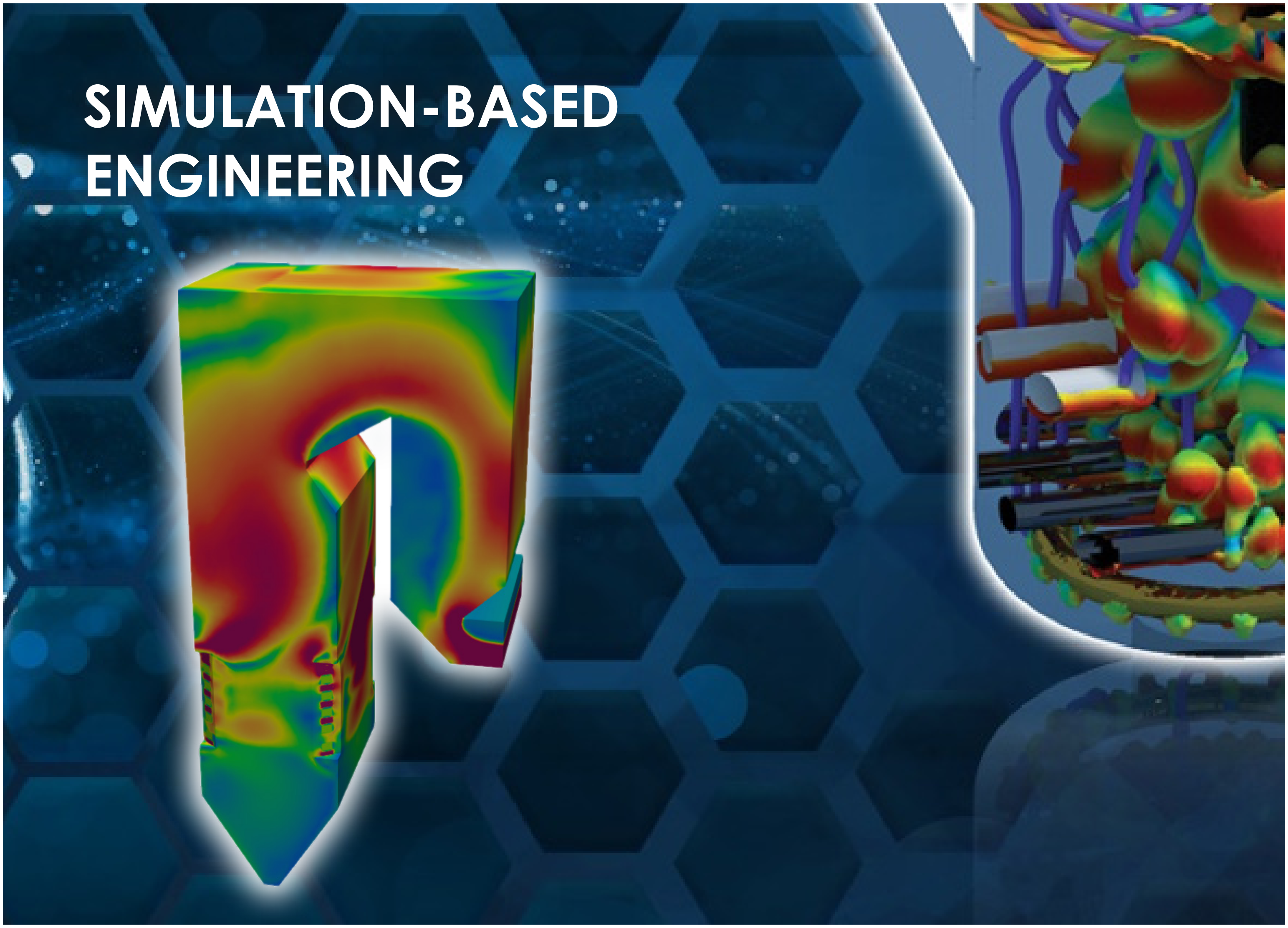
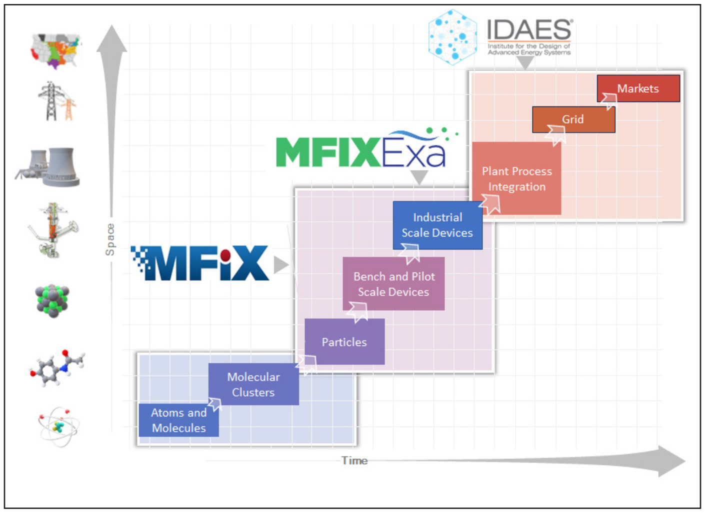
SIMULATION-BASED ENGINEERING



Program 134, July 2024

NATIONAL ENERGY TECHNOLOGY LABORATORY

The Simulation-Based Engineering (SBE) program, within the Hydrogen with Carbon Management portfolio, supports the development and application of new, innovative, physics- and chemistry-based models and computational tools at multiple scales (i.e., atomistic, device, process, grid and market) to accelerate development and deployment of clean advanced energy technologies. Research in this area provides the basis for the simulation of engineered devices and systems to better predict and optimize the performance of energy generation units. Computational design methods and concepts are vital to significantly improve performance, reduce the costs and emissions of energy power systems and enable the development, analysis and optimization of new systems and capabilities. Current technologies of focus include integrated energy systems, gasification of sustainably sourced carbon-based feedstocks and hydrogen production to support the DOE's Hydrogen Shot goals. SBE also supports technologies for carbon capture (both point source capture and carbon dioxide removal), utilization and reliable storage and transport to support both industrial and domestic carbon management goals.



NETL's SBE program combines technical knowledge, software development, computational power, data repositories, experimental facilities and unique partnerships to support research into timely and accurate solutions for complex advanced energy systems. Analysis and visualization tools are manipulated to gain scientific insights into complex, uncertain, high-dimensional and high-volume datasets. The information generated is then collected, processed and used to inform research that combines theory, computational modeling, advanced optimization, experiments and industrial input with a focus on the following three main research areas:

- **Multiphase Flow Science**
- **Advanced Process Simulation**
- **Computational Materials Design**

MULTIPHASE FLOW SCIENCE — NETL has developed the Multiphase Flow with Interphase eXchanges (MFiX) software suite, which is the world's leading open-source design software for comparing, implementing and evaluating multiphase flow constitutive models. These tools provide an accurate, validated and cost-effective capability to design, optimize, scale up and troubleshoot a diverse range of multiphase flow applications. MFiX has been utilized to examine complex energy applications including gasification of biomass and municipal solid waste (MSW) for hydrogen production (negative carbon emission), carbon capture using solid sorbents or liquid solvents, chemical-looping combustion of gaseous and solid fuels, as well as bioenergy production from biomass. The MFiX Software Suite has over 8,900 registered users and is the national leading platform for computational fluid dynamics code.

MFiX

NETL Multiphase Flow Science flagship computational fluid dynamics (CFD) code.

Presents a versitile toolset for characterizing performance of energy conversion processes.

Accelerates reactor development and reduce cost by using multiphase flow modeling and simulation tools.

Optimizes performance equipment and unit operation enabling more throughput and less process downtime.

Reduces design risks and ROI risk through validation against experiments and predictive science-based calculations.

PORTFOLIO SUITE

- **MFIX-TFM (Two-Fluid Model)**
- **MFIX-DEM (Discrete Element Model)**
- **MFIX-PIC (Multiphase Particle-In-Cell)**
- **MFIX Exa (Exascale)**
- **C3M multiphase chemistry management software**

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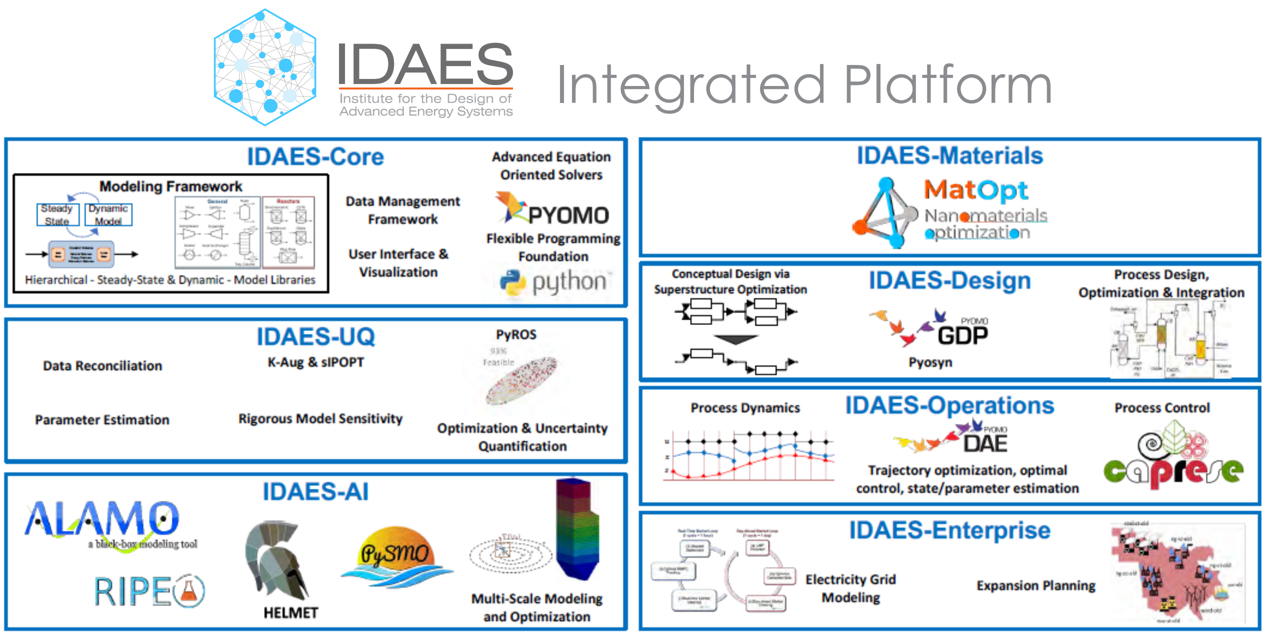
ADVANCED PROCESS SIMULATION — NETL's Institute for the Design of Advanced Energy Systems (IDAES) optimizes the design and operation of complex interacting technologies and systems by providing rigorous modeling capabilities to increase efficiency, lower costs, increase revenue and improve sustainability of power generation and electricity distribution. IDAES represents a paradigm shift as the only fully equation-oriented platform with integrated support for steady-state design, optimization, dynamic operations, data reconciliation, parameter estimation and uncertainty quantification of complex energy and chemical processes. IDAES uniquely supports the process modeling lifecycle, from conceptual design to dynamic optimization and control. IDAES enables users to efficiently search vast complex design spaces that cannot be adequately explored with existing tools to discover the lowest cost and most environmentally sustainable solutions. The extensible open platform empowers users to create models of novel processes and rapidly develop custom analyses, workflows and end-user applications.



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COMPUTATIONAL MATERIALS DESIGN — Computational materials design utilizes modeling tools to enable rapid design and simulation of new and novel materials suitable for extreme service conditions. Computational methods are also used to provide validated models that are capable of simulating and predicting long-term performance and failure mechanisms of the newly developed materials with specific emphasis on durability, availability and cost. Research supports the U.S. DOE Office of Fossil Energy and Carbon Management by addressing material integrity challenges associated with enabling affordable and durable alloys need to meet our Nation's energy and decarbonization goals.

eXtremeMAT — Harnesses unparalleled capabilities for materials design, high-performance computing, manufacturing and characterization that exists across the U.S. DOE complex to accelerate the development of materials for service in extreme environments. Specifically, this mission-focused team aims to improve both heat-resistant alloys and models for predicting long-term material performance. https://edx.netl.doe.gov/extrememat/

SOLUTIONS TO PROBLEMS BEYOND EXPERIMENTAL BOUNDARIES:

- The MFIX Suite provides accurate, customizable high-fidelity models deployable at high performance and Exa computing scales.
- MFIX simulations reduce development time of advanced technologies critical for the DOE to meet its low-cost high-efficiency goals.
- IDAES has been adopted as the core modeling and optimization platform for several multi-institutional initiatives including the Grid Modernization Laboratory Consortium's DISPATCHES, the National Alliance for Water Innovation's WaterTAP and the Office of Fossil Energy and Carbon Management's PrOMMiS with applications ranging from hybrid energy systems and water desalination to rare earth element/critical mineral processing.
- The ***eXtremeMAT*** computational framework incorporates complex stress states representative of real service conditions and microstructural evolution (coarsening) during service of real alloys in predictive models and has been used to successfully predict the creep performance of stainless steels.
- ***eXtremeMAT-H2*** incorporates the impact of hydrogen containing environments on alloy performance at high temperatures, under complex loads, and long service times.
- Models developed with comprehensive uncertainty quantification will reduce the risk of modification and optimization.
- NETL's Joule supercomputer is one of the world's fastest and most energy-efficient, intended to help energy researchers discover new materials, optimize designs, and better predict operational characteristics.

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.

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