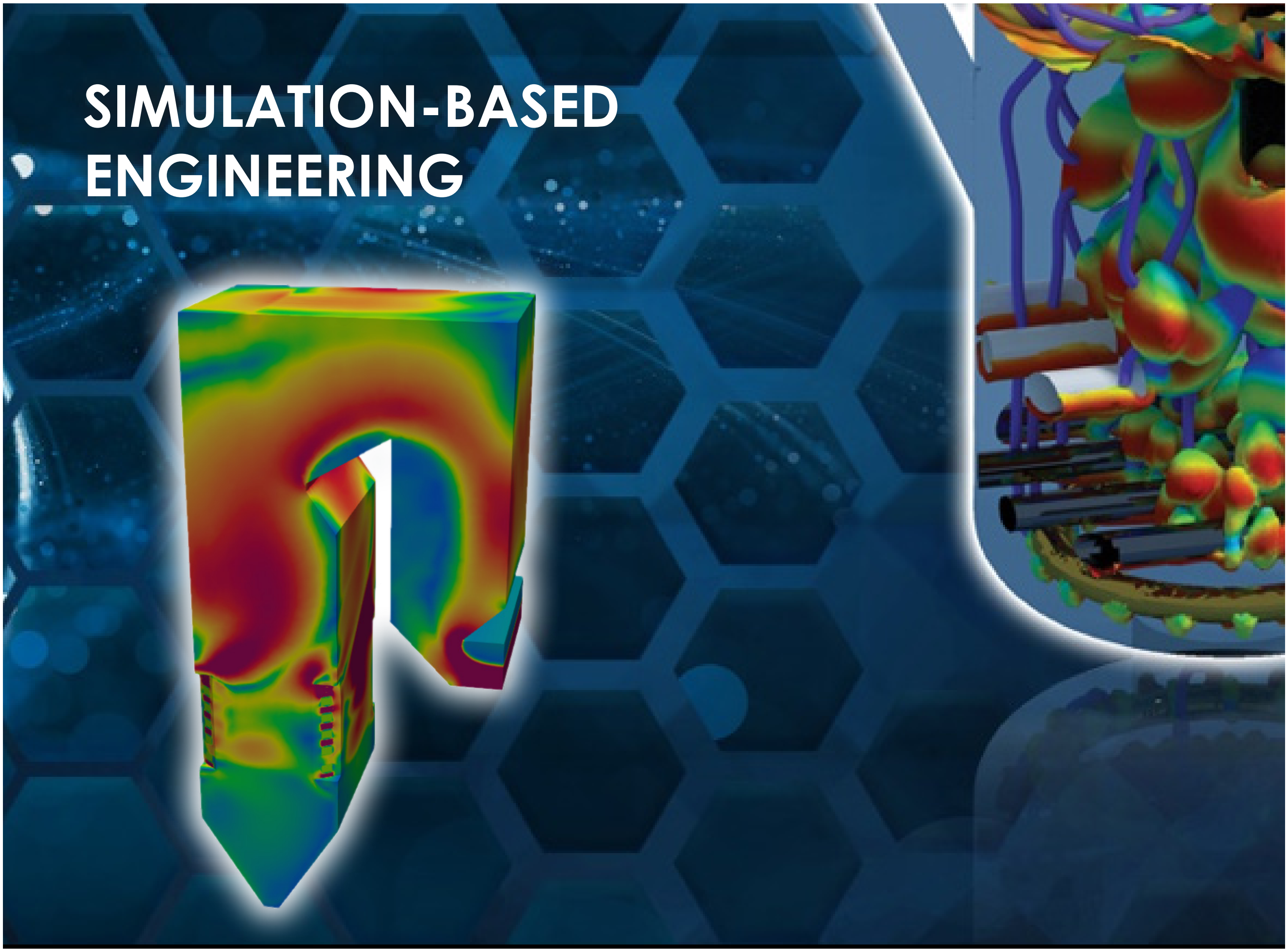
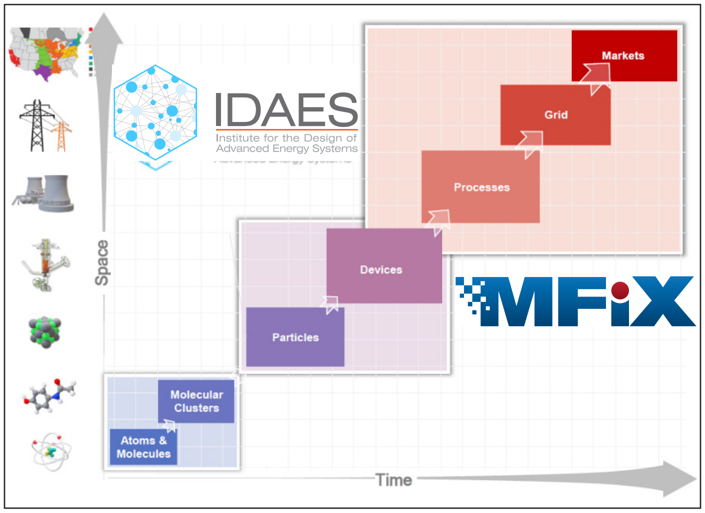
SIMULATION-BASED ENGINEERING



NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

The Simulation-Based Engineering (SBE) program, within the Crosscutting Research 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) in order to accelerate development and deployment of clean, advanced fossil fuel technologies. Research in this area provides the basis for the simulation of engineered devices and systems to better predict and optimize the performance of fossil energy electricity generation units. Computational design methods and concepts are vital to significantly improve performance, reduce the costs and emissions of fossil energy power systems, and enable the development, analysis, and optimization of new systems and capabilities. Current technologies of focus include integrated energy systems, advanced ultra-supercritical operation, biomass gasification, hydrogen storage and combustion, as well as carbon capture, utilization, and sequestration.



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 fossil 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 Modeling and Optimization**
- **Computational Design of Materials and Components**

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 an extremely diverse range of multiphase flow applications. MFiX has been utilized for complex fossil energy applications including gasification with biomass for hydrogen production (negative carbon emission), carbon capture using solid sorbents or liquid solvents, and chemical-looping combustion of gaseous and solid fuels. MFiX Software Suite has over 6,700 registered users and is the national leading platform for computational fluid dynamics code.

NETL MFS' flagship computational fluid dynamics (CFD) code.

Versatile toolset for understanding the behavior and characterizing the performance of energy conversion processes.

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

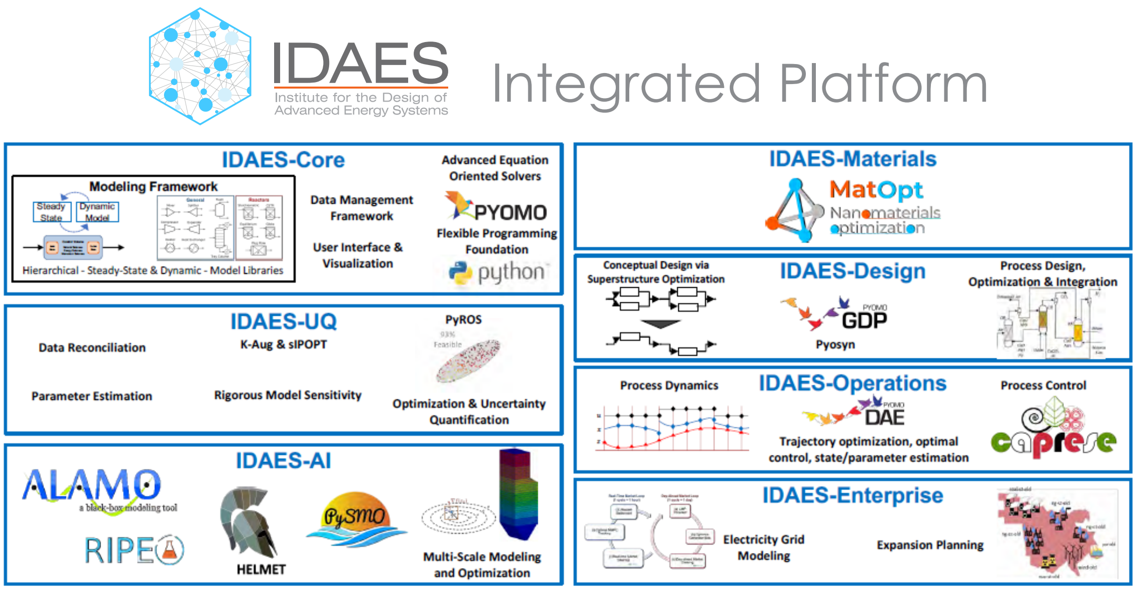
Optimizes performance for equipment and unit operations, enabling more throughput and less process downtime.

Reduces design risks when validated by predictive science-based calculations, lowering risk in obtaining return on investment.

PORTFOLIO SUITE

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

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, 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.



COMPUTATIONAL DESIGN OF MATERIALS AND COMPONENTS — Computational materials design utilizes modeling tools to enable rapid design and simulation of new and novel alloys suitable for high-temperature, high-pressure, corrosive environments of an advanced energy system. Computational methods are also used to provide validated models capable of simulating and predicting long-term performance and failure mechanisms of the newly developed materials with specific emphasis on durability, availability, and cost. Similarly, component-scale modeling develops insight into fossil plant challenges and mitigation solutions using novel modeling tools. The program utilizes physically informed models of industrial components under cyclic loading, long-duration stress, and high-temperature exposure to generate practical and cost-effective solutions to reduce plant failures and extend plant life.

SOLUTIONS TO PROBLEMS BEYOND EXPERIMENTAL BOUNDARIES:

- NETL researchers work closely with stakeholders and partners to outline issues, emerging trends, and areas of need.
- MFiX provides accurate, high-fidelity models with advanced computing to reduce the time of development of advanced technologies critical for the DOE to meet its low-cost, high-efficiency goals.
- IDAES is the core platform for the Grid Modernization Laboratory Consortium's (GMLC) DISPATCHES project to develop and demonstrate an open, transparent, multi-lab computational platform to support the design, optimization, and analysis of tightly coupled hybrid systems with zero or negative CO2 emissions. It is also the computational platform for the National Alliance for Water Innovation (NAWI) process modeling library, ProteusLib.
- 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.

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