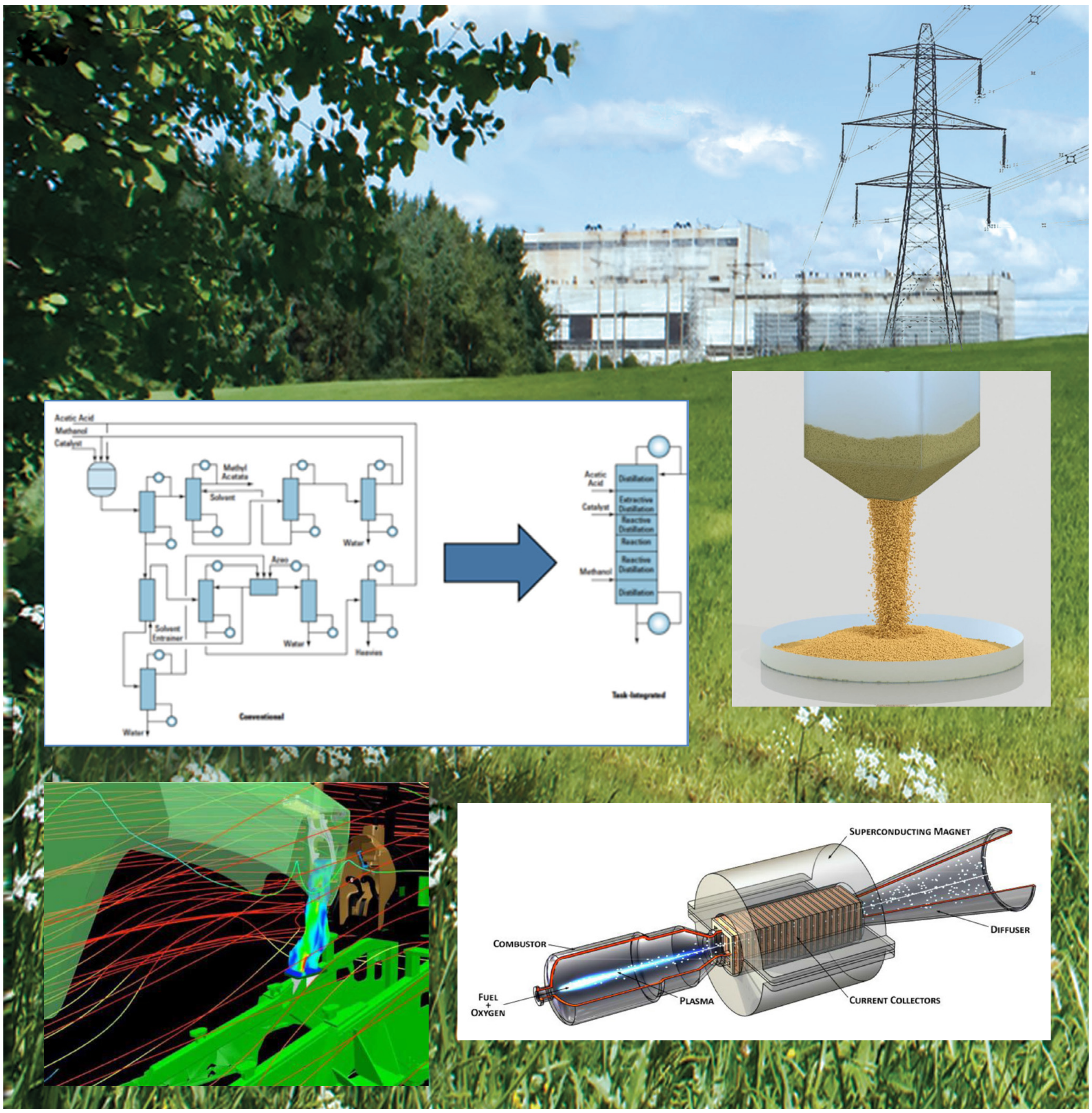
NATIONAL ENERGY TECHNOLOGY LABORATORY

# CROSSCUTTING RESEARCH PROGRAM

## SIMULATION-BASED ENGINEERING PROJECT PORTFOLIO




April 2018


U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

# DISCLAIMER

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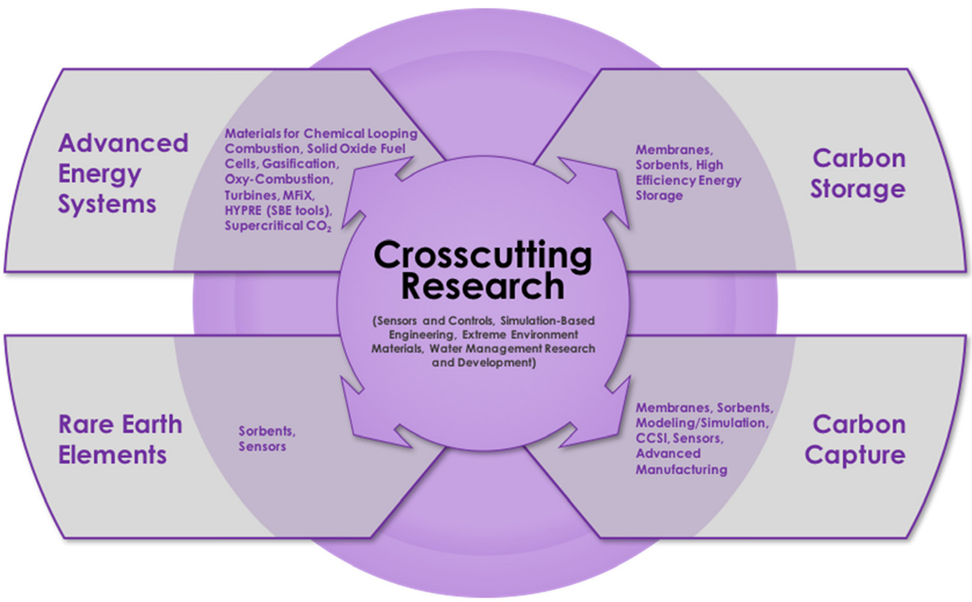
# INTRODUCTION

The Crosscutting Research Program develops a range of innovative and enabling technologies that are key to improving existing power systems and essential for accelerating the development of a new generation of highly efficient, environmentally benign fossil fuel-based power systems. The mission space is focused on bridging the gap between fundamental and applied research and development (R&D) efforts. Technologies that successfully bridge this gap are intended to offer viable step-change improvements in power system efficiency, reliability, costs, and environmental impacts.

The research fundamental to the Crosscutting Research Program overlaps and benefits other Office of Fossil Energy (FE) program areas—rare earth elements, carbon capture, carbon storage, and advanced energy systems—as shown in the figure below.




**Crosscutting Research technology overlaps with other Fossil Energy Program Areas.**

The Crosscutting Research Program executes R&D efforts by partnering and collaborating with research institutions and the power generation industry throughout the United States and in select international locations. The Crosscutting Research Program also sponsors one of the longest running and most important university training and research programs to reinforce the research-based education of students at U.S. universities and colleges with emphasis on fossil energy science. The major objective for this program is to produce tools, techniques, and technologies that map to the Clean Coal Research Program efforts.

The Crosscutting Research Program is comprised of three focus areas: Coal Utilization Sciences, Plant Optimization Technologies, and University Training and Research. A description of each area follows.

**Coal Utilization Sciences:** The Coal Utilization Sciences technology area research effort is focused on modeling and simulation technologies that lead to a suite of products capable of designing and simulating the operation of next-generation, near-zero-emissions power systems such as gasification and oxy-combustion. Models can also solve current plant operational and lifetime issues. These products are based on validated models and highly detailed representations of equipment and processes.

**Plant Optimization Technologies:** The Plant Optimization Technologies technology area exists to improve availability, efficiency and environmental performance of coal-based fossil energy power generation plants. Research is focused on sensors and control systems, materials, and water management as the basis for successful implementation of advanced power generation systems in the harsh coal-fired environment. This area also explores novel concepts such as direct power extraction and the application of additive manufacturing towards constructing complex components (e.g., turbine blades with embedded sensing capabilities).

**University Training and Research:** The University Training and Research (UTR) program awards research-based educational grants to U.S. universities and colleges in areas that benefit the FE and the Crosscutting Research Program. UTR is the umbrella program under which the University Coal Research (UCR) and Historically Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) initiatives operate. These grant programs address the scientific and technical issues key to achieving Fossil Energy's goals and build our nation's capabilities in energy science and engineering by providing hands-on research experience to future generations of scientists and engineers. The program also coordinates with and seeks opportunities to partner with State and Tribal governments and engage industry, universities, and non-governmental organizations (NGOs) on the responsible use of fossil fuels nationally and internationally.

In addition to the Crosscutting Research Program listed above, the National Energy Technology Laboratory (NETL) uses its participation in the U.S. Department of Energy's (DOE) Office of Science **Small Business Innovation Research (SBIR) Program** to leverage funding, enhance the research portfolio, and, most importantly, facilitate a pathway to commercialization. SBIR is a highly competitive program that encourages small businesses to explore technological potential and provides the incentive to profit from commercialization. By including qualified small businesses in the nation's R&D arena, high-tech innovation is stimulated and the United States gains entrepreneurial spirit to meet specific research and development needs. SBIR targets the entrepreneurial sector because that is where most innovation and innovators thrive. By reserving a specific percentage of Federal R&D funds for small business, SBIR protects small businesses and enables competition on the same level as larger businesses. SBIR funds the critical startup and development stages and encourages the commercialization of the technology, product, or service which, in turn, stimulates the U.S. economy. Since its inception in 1982 as part of the Small Business Innovation Development Act, SBIR has helped thousands of small businesses compete for Federal research and development awards. These contributions have enhanced the nation's defense, protected the environment, advanced health care, and improved our ability to manage information and manipulate data.

The Crosscutting Research Program fosters the development of innovative power systems by conducting research in these key technology areas:

**Sensors and Controls:** The basis for this research area is to make available new classes of sensors and measurement tools that manage complexity; permit low cost, robust monitoring; and enable real-time optimization of fully integrated, highly efficient power-generation systems. Sensor development focuses on measurements to be made in high temperature, high pressure, and/or corrosive environments of a power system or underground injection system. Harsh environment sensing concepts and approaches focus on low cost, dense distribution of sensors; exploration of sensor networking using passive and active wireless communication; and thermoelectric and vibration energy harvesting approaches. Advanced manufacturing techniques focus on how to lower cost and improve fabrication of sensors. Controls research centers on self-organizing information networks and distributed intelligence for process control and decision making.

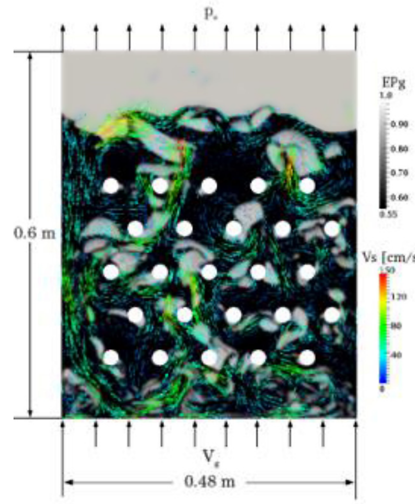
**High Performance Materials:** Materials development under the Crosscutting Research Program focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems and on functional materials, which are designed to perform specified non-structural tasks (e.g., shape memory materials or barrier coatings). Computational tools in predictive performance, failure mechanisms, and molecular design of materials are also being developed to support highly-focused efforts in materials development and reduce the time and cost to develop new materials. Advanced manufacturing development is represented under High Performance Materials in two capacities: first, the need for advancements in feedstocks such as metal powders for superalloys and second, as a set of methods for producing high-performance materials.

**Simulation-Based Engineering:** This key technology area comprises the expertise and capability to computationally represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant. Science-based models of the physical phenomena occurring in fossil fuel conversion processes and development of multiscale, multi-physics simulation capabilities are just some of the tools and capabilities in Simulation-Based Engineering. This key technology area enables the development of innovative, advanced energy systems by developing and utilizing advanced process systems, engineering tools and approaches, and the transformation of computationally intensive models into reduced order, fast, user-enabled models for the purposes of study, development, and validation. These tools will be used to optimize data handling and exploit information technology in the design of advanced energy systems with carbon capture.

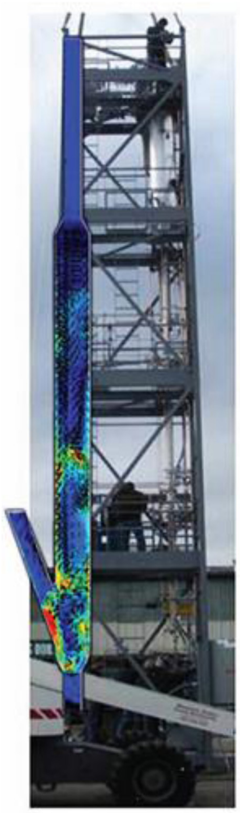
**Water Management Research and Development:** Water research encompasses the need to reduce the amount of freshwater used by power plants and to minimize any potential impacts of plant operations on water quality. Research in effluent treatment and water quality sensing, field testing of technologies and processes for treating water produced by injection of carbon dioxide into deep saline aquifers, and exploration of water-limited cooling and innovative multi-stage filtration technologies are being conducted. Data modeling and analysis is being employed to examine existing water availability data on a regional basis. The vision for this program area is to develop a 21st-century America that can count on abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential for continued security and economic health. To accomplish this, Crosscutting Research is needed to lead a critical national effort directed at removing barriers to sustainable, efficient water and energy use, developing technology solutions, and enhancing our understanding of the intimate relationship between energy and water resources.

# SIMULATION-BASED ENGINEERING

Modeling efforts stem from the motivation to reduce costs and time delays resulting from the use of expensive lab set-ups in research and physical prototypes in the design and engineering phase of projects. Improvements are being sought in all aspects of modeling from algorithms to software engineering. NETL's Simulation-Based Engineering area combines the technical knowledge, software development, computational power, data repository, experimental facilities, and unique partnerships to support research to provide timely and accurate solutions for complex power systems. Understanding the performance of complex flows and components used in advanced power systems and having the means to impact their design early in the development process provides significant advantages in product design. Computational models can be used to simulate the device and understand its performance before the design is finalized. During new technology development—for instance, the development of a new sorbent adsorber/desorber reactor for carbon dioxide capture—empirical scale-up information is not available because the device has not yet been built at the scale required. Traditional scale-up methods do not work well for many of the components of complex power systems. Therefore, science-based models with quantified uncertainty are important tools for reducing the cost and time required to develop these components.




**The simulation of a bubbling fluidized bed with heat transfer tubes used for model validation.**



**CFD model of a pilot-scale $CO_2$ adsorber (shown in the background).**

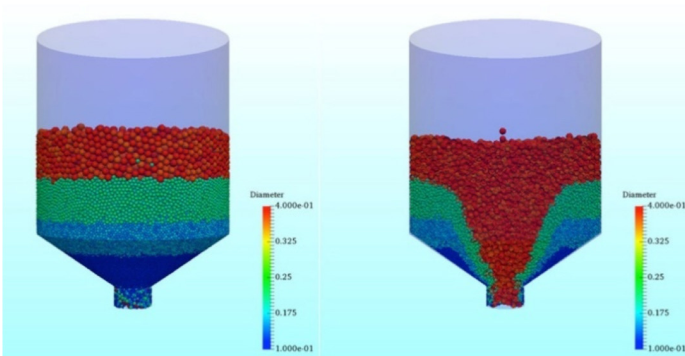
Research through simulation-based engineering develops accurate and timely computational models of complex reacting flows and components relevant to advanced power systems. Model development and refinement is achieved through in-house research and partnerships to utilize expertise throughout the nation, such as NETL's University Training and Research programs. Partnerships have also been formed with other national laboratories through the Institute for the Design of Advanced Energy Systems (IDAES) and Carbon Capture Simulation Initiative (CCSI) tool set.

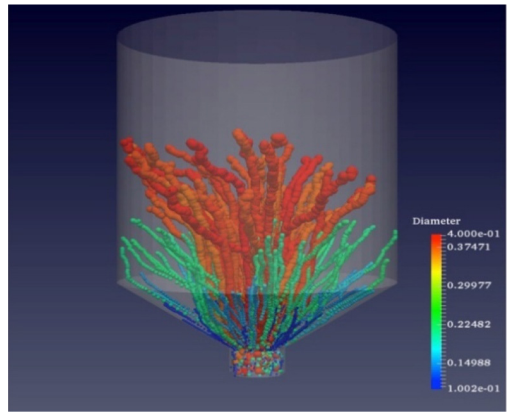
The vast computational resources available to NETL ensure timely solutions to the most complex problems. The NETL Joule Supercomputer is one of the world's fastest and most energy-efficient, intended to help energy researchers discover new materials, optimize designs, and better predict operational characteristics. Speed-up is also achieved through research in modern graphical processing unit computing as well as the implementation of reduced order models when appropriate. Simulation-based engineering also exploits on-site, highly instrumented experimental facilities to validate model enhancements. Models are made available to the public through the laboratory's computational fluid dynamics (CFD) code Multiphase Flow with Interphase eXchanges (MFiX), developed specifically for modeling reacting multiphase systems.

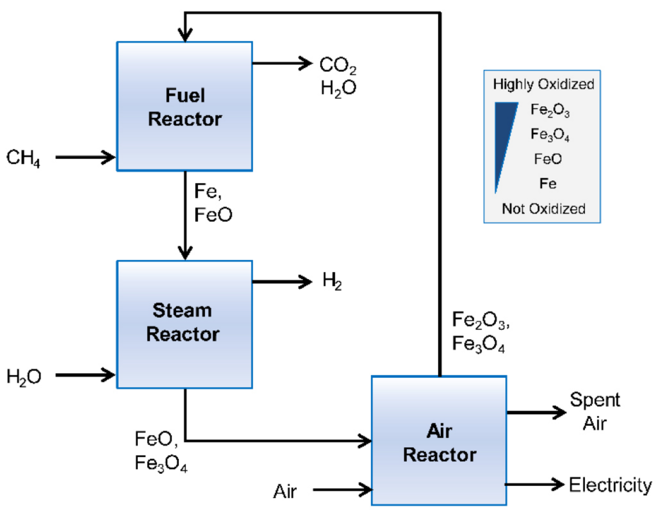
Simulation-Based Engineering personnel work closely with stakeholders and partners to outline issues, emerging trends, and areas of need. NETL has sponsored multiphase flow workshops annually to bring together industry and academia to identify R&D priorities and ensure that key technologies will be available to meet the demands of future advanced power systems.

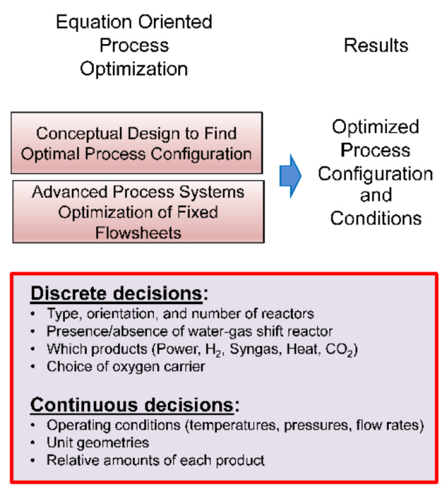
The research areas under Simulation-Based Engineering are CFD: Multiphase Flows, Systems Engineering, and Materials.

# PROJECTS BY RESEARCH AREA

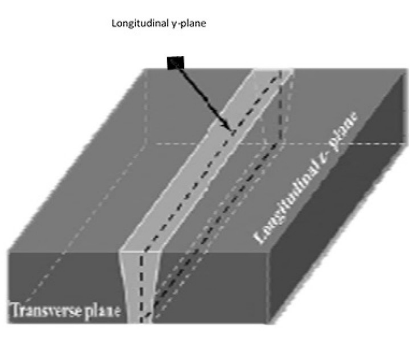


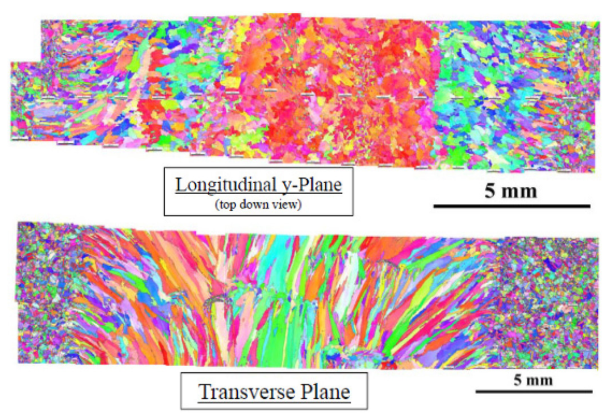



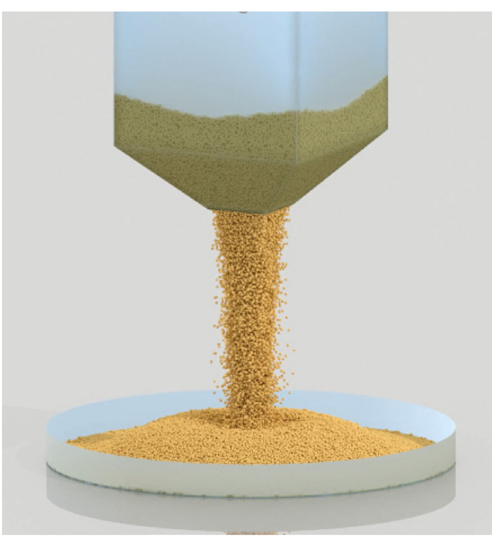


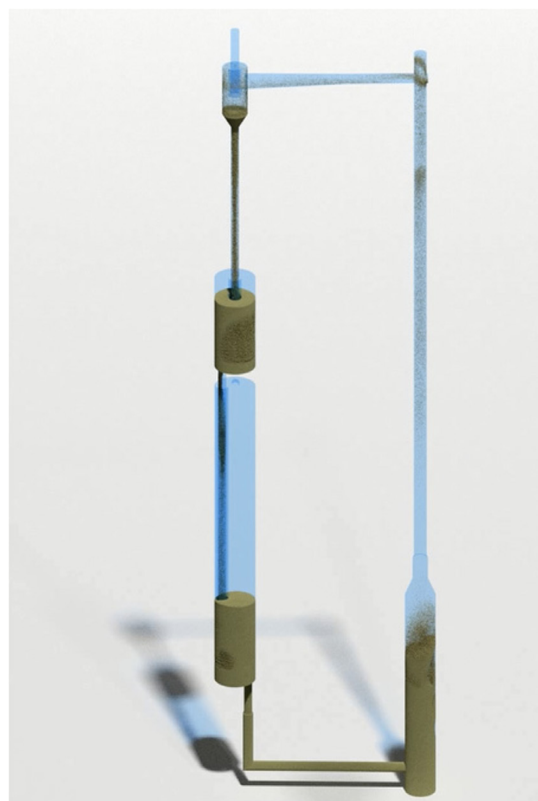


# CFD: MULTIPHASE FLOW





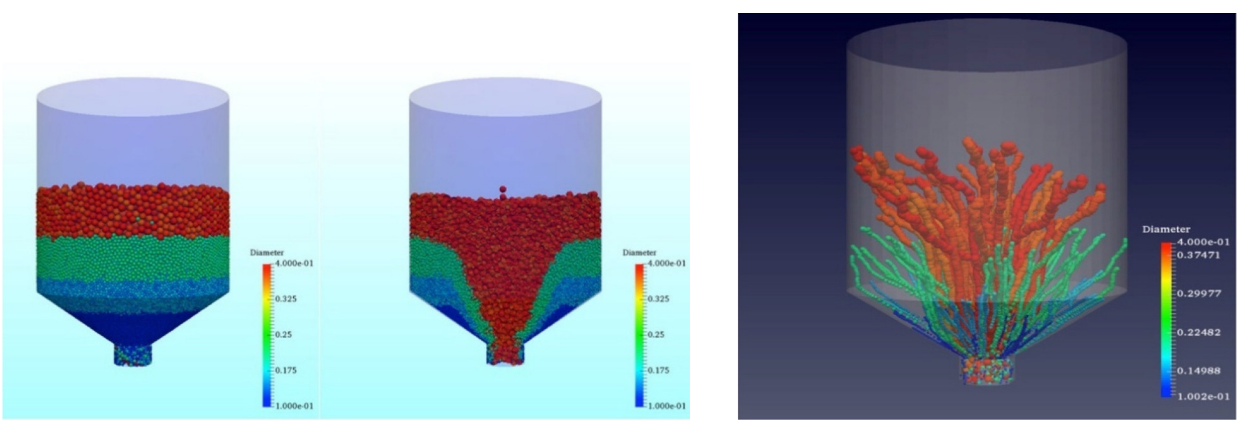


# MFiX-DEM PHI: Performance and Capability Improvements Towards Industrial Grade Open-Source DEM Framework with Integrated Uncertainty Quantification

| Performer | Arizona State University | Lawrence Livermore National Laboratory | Sandia National Laboratories |
|---|---|---|---|
| **Award Number** | FE0026393 | FWP-FEW0199 | FWP-15-018146 |
| **Project Duration** | 09/09/2015-02/28/2018 | 08/28/2015-02/28/2018 | 08/01/2015-02/28/2018 |
| **Total Project Value** | $703,385 | $140,000 | $94,375 |
| **Total Value (All)** | $937,760 | | |
| **Technology Area** | Coal Utilization Sciences | | |

Arizona State University, along with the Lawrence Livermore National Laboratory and Sandia National Laboratories, worked collaboratively for the enhancement of an open source solver for computational fluid dynamics (CFD) coupled with a discrete element method (DEM) named MFiX-DEM, which is developed and maintained by the National Energy Technology Laboratory. The objectives of the project were to improve the physical modeling capabilities of MFiX-DEM while tightly integrating these improvements with an intuitive graphical user interface driven by an uncertainty quantification framework, and to effectively lower the barrier for industrial adoption of MFiX-DEM. To achieve these objectives, as part of the Phase 1 activities, the MFiX-DEM Phi team has been collaborating with two major global corporations, ExxonMobil and Procter & Gamble that have diverse multiphase flow application areas ranging from oil and refineries to consumer products.

The relevance and potential impact of MFiX-DEM Phi lies in tools that industry can use to solve problems of realistic size with modest high-performance computing (HPC) resources within an acceptable timeframe. This work has the potential to transform the way multiphase flow-based engineering systems are designed and evaluated by providing a user-friendly tool that offers integrated uncertainty quantification; enhanced physical modeling capabilities such as particle size distributions and heat transfer; and improved performance through code modernization. These contributions will provide the ability to solve industrial-scale problems by taking advantage of advanced HPC systems that will be ubiquitous in the near future but more importantly enable industrial users to assess the credibility of their simulation results through an intuitively easy-to-use uncertainty quantification framework.




**Hopper bin discharge simulation of stacked multilayer phase packing with user prescribed polydispersity (left) and time history ("trajectory") plot of select particles from each layer (right).**

# RIC Field Work Proposal – Virtual Reactor Optimization Task 4.1: MFiX Suite Multiphase Code Development and Validation

| | |
|---|---|
| **Performer** | National Energy Technology Laboratory – Research and Innovation Center |
| **Award Number** | RIC Advanced Reaction Systems FWP – 1022405 |
| **Project Duration** | 01/01/2017– 03/31/2018 |
| **Total Project Value** | $3,089,600 |
| **Technology Area** | Coal Utilization Sciences |

Design and optimization of complex reactors for fossil energy applications is a challenging and expensive process. Understanding the performance of complex multiphase flow reactors used in fossil energy technology and having the means to impact their design early in the developmental process is important for two reasons. First, about 75 percent of the manufacturing cost of any product is committed at the conceptual design stage, even when the incurred cost might be very small. Once the conceptual design stage is completed, opportunities for cost savings are substantially diminished. Second, during innovative technology development, empirical scale-up information is not available because reactors at large scales have not been built. It is well known that traditional scale-up methods do not work well for multiphase flow reactors, such as the ones used for fossil energy applications. Given these challenges, computational models can be used to simulate the device and understand its performance before the design is finalized, which is important for reducing risk and cost. Science-based models are critical tools for reducing the cost and time required for development. The objectives of this work are to:

- Develop, validate, apply, publicly distribute, and support the Multiphase Flow with Interphase eXchanges (MFiX) suite, a multiphase flow software suite capable of modeling large-scale, reactor systems that include chemical reactions and complex geometries. These modeling tools will support the design and optimization of novel reactor systems that will meet Advanced Reaction Systems (ARS) Field Work Proposal (FWP) and Office of Fossil Energy (FE) programmatic goals.

- Continue development and application of the Software Quality Assurance Program for the MFiX suite to ensure that the software provides physically accurate predictions. The Quality Assurance Program includes verification, validation, and uncertainty quantification processes and uses the capabilities of the multiphase flow analysis laboratory facilities for generation of high-quality validation data.

NETL researchers and the MFiX suite of codes provide the FE program with this critical modeling capability. The MFiX suite includes the following set of complementary modeling tools that can be brought to bear on fossil energy technologies:

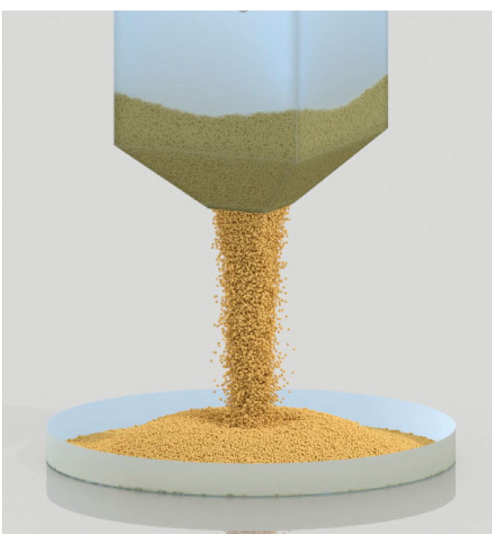
*MFiX-TFM (Two-Fluid Model):* An Eulerian-Eulerian code capable of dealing with the range of small-scale through industry-scale reacting simulations. It is presently the most mature code and includes a broad range of capabilities for dense reacting multiphase flow. The approximation of the solid phase as a continuum allows for faster simulation time but it also introduces the need for more complex model closures to accurately represent solid phase behavior. Development of faster and more accurate algorithms to accomplish this is one of the key research program objectives for this approach.

*MFiX-DEM (Discrete Element Model):* An Eulerian-Lagrangian code that treats the fluid phase as a continuum and models the individual particles of the solids. While the treatment of individual particles can provide higher fidelity over a broad range of flow regimes (from dilute to pack), it is also very challenging when dealing with very large numbers of particles for large-scale simulations. These large-scale applications require high-performance computing resources and substantial amounts of computer time. Therefore, code optimization and speed-up are critical research fronts to support industrial-scale applications.

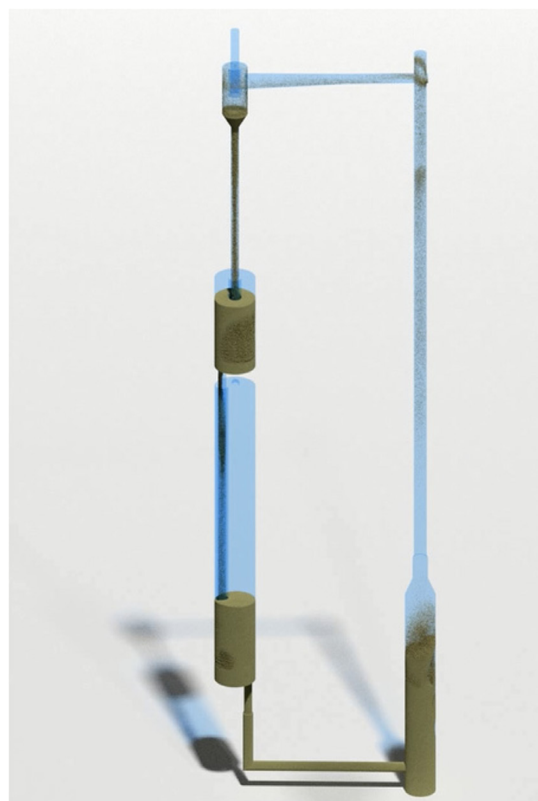
*MFiX-MPIC (Multiphase Particle-In-Cell):* An Eulerian-Lagrangian code that treats the fluid phase as a continuum and models solids as discrete "parcels" of particles, with each parcel representing a group of real particles with the same physical characteristics. This is an emerging capability that will be brought to maturity for use in ARS reactor simulations over the course of the proposed work. The MFiX-MPIC approach greatly reduces the computational cost. However, modeling approximations are required for the MPIC technique, which will affect accuracy. Development, validation, and optimization of these modeling approximations are critical research fronts.

Science-based models with quantified uncertainty are critical tools for reducing the risk, cost, and time required for development of novel fossil energy reactors. In this research effort, NETL is providing an advanced suite of multiphase flow CFD models that enable this capability. These models provide detailed predictions of reactor performance including temperature, velocities, chemical composition, reaction rates, and heat transfer for both fluid and solid phases in the reactors.

In contrast to expensive, proprietary commercial CFD software, the MFiX suite and associated toolsets are open-source codes that are developed, validated, and supported in-house by NETL's software development and application specialists. As open-source codes, the MFiX suite can be customized for novel applications. The MFiX Suite is available on NETL's Joule supercomputer, enabling advanced, large-scale, challenging, computer-intensive applications. There are over 4,600 registered users of the MFiX Suite and associated toolsets including industry, academic, and national laboratories. User applications span a broad range of topics, including chemical process, energy conversion, and even volcanology. Members of the user group exchange information through support mailing lists which helps to ensure that code problems are found and addressed quickly.



**MFIX-DEM simulation of granular solids discharge from a hopper.**



**MFIX-DEM simulation of a chemical looping reactor.**

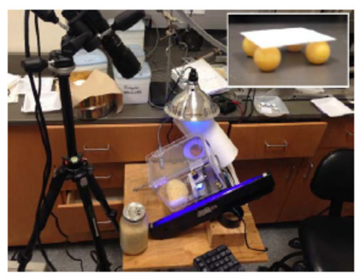
# MFiX-DEM Enhancement for Industry-Relevant Flows

| | | |
|---|---|---|
| **Performer** | University of Colorado | National Renewable Energy Laboratory |
| **Award Number** | FE0026298 | FWP – DOW4659 |
| **Project Duration** | 09/01/2015 – 08/31/2020 | 10/01/2015 – 08/31/2020 |
| **Total Project Value** | $3,778,002 | $899,419 |
| **Total Value (All)** | $4,677,421 | |
| **Collaborator** | Particulate Solid Research, Inc. | |
| **Technology Area** | Coal Utilization Sciences | |

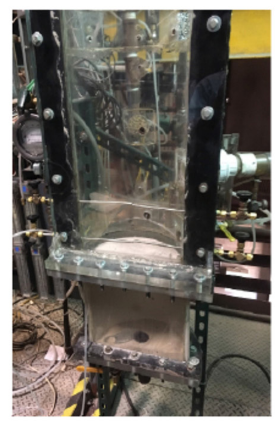
This project will improve performance of the Multiphase Flow with Interphase eXchanges– discrete element method (MFiX-DEM) code to enable a transformative shift for industrial use. The proposed approach will enhance MFiX-DEM by using a state-of-the-art profiling methodology developed by our team members to comprehensively and continuously identify numerical and algorithmic bottlenecks. Both serial and parallelization bottlenecks will be overcome via vectorization, cache utilization, algorithmic improvements, and implementation of hybrid message passing interface/OpenMP parallelization methods that synergize with current heterogeneous high-performance computing (HPC) architectures and accelerators. Optimizing MFiX-DEM and implementing parallelization for accelerated HPC systems will enable simulations of industrially relevant problems on machines that industry is likely to have in the coming years.

The goal is to achieve an increase in performance of two orders of magnitude; a refined estimate will result from the profiling effort. Based on preliminary findings and recent work, a realistic quantitative goal for Phase 1 is an order-of-magnitude performance improvement and demonstration on an industrially-relevant simulation involving $10^8$ particles. Regarding the latter, over thirty Particulate Solid Research Inc. consortium member companies will be surveyed during the beginning of the project to identify industrial needs. New experiments will be performed involving ~$10^8$ particles in a system of industrial relevance, and this experiment will be used to demonstrate the enhanced MFiX code. Uncertainty quantification (UQ) will also be performed by coupling the freely available UQ toolkit Problem Solving environment for Uncertainty Analysis and Design Exploration (PSUADE) with an enhanced version of MFiX. Uncertainty quantification using the enhanced MFiX code on larger and industrially relevant systems will be demonstrated.

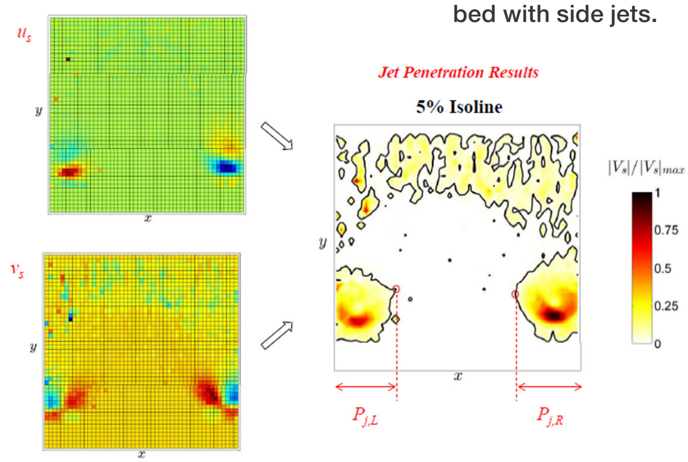
The immediate outcome will be an enhanced DEM tool implemented into the open-source MFiX framework. The enhanced DEM model will be optimized for computational efficiency and will contain parallelization methods that leverage advances in heterogeneous HPC architectures with accelerators.



**Horizontal jet experiments particle characterization.**



**Semi-circular fluidized bed with side jets.**




**Horizontal jet experiments particle tracking post-processing.**

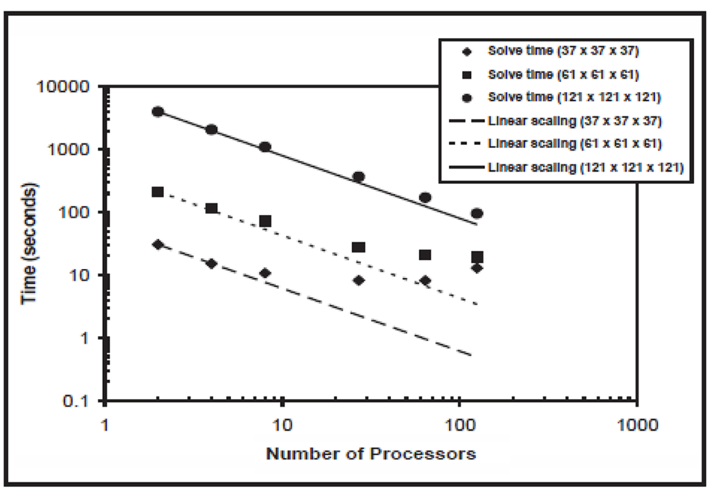
# Interfacing MFiX with PETSc and HYPRE Linear Solver Libraries

| | |
|---|---|
| **Performer** | University of North Dakota |
| **Award Number** | FE0026191 |
| **Project Duration** | 09/01/2015 – 08/31/2018 |
| **Total Project Value** | $400,000 |
| **Collaborator** | University of Utah |
| **Technology Area** | University Training and Research |

High computational cost associated with the solution of large, sparse, poorly conditioned matrices is a serious impediment to increasing the utility of computational fluid dynamics models for resolving multiphase flows. This project will interface NETL's Multiphase Flow with Interphase Exchanges (MFiX) code with Portable Extensible Toolkit for Scientific Computation (PETSc) and High Performance Preconditioners (HYPRE) linear solver libraries with the goal of reducing the time to solution for the large, sparse, and often ill-conditioned matrix equations resulting during the solution process. The lack of robust convergence associated with the current iterative methods in MFiX can be alleviated through appropriate preconditioning techniques to Krylov subspace solvers and multigrid methods accessible from these third-party solver libraries.

The overall objective of this project is to first establish a robust well-abstracted solver interface that will present an extensible back-end enabling MFiX to successfully interface with various solver libraries. Next, this extensibility will be demonstrated by interfacing MFiX with PETSc and HYPRE linear solver libraries with the goal of reducing the time to solution for large, sparse, linearized matrix equations resulting from the discretization of multiphase transport equations.

This project could reduce the time to solution by at least 50 percent when compared to current linear solver options in MFiX. It also could show that near linear scaling in parallel performance can be achieved to at least 1000 processors, which could translate to achieving good scalability on current high-performance computing systems such as the DOE leadership computing facilities as well as enabling the portability of MFiX with new hardware technologies.




PETSc relative solve times for solution to the inhomogeneous Helmholtz Equation (3D) (Septadiagonal matrix, uniprocessor)

$$\nabla^2 A + k^2 A = -f$$

Stand alone solver timing studies

| Degrees of Freedom | CG | GMRES | BiCGSTAB |
|---|---|---|---|
| 150K | 1.56 | 11.11 | 2.16 |
| 600K | 23.45 | 700.00 | 35.56 |

Best stand alone solver with pre-conditioning options in brackets

| Degrees of Freedom | CG (Point Jacobi) | CG (Block Jacobi) | CG (ILU) | CG (SOR) |
|---|---|---|---|---|
| 150K | 1.29 | 1.06 | 1.06 | 1.00 |
| 600K | 25.24 | 19.31 | 18.01 | 17.87 |
| 1.2M | 57.64 | 42.94 | 41.76 | 40.00 |

**Variations in run time with the number of processors for different fixed problem sizes (indicated within brackets) when solving a non-symmetric matrix in PETSc.**

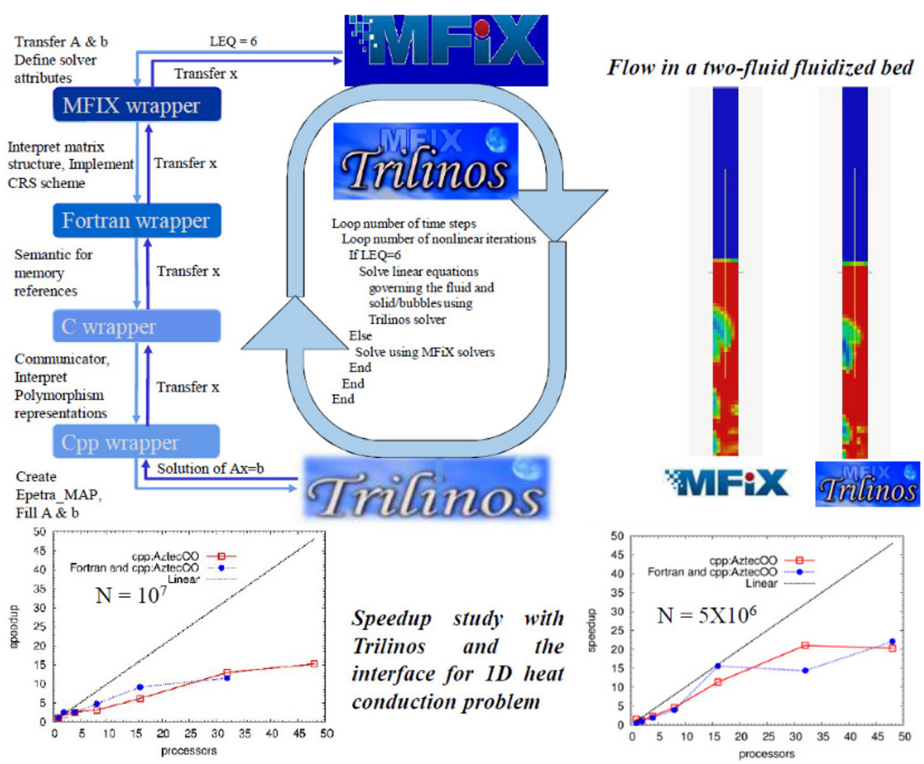
# High Fidelity Multiphase Computational Fluid Dynamic Model for Fluidized Bed Experiments with Trilinos

| **Performer** | University of Texas at El Paso | Sandia National Laboratories |
|---|---|---|
| **Award Number** | FE0026220 | FWP-15-018068 |
| **Project Duration** | 09/09/2015-08/31/2018 | 10/01/2015-08/31/2018 |
| **Total Project Value** | $339,999 | $60,000 |
| **Total Value (All)** | $399,999 | |
| **Technology Area** | University Training and Research | |

Multiphase CFD software is critical for understanding the complex thermal-fluid behavior of fossil fuel reactors and is increasingly being used in their design and scale-up. The goal of this project is to develop a high-fidelity and user friendly multiphase simulator based on the Multiphase Flow with Interphase eXchanges (MFiX) software package, a multiphase CFD software developed by the Department of Energy and widely used by the fossil fuel reactor communities.

This work will leverage the linear solver libraries from Trilinos open-source software packages developed by Sandia National Laboratories. Trilinos packages provide easy-to-use and scalable applied mathematics libraries suitable for massively parallel computers and are kept up to date for the latest hardware including graphics processing unit (GPU) acceleration. To achieve this, project personnel will devise a framework to integrate the MFiX linear solvers with the Trilinos linear solver packages (Trilinos MFiX), evaluate the performance of the state-of-the-art preconditions and linear solvers, and test Trilinos MFiX with the MFiX suite on massively parallel and cloud-based computers with and without GPU acceleration.

Integrating Trilinos into MFiX will incorporate advanced modeling capabilities into MFiX as well as enable efficient use of existing resources from various DOE labs; reduce development costs without compromising competitiveness; and potentially simplify the addition of new physics-based features such as new drag models based on theoretical, numerical, or table-based drag coefficients



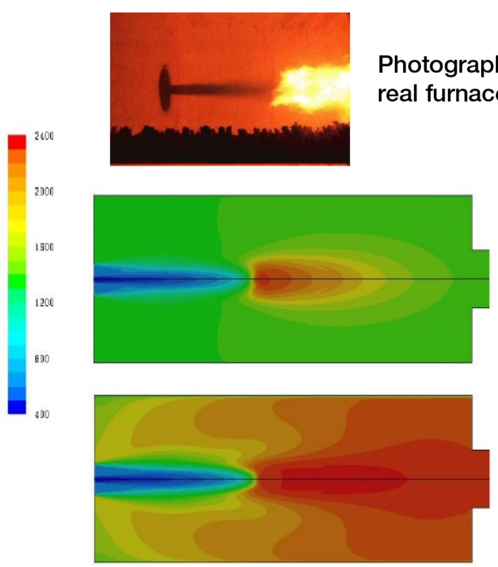

Overview of MFiX – Trilinos integration.

# Implementing General Framework in MFiX for Radiative Heat Transfer in Gas-Solid Reacting Flows

| | |
|---|---|
| **Performer** | University of Wyoming |
| **Award Number** | FE0030485 |
| **Project Duration** | 08/01/2017 – 07/31/2020 |
| **Total Project Value** | $400,000 |
| **Technology Area** | University Training and Research |

The objectives of this research are to (1) develop and implement a general framework to support the integration of modern gas radiation models for gas-solid reacting flows; (2) implement a methodology for developing new multiphase radiation models with accuracy and efficiency commensurate to the different importance in a variety of energy related applications; (3) reduce the computational cost of existing high-fidelity models via systematic optimization; and (4) demonstrate the accuracy and efficiency of the radiation models under typical gas-solids reacting flow conditions.

This project aims to have a significant impact on the development of the National Energy Technology Laboratory's Multiphase Flow with Interphase Exchanges software (MFiX) and future research of gas-solid reacting flows. Fundamental knowledge of radiation transport and predictive models developed for these processes could shorten design time and reduce design cost of new energy conversion technologies.



**Photograph of real furnace.**

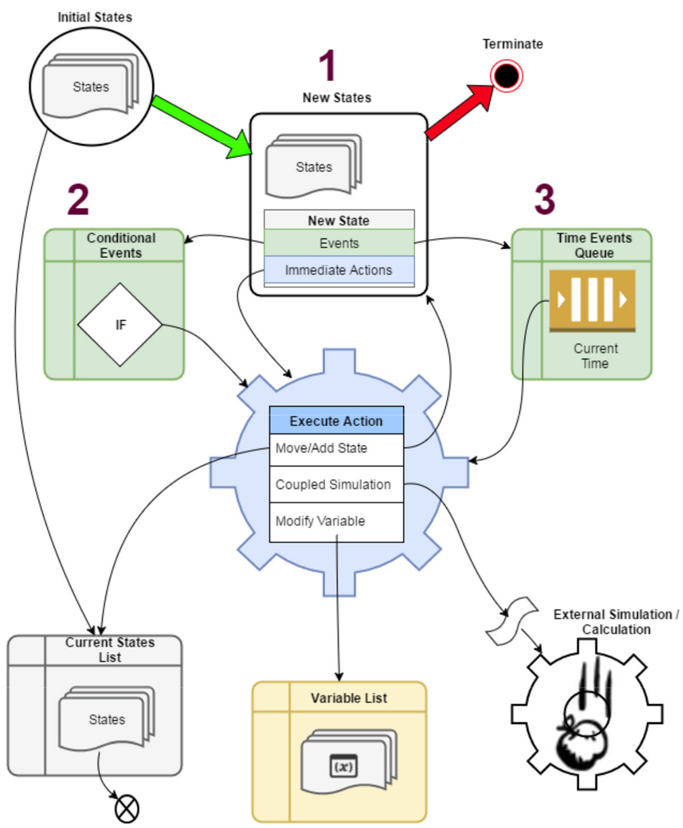
**Computational fluid dynamics (CFD) including thermal radiation.**

**CFD without thermal radiation.**

**Relevance of radiative heat transfer in pulverized coal combustion.**

# SYSTEMS ENGINEERING

| PERFORMER(S) | PROJECT TITLE | PAGE |
|---|---|---|
| Idaho National Laboratory | Event Model Risk Assessment Using Linked Diagrams (EMRALD) | 19 |
| National Energy Technology Laboratory; Lawrence Berkeley National Laboratory; Sandia National Laboratories | Institute for the Design of Advanced Energy Systems | 20 |



# Event Model Risk Assessment Using Linked Diagrams (EMRALD)

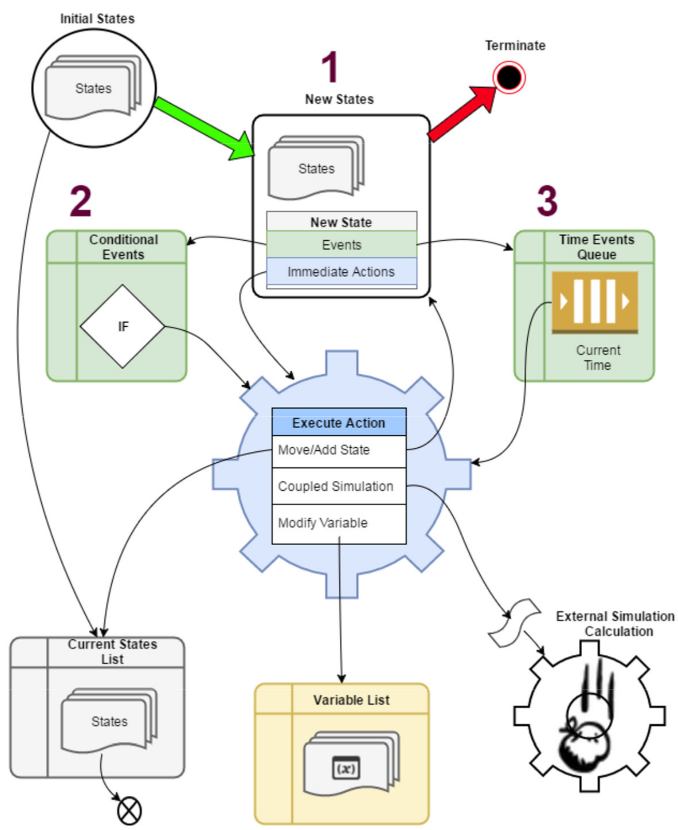
| | |
|---|---|
| **Performer** | Idaho National Laboratory |
| **Award Number** | TCF-17-13410 |
| **Project Duration** | 10/01/2017- 09/30/2018 |
| **Total Project Value** | $123,812 |
| **Technology Area** | Plant Optimization Technologies |

Modern industry has moved from physical testing to physics-based computer models for testing designs and stress cases. As variations of those tests produce differing results, a probabilistic approach is needed to sample, map, and assess the data. Secondly, these systems will be placed in a real environment where they interact with other systems and operators. Engineers and analysts could optimize reliability, and safety efforts, if simulations probabilistically showed how their system performed when integrated into an operating environment. EMRALD is a simulation tool that can calculate numerous system probabilities and couple with other physics simulations to perform dynamic probabilistic risk assessment (PRA).

Traditional PRA tools provide a static assessment of a given model that is sufficient for several applications. However, a large number of problems are best resolved with consideration of time-dependent or dynamic behavior such as operator actions. EMRALD has a unique ability to model complex interactions and yet keep the model simple by combining concepts from traditional PRA, such as logic trees and state transition diagrams. EMRALD uses a state-based PRA model to perform a three-phase discrete event simulation, which makes both time-dependent modeling and coupling with other simulations possible.

An EMRALD model consists of states, events, and actions that drive the condition of the model over time. Although the methodology is different from traditional PRA, it is designed so that some sections of the modeling are similar and equivalent to traditional PRA models. This overall design concept enables easy use for both experienced PRA modelers and those unfamiliar with traditional PRA modeling but understand flow diagrams. Additionally, most information in traditional PRA models could be automatically converted into an EMRALD model.

This software technology was originally designed for system risk and reliability and has shown many uses including coupling seismic data, flooding simulations, and thermal hydraulics simulations for overall dynamic PRA results. EMRALD could be used in fields where event times or operator actions are critical to the reliability of the overall system or preventing the loss of life. Such systems range from the power grid with all the dynamic conditions involved in control room operations to human protection systems on oil rigs. EMRALD would provide each an overall summary of failure probabilities with the ability to drill down and view specific sequences of events for high-probability failures, thus showing where to optimize mitigation efforts to maximize safety and reliability.




**Execution of an EMRALD model based on three-phase discrete event simulation. (Phase 1) While there are states in the "New States" list add events to the Time Queue or Conditional Events. (Phase 2) If any Conditional Events criteria are met, execute that event's actions and go to Phase 1. (Phase 3) Jump to the next chronological event, process its actions, and go to Phase 1.**

# Institute for the Design of Advanced Energy Systems

| Performer | National Energy Technology Laboratory–Research & Innovation Center | Lawrence Berkeley National Laboratory | Sandia National Laboratories |
|---|---|---|---|
| Award Number | FWP-1022423 | FWP-CS IDAES FY18 | FWP-16-018847 |
| Project Duration | 01/01/2018-12/31/2018 | 01/01/2018-12/31/2018 | 01/01/2018-12/31/2018 |
| Total Project Value | $1,400,860 | $2,494,140 | $1,905,000 |
| Total Value (All) | $5,800,000 | | |
| Collaborators | Carnegie Mellon University; West Virginia University | | |
| Technology Area | Coal Utilization Sciences | | |

National Energy Technology Laboratory (NETL) Institute for the Design of Advanced Energy Systems (IDAES) seeks to be the premier resource for the identification, synthesis, optimization, and analysis of innovative advanced energy systems at scales ranging from process to system to market.

IDAES was formed in 2016 to develop new advanced process systems engineering capabilities to support the design and optimization of innovative new processes that go beyond current equipment/process constraints. IDAES was formed to address the gaps between state-of-the-art simulation packages, such as Aspen Plus®, general PROcess Modeling System (gPROMS), Process Simulation (ProSim), PRO/II®, and general algebraic modeling languages (AMLs), such as General Algebraic Modeling System (GAMS), A Mathematical Programming Language (AMPL), and Advanced Interactive Multidimensional Modeling System (AIMMS). Major strengths of commercial simulation packages are their libraries of unit models and thermo-physical properties. Such simulation packages, however, often have difficulty optimizing flowsheets and have limited support for incorporating models of non-standard dynamic units, such as solids handling. In addition, these packages do not directly support uncertainty quantification. AMLs, on the other hand, are eminently flexible and readily support large-scale optimization, but considerable work is required to construct process models, which are often only useful for a one-time application. Moreover, AMLs currently lack the ability to integrate with process model libraries that incorporate thermodynamic equilibria, transport, kinetic phenomena, and complex behavior at multiple time and length scales.

The IDAES process systems engineering framework addresses the capability gap between state-of-the-art simulation packages and AMLs by integrating an extensible, equation-oriented process model library within the open-source, DOE-funded Pyomo AML (Hart et al., 2017), which addresses challenges in formulating, manipulating, and solving large, complex, structured optimization problems. The IDAES framework now includes tools for: (1) process synthesis and conceptual design, including process intensification, (2) process design and optimization, including process integration, (3) process control and dynamic optimization, (4) using advanced solvers and computer architectures, (5) automated development of thermodynamic, physical property, and kinetic submodels from experimental data, (6) integration of multi-scale models, (7) comprehensive, end-to-end uncertainty quantification, including stochastic optimization, (8) maintaining complete provenance information, and (9) the ability to support multiple scales, from materials to process to market.

IDAES and its capabilities will be deployed to improve the efficiency and reliability of the existing fleet of coal-fired power plants while accelerating the development of a broad range of advanced fossil energy systems, including chemical looping combustion and other transformational $CO_2$ capture technologies. IDAES will bring many benefits to the DOE, including the ability to (1) suggest promising opportunities for retrofitting existing plants with new technologies, (2) identify novel new advanced energy systems for further development, (3) analyze various concepts to increase the ability to technically differentiate alternatives, and (4) support ongoing development, scale up, and deployment of new energy technology. Specific benefits include the following:

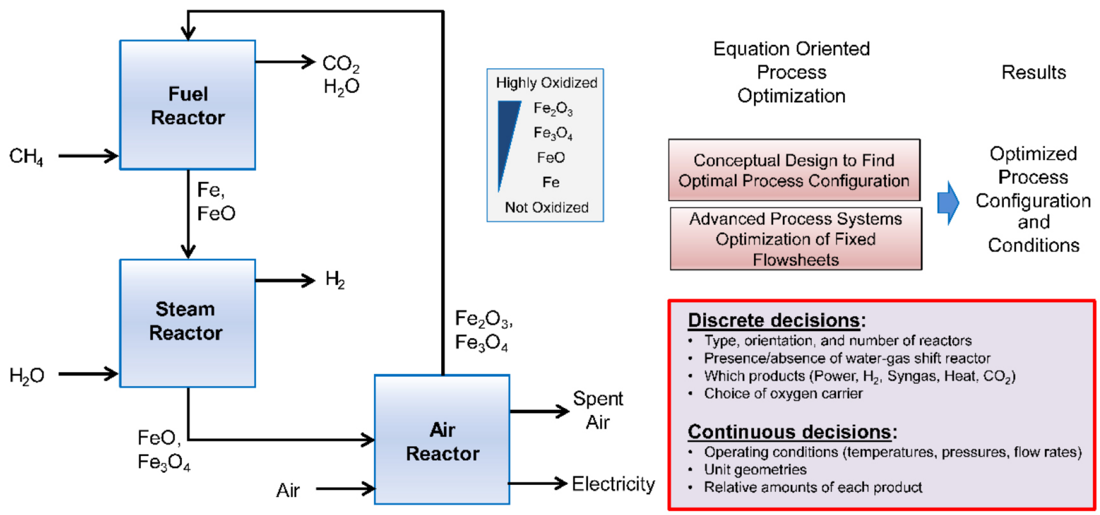
- Systematic identification, evaluation, and prioritization of R&D concepts throughout the development cycle, including identification of gaps and enabling technologies, to enable new technologies to be successfully deployed in the market and to enable existing assets to remain economically competitive.

- Key analytical support for Fossil Energy portfolio analysis and definition of component and technology goals based on both plant-level and broader life cycle, infrastructure and market needs.

- Support for the development of new energy technologies through the use of models and computational approaches to reduce technical risk and maximize learning at each stage of the development process, enabling increased rate of maturation.

- An optimization framework that can be extended to other complex energy challenges, including optimization of base and intermittent energy generation sources within the grid, an effective and efficient distribution system, and approaches to manage the water-energy-food challenges looming into the 21st century.

- For policy makers, an unbiased, science-based, holistic understanding of the trade-offs between various energy technologies and future scenarios.



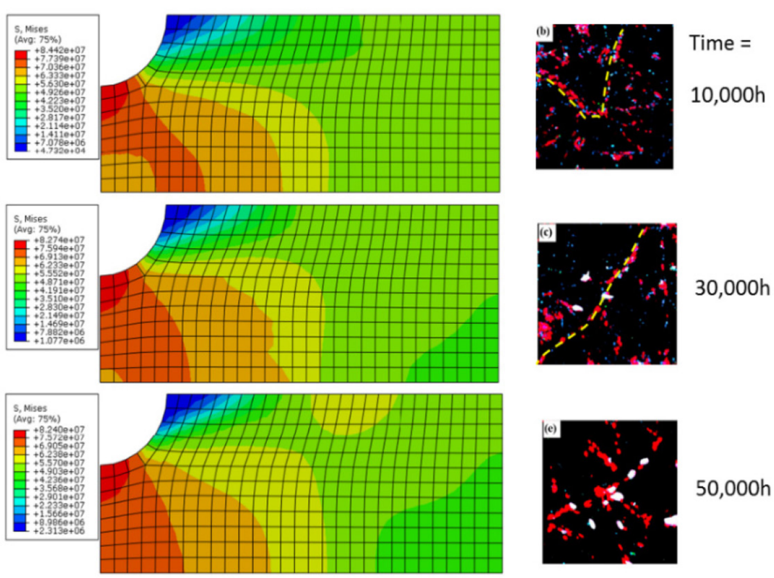

**Conceptual design of chemical looping systems.**

IDAES
Institute for the Design of Advanced Energy Systems

NATIONAL ENERGY TECHNOLOGY LABORATORY   BERKELEY LAB   Sandia National Laboratories   Carnegie Mellon   West Virginia University

# MATERIALS





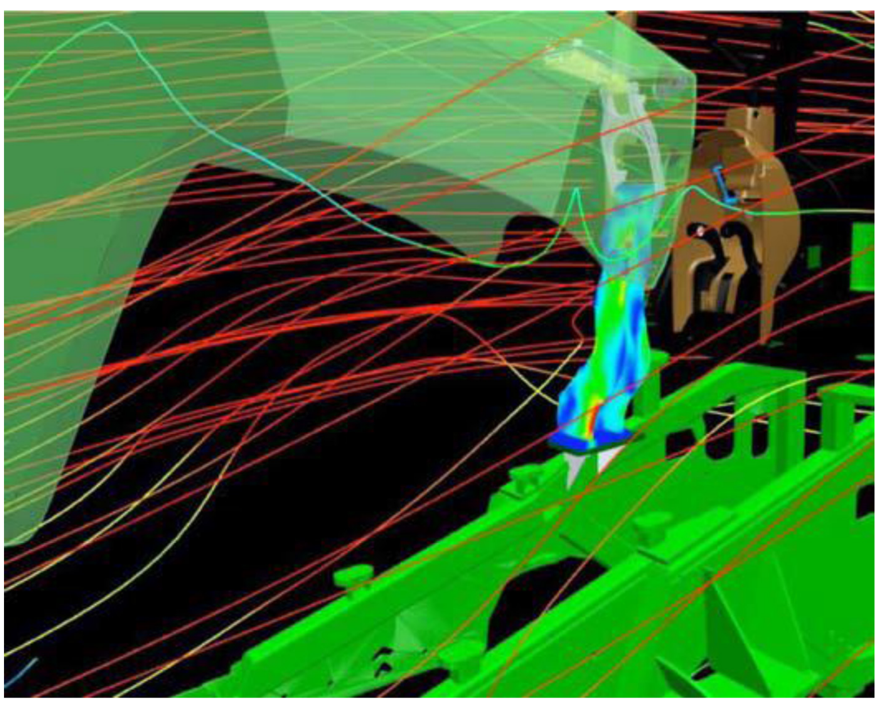
# Computational System Dynamics (Computational Design of Multiscale Systems)

| | |
|---|---|
| **Performer** | Ames Laboratory |
| **Award Number** | FWP-AL-14-450-012 |
| **Project Duration** | 10/01/2014 – 09/30/2018 |
| **Total Project Value** | $791,000 |
| **Technology Area** | Coal Utilization Sciences |

NETL partnered with Ames Laboratory to develop computational algorithms, strategies, and an informational framework needed to design materials in an integrated manner across length and time scales, creating the ability to design and tailor material properties for specific applications. The overall objective of the project is to provide a capability to assess degradation mechanisms and improve the reliability of refractory alloys for coal gasification and related processes.

The project will investigate potential alloy formulations using progressively more accurate thermodynamic methods; conduct critical experiments to test the accuracy of the calculations; evaluate each alloy's key mechanical, thermal, and oxidation properties; and screen alloys showing the greatest potential for high-performance thermochemical stability using state-of-the-art thermal analysis, high-temperature X-ray diffraction analysis, and microstructural evaluation with electron microscopy.

The resulting tool will allow researchers to reduce possible alloy formulations from tens of thousands to a manageable number of combinations that are most likely to succeed.



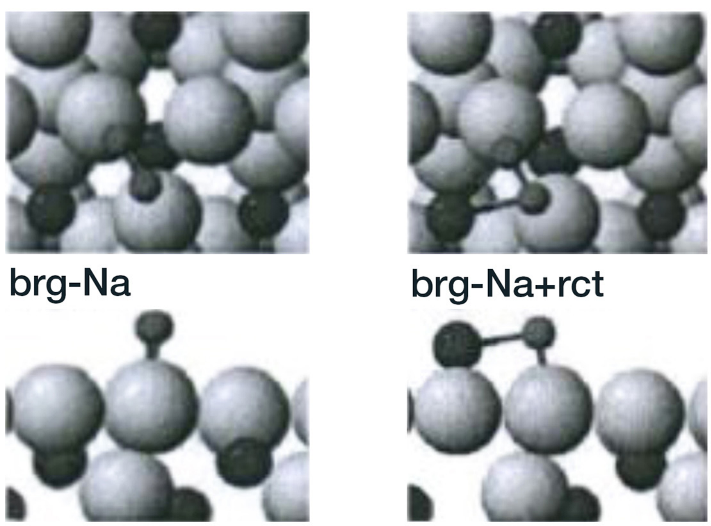
**Graphic output from Virtual Engineering (VE) -suite of a simulation of the response of part of a component to an external load.**

# The SMARTER Project (Science of Multicomponent Alloys: Roadmap for Theoretical and Experimental Research)

| | |
|---|---|
| **Performer** | Ames Laboratory |
| **Award Number** | FWP-AL-14-510-075 |
| **Project Duration** | 04/01/2015 – 09/30/2018 |
| **Total Project Value** | $510,000 |
| **Technology Area** | Coal Utilization Sciences |

NETL is partnering with Ames Laboratory to propose a new methodology to speed the discovery and optimization of chemically complex alloys and leverage theoretical and experimental capabilities for assessing their long-term stability. Near equiatomic alloys have a high degree of chemical disorder in a single high-temperature phase leading to high mechanical strength. These disordered alloys have potential for fossil energy use in high-temperature applications; however, their long-term stability in harsh combustion environments has not yet been explored.

Near equiatomic alloys offer excellent promise as structural materials for use in several commercial applications, including gas turbines for power generation, advanced ultrasupercritical boiler walls, aerospace engines, and nuclear reactor walls.



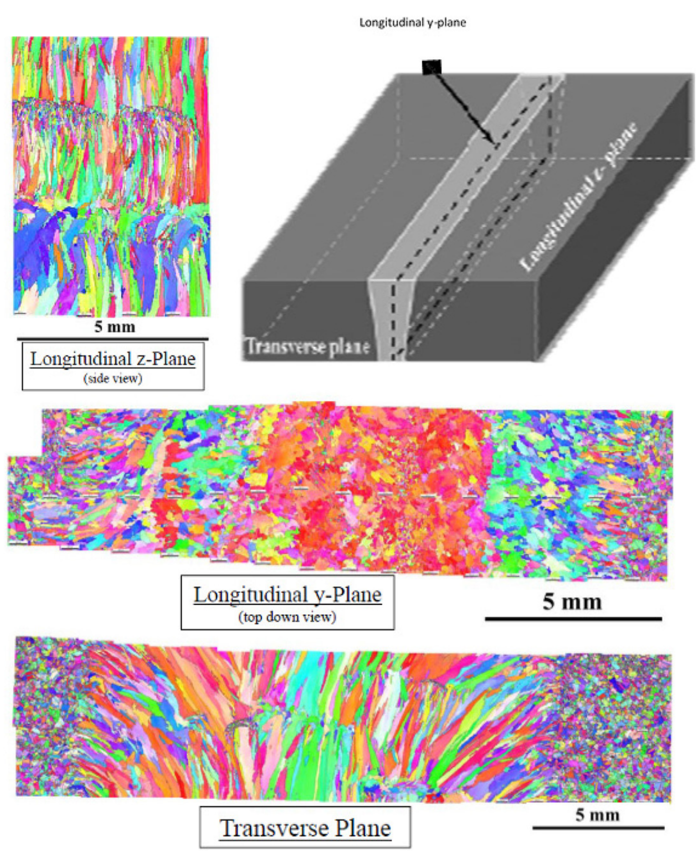

**$O_2$ adsorption on $NaAu_2$ (111) surface at the brg-Na site (left) and the same site with reconstruction of surface Na pop-up (right).**

# Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications

| | |
|---|---|
| **Performer** | Idaho National Laboratory |
| **Award Number** | FWP-B000-14029 |
| **Project Duration** | 06/01/2015 – 09/30/2018 |
| **Total Project Value** | $955,000 |
| **Technology Area** | Coal Utilization Sciences |

Idaho National Laboratory (INL) will improve the capability to perform accurate and rapid computational modeling of the long-term mechanical behavior of nickel superalloy weldments that will be used in advanced fossil energy power cycles. An improved capability to predict the long-term behavior of weldments will allow materials scientists and structural component designers to optimize the use of advanced materials in advanced fossil energy applications. In this project INL will develop a microstructure-based creep model for nickel superalloys and add it to a computational platform, Multiphysics Object-Oriented Simulation Environment (MOOSE), that INL has developed for multi-scale simulation of the behavior of high-temperature materials in nuclear power plant applications.

This project will develop improved computational methods to predict the long-term behavior of advanced materials and structural components in fossil energy power plants that will reduce the time and expense of developing and qualifying new materials and enable a more cost-effective use of advanced materials at higher operating temperatures and pressures, which will result in higher-efficiency fossil fuel based power systems.



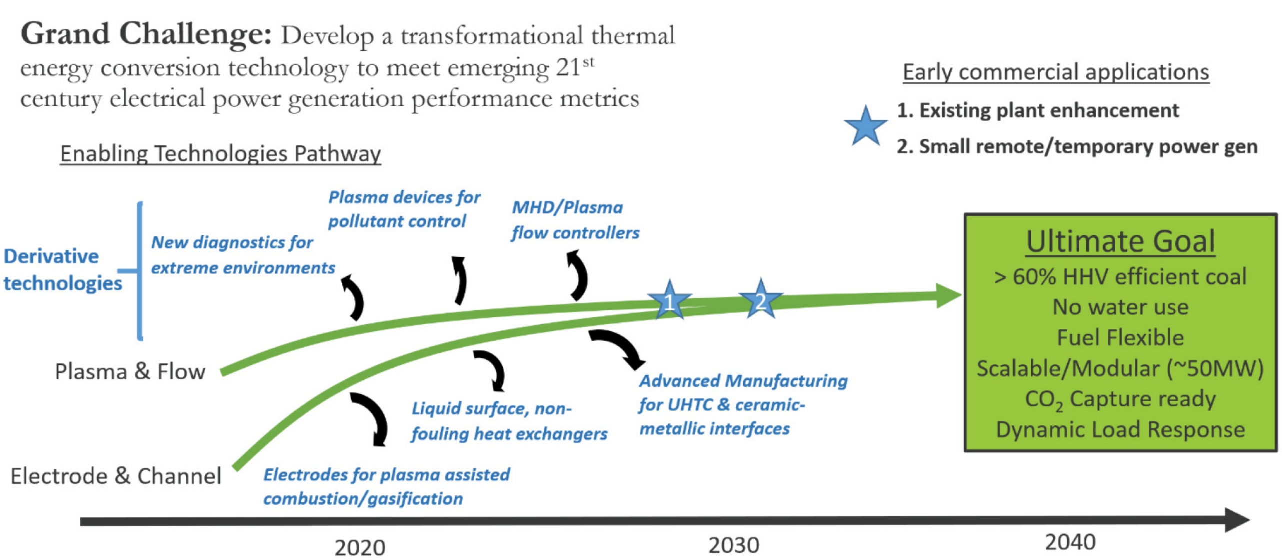

**Microstructure of base metal, heat affected zone, and weld metal.**

# Direct Power Extraction

| | |
|---|---|
| **Performer** | National Energy Technology Laboratory – Research and Innovation Center |
| **Award Number** | RIC Advanced Combustion FWP – 1022401 |
| **Project Duration** | 01/01/2018 – 03/31/2018 |
| **Total Project Value** | $1,229,000 |
| **Technology Area** | Coal Utilization Sciences |

This early stage R&D plan describes a multi-year plan to conclusively determine the viability of magnetohydrodynamic (MHD) power generation for future fossil-derived electrical power generation with and without carbon capture. An MHD power generator directly converts the kinetic energy of a working fluid into electrical power. Succinctly, MHD replaces conventional mechanical conversion steps (i.e., momentum transfer in a turbine) with the direct power extraction (DPE) concept. Consequently, the maximum efficiencies are inherently higher than those of conventional turbine-based fossil conversion systems. Historic MHD research has established key facts: A combined cycle system with fossil-based MHD power generators could in theory exceed 60 percent higher heating value thermal efficiency, and constructed MHD power generators have yielded expected power performance. Today, it is apparent that MHD-derived power complements the oxy-fuel approach for carbon capture. It is generally clear that material durability and overall systems costs were key issues that hampered commercialization following past U.S. Department of Energy R&D into MHD power generation. Since then, advantageous technology improvements related to magnets and other key technologies have been developed, and oxy-fuel products can yield about twice the MHD power density compared to legacy pre-heated air or enriched-air open cycle systems. On balance, a devoted and focused technical effort will allow the Office of Fossil Energy to critically evaluate the promise of this potentially high-efficiency technology. Technology development will be focused on the establishment of the theoretical and practical performance of MHD energy conversion systems and experimental validation of the performance and reliability of key components for those systems.

The high-level goal of this work is to conclusively determine the viability of MHD power generation for future fossil-derived electrical power generation. To meet this goal, this work proposal will execute the appropriate techno-economic analysis, develop and verify the required simulation tools for this analysis, and experimentally validate device scale simulations. Systems which utilized DPE are being analyzed and ranked according to efficiency, cost, and various other qualitative factors. Simulations are

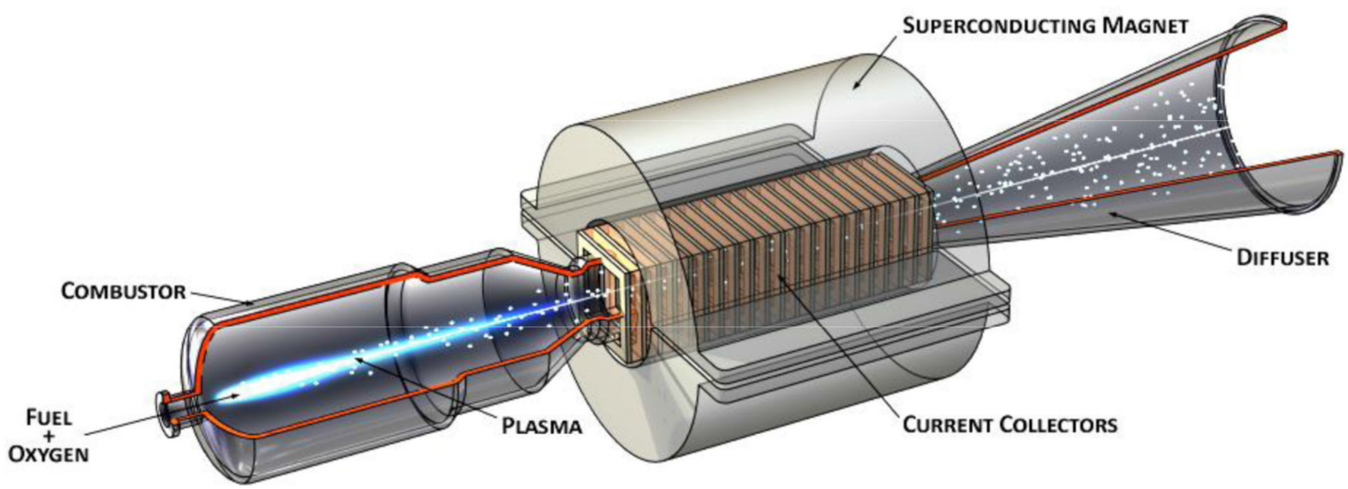



**Conceptual roadmap for continued DPE technology development with near term spin-offs.**

being developed and utilized to accurately predict MHD generator performance. Experiments are performed to validate those simulations to increase our confidence in the performance predictions. Standard and novel materials are being developed, simulated, and tested for use as MHD channel materials. This effort focuses on developing and utilizing fundamentals to be useful in a technology viability assessment, and not focused on demonstrations or detailed optimizations of the technology.

This activity will also define a technology development roadmap, as conceptually shown in the figure. This will include consideration of near term technology spin-offs, and efforts toward developing an early commercial application of DPE. Ideas for existing plant retrofits to enhance plant efficiency and remote or temporary power generation applications will be developed in this activity.

In addition to conclusively answering the primary question of technical viability, the project will produce and transfer significant research on fossil energy-relevant topics including mass and thermal flow modeling in aggressive operating environments, functional material development for aggressive applications, and in situ measurement techniques for reactive flow streams, among others.



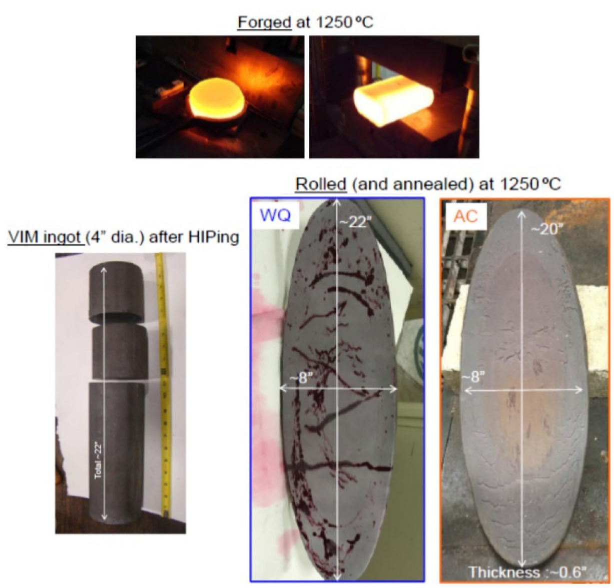

**An oxy-fuel fired open cycle MHD power generator. A diffuser is used to slow the flow down prior to it entering a bottoming cycle.**

# Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications

| | |
|---|---|
| **Performer** | Oak Ridge National Laboratory |
| **Award Number** | FWP-FEAA114 |
| **Project Duration** | 10/01/2013 – 09/30/2018 |
| **Total Project Value** | $1,934,000 |
| **Technology Area** | Plant Optimization Technologies |

NETL is partnering with Oak Ridge National Laboratory to identify and apply breakthrough alloy design concepts and strategies for incorporating improved creep strength, environmental resistance, and weldability into the classes of alloys intended for use in heat exchanger tubes in fossil-fueled power generation systems at higher temperatures than are possible with currently available alloys. This work will develop stable microstructures with dispersion of strengthening second-phase precipitates based on guidance from computational thermodynamics and modeling of inter-diffusion, including new directions suggested by ongoing modeling studies in other Crosscutting Research projects; apply mechanistic understanding of the development and evolution of microstructures associated with strengthening phases, and of the influences of and interactions with the concentration and distribution of specific elements necessary to form an inherently protective outer oxide layer; and use advanced analytical techniques, and especially their evolution, as a function of time, temperature, and external environment.

Higher performance from alloys used in fossil-fueled power generation systems at higher temperatures will lead to improvements in efficiency and operational flexibility and result in lower operating costs.



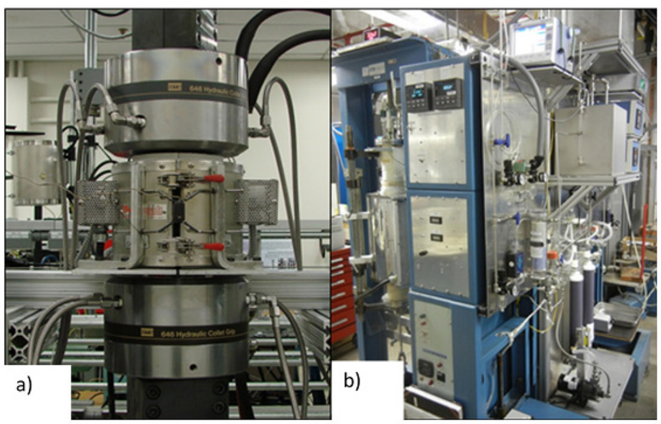

Scale-up efforts (Fe-30Cr-3Al-2Nb-0.2Si-0.12Y).

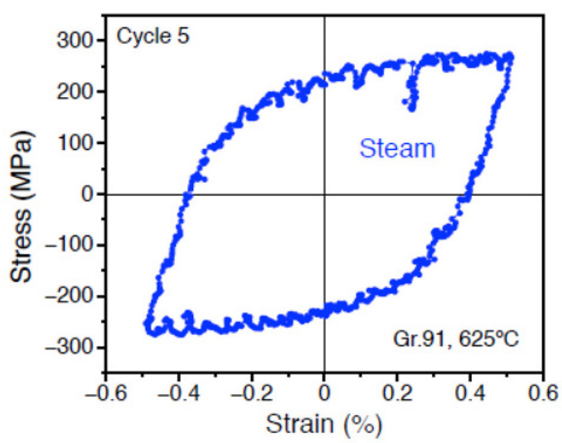
# Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes under Fossil Energy Service Conditions

| | |
|---|---|
| **Performer** | Oak Ridge National Laboratory |
| **Award Number** | FWP-FEAA115 |
| **Project Duration** | 10/01/2013 – 09/30/2018 |
| **Total Project Value** | $1,500,000 |
| **Technology Area** | Coal Utilization Sciences |

NETL is partnering with Oak Ridge National Laboratory to generate pertinent creep-fatigue data and develop new lifetime models to help accurately predict the lifetimes of fossil fuel power plant components that are subjected to flexible operation (e.g., load cycle following of renewable power generation). Such flexible operation can cause thermal-mechanical fatigue of components over long periods, resulting in their premature failure. Most existing coal-fired power plants were not designed for this type of operation, and new advanced fossil fuel plants may need to include flexible operation in their thermal/mechanical design.

Improvements to creep-fatigue data and lifetime models will advance the development of advanced power plant designs, improve efficiency and operational flexibility, and reduce operating costs.




**a) Servo-hydraulic creep-fatigue machine.**

**b) Thermal cyclic creep machines allowing testing in steam.**

**Bottom: Stress-strain curve, 9Cr-1Mo ferritic steel, 625 °C, fully reversed 1% total deformation, steam.**

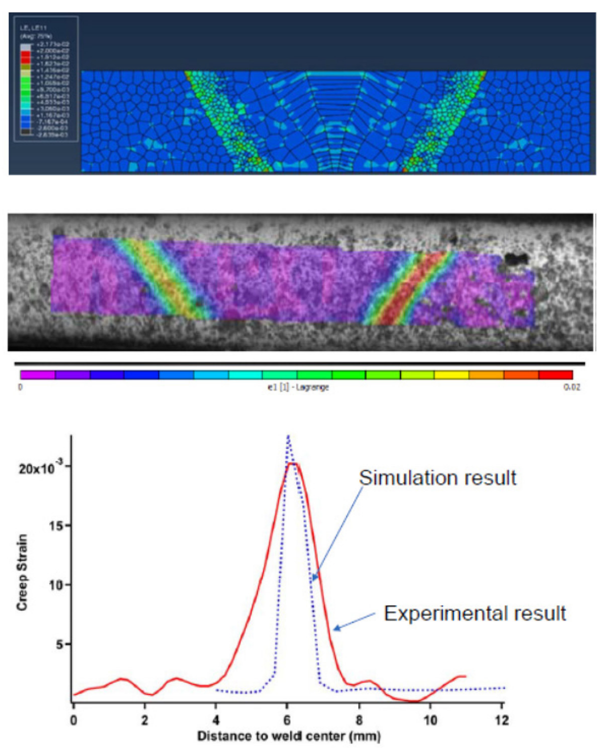
# Weldability of Creep Resistant Alloys for Advanced Power Plants

| | |
|---|---|
| **Performer** | Oak Ridge National Laboratory |
| **Award Number** | FWP-FEAA118 |
| **Project Duration** | 10/01/2013 – 09/30/2018 |
| **Total Project Value** | $1,450,000 |
| **Technology Area** | Coal Utilization Sciences |

NETL is partnering with Oak Ridge National Laboratory (ORNL) to develop practical engineering solutions to two key issues regarding the weldability of high-temperature creep-resistant alloys used in advanced fossil energy power plants: (1) the reduced creep strength of the weld region versus the base metal and (2) welding of dissimilar metals.

The work will develop fundamental mechanistic understanding of the weld failure process using advanced in-situ neutron and synchrotron experimental techniques and a state-of-the-art integrated computational welding engineering (ICWE) modeling tool developed at ORNL; apply the ICWE modeling tool to simulate the microstructure and property variations in the weld region; develop an improved weld creep testing technique using digital image correlation to accurately measure the localized non-uniform deformation of a weld under high-temperature creep testing conditions; determine the local creep and creep-fatigue constitutive behavior in different regions of a weld; and develop new welding and post-heat treatment practices to improve the creep resistance of similar and dissimilar metal weldments.

The research will promote the design of advanced power plants capable of operating at higher temperatures and pressures, thus improving their efficiency and operational flexibility and reducing capital and operating costs.

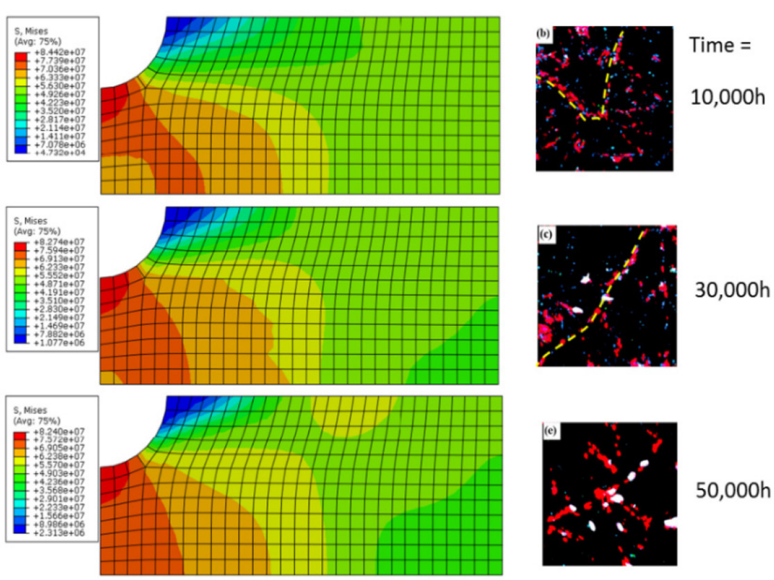



**Top: Modeling result.**
**Middle: Experimental result.**
**Bottom: Simulation result shows agreement with experiments.**

# Improved Models of Long Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants (Crosscutting Technology Research)

| | |
|---|---|
| **Performer** | QuesTek Innovations LLC |
| **Award Number** | SC0015922 |
| **Project Duration** | 06/13/2016 – 07/30/2019 |
| **Total Project Value** | $1,164,586 |
| **Technology Area** | Plant Optimization Technologies |

NETL is partnering with QuesTek Innovations LLC to develop a robust creep modeling toolkit to predict the long-term creep performance of materials for base alloys and weldments in fossil energy systems under wide thermal and mechanical conditions. Precipitation modeling using thermodynamic databases will provide fundamental quantities that will be used as inputs for upscaling strategies/methods. The goal is to establish microstructure-sensitive models that capture the different creep mechanisms observed in ferritic steels and integrate the models into QuesTek's Defense Advanced Research Projects Agency - Accelerated Insertion of Materials (DARPA-AIM) efforts to predict the variability of the creep strength as a function of the microstructure and service conditions. In the Phase I effort, the methods proposed have been demonstrated to predict creep life near 100,000 hours for P91 ferritic steels with microstructure inputs obtained from the National Institute of Material Science. In Phase II, the tools will be expanded and exercised in wider operating conditions including different temperatures and applied stresses in order to predict creep behaviors with over 300,000 hours creep life. Integration of precipitate evolution schemes into the long-term material behavior (i.e., stability of microstructure and the different phases over long periods), along with a refined uncertainty quantification of various material and process parameters, will be assessed and calibrated in Phase II. Additionally, the methodology developed would be applicable to alternative material systems and microstructures through additional modules that capture the relevant mechanisms of creep. Accurate and efficient quantification of material properties for advanced ultrasupercritical (AUSC) boilers will directly enhance the success of DOE's crosscutting research and new alloy development program and provide significant public benefits.



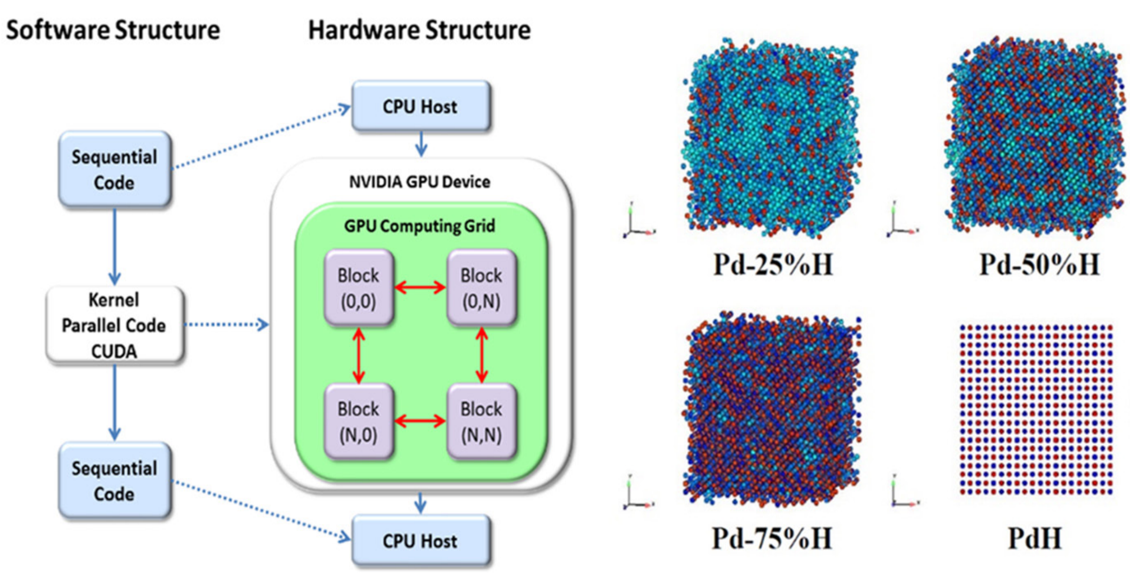

**Model prediction with microstructure evolution.**

# Large-Scale, Graphics Processing Unit (GPU)-Enhanced Density Functional Tight Binding (DFTB) Approaches for Probing Multi-Component Alloys

| | |
|---|---|
| **Performer** | Regents of the University of California at Riverside |
| **Award Number** | FE0030582 |
| **Project Duration** | 08/01/2017 – 07/31/2020 |
| **Total Project Value** | $250,000 |
| **Technology Area** | University Training and Research |

The objectives of this project are to develop, analyze, and introduce (1) accurate intermolecular potentials and (2) graphics processing unit enhancements to the density functional tight binding approach for high-throughput ab initio molecular dynamics calculations of multi-component alloys at elevated temperatures. Specifically, this transformative approach utilizes two complementary pathways that will employ a high degree of coordination and communication between them to realize a final, rigorously sound, and validated computational capability upon completion.

The capabilities developed in this project will provide accurate, efficient, and reduced cost assessment of alloy structural performance at elevated temperature and pressure operational conditions in advanced fossil energy power plants.




Large-scale simulations of alloy systems.

# ABBREVIATIONS

AIMMS . . . . . . . . . advanced interactive multidimensional modeling system

AMLs . . . . . . . . . . . . . . . . algebraic modeling languages

AMPL. . . . . . . . . a mathematical programming language

ARS . . . . . . . . . . . . . . . . . . Advanced Reaction Systems

AUSC. . . . . . . . . . . . . . . . . . .advanced ultrasupercritical

CCSI . . . . . . . . . . . . Carbon Capture Simulation Initiative

CFD . . . . . . . . . . . . . . . . . . computational fluid dynamics

DARPA-AIM . . . . . . . . . . . . Defense Advanced Research Projects Agency - Accelerated Insertion of Materials

DEM. . . . . . . . . . . . . . . . . . . . . discrete element method

DFTB . . . . . . . . . . . . . . . . density functional tight binding

DOE . . . . . . . . . . . . . . . . . . . . . . . Department of Energy

DPE . . . . . . . . . . . . . . . . . . . . . . .direct power extraction

EMRALD . . . . . . . . . . . . . . event model risk assessment using linked diagrams

FE . . . . . . . . . . . . . . . . . . . Office of Fossil Energy (DOE)

FWP . . . . . . . . . . . . . . . . . . . . . . . . Field Work Proposal

GAMS . . . . . . . . . . . .general algebraic modeling system

gPROMS . . . . . . . . . . general process modeling system

GPU . . . . . . . . . . . . . . . . . . . . .graphics processing unit

HBCU. . . . . . .Historically Black Colleges and Universities

HPC . . . . . . . . . . . . . . . . . . high performance computing

HYPRE. . . . . . . . . . . . high performance preconditioners

ICWE . . . . integrated computational welding engineering

IDAES. . . . . . . . . . . . . . . . . . . . Institute for the Design of Advanced Energy Systems

INL . . . . . . . . . . . . . . . . . . . . . Idaho National Laboratory

MFiX. . . . . . .Multiphase Flow with Interphase eXchanges

MHD. . . . . . . . . . . . . . . . . . . . . . .magnetohydrodynamic

MOOSE . . . . . . . . . . . . . . . . multiphysics object-oriented simulation environment

MPIC . . . . . . . . . . . . . . . . . . . .multiphase particle-in-cell

NETL . . . . . . . . . National Energy Technology Laboratory

NGOs. . . . . . . . . . . . . . . .non-governmental organizations

OMI . . . . . . . . . . . . . . . . . . . . . other minority institutions

ORNL. . . . . . . . . . . . . . . . .Oak Ridge National Laboratory

PETSc . . . . . . . . . . . . . . . . . . .portable extensible toolkit for scientific computation

PRA . . . . . . . . . . . . . . . . . . probabilistic risk assessment

ProSim . . . . . . . . . . . . . . . . . . . . . . . . process simulation

PSUADE. . . . . . . . . . . . .problem solving environment for uncertainty analysis and design exploration

R&D . . . . . . . . . . . . . . . . . . . .research and development

SBIR. . . . . . . . . . . . Small Business Innovation Research

TFM . . . . . . . . . . . . . . . . . . . . . . . . . . . . two-fluid model

U.S. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . United States

UCR . . . . . . . . . . . . . . . . . . . . . University Coal Research

UQ . . . . . . . . . . . . . . . . . . . . . . uncertainty quantification

UTR . . . . . . . . . . . . . . . University Training and Research

VE . . . . . . . . . . . . . . . . . . . . . . . . . . Virtual Engineering

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