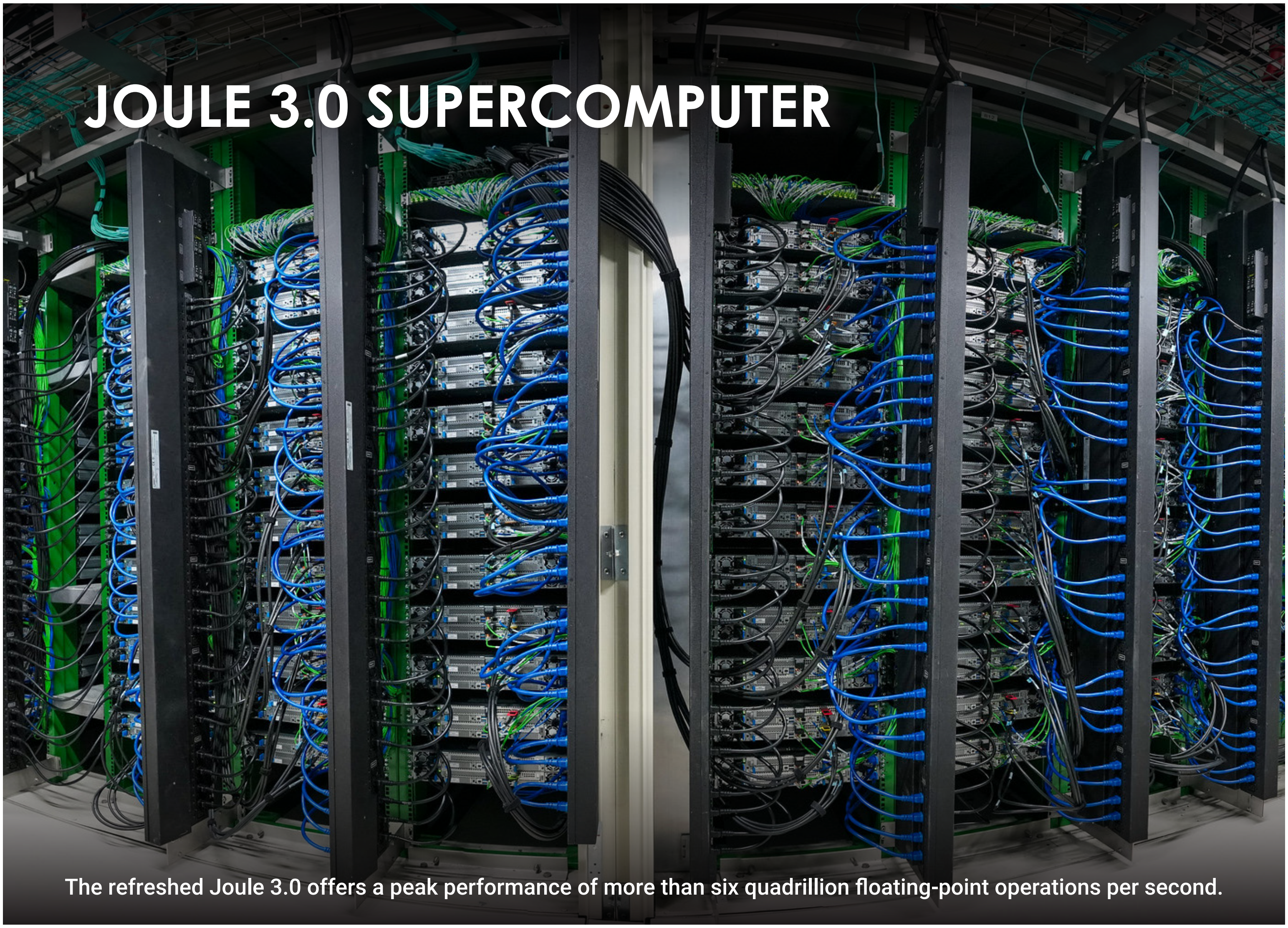
JOULE 3.0 SUPERCOMPUTER



The refreshed Joule 3.0 offers a peak performance of more than six quadrillion floating-point operations per second.

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NATIONAL ENERGY TECHNOLOGY LABORATORY

INTRODUCTION

NETL is home to Joule — among the world's fastest high-performance computers — and advanced visualization centers that serve the organization's research and development needs. The third generation of Joule supercomputer underwent a $21.66 million refresh in June 2024, resulting in a nearly a 40% increase in computing capacity. As of November 2024, Joule 3.0 is ranked 24th among DOE National Laboratory supercomputers, 65th in the United States, and 215th globally on the TOP500 list, as well as 101st worldwide on the HPCG ranking. The TOP500 ranking, based on the High-Performance LINPACK (HPL) benchmark, measures raw computational performance and peak processing speed. In contrast, the High-Performance Conjugate Gradient (HPCG) benchmark focuses on real-world application performance by assessing memory bandwidth, communication efficiency, and latency, providing a more practical evaluation of the system's effectiveness in solving complex problems.

Joule supercomputer 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 clean energy goals calling for net-zero carbon emissions in the electricity sector by 2035 and economy-wide net-zero emissions by 2050. 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 reduce the cost and time of technology development at every stage, speeding the discovery of new materials, increasing the reliability and performance of novel devices, and reducing the risk inherent in scale-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 as it responsibly transitions to greater reliance on renewable energy sources.

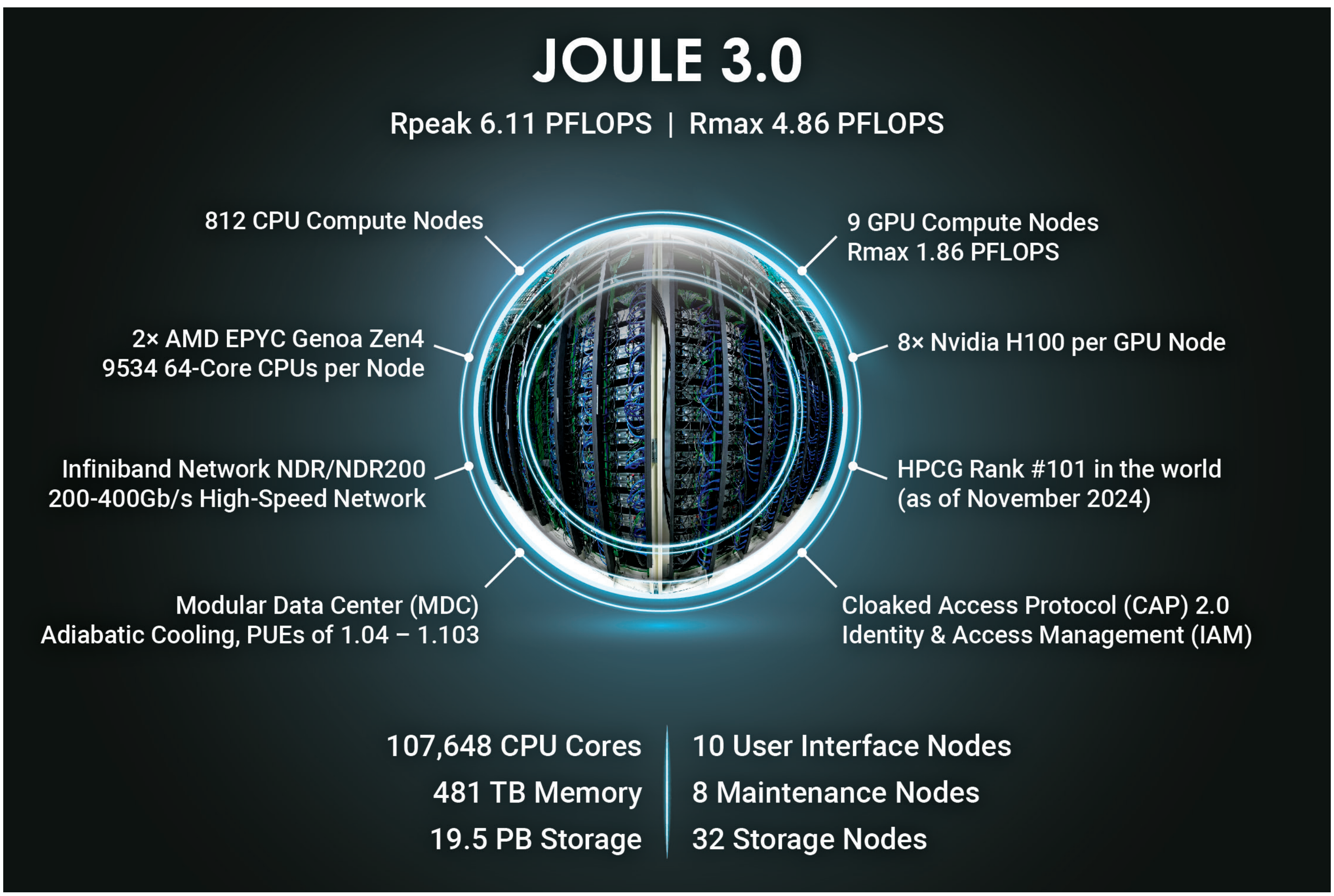
COMPUTATIONAL CAPABILITIES

Joule 3.0 is a 6.11 PFLOPS supercomputer that enables the numerical simulation of complex physical phenomena. The system includes 107,648 central processing unit (CPU) cores and 72 graphics processing units (GPUs).

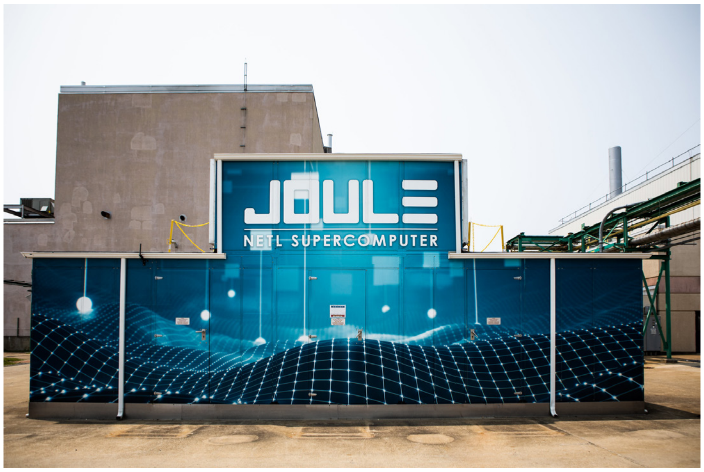
Joule 3.0 provides capabilities for running modeling tools at various scales ranging from molecules to devices to entire power plants and natural fuel reservoirs. Facilities associated with Joule allow enhanced visualization, data analysis and data storage capabilities that enable researchers to discover new materials, optimize designs and predict operational characteristics.

JOULE – FULLY UTILIZED, HIGHLY EFFICIENT AND RELIABLE

Joule 3.0 is housed in an energy-efficient Modular Data Center (MDC). Joule routinely runs an average utilization of >90% with peak utilization of 99.9%. Joule 3.0 is extremely efficient in power use with a Power Utilization Effectiveness (PUE) of 1 .0 4 – 1.103. 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 takes less than 10% of the power consumed to cool the equipment, a feat achieved using 48 variable-speed fans to move ambient air augmented with evaporative media.



Rpeak: theoretical peak performance | Rmax: maximum performance measured



IMPACTS ON RESEARCH INTO A BROAD SPECTRUM OF FOSSIL ENERGY AND CARBON MANAGEMENT TECHNOLOGIES

Joule is revolutionizing reactor design by leveraging advanced computational fluid dynamics (CFD) simulations to develop scalable, high-efficiency gasifiers and chemical reactors. This approach, which relies on intensive multiphase CFD simulations, demands significant computational resources to ensure that reactor performance can be consistently replicated. Additionally, Joule supports essential combustion research for power generation, including pressure-gain combustion and high-pressure oxy-combustion in supercritical carbon dioxide (CO_2) cycles, guiding researchers in optimizing these processes to enhance power production.

Joule enhances Quantum Computing capabilities by serving as a robust platform for advanced simulations. The Quantum for Energy Systems and Technologies (QUEST) team successfully deployed IBM Qiskit-based quantum computing simulators by Joule's computational power. Molecular reaction energies — including electronic and vibrational components — were assessed through quantum computing and the simulations were executed on Joule supercomputer and the IBM Quantum Platform, demonstrating the ability of quantum computing to overcome memory limitations faced by classical systems and showcasing Joule's critical role in enabling cutting-edge quantum research.

Joule also improves the efficiency of rare earth element extraction from coal and other materials. In materials science, Joule's simulations accelerate the screening of high-temperature alloys for energy applications, such as gas turbines, identifying top-performing materials among thousands of alloy compositions. With over 140,000 alloys screened, Joule has identified 400 promising candidates, expediting experimental validation.

Joule extends NETL's research into wave simulations, offering valuable data for extreme wave event prediction in the Gulf of Mexico by analyzing 200 GB of metocean data. The supercomputer also improves CO_2 storage studies by providing enhanced accuracy in evaluating subsurface geological formations.

Fuel cell research benefits from Joule's ability to simulate models that enhance power output and longevity while reducing costs. Joule's thermodynamic modeling capabilities have advanced solid oxide fuel cell and electrolysis cell applications, optimizing electrode behavior across various conditions for efficient clean energy production. By refining materials such as water sorption agents and catalysts, Joule plays a crucial role in developing NETL's energy technologies, underscoring the power of high-performance computing in advancing innovative solutions.

A CRITICAL RESOURCE FOR NETL RESEARCHERS AND COLLABORATORS

The Joule supercomputer facilities at NETL enhance collaboration through secure access and centralized control using Cloaked Access Protocol (CAP) 2.0. Additionally, Joule serves as a regional asset supporting research partnerships with institutions like West Virginia University, University of Pittsburgh, and Oregon State University. For example, a team from Oregon State used Joule to analyze geophysical data from the Newberry Enhanced Geothermal System, advancing an NETL project in collaboration with the DOE's Geothermal Technologies Office.

AI and machine learning initiatives at NETL, such as Science-based Artificial Intelligence/Machine Learning Institute (SAMI) and the Science-informed Machine Learning to Accelerate Real-Time Subsurface Decision Making (SMART) projects, use Joule to drive progress across sectors, including energy, defense and healthcare, with specific gains in oil and gas exploration and carbon storage.

Joule plays a crucial role in NETL's research efforts and is essential for many DOE-supported projects. Researchers rely on Joule for faster evaluations of materials and technologies, yielding insights and accelerating progress that would otherwise be costly or slow through traditional experiments alone. NETL uses Joule to speed the progress through the Technology Readiness Level (TRL) process. Faster results allow NETL to eliminate years from the TRL process enabling researchers and their industrial partners to get new technologies to improve efficiency and reduce the effects of burning fossil fuels to market faster.

For a full accounting of Joule functionality and capabilities please see https://hpc.netl.doe.gov/ or contact the HPC-Support@netl.doe.gov.

www.NETL.DOE.gov

NETL is a U.S. Department of Energy national laboratory that drives innovation and delivers solutions for a clean and secure energy future by advancing carbon management and resource sustainability technologies. Through its expertise and research facilities, NETL is advancing innovations to enable environmental sustainability for all Americans. Using the power of workforce inclusivity and diversity, innovators at NETL's research laboratories in Albany, Oregon; Morgantown, West Virginia; and Pittsburgh, Pennsylvania, conduct a broad range of research activities that support DOE's mission to ensure America's security and prosperity by addressing its energy and environmental challenges through science and technology solutions.

Contacts

Mi Kyung Kang
Computer Engineer | HPC Lead
Computational Sciences & Engineering
MiKyung.Kang@netl.doe.gov

Chris Guenther
ACAI Team Supervisor
Computational Sciences & Engineering
Chris.Guenther@netl.doe.gov

Tammie Borders
Associate Director
Computational Sciences & Engineering
Tammie.Borders@netl.doe.gov