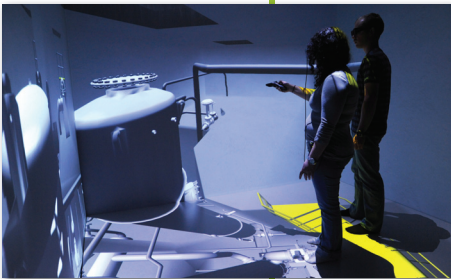
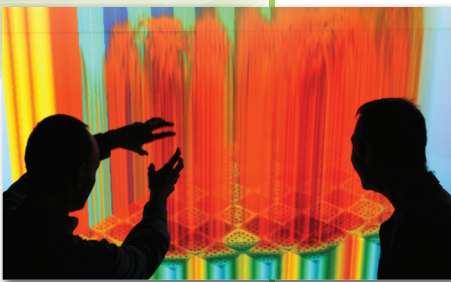


# ENERGY INNOVATION HUB FOR MODELING AND SIMULATION

*The U.S. Department of Energy's Office of Nuclear Energy*

*The Energy Innovation Hub for Modeling and Simulation will apply advanced modeling and simulation capabilities to find new ways to address nuclear energy safety, waste management, and operations.*

In early 2010, the Department of Energy (DOE) Office of Nuclear Energy (NE) held an open competition for a team to operate the Nuclear Energy Modeling and Simulation Hub. The results of the competition were announced in May 2010. The team chosen to operate the NE Hub is known as the Consortium for Advanced Simulation of Light Water Reactors (CASL). The team consists of four DOE laboratories (Oak Ridge, Idaho, Los Alamos, and Sandia), three universities (MIT, North Carolina State, Michigan), and three industry partners (Westinghouse, Tennessee Valley Authority (TVA), and the Energy Power Research Institute (EPRI)). The CASL team is applying advanced modeling and simulation (M&S) capabilities to develop a "virtual reactor" to simulate the Westinghouse-built, TVA-operated reactors at Sequoyia and Watts Bar. With the advent of very high-powered computing, advanced M&S can provide faster and more detailed insights into the operation of nuclear power plants. The immediate goal of the Hub is to find ways to improve the reliability, safety, and power output of nuclear reactor fuel during normal operation.



## OBJECTIVES

The Hub will achieve its goal of improving existing nuclear energy operations with advanced modeling and simulation through the following key objectives:

- Enable the use of leadership-class computing for engineering design and analysis to achieve reactor power uprates, life extensions, and higher fuel burnup.
- Develop a highly integrated multiphysics M&S environment for engineering analysis through increased fidelity methods (e.g., neutron transport and computational fluid dynamics (CFD), rather than diffusion theory and subchannel methods).
- Educate today's reactor engineers in the use of advanced M&S through direct engagement in CASL activities and develop the next generation of engineers through curricula at partner universities.
- Promote an enhanced scientific basis and understanding by replacing empirically based design and analysis tools with predictive capabilities.
- Incorporate uncertainty quantification (UQ) as a basis for developing priorities and supporting application of the Virtual Reactor tools for predictive simulation.

## Program Budget

EIH – Modeling and Simulation  
(\$ in Millions)

FY 2012  
Request  
\$24.3

- Engage the Nuclear Regulatory Commission to obtain guidance on the use and deployment of the CASL Virtual Reactor tools to support licensing applications.

## THE VIRTUAL REACTOR

The Energy Innovation Hub for Modeling and Simulation is developing advanced modeling and simulation capabilities to create a usable environment for predictive simulation of light water reactors (LWRs). This environment, designated the Virtual Reactor (VR), will incorporate science-based models, state-of-the-art numerical methods, modern computational science and engineering practices, and UQ and validation against data from operating pressurized water reactors (PWRs). It will couple state-of-the-art fuel performance, neutronics, thermal-hydraulics, and structural models with existing tools for systems and safety analysis and will be designed for implementation on both today's leadership-class computers and the advanced architecture platforms now under development by DOE.

## CHALLENGES

To accomplish the vision for the Virtual Reactor simulation tool, the Hub will focus on a set of challenges that encompass the key phenomena limiting the performance of PWRs, with the expectation that much of the capability developed will be applicable to other types of reactors. Broadly, the Hub's mission is to develop and apply modeling and simulation capabilities to address three critical areas of performance for nuclear power plants:

- Capital and operating costs per unit energy, which can be reduced by enabling power uprates and lifetime extension for existing plants and increasing the rated powers and lifetimes of new Generation III+ plants;
- Nuclear waste volume generated, which can be reduced by enabling higher fuel burnups; and
- Nuclear safety, which can be enhanced by enabling high-fidelity predictive capability for component performance through failure.

## SCOPE

To develop the Virtual Reactor, CASL has organized the Hub into five technical focus areas:

**Advanced Modeling Applications (AMA)** — AMA is the primary interface of the Virtual Reactor with the applications related to existing physical reactors, the challenge problems, and full-scale validation. AMA will provide necessary direction to the Virtual Reactor by developing the set of functional requirements, prioritizing the modeling needs, and performing assessments of capability.

**Virtual Reactor Integration (VRI)** — VRI develops the Virtual Reactor tools integrating the models, methods, and data developed by other focus areas within a software framework. VRI will collaborate with AMA to deliver usable tools for performing analysis, guided by the functional requirements developed by AMA.

**Models and Numerical Methods (MNM)** — MNM advances existing and develops new fundamental modeling capabilities for nuclear analysis and associated integration with solver environments utilizing large-scale parallel systems. The primary mission of MNM is to deliver radiation transport and thermal-hydraulics components that meet the rigorous physical model and numerical algorithm requirements of the Virtual Reactor.

**Materials Performance and Optimization (MPO)** — MPO develops improved materials performance models for fuels, cladding, and structural materials to provide better prediction of fuel and material failure. The science work performed by MPO will provide the means to reduce reliance on empirical correlations and enable the use of an expanded range of materials and fuel forms.

**Validation and Uncertainty Quantification (VUQ)** — The quantification of uncertainties and associated validation of the Virtual Reactor models and integrated systems are essential to the application of M&S to reactors. Improvements in the determination of operating and safety margins will directly contribute to the ability to uprate reactors and extend their lifetimes. The methods proposed under VUQ will significantly advance state-of-the-art nuclear analysis and support the transition from integral experiments to the integration of small-scale separate-effect experiments.

## PLANNED PROGRAM ACCOMPLISHMENTS

### FY 2011

- Apply the virtual reactor simulation code (VERA) to model the formation of deposits on reactor fuel cladding and mechanical fretting within fuel assemblies to assess the potential for power uprates and higher fuel burnup. The analysis will be based on coupled neutronics (transport) and thermal-hydraulics.
- Issue a major release of the VERA to CASL partners and the broader nuclear energy community. Emphasis will be on the code-coupling infrastructure and initial physics capabilities (transport, thermal hydraulics, mechanics, fuel performance, coolant chemistry) in support of fuel performance analysis.
- Complete and document the VERA requirements by developing the functional and user requirements to support VERA development activities.
- Release initial CASL UQ capability within VERA—in particular, the CASL mathematical data assimilation framework with the required new numerical algorithms for quantifying nonlinear effects up to and including fourth-order uncertainties.

*CASL connects fundamental research and technology development through an integrated partnership of government, academia, and industry that extends across the nuclear energy enterprise.*



## **FY 2012**

- Apply VERA to the following problems: prediction of departure from nucleate boiling, calculation of radionuclide source terms, prediction of deposits on fuel, and calculation of Grid-to-Rod Fretting (fuel rod vibration).
- Compare the virtual reactor analysis with the Physical Reactor; the physical reactor model development will be completed and an initial qualification of results of VERA analysis with operational data from the physical reactor will occur.
- Release the second generation of VERA to CASL partners and the broader nuclear energy community. Capabilities delivered in VERA include higher-fidelity versions of the initial physics capabilities (transport, thermal hydraulics, mechanics, fuel performance, and coolant chemistry), but with improved predictability afforded by the addition of new science-based models for fuel and structural material performance and response (fuel/clad microstructure, corrosion chemistry, foreign material deposition and growth, and brittle failure).
- Deliver capability for coupling sensitivity results from each VERA component for full system response sensitivities and broadened UQ support within VERA to address epistemic and modeling bias uncertainties.
- Add advanced fluid modeling capabilities to VERA, including computational fluid dynamics and incompressible, single-phase flow with sub-cooled boiling flow capability.