

# The Consortium for Advanced Simulation of Light Water Reactors

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Ronaldo Szilard  
Douglas Kothe  
Paul Turinsky

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## The Consortium for Advanced Simulation of Light Water Reactors

Ronaldo Szilard<sup>a</sup>, Douglas Kothe<sup>b</sup>, Paul Turinsky<sup>c</sup>

<sup>a</sup> *Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3870, USA*  
Tel: +1 (208)526-8376, Fax: +1 (208)526-0528, Email: [Ronaldo.Szilard@inl.gov](mailto:Ronaldo.Szilard@inl.gov)

<sup>b</sup> *Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6290, USA*

<sup>c</sup> *Department of Nuclear Engineering, North Carolina State University, Raleigh, NC 27695-7909, USA*

### ABSTRACT

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is a DOE Energy Innovation Hub for modeling and simulation of nuclear reactors. It brings together an exceptionally capable team from national laboratories, industry and academia that will apply existing modeling and simulation capabilities and develop advanced capabilities to create a usable environment for predictive simulation of light water reactors (LWRs). This environment, designated as the Virtual Environment for Reactor Applications (VERA), will incorporate science-based models as appropriate, state-of-the-art numerical methods, modern computational science and engineering practices, and uncertainty quantification (UQ), and be qualified using data from operating pressurized water reactors (PWRs). It will couple state-of-the-art fuel performance, neutronics, thermal-hydraulics (T-H), 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 computers that will be commercially available and attractive to the nuclear industry in half a decade. CASL focuses on a set of challenge problems such as CRUD induced power shift and localized corrosion, grid-to-rod fretting fuel failures, pellet clad interaction, fuel assembly distortion, etc. that encompass the key phenomena limiting the performance of PWRs. CASL will also develop capabilities to better predict fuel performance during abnormal conditions such as experienced during LOCA and RIA. It is expected that much of the capability developed will be applicable to other types of reactors. CASL's mission is to develop and apply modeling and simulation capabilities to address three critical areas of performance for nuclear power plants: 1) reduce capital and operating costs per unit energy by enabling power uprates and plant lifetime extension, 2). reduce nuclear waste volume generated by enabling higher fuel burnup, and 3). enhance nuclear safety by enabling high-fidelity predictive capability for component performance.

### 1. INTRODUCTION

Modeling and simulation have played significant roles in terms of improved understanding, reliability, safety and reduced costs of nuclear energy systems. The U.S. Department of Energy is now embarking on major efforts to develop high-performance computer simulation capabilities for broad application to nuclear energy systems.<sup>1</sup> The Consortium for Advanced Simulation of Light Water Reactors (CASL)<sup>2</sup> has been established as the first U.S. Department of Energy (DOE) Energy Innovation Hub for Modeling and Simulation for Nuclear Reactors. CASL started its operations on July 1, 2010, at its Oak Ridge National Laboratory (ORNL) headquarters with full participation from its ten core partners (ORNL, Idaho National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, Electric Power Research Institute,

Westinghouse Electric Company, Tennessee Valley Authority (TVA), North Carolina State University, University of Michigan, and Massachusetts Institute of Technology).

CASL's mission is to develop and apply models, methods, data, and understanding while addressing three critical areas of performance for nuclear power plants (NPPs):

- Reducing capital and operating costs per unit of energy by enabling power uprates and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new Generation III+ NPPs,
- Reducing nuclear waste volume generated by enabling higher fuel burnup, and
- Assuring nuclear safety by enabling high-fidelity predictive capability for component performance through failure.

CASL will apply existing modeling and simulation (M&S) capabilities and develop advanced capabilities to create a usable environment for predictive simulation of light water reactors. This environment, designated the Virtual Environment for Reactor Applications (VERA), will incorporate science-based models as appropriate, state-of-the-art numerical methods, modern computational science and engineering practices, and uncertainty quantification (UQ), and be qualified using data from operating pressurized water reactors (PWRs), single-effect experiments, and integral tests. It will couple state-of-the-art fuel performance, neutronics, thermal-hydraulics, and structure models with existing tools for systems and safety analysis and will be designed for implementation on today's leadership-class computers and computers that will be commercially available and attractive to the nuclear industry in half a decade. Such a capability is envisioned to help quantify design margins as well as reducing the level of conservatism that must be applied to account for the shortcomings of current design and analysis approaches. The goal is for VERA to help support the more rapid introduction of new products through the employment of science-based, predictive M&S to address three key issues for nuclear energy: cost, reduction in amount of used nuclear fuel, and safety. The first two can be enabled by power uprates, lifetime extension, and higher burnup while assuring the third, safety.

Power uprates have reduced the cost of nuclear-power-generated electricity by increasing the revenue generated for a given capital investment. Since 1977, power uprates at existing plants have delivered over 6 GWe to the U.S.'s grid<sup>3</sup>, equivalent to building an additional five to six NPPs for a fraction of the cost of constructing new reactors. This has been achieved not only by plant and fuel modifications but also by application of best-estimate M&S capabilities, which have enabled the recovery of conservatism in safety analysis. The vendor and/or utility must have confidence that the power uprate will not cause accelerated damage to the NPP system, structure and components (SSC) during normal operations. Key concerns are integrity of fuel (due to increased fuel duty) and the steam generator (due to increased steam loads).

Lifetime extension requires the ability to predict with confidence the onset of SSC degradation so that corrective maintenance actions can be taken. Monitoring and inspection of SSC in combination with a predictive capability are necessary. Key concerns are the integrity of the reactor vessel and internals; these concerns are due to increased radiation damage, thermal fatigue, mechanical fatigue and aging. Performance questions about SSC outside the vessel (such as the effects of aging on the containment and piping) also need consideration and are being addressed in another DOE program, i.e. Light Water Reactor Sustainability Program. A mature and predictive VERA simulation capability will allow CASL to address this issue in depth.

Higher fuel burnup is also necessary to support power uprates. For a certain percentage increase in power rating without a coincident increase in the fuel burnup limit, the need for additional fuel assemblies would also increase the fuel cost, reducing the savings associated with power uprates. More important, higher fuel burnup supports a reduction in the amount of used nuclear fuel. Higher fuel burnup challenges cladding integrity; key concerns are fretting, corrosion, corrosion-related unidentified deposits (CRUD), hydriding, creep, and cladding-fuel mechanical interactions. For normal operation, this implies cladding integrity; for accident conditions, acceptable levels of degradation of the cladding fission product barrier must be demonstrated.

## 2. CASL Challenge Problems

The specific applications driving VERA development are targeted *challenge problems* that are focused on enabling power uprates and plant lifetime extension, and higher fuel burn-up, as well as providing a significant improvement in the predictive M&S capability to address the key phenomena currently limiting the performance of PWRs, with the recognition that much of the capability developed will be broadly applicable to other types of reactors. A review of challenges to reactor power level, burnup, and lifetime indicates ten key limiting phenomena, as shown in Table 1.

**Table 1. Key Phenomena Limiting Improved Reactor Performance**

Phenomena	Power Uprate	Higher Burn-up	Life Extension
<b><i>Operational</i></b>			
CRUD-Induced Power Shift (CIPS)	X	X	
CRUD-Induced Localized Corrosion (CILC)	X	X	
Grid-to-Rod Fretting Failure (GTRF)		X	
Pellet Clad Interaction (PCI)	X	X	
Fuel Assembly Distortion (FAD)	X	X	
<b><i>Safety</i></b>			
Departure from Nucleate Boiling (DNB)	X		
Cladding Integrity during Loss of Coolant Accidents (LOCAs)	X	X	
Cladding Integrity during Reactivity Insertion Accidents (RIA)	X	X	
Reactor Vessel Integrity	X		X
Reactor Internals Integrity	X		X

From these limiting phenomena, ten CASL challenge problems have been defined, and these drive requirements for VERA development and application. Each challenge problem carries its own unique set of functional science and engineering requirements, and these requirements provide a means to prioritize CASL activities. A hierarchy of milestones linked to these requirements provides a means of tracking and assessing progress. The description of the ten challenge problems are as follows:

1). CRUD: Two phenomena are considered associated with CRUD - CRUD Induced Power Shift (CIPS) and CRUD Induced Local Corrosion (CILC). CIPS can be explained as CRUD

deposition in high power density regions with subcooled boiling that causes deviation in axial power shape by accumulation of boron in the CRUD layer. CILC causes clad corrosion and failure due to CRUD deposition that in turn elevates the clad surface temperature. Both CIPS and CILC would limit power uprates which yield higher power density and an increased potential for CRUD growth, axial power offsets, and clad failures.

2). Grid-to-Rod Fretting (GTRF): GTRF has been the leading cause of fuel failure in PWRs. It causes clad failure due to flow vibration-induced rod-spring interactions amplified by irradiation-induced grid spacer growth and spring relaxation along with changes in the fuel rod radius. Power uprates and burnup increase the potential for fretting failures.

3). Internals Lifetime: Thermal fatigue, mechanical fatigue, radiation damage, and stress corrosion cracking all cause damage to core internals packages. Replacement cost of internals is high, making lifetime extension less economically attractive.

4). Departure from Nucleate Boiling (DNB): DNB results from local clad surface dryout causing dramatic reduction in heat transfer capability during certain accident transients (e.g., overpower and low coolant flow). Power uprates require improved quantification of margins for DNB limits. CASL's focus is on modeling subcooled boiling to better understand and predict the onset of DNB.

5). Fuel Assembly Distortion (FAD): Excessive axial forces caused by radiation-induced swelling induce fuel assembly distortion and component structural failure. FAD has a high adverse impact on plant performance. Power uprates and increased burnup may increase fuel distortions and alter the core power distributions and fuel handling scenarios.

6). Advanced Fuel Forms: New fuel forms will enable power uprates, higher fuel burnup, and lower fuel cycle costs than can be achieved by incremental modifications of current fuel forms, i.e., zirconium alloy cladding, UO<sub>2</sub> fuel pellet, and cylindrical geometry. Advanced analytical tools are required to examine new cladding material, fuel material and fuel pin geometries.

7). Loss of Coolant Accident (LOCA): Realistic LOCA analyses (10 CFR 50.46) can enable power uprates that would not have been achievable with previously licensed evaluation models. CASL's focus is on modeling fuel performance under the core conditions experienced during LOCA.

8). Reactivity Insertion Accident (RIA): RIA can cause clad failure due to rapid heating of the pellet, leading to pellet disintegration caused by the rim effect. Higher fuel burnup increases the rim effect. Power uprates may lead to increased energy release during RIA. This phenomenon currently is not limiting but may change with further test data such as CABRI data and proposed regulatory criteria. The Cabri Water Loop Project is investigating the ability of high burn-up fuel to withstand the sharp power peaks that can occur in power reactors due to rapid reactivity insertion in the core.<sup>4</sup> CASL is addressing not only the core neutronics and thermal-hydraulic response to an RIA, but also the fuel response.

9). Pellet Clad Interaction (PCI): PCI causes clad failure due to pressure and radiation-induced fuel rod/cladding contact enhanced by stress corrosion cracking and fuel defects. Power uprates and increased burnup increase fuel/clad contact and the likelihood for fuel failures. Currently it only limits power ramp rates during normal operation, which are infrequent but can be costly when returning from an outage.

10). Reactor Vessel Lifetime: Radiation damage results in increased temperature for the onset of brittle failure, making failure more likely due to thermal shock stresses with Safety Injection System (SIS). Increased power rating and lifetime both increase radiation damage to the vessel. Low leakage loading patterns and proposed revised NRC rule indicate that expected vessel lifetime exceeds 80 years for most PWRs so is not of immediate concern, but conjectures about late blooming effects could change this situation if found valid. CASL's focus is on enhanced modeling of radiation field and thermal-hydraulics associated with the vessel, dependent upon other DOR program for material degradation models.

These ten challenge problems fall into six categories: CRUD, Grid-to-Rod Fretting Failure/Fuel Assembly Distortion (GTRF/FAD), Safety, Advanced Fuel (AF), Lifetime Extension (LE) and Operational Reactor (OR). By addressing these identified challenges through predictive simulations with quantified uncertainties, VERA will

- Facilitate improved quantification of design margins to support decision making concerning power uprates, lifetime extension, and higher fuel burnup for existing NPPs and fuel designs;
- Facilitate the introduction of new fuel designs with the enhanced performance characteristics necessary to further support power uprates and higher fuel burnup for existing; and
- Fundamentally impact the nuclear steam supply system design for future-generation NPPs.

### **3. CASL Execution and Implementation**

The CASL vision is to develop and embody VERA with predictive capability, by coupling state-of-the-art fuel performance, neutronics, thermal hydraulics (T-H), and structural models with existing system/safety analysis tools. To achieve this vision, CASL aims at carrying out the following activities:

- Enable the use of leadership-class computing for engineering design and analysis to achieve reactor power uprates, life extensions, and higher fuel burnup.
- Promote an enhanced scientific basis and understanding by replacing empirically based design and analysis tools with predictive capabilities.
- 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].
- Incorporate uncertainty quantification (UQ) as a basis for developing priorities and supporting application of VERA for predictive simulation.
- 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.
- Engage the nuclear regulator [the Nuclear Regulatory Commission (NRC)] to obtain guidance and direction on the use and deployment of VERA to support licensing applications.

To provide solutions to the challenge problems, CASL will execute in six technical focus areas (FAs) to ensure that VERA (1) is equipped with the necessary physical and analytical models and multiphysics integrators; (2) functions as a comprehensive, usable, and extensible system for addressing essential issues for NPP design and operation; and (3) incorporates the V&V, qualification and UQ needed for credible predictive M&S. The utility of VERA to reactor designers, nuclear power plant operators, nuclear regulators, and a new generation of nuclear

energy professionals is an important CASL performance metric. The six technical focus areas are described as follows:

1). *Materials Performance and Optimization (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 the reliance on empirical correlations and to enable the use of an expanded range of materials and fuel forms.

2). *Radiation Transport Methods (RTM)* – Develop next-generation neutron transport simulation tools to VERA, which consist of the primary development path based on 3D full-core discrete ordinates (Sn) transport, the legacy path based on full core, two-dimensional/one-dimensional (2D/1D) or to be developed 3D method of characteristic (MOC) transport, and the advanced development path based on hybrid Monte Carlo.

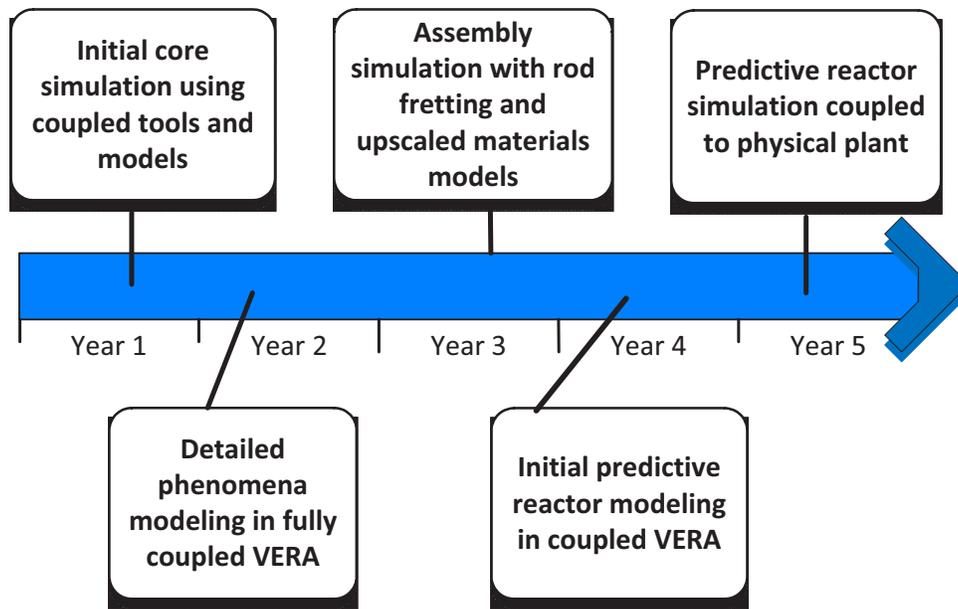


Figure 1. CASL evolving simulation capability roadmap

3). *Thermal Hydraulics Methods (THM)* – Advance existing and develop new modeling capabilities for thermal-hydraulics (T-H) analysis and its integration with solver environments deployed on large-scale parallel computers. With a strong focus on subcooled boiling, various CFD (e.g. RANS, URANS, LES and DNS) and ITM are being assessed for applicability to model the challenge problem requirements. The primary mission of THM is to deliver T-H components that meet the rigorous physical model and numerical algorithm requirements of VERA. Within the umbrella of validation and uncertainty quantification (VUQ), THM collaborates closely with MPO for sub-grid material and chemistry models, with RTM for coupling issues with radiation transport, and connects to virtual reactor integration (VRI) for integration and development of VERA.

4). *Virtual Reactor Integration (VRI)* – Develops VERA tools integrating the models, methods, and data developed by other FAs within a software framework, in addition to the fluid-structure interaction capabilities developed within VRI. Capability to replace VERA

simulation modules with user (proprietary) modules is being required. VRI collaborates with advanced modeling applications (AMAs) to deliver usable tools for performing the analyses, guided by the functional requirements developed by AMA.

5). *Validation and Uncertainty Quantification (VUQ)* – The quantification of uncertainties and associated V&V of VERA models and integrated systems are essential to the application of modeling and simulation to reactor applications. Improvements in the determination of operating and safety margins will directly contribute to the ability to make informed decisions to uprate reactors and extend their lifetimes, and increase fuel discharge burnup. The methods proposed under VUQ will significantly advance the state of the art of nuclear analysis and will support further complementing integral experiments with small-scale separate-effect experiments.

6). *Advanced Modeling Applications (AMA)* – The primary interface of CASL research and development (R&D) with the applications related to existing physical reactors, the challenge problems, and full-scale qualification. In addition, AMA will provide the necessary direction to models and methods development to be incorporated into VERA by providing the functional requirements, prioritizing the modeling needs, and performing assessments of capability. AMA also defines the overall verification and validation (V&V) and qualification requirements and engages with the NRC to provide confidence of regulatory acceptance of VERA capabilities.

Figure 1 shows the roadmap for the evolving simulation capability of VERA over a 5 year period. This roadmap supports the overall CASL objective to enable solution of the challenge problems.

#### **4. Collaboration and Ideation**

Early on it was recognized to address the challenge problems, a very talented staff composed of scientists and engineers would be required that does not exist at any single organization; hence, multiple organizations would need to partner to obtain the talent pool required. To facilitate collaboration and ideation among CASL's many partners, CASL adopts a virtual one-roof approach by widespread implementation of state-of-the-art collaboration technology. CASL's virtual one-roof strategy is dependent upon the development and maturation of the Virtual Office, Community, and Computing (VOCC) and computing/networking infrastructure. The VOCC consists of a unique set of infrastructure integrated in a special way so as to promote collaboration and critical thinking. Critical thinking leads to insight and insight leads to innovation. "Innovation at the speed of insight" means a more rapid deployment of predictive simulation capability to the LWR industry. CASL is not only working to reduce the capital and operating costs per energy unit for the installed base but also reducing the time and cost required for industry to drive LWR innovations and solutions to future designs with market functionality.

The key infrastructure components making up the VOCC collaboration laboratory are an immersive visualization system, an advanced telepresence (tele-immersion) system, an interactive multi-touch design system, and an ideation studio. Seamless integration of each unique component into a central information processor allows for sharing of visual LWR model and simulation information (2D and 3D). VOCC's telepresence and desktop video exchange technology will significantly increase CASL's colocation opportunities. Colocation, whether physical or virtual, spurs collaboration, resulting in a convergence of disparate knowledge

spaces. Collaboration takes place when human dynamics (human perception, perspective, and cognition) and information or data can be colocated physically or virtually with visually immersive, 3D design modeling systems. Collectively, these components form a virtual cognitive laboratory representing a collective design conscious of LWR design/operations knowledge and capability. By singularly locating this design knowledge and insight, we can guarantee rapid movement of technology and engineering practice into U.S. industry design/build centers.

VOCC does not represent “merely another computer architecture”. It represents an intellectual paradigm in which CASL and its partner sites will conduct daily Focus Area work tasks. Also prominent in its unique scalable integration design is the ability to quickly leverage collaboration infrastructure and tools located at other partner sites. Collectively, its architectural components form a virtual cognitive laboratory representing a collective design conscious of design knowledge and capability that can be generically used for a variety of applications beyond nuclear power—including automotive, fossil power plant, solar, wind, and geothermal, to name a few. So VOCC in its own right will make a substantial contribution to advancing science and technology decision making.

## 5. CONCLUSIONS

CASL connects fundamental research and technology development through an integrated partnership of government, academia, and industry that extends across the nuclear energy enterprise. The CASL partner institutions possess the interdisciplinary expertise necessary to apply existing M&S capabilities to real-world reactor design issues and to develop new system-focused capabilities that will provide the foundation for advances in nuclear energy technology. CASL’s organization and management plan have been designed to promote collaboration and synergy among the partner institutions, taking advantage of the breadth and depth of their expertise and capitalizing on their shared focus on delivering solutions.

To deliver on its mission within the prescribed time and budget constraints, CASL places priority on improved simulation of PWR cores, internals, and vessels. The developed CASL capability (VERA) will be tightly coupled to an existing and evolving out-of-vessel simulation capability. VERA, as developed, will be applicable to other NPP types, in particular boiling water reactors (BWRs) and LWR-based small modular reactors (SMRs).

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