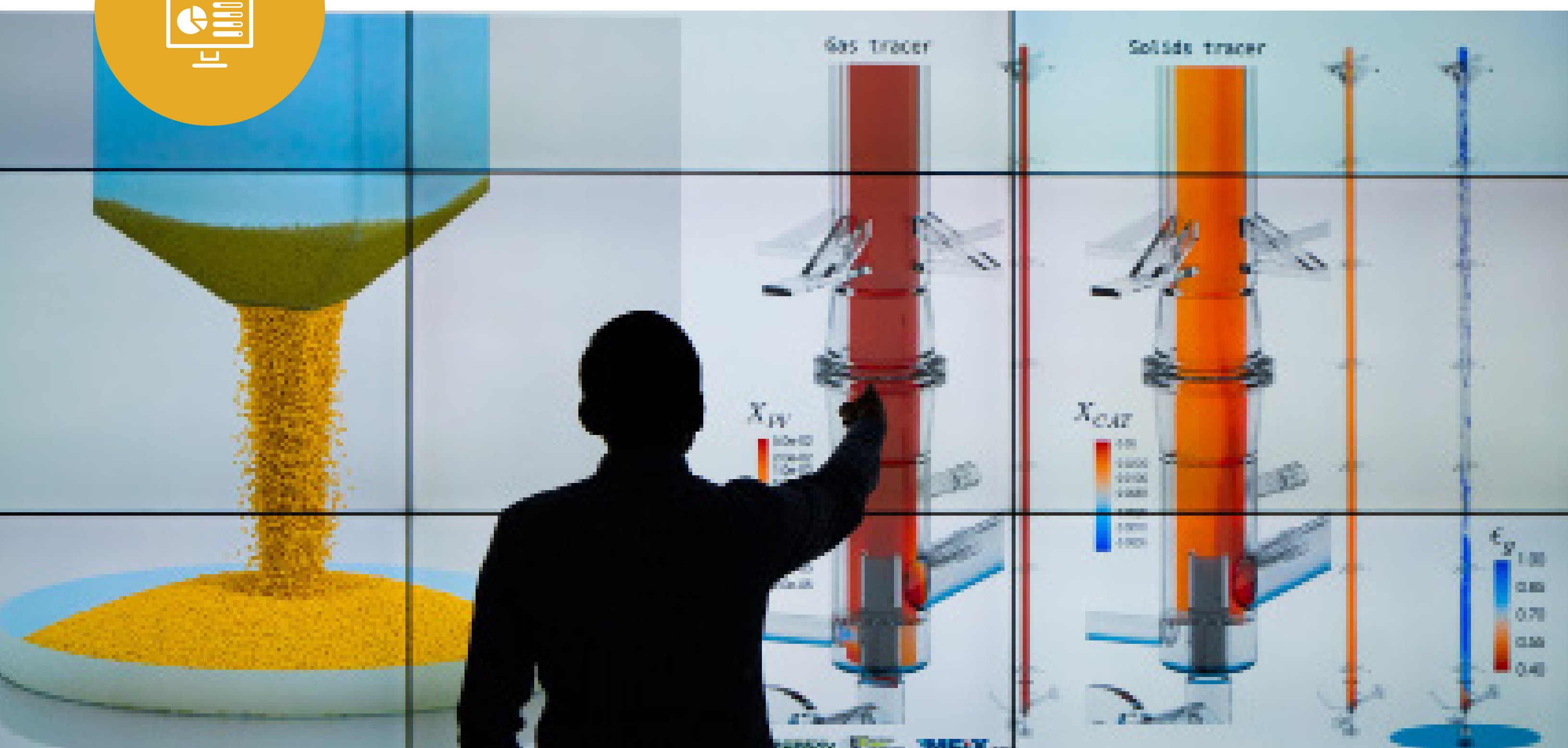
NETL Core Competencies

Computational Science & Engineering

Science-based Simulations to Accelerate Innovation

Traditional experimentation methods have historically been at the heart of effective and productive research and innovation. However, the advent of computational simulation and multiscale modeling — with data analytics — now facilitates faster technology development at lower costs that cannot be achieved by traditional experimentation methods alone. At NETL, world-class facilities matched with an experienced team of experts support research across the Laboratory that analyzes and predicts performance on a diverse set of energy research projects. The unique computational capabilities combine theory, computational modeling, advanced optimization, experiments, and industrial input to address complexities and advance energy processes. NETL utilizes these capabilities to achieve novel fossil energy innovation (Including fuel cell development, gasification and combustion reactors, functional materials for carbon capture, and the extraction of rare earth elements from coal and coal by-products) in an efficient way while saving time, money, and materials.



1

JOULE 2.0 Supercomputer

Enabling Complex Models & Simulations of Complex Energy Systems

The NETL supercomputer is a 3.275 PFLOP supercomputer that can perform more than three quadrillion calculations per second and ranks as the 21st fastest in the U.S. and 55th fastest in the world. The recent upgrade represents a nearly 10-fold increase in speed over the original Joule supercomputer. Joule 2.0 enables the numerical simulation of complex physical phenomena. Joule 2.0 provides computational throughput to run high-fidelity modeling tools at various scales ranging from molecules to devices to entire power plants and natural fuel reservoirs. Facilities associated with Joule allow for enhanced visualization and data analysis, as well as data storage capabilities that enable researchers to discover new materials, optimize designs, and predict operational characteristics with minimized financial and safety risks.

2

Center for Artifical Intelligence & Machine Learning (CAML)

Developing Next-Generation Energy Technologies Using Simulations

The Center is specifically designed to house, move, and process multiple petabytes of data using a variety of cutting-edge algorithms developed inhouse and with corporate and university research partners. Scale and performance of CDAML will accelerate ability to process data more efficiently than any other NETL resource. Integrated 1.1 PFLOPS graphics processing units (GPU) performance and 50 TFLOPS central processing units (CPU) performance enhances machine learning and data analytic capabilities. The Data Analytic Center of Excellence is specifically designed to house, move, and process multiple petabytes of data using a variety of cutting-edge algorithms developed inhouse and with corporate and university research partners.

3

Multiphase Computational Fluid Dinamics Modeling

Assisting the Scale-Up of Existing Technologies

Modeling and simulation allows for the rapid scale-up of technologies, reducing or even avoiding costly intermediate- scale testing. New designs can be tested with the help of simulations to ensure reliable operation under a variety of operating conditions. NETL has improved the multi-phase computational fluid dynamics (CFD) models that underpin the simulation of several advanced energy technologies, adapting methods developed for fossil systems to other applications

4

Institute for the Design of Advanced Energy Systems (IDAES)

Simulation Based Computational Tools to Optimze Energy Systems

Advancing new effective energy technologies and processes can be lengthy and costly because experimental scientists are often unable to observe and measure aspects of design research. IDAES develops accelerates development of a broad range of advanced fossil energy systems and consists of experts from NETL, Sandia and Lawrence Berkeley National Laboratories, Carnegie Mellon University and West Virginia University. Pooling skills and resources, the Institute is pioneering development of new computational tools that can be used to optimize the performance of power plants at multiple scales over a full range of operating conditions — both supporting the existing fleet and enabling the design and scale up of transformative advanced coal energy systems. IDAES develops a rigorous computational approach for creating new concepts in power systems, biofuels, green chemistry and environmental management.

5

Energy Data Exchange (EDX)

NETLS Data Driven Tool for Science-Based Decision Making

EDX is the Department of Energy Office of Fossil Energy's virtual platform for public curation of data and tools. Maintained and developed by NETL researchers and technical computing teams, EDX supports private collaboration for ongoing research and tech transfer of finalized DOE NETL research products. EDX supports research by coordinating historical and current data and information from a wide range of sources to facilitate access to research that crosscuts multiple NETL projects; provides external access to technical products and data published by NETL-affiliated research teams; and collaborates with a variety of organizations and institutions in a secure environment through collaborative workspaces. Primary users of EDX are NETL and its affiliated research teams and non-NETL fossil energy researchers who are actively engaged in work relevant to a broad spectrum of energy and environmental research and development programs.

6

National Risk Assessment Partnership (NRAP)

Computational Tools to Inform About Long-Term Risks at Specific Geological Storage Sites

The effectiveness of carbon storage depends on the ability of a specific site to store CO_2 permanently. Carbon storage risk analysis is complicated by variables such as geology, existing wellbores, and subsurface faults or fractures. In addition, the characteristics and associated risks of sites change over time. NRAP was formed to develop and deploy advanced computational tools to accelerate commercialization of carbon storage technologies. The computational tools calculate risk profiles to quantify the likelihood of long-term risks and liabilities and help design efficient monitoring programs for risk-based standards.

7

Muiltiphase Flow with Interface Exchanges (MFIX)

Open-Source Software Simulates Multiphase Flow Processes

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8

Main Computational Materials Engineering & Melecular Science

Understanding and Predicting Performance at Atomic & Melecular Levels

NETL's Computational Materials Engineering Team uses state-of-the-art capabilities to model materials behavior and provide insights that enable their use in new fossil energy technologies. NETL's Joule supercomputer, and multi-scaled modeling capabilities are used to characterize materials' properties. For example, computational modeling was used to understand how high-entropy alloys are formed and how their properties conform to the high-temperatures of next generation fossil energy applications. NETL also demonstrated a computational methodology to identify mixed-matrix membranes for gas separations for post-combustion carbon capture — knowledge that could help decrease the cost of carbon capture from $63 to $48 per tonne of CO_2 removed.

U.S. Department of ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Computational Science & Engineering

- **JOULE 2.0 Supercomputer – Morgantown**
- **Center for Data Analytics & Machine Learning (CDAML) – Pittsburgh**
- **Multiphase Computational Fluid Dynamics Modeling – Morgantown**
- **Multiphase Flow with Interphase Exchanges (MFIX) – Morgantown**
- **Computational Materials Engineering & Molecular Science – Albany**
- **Energy Data Exchange (EDX) – Albany, Morgantown, Pittsburgh**
- **Institute for the Design of Advanced Energy Systems (IDAES) – Albany, Morgantown, Pittsburgh**
- **National Risk Assessment Partnership (NRAP) – Albany, Morgantown, Pittsburgh**

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