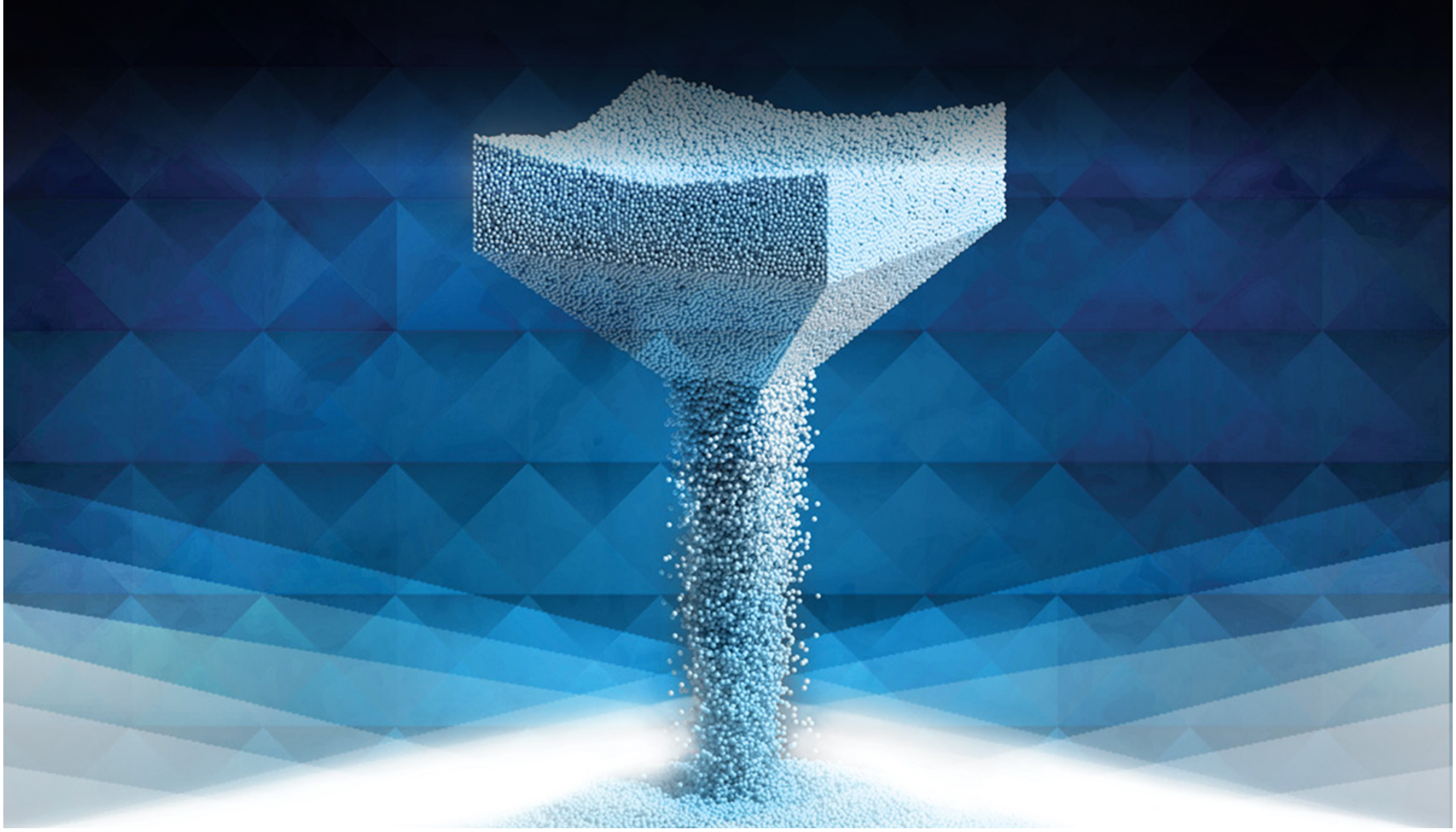
COMPUTATIONAL DEVICE ENGINEERING TEAM



NATIONAL ENERGY TECHNOLOGY LABORATORY

BACKGROUND

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory's (NETL) Computational Science & Engineering (CSE) Directorate is recognized for its ability to develop science-based simulation models, mathematical methods and algorithms, and software tools to address the technical barriers in the development of next-generation technologies. This competency works in collaboration with other capabilities at NETL to generate information and scientific understanding beyond the reach of experiments alone through the integration of experimental information with computational sciences across different time and length scales. The CSE Directorate is organized into three teams that collectively maintain NETL's computational science and engineering competency: 1) Computational Materials Engineering, 2) Computational Device Engineering, and 3) Data Analytics.

COMPUTATIONAL DEVICE ENGINEERING TEAM

The Computational Device Engineering (CDE) Team at NETL provides national laboratory expertise in multiphase flow science through computational and experimental research and development (R&D) coupled with high-performance computing to support DOE's Office of Fossil Energy and Carbon Management R&D programs. For more than 30 years, NETL's work in multiphase flow science has served as one of the cornerstones of the Laboratory's research portfolio. Multiphase flow refers to the simultaneous flow of gases, liquids, and solid materials. For example, in mixed feed stock combustion and gasification processes encountered in fluidized bed boilers and entrained flow gasifiers, energy dense particles react with and devolve into gases under a wide range of flow conditions and chemistries. Multiphase flow occurs in many other energy system processes including bioenergy production from biomass, waste treatment and emissions control units, carbon dioxide (CO_2) capture systems involving gas-phase CO_2 captured by solid-phase sorbents, liquid-phase solvents, and direct air capture systems. Multiphase flow challenges are complex and require sophisticated computational approaches and suitable validation against experimental results to yield robust solutions.

NETL's CDE Team is part of a global community researching multiphase flow towards the development of future energy conversion systems that will run more efficiently, delivering reliable energy globally. This work is dynamic, as computational science evolves rapidly. Faster and more complex computing systems appear every day to underpin increasingly realistic mathematical models and computer simulations of energy systems.

Supercomputers that broke ground just a few years ago will soon be replaced by systems operating at the exa-scale (one quintillion floating-point operations each second), representing a thousand-fold increase in computational speed. This surge of processing power will open doors to breakthroughs across the scientific community, and NETL is involved in DOE's Exascale Computing Project, a multi-year effort to maximize the benefits of high-performance computing for U.S. economic competitiveness, national security, and scientific discovery.

CAPABILITIES

The CDE team's software portfolio features physics-based modeling tools to guide the design, operation, and troubleshooting of multiphase flow devices, with an emphasis on energy production technologies (e.g., gasifiers, CO_2 capture devices, and chemical looping).

OPEN-SOURCE SOFTWARE FOR SIMULATING MULTIPHASE FLOW PROCESSES – The Multiphase Flow with Interphase eXchanges (MFiX) suite is a physics-based software for design, optimization and scale-up of multiphase reactors in advanced power plants and the chemical industry. The scale-up of multiphase reactors is notoriously difficult; engineers struggle to predict commercial-scale (large) reactor performance merely based on pilot-scale (small) reactor performance. To that end, the MFiX suite of software provides multiple Eulerian-Eulerian and Eulerian-Lagrangian computational frameworks that can be used to characterize and quantify the performance of multiphase reactors at any scale (Figure 1).

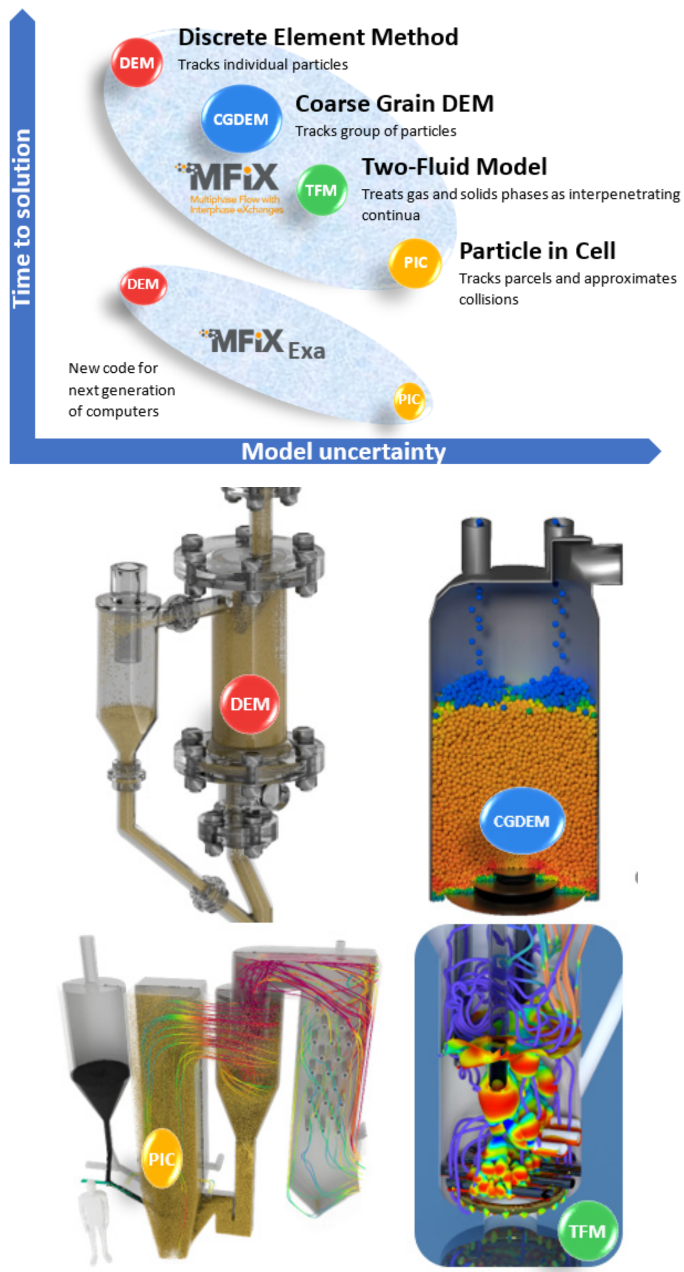


Figure 1. MFiX suite of multiphase CFD software.

MFIX-EXA SOFTWARE – MFIX-Exa is a U.S. Department of Energy Exascale Computing Project (ECP) application code being developed to use computer modeling and the next generation of supercomputers to support the design, optimization, and decarbonization of pilot and commercial scale gas-solid reactors. The fundamental physics models in MFIX-Exa follow those of the original MFiX code, but new algorithmic approaches built on top of AMReX, a software framework developed at LBNL for massively parallel, block-structured adaptive mesh refinement codes, enables MFIX-Exa to leverage emerging exascale machines.

MULTIPHASE FLOW ANALYSIS LABORATORY (MFAL) – The CDE Team's MFAL provides a powerful combination of high-quality experimentation closely aligned with multiphase modeling activities. The MFAL operates to obtain accurate, high-fidelity data that measures key performance parameters in multiphase flows that are subsequently used in MFiX simulation. Bench-scale circulating fluidized beds, fixed, and moving beds are fully instrumented to collect key data parameters. Furthermore, these set-ups employ novel diagnostic techniques and tools such as Laser Doppler Velocimetry, Particle Image Velocimetry, and image analysis to deepen understanding of how these complex flows develop and evolve. Furthermore, 3D printing is used to explore and validate the effect of geometric design changes offered through computational investigations, creating a synergistic research loop between simulation and experimentation.

HIGH PERFORMANCE COMPUTING – NETL is a leader in applying high-performance computing to computationally demanding multiphase flow science. The CDE Team has considerable expertise in applying high-performance computing to challenging industrial-scale problems.

NETL's High Performance Computing (HPC) system, JOULE, provides state of the art computing power for computationally intensive multiphase flow simulations, along with advanced visualization tools for post processing and analysis of data.

MFIX USERS AND PUBLICATIONS – CDE team scientists and engineers routinely publish and present their research in peer-reviewed journals and at conferences and symposia. The MFiX community consists of over 7,500 registered users across the globe in academia, industry, and national laboratories, with North America leading the way (Figure 2).

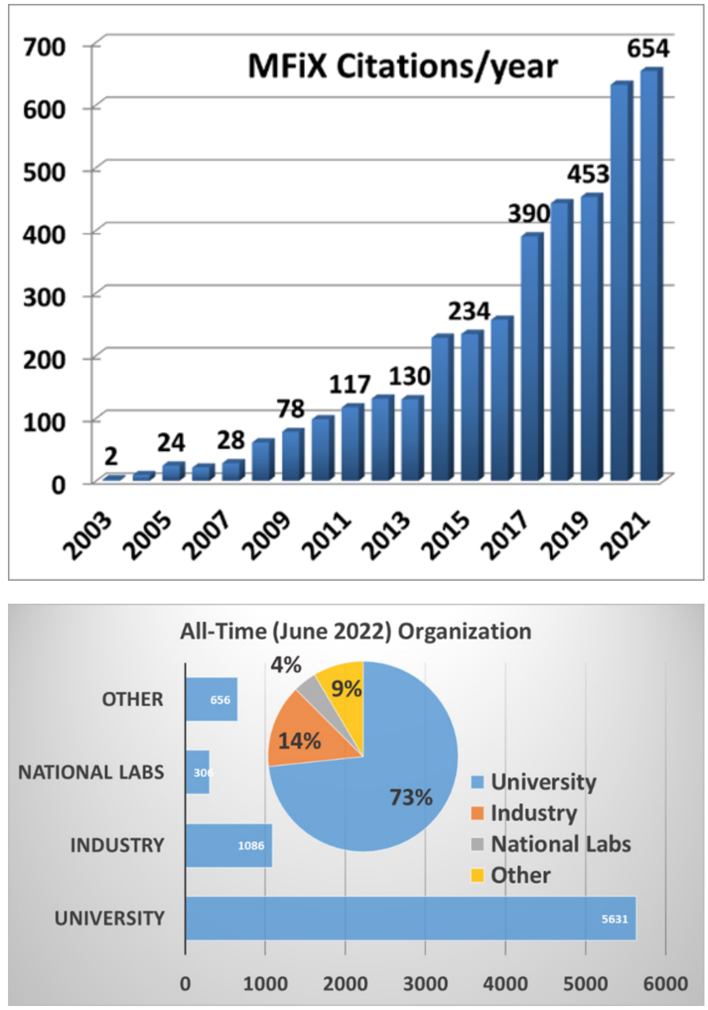


Figure 2. MFiX outreach.

NETL is a U.S. Department of Energy national laboratory that drives innovation and delivers technological solutions for an environmentally sustainable and prosperous energy future. By leveraging its world-class talent and research facilities, NETL is ensuring affordable, abundant and reliable energy that drives a robust economy and national security, while developing technologies to manage carbon across the full life cycle, enabling environmental sustainability for all Americans.

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