A Project Summary

Power uprates and plant life extension

Engineering design and analysis

Science-enabling high performance computing

Fundamental science

Plant operational data
Oak Ridge National Laboratory

in partnership with
Electric Power Research Institute
Idaho National Laboratory
Los Alamos National Laboratory
Massachusetts Institute of Technology
North Carolina State University
Sandia National Laboratories
Tennessee Valley Authority
University of Michigan
Westinghouse Electric Company

and individual contributions from
ASCOMP GmbH
CD-adapco, Inc
City University of New York
Florida State University
Imperial College London
Rensselaer Polytechnic Institute
Southern States Energy Board
Texas A&M University
University of Florida
University of Tennessee
University of Wisconsin
Worcester Polytechnic Institute
SUMMARY OF PROJECT OBJECTIVES

The Consortium for Advanced Simulation of Light Water Reactors (CASL) brings together an exceptionally capable team that 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 (LWRs). This environment, designated the Virtual Reactor (VR), will:

- 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 UQ as a basis for developing priorities and supporting application of the VR tools for predictive simulation.

CASL will further 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 and engage the nuclear regulator (NRC) to obtain guidance and direction on the use and deployment of the CASL VR tools to support licensing applications.

CASL will focus on a set of challenge problems 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, CASL’s mission is to develop and apply M&S capabilities to address three critical areas of performance for nuclear power plants (NPPs):

- capital and operating costs per unit energy, which can be reduced by enabling power uprates and lifetime extension for existing NPPs and by increasing the rated powers and lifetimes of new Generation III+ NPPs;
- 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.

Work to develop the VR will be executed in five focus areas (FAs, see below) selected to ensure that the VR: (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 validation and UQ needed for credible predictive M&S. CASL’s management plan also includes tasks designed to ensure the utility of the VR to reactor designers, NPP operators, nuclear regulators, and a new generation of nuclear energy professionals.

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.

The CASL lead institution, Oak Ridge National Laboratory (ORNL), was founded to develop the world’s first nuclear fuel cycle and today is DOE’s largest science and energy laboratory, with world-leading capabilities in computing and computational science and substantial programs and assets in nuclear energy research and development (R&D), as well as a record of accomplishment in leading large-scale scientific collaborations. The participation of Idaho National Laboratory (INL), Los Alamos National Laboratory (LANL), and Sandia National Laboratories as CASL partners provides exceptional strengths in fundamental science, nuclear energy R&D, transformational high-performance computing (HPC) technology, and development of models and algorithms for the solution of complex problems. Academic partners North Carolina State University (NCSU), the University of Michigan (UM), and the Massachusetts Institute of Technology (MIT) are leaders in nuclear engineering R&D and education. The Electric Power Research Institute (EPRI) conducts R&D to ensure that nuclear power remains a safe and economically feasible generation option and provides CASL with connections to nuclear power plant operators, regulatory agencies, and other research organizations. Westinghouse Electric Company (WEC), a pioneer in nuclear power, has a long and successful history of supplying leading-edge nuclear technology. The Tennessee Valley Authority (TVA) operates six reactors that provide more than 6,900 MW of electricity to the grid and is engaged in a $2.5 billion project to complete a second PWR at its Watts Bar Nuclear Plant.

To deliver on its mission within the prescribed time and budget constraints, CASL will place near-term priority on improved simulation of the reactor core, internals, and vessel for a pressurized water reactor (PWR). The developed capability will be tightly coupled to an existing and evolving out-of-vessel simulation capability. Much of the CASL VR to be developed will be applicable to other NPP types, in particular boiling water reactors (BWRs). During its second 5 years of operation, CASL activities will expand to include structures, systems, and components (SSC) beyond the reactor vessel and will more directly consider BWRs and small modular reactors (SMR).
CASL FOCUSES ON KEY NUCLEAR ENERGY CHALLENGES

CASL will focus on three key issues for nuclear energy: cost, reduction in amount of used nuclear fuel, and safety. All three can be enabled by power uprates, lifetime extension, and higher burnup through predictive simulation.

Power uprates have reduced the cost of nuclear-power-generated electricity by increasing the revenue generated for a given capital investment. Since 1997, power uprates at existing plants have delivered an additional 5 GWe to our nation’s grid, equivalent to building an additional five to six NPPs for approximately 20% 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 that have enabled the recovery of conservatism in safety analysis. Additional advances in M&S are needed to enable further uprates (on the order of 20 GWe being possible). In fact, many limits must be overcome to support a power uprate. The vendor and/or utility must have confidence that the power uprate will not cause accelerated damage to the NPP SSC during normal operations. Key concerns are integrity of fuel (due to increased fuel duty) and steam generator (due to increased steam loads). The fuel element is the single NPP component affecting all three performance enablers noted above, and its integrity is the most important of the three fission product barriers (the other two being the primary system and containment). Other components on the secondary side are more amenable to economically attractive modifications. The regulator also needs confidence that mandated safety limits will not be violated during accident conditions.

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 due to increased radiation damage and aging. Performance questions about SSC outside the vessel (such as the effects of aging on the containment and piping) also need consideration, which the developed VR simulation capability will allow CASL to address in depth during its second 5 years.

Higher fuel burnups are also necessary to support power uprates. For a 20% increase in power rating without a coincident increase in the fuel burnup limit, the need for additional fuel assemblies increases cost by about 6%, reducing the savings associated with power uprates. More importantly, higher fuel burnups support a reduction in the amount of used nuclear fuel. Higher fuel burnups challenge cladding integrity; key concerns are fretting, corrosion, corrosion-related unidentified deposits (CRUD), hydriding, creep, and cladding-fuel mechanical interactions. For normal operations, this implies cladding integrity; for accident conditions, acceptable levels of degradation of the cladding fission product barrier must be demonstrated.

To provide the greatest impact within the first 5 years, CASL will focus on the performance of the reactor core, reactor vessel, and in-vessel components of PWRs. An expert review of challenges to reactor power level, burnup, and lifetime indicates ten key limiting phenomena, as presented in the table below. From these limiting phenomena, ten challenge problems have been defined to drive requirements for the VR. These were further prioritized such that CASL, within the 5 year time frame, will focus on six of these challenge problems and address selected key aspects of the others. 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.

### Key Phenomena Limiting Improved Reactor Performance

<table>
<thead>
<tr>
<th>Phenomena</th>
<th>Power Uprate</th>
<th>Higher Burnup</th>
<th>Life Extension</th>
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</thead>
<tbody>
<tr>
<td><strong>Operational</strong></td>
<td></td>
<td></td>
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<tr>
<td>CRUD-Induced Power Shift (CIPS)</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>CRUD-Induced Localized Corrosion (CILC)</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Grid-to-Rod Fretting Failure (GTRF)</td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Pellet Clad Interaction (PCI)</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Fuel Assembly Distortion (FAD)</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td><strong>Safety</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Departure from Nucleate Boiling (DNB)</td>
<td>X</td>
<td></td>
<td></td>
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<tr>
<td>Cladding Integrity during Loss of Coolant Accidents (LOCA)</td>
<td>X</td>
<td>X</td>
<td></td>
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<tr>
<td>Cladding Integrity during Reactivity Insertion Accidents (RIA)</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Reactor Vessel Integrity</td>
<td>X</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Reactor Internals Integrity</td>
<td>X</td>
<td></td>
<td>X</td>
</tr>
</tbody>
</table>

**A MILESTONE DRIVEN APPROACH**

Level 1 (L1) milestones (below) have been grouped into six categories: CRUD, GTRF/FAD, Safety, Advanced Fuel (AF), Lifetime Extension (LE) and Operational Reactor (OR). These categories establish the linkages between the application-oriented L1 milestones and the discipline-oriented FA projects. The OR category connects the VR to physical reactors through qualification against data from operating plants.

The VR will address these identified challenges through predictive simulations with quantified uncertainties. As a result, the VR will

- facilitate improved quantification of design margins to support power uprates, lifetime extension, and higher fuel burnups for existing NPPs and fuel designs;
- facilitate the introduction of new fuel designs with the enhanced performance characteristics necessary to further support the power uprates and higher fuel burnups for existing NPPs allowed by the reduction in uncertainty of design margins; and
- fundamentally impact the nuclear steam supply system design for future-generation NPPs.

To meet these milestones, CASL has been organized into five technical focus areas (FAs) to perform the necessary work ranging from basic science, model development, and software engineering, to applications:

*Advanced Modeling Applications (AMA)* – The primary interface of the CASL VR with the applications related to existing physical reactors, the challenge problems, and full-scale validation. In addition, AMA will provide the necessary direction to the VR development by
developing the set of functional requirements, prioritizing the modeling needs, and performing assessments of capability.

**CASL Level 1 Milestones**

<table>
<thead>
<tr>
<th>Year</th>
<th>VR Capability</th>
<th>L1 Milestone Category</th>
<th>L1 Milestone</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Initial core simulation using coupled tools and models</td>
<td>CRUD</td>
<td>Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate quantities relevant to CRUD initiation and growth</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GTRF/FAD</td>
<td>Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting</td>
</tr>
<tr>
<td>2</td>
<td>Detailed phenomena modeling in fully coupled VR</td>
<td>CRUD</td>
<td>Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GTRF/FAD</td>
<td>Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration</td>
</tr>
<tr>
<td>3</td>
<td>Assembly simulation with rod fretting and upscaled materials models</td>
<td>CRUD</td>
<td>Model boron uptake from reactor coolant into CRUD on fuel rods</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GTRF/FAD</td>
<td>Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods</td>
</tr>
<tr>
<td></td>
<td>Safety</td>
<td>Initial modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients</td>
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<td></td>
<td></td>
<td>OR</td>
<td>Initial modeling of reactor operation; qualify with operational data</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CRUD</td>
<td>Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape</td>
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<tr>
<td></td>
<td></td>
<td>GTRF/FAD</td>
<td>Calculate fuel rod material wear resulting from GTRF</td>
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<td></td>
<td></td>
<td>LE</td>
<td>Model reactor vessel fluence and material property changes that result in material degradation and limit vessel performance</td>
</tr>
<tr>
<td>4</td>
<td>Initial predictive reactor modeling in coupled VR</td>
<td>CRUD</td>
<td>Analyses to mitigate CRUD formation and minimize CIPS</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GTRF/FAD</td>
<td>Analyze grid geometry and spring materials to mitigate materials changes and wear</td>
</tr>
<tr>
<td></td>
<td>Safety</td>
<td>Improved modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LE</td>
<td>Model mechanical and thermal stresses and fatigue that result in material failures of core internals</td>
</tr>
<tr>
<td></td>
<td></td>
<td>AF</td>
<td>Demonstrate the impact of new fuel forms (clad materials, fuel materials, and fuel geometries) for use in current reactor core configurations</td>
</tr>
<tr>
<td>5</td>
<td>Predictive reactor simulation coupled to physical plant</td>
<td>CRUD</td>
<td>Improved simulation of reactor operation; qualify with operational data</td>
</tr>
</tbody>
</table>

**Virtual Reactor Integration (VRI)** – Develops the CASL VR tools integrating the models, methods, and data developed by other FAs within a software framework. VRI will collaborate with AMA to deliver usable tools for performing the analyses, guided by the functional requirements developed by AMA.

**Models and Numerical Methods (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 T-H components that meet the rigorous physical model and numerical algorithm requirements of the VR. MNM will collaborate closely with MPO for sub-grid material and chemistry models and will connect to VRI for integration and development of the CASL VR.

**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.

*Validation and Uncertainty Quantification (VUQ)* – The quantification of uncertainties and associated validation of the VR models and integrated system 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 uprate reactors and extend their lifetimes. The methods proposed under VUQ will significantly advance the state of the art of nuclear analysis and support the transition from integral experiments to the integration of small-scale separate-effect experiments.

In addition to these focus areas, CASL implements a management strategy distinguished by collaboration, central leadership, and multidisciplinary teams executing a single milestone-driven plan, and integrated co-dependent projects. The CASL streamlined management structure includes collocation at CASL, use of technology to achieve multidisciplinary collaboration, face-to-face meetings, and a Virtual Office, Community, and Computing (VOCC) project that integrates both the latest and emerging technologies to build an extended “virtual one roof.” CASL has a strong management philosophy, and with significant input provided by independent scientific and industry councils.

Integration of all the CASL milestones and FAs will lead to the development of a state-of-the-art *pellet-to-plant* VR simulation environment, with high-resolution representation of a physical reactor on the computational platforms of today and the future, creating distinct technological innovation and paving the way for a nuclear power industrial revolution.

**CASL INTEGRATION AND IMPACT**

CASL is designed to create a user environment for predictive simulation (the VR) that can be used to address essential issues in NPP design and operation. The primary challenge to satisfying the major objective to “after five years… produce a multi-physics computational environment that can be used… for calculations of both normal and off-normal conditions” is the development of superior physical and analytical models and multi-physics integrators. CASL will address this challenge through the five FAs, validating the VR models against single and multiple effects experiments and then against operating reactor data from the TVA PWR fleet. The resulting VR will couple state-of-the art neutronics, T-H, structural, and fuel performance modules, linked with existing systems and safety analysis simulation tools, to model NPP performance in a high-performance computational environment that enables engineers to simulate physical reactors.

In satisfying the goal of overcoming “potential roadblocks and bottlenecks… in order to implement a sustainable and commercially viable technology,” the CASL VR will take as its starting point a select set of mature and validated neutronics and T-H codes developed by the CASL partners, some of which have been used to design and license the U.S. PWR operating fleet. The availability of this code suite enables CASL to jumpstart operation of the VR while developing the improvements and capabilities needed to deliver the HPC-based multiphysics VR.
The CASL technical vision

Implementation of a sustainable and commercially viable technology, through achievement of an NRC-licensed application of the VR, will be facilitated through engagement with the NRC. As discussed below, an existing MOU between CASL partner EPRI and the NRC Office of Nuclear Regulatory Research (RES) will be expanded to secure NRC review and guidance of key additions to the VR. CASL will also draw on the availability of the WEC code suite, the ability to validate the VR against the TVA reactors, the established interface with RES, and on WEC’s record of success in licensing to achieve its goal of delivering high-fidelity predictive capabilities in the shortest possible time.

Accomplishing these goals is made possible both by the robust interaction with industry that is a CASL hallmark and by the breadth and depth of scientific and technological expertise under CASL’s “virtual roof.” CASL combines “exceptional skill and creativity in general energy technology research with cutting-edge expertise in the specific problems to be addressed” both by including researchers specializing in nuclear energy and by drawing on “strong partnerships and working relationships” that have not had to be developed for this purpose, since some collaborations have been in place for as much as 60 years. These relationships will help CASL to achieve synergies in attacking the complex problems posed by nuclear energy M&S. The breadth of perspectives within CASL will also provide advantages in “understanding and achieving effective technology transfer and eventual large-scale commercialization and deployment of cost-effective technologies.”

The CASL partnership is exceptionally well positioned to meet the objective of utilizing “existing advanced M&S capabilities” developed with support from DOE programs. Many of these capabilities were developed by CASL partners, whose considerable expertise will now be focused on integrating them into the VR.
CASL will also build on current investments being made by DOE’s Office of Nuclear Energy (DOE/NE). For example, the Light Water Reactor Sustainability (LWRS) program, led by INL, addresses the first objective in the DOE/NE R&D Roadmap: extending the life, improving the performance, and maintaining the safety of the current U.S. NPP fleet by addressing long-term operational challenges faced by U.S. nuclear utilities. The alignment between CASL and LWRS technical activities is shown in the above figure. Of greater significance, CASL will simultaneously address the second objective in the DOE/NE R&D Roadmap: enabling new builds and improving the affordability of nuclear power.

The CASL VR will initially be used to address issues for existing reactors (e.g., life extensions and power uprates); the CASL challenge problems have been selected principally to demonstrate the capability of the VR to enable power uprates and life extensions, with increased fuel burnup included because it is strongly linked to power uprates. Demonstration of the capability is not, however, synonymous with its actual realization. Even if the enhanced computational capability of the VR indicates that power can be safely increased, the reactor hardware (chiefly the fuel) must be physically able to deliver such a power increase, and this will have implications for current fuel designs.
Through improvements in M&S capability using a science-based approach, CASL will enable exploration of advanced fuel design features. These advanced features may range from modifications of the current compositions of the zirconium-based alloys now used for cladding to the development of entirely new cladding materials, new fuel materials with higher densities and improved thermal properties, and changes in the fuel geometry and configuration. The use of these advanced materials and geometries offer the opportunity for transformational improvements in nuclear fuels. This is just one example of how the CASL-built VR capability will progress from analyses of operating reactors to design improvements. Other examples include improved designs of the reactor internals (for life extension) and steam generators (for power uprates).

Finally, a third application of the VR will contribute to satisfying the remaining three DOE/NE R&D Roadmap objectives:

- enable the transition away from fossil fuels by producing process heat for use in the transportation and industrial sectors,
- enable sustainable fuel cycles, and
- understand and minimize proliferation risk.

Introduction of new reactor designs is a long and expensive process. The major stumbling block has been the required construction and operation of a prototype reactor. The CASL VR will shorten the time required to build a new reactor design and allow the deployment of high-temperature reactors for process heat and of fast-spectrum reactors to close the fuel cycle. Thus the key impact of the CASL VR and related activities will be the ability to address technology issues concerning nuclear energy in the short, mid, and long term.

CASL will apply a remarkable set of assets to produce a usable tool for addressing practical problems for the nuclear energy industry:

- a group of partners with unparalleled collective institutional knowledge, nuclear science and engineering talent, and record of LWR regulatory and design accomplishments;
- intimate knowledge and understanding of operating NPP challenges; and
- a clear, milestone-driven technical strategy for solving real-world reactor problems.

CASL’s success in delivering the VR will directly contribute to three overarching goals:

- maximize the value of the U.S. investment in its existing NPPs;
- enable the development and deployment of transformational nuclear energy systems; and
- improve the ability of the U.S. industry to compete in worldwide market.

Thus, the VR is the heart of the CASL proposal. As a suite of M&S tools and methods for integration of multiple tools and for use in gaining an understanding of processes and material evolution, the VR will enable enhanced engineering design and operations.
KEY TECHNICAL ELEMENTS

Computational Science

Current M&S practice in the nuclear energy industry is depicted on the figure below. Sets of proprietary tools are executed separately, primarily on desktop workstations. These tools are separately calibrated to different sets of proprietary data and are supported by large experimental programs. They are limited in making science-based predictions of behavior that extend beyond their calibrated range. Arrows indicate communication flow, which typically occurs via separate files, and some aspects are simplified. Simulation results from this collection of tools generally do not follow from a coupled, nonlinearly consistent solution. The CASL-enabled work flow is depicted in the figure below. It shows a coupled, multi-physics 3D predictive simulation tool replacing most of the tools on the figure below, coupled to ex-vessel systems and containment. The VR will be a component-based software system that enables assembly of a family of highly optimized M&S codes that can be used by reactor analysts, operators, and designers to answer fundamental nuclear engineering questions well beyond the current CASL mission.

Traditional and CASL-Enabled Reactor Design Work Flow

Over the past decade HPC has enabled a paradigm shift in science-based M&S. Petascale computing is being applied to real-world problems at the Oak Ridge Leadership Computing Facility (OLCF) and on the LANL Roadrunner system. Predictive M&S for nuclear reactor designs and analyses requires these types of resources. For example, recent neutron transport simulations at ORNL of highly resolved PWR assemblies in a full-core model requiring 10 trillion degree-of-freedom solutions have become routine on supercomputing systems, and will soon be possible on high-end desktops (Figure below). A complete core-to-vessel multiphysics simulation will require more resources, but the VR will be designed to exploit advanced computing platforms like those at the OLCF and LANL so that first-principles design tools can be developed, tested, and brought to desktops, transforming the reactor design and analysis process.

A cross-cutting issue that will impact the entire range of computational efforts over the lifetime of CASL is the dramatic shift occurring in computer architectures, with rapid increases in the number of cores in CPUs and increasing use of specialized processing units [such as graphical processing units (GPUs)] as computational accelerators. As a result, applications must be
designed for multiple levels of memory hierarchy and massive thread parallelism. While we can expect peak performance at the desktop exceeding 10 trillion operations per second (teraflnop/s, TF/s) and leadership platform performance of several hundred quadrillion operations per second (petafllops/s, PF/s) during the next 5 years, it will be challenging for applications to achieve a significant fraction of these peak performance numbers, particularly existing applications that have not been designed to perform well on such machines.

CASL partners, in particular ORNL, LANL, and SNL, are at the forefront of these changes and are exceptionally well equipped to ensure that new software components in the VR are designed and implemented to perform efficiently on both existing and future computing platforms, from the desktop to leadership-class systems. In 1997, SNL fielded the first supercomputer to break the 1 TF/s barrier. In 2008, LANL deployed the first supercomputer to break the 1 PF/s barrier, the Roadrunner platform (a hybrid architecture combining traditional and a modified version of the chip created for the Sony Playstation 3). Today, ORNL supercomputers occupy the first and third positions on the Top500 list of the world’s most powerful supercomputers. Staff at these three institutions formed and are participating in the Hybrid Multicore Consortium (announced at the Supercomputing 2009 conference), which is focused on collaborations in computer science, numerical methods, and tool development to enable applications to extract performance on future advanced architectures at multiple scales (desktop to petascale). This expertise is unique and will allow CASL to deliver a suite of components that will transform M&S for nuclear energy applications. CASL will bring high-fidelity methods such as transport and CFD, used in production at national laboratories for years, into the workflows of designers of existing and future nuclear energy systems. Designers will be able to consider not only best-estimate predictive performance but also the uncertainty in the predicted performance when making design decisions.

Development of the CASL VR will follow two paths. The first is rapid delivery of an initial capability, based on integration of existing tools, to end users. The second builds on this framework technology to enhance the VR suite, providing next-generation M&S capability to the same design community. The CASL challenge problem definitions drive requirements for the VR and set measurable milestones for its development. While focus is essential for timely delivery of a valued product, ultimately, the CASL VR will embody a breadth of capabilities able to address a broad array of practical issues for the nuclear industry. As a result, CASL will design end-user simulation tools that can meet current challenges in nuclear reactor analysis while developing and testing transformational concepts that can be used to revolutionize the reactor design process. Frequent releases and constant
interaction between CASL code developers and industry designers at Westinghouse and EPRI will result in a fundamental change in design and analysis work flows.

**Industrial Partnerships and Access to Critical Data**

The physical reactor selected as the focus of CASL is the Westinghouse four-loop PWR. TVA operates three reactors of this type, two at the Sequoyah Nuclear Plant and one at the Watts Bar Nuclear Plant. A fourth reactor, Watts Bar 2, is under construction and will become operational by 2012.

PWRs are an excellent choice for the initial CASL focus as they represent over 60% of the U.S. and the world’s nuclear fleet and a large fraction of the proposed NPPs to be built in the coming decade. In addition, many of the CASL developments can be applied to BWRs and other advanced reactors, which both represent fruitful areas for future activities, perhaps in the second 5 years. As a CASL member, TVA will provide reactor design and operational data for its three operational reactors and selected test data from the Watts Bar 2 reactor, to support the validation of the VR models.

Validation of the VR against operating reactors is critical for the success of this initiative. The selection of TVA’s four-loop Westinghouse PWRs as CASL’s physical reactors provides the VR with access to the wealth of experience gained in designing and operating these Generation II reactors. One of the five CASL technical FAs, VUQ, is dedicated to validation and UQ. The VUQ research plan, which supports validation activities in other FAs. In addition, AMA Projects will coordinate the collection of data for validation of VR simulation results for the selected challenge problems.

**NRC Engagement**

CASL will follow a strategy of close engagement with the NRC throughout the development of the VR, keeping in mind that the CASL effort is not aimed at licensing a reactor application but instead is a research activity eventually leading to applications. CASL will leverage the existing memorandum of understanding (MOU) between the NRC Office of Nuclear Regulatory Research (RES) and one of its partners, EPRI, to build a collaborative relationship leading to higher confidence that future licensing applications incorporating M&S, particularly those based on CASL models and tools, will result in timely, positive decisions.

**Education, Training, and Outreach**

A comprehensive education, training, and outreach (ETO) program will catalyze CASL engagement with undergraduate and graduate students, postdoctoral associates, faculty, practicing scientists and engineers, and regulators. Of particular note, CASL will take full advantage of EPRI’s membership in the CASL consortium to inject much-needed computational science and engineering into the current and future nuclear energy workforce, dramatically increasing the competitiveness of the U.S. nuclear industry.
TECHNICAL INNOVATION

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- a group of partners with unparalleled collective institutional knowledge, nuclear science and engineering talent, and record of LWR regulatory and design accomplishments;
- intimate knowledge and understanding of operating NPP challenges; and
- a clear, milestone-driven technical strategy for solving real-world reactor problems.

CASL’s success in delivering the VR will directly contribute to three overarching goals:

- maximize the value of the U.S. investment in its existing NPPs;
- enable the development and deployment of transformational nuclear energy systems; and
- improve the ability of the U.S. industry to compete in worldwide market.

CASL will also enable innovative advances in computer and computational science, applied mathematics, materials science, chemistry, nuclear engineering, and mechanical engineering. Specific CASL innovation targets are shown in the table below.

<table>
<thead>
<tr>
<th>Focus Area</th>
<th>Innovation Target</th>
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<tbody>
<tr>
<td>AMA</td>
<td>Embedding coupled physics VR tools and HPC in bench engineering reactor design and analysis processes, with advanced visualization, optimization, and UQ</td>
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<td></td>
<td>Systematic automatic analysis of uncertainties supporting best-estimate analysis approaches</td>
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<td></td>
<td>Physics-based analysis methods and tools to predict margin to failure and new operational phenomena</td>
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<td>VRI</td>
<td>Unified, portable extensible software environment supporting flexible coupling of multiscale physics and chemistry components and integral UQ</td>
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<td>Broadly applicable, verified software components that can be flexibly assembled into multiple applications for predictive simulation of physical phenomena</td>
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<td></td>
<td>Efficient, numerically stable, and scalable physics component coupling methods</td>
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<td>MNM</td>
<td>Hybrid Monte Carlo and deterministic transport methods with improved source convergence</td>
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<td></td>
<td>First-principles T-H code coupling, fuel assembly-level multiphase flow, subgrid-level flow, and heat transfer</td>
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<td></td>
<td>Optimized, portable, and extensible algorithms and software implementations for advanced architectures</td>
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<td></td>
<td>Microstructural evolution and performance prediction of fuel and clad (both existing and innovative designs) under normal and accident conditions</td>
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<tr>
<td>MPO</td>
<td>Fundamental understanding of corrosion mechanisms of nuclear materials</td>
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<td></td>
<td>Prediction of radiation, thermal, and chemical contributions to failure modes in fuel, reactor pressure vessel, and reactor internals</td>
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<tr>
<td>VUQ</td>
<td>Generalized high-order data assimilation and model calibration methods for both data and modeling errors</td>
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<td></td>
<td>Time-dependent global, dynamically adaptable sensitivity analysis and model calibration methods</td>
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<td></td>
<td>UQ methods for multiple coupled models, bridging lower-length scale models into macroscale codes</td>
</tr>
</tbody>
</table>

A Collaborative Scientific Consortium

CASL provides a unique opportunity not only to advance the use of nuclear power in the United States but also to advance the state of distance collaboration – a key element in an increasingly
global society. CASL has a clear commitment to the use of state-of-the-art technology and frequent virtual meetings to enable long distance collaboration.

An unprecedented alliance of national laboratories, universities, and private industries are wholly and singularly committed to accomplishing the compelling CASL vision. ORNL is the lead institution for CASL, the CASL Director is an ORNL employee and single Principal Investigator. The senior management team (Office of the Director) has >90% residency at CASL. CASL will follow ORNL management, administrative, and operational procedures and processes as established under the UT-Battelle contract.

CASL draws heavily on the ORNL experiences such as SNS and BESC in executing large technical programs that require integration of multiple technical disciplines across several institutional partners. CASL selected each partner to maximize the probability of successfully achieving the goals and objectives for the DOE for the M&S hub. CASL integrates world-class basic and applied research capabilities with experience in all aspects of the CASL mission. CASL’s leading-edge scientific research institutions along with CASL’s nuclear energy design and engineering industries and utility owner/operators ensures that CASL deliverables are well informed by commercial needs and that CASL tools, scientific discovery, and innovations have near-term real-world impact. CASL’s industrial partners bring unique applied research experience and operational reactor and plant data which focuses CASL’s scientific activities on real-world challenge problems. The national laboratories bring a cross-disciplinary approach, with strong capabilities in technology development, applications understanding, particularly in the application of the physical and computational sciences, experience in managing large-scale projects, and large-scale HPC. The universities further enhance this science base, with key capabilities in relevant domain science.

**CASL Organizational Structure**

The figure below shows the proposed CASL organization structure enabling efficient execution and innovation. Major features include:

- Central, integrated management working predominately from a single location at ORNL: Director with full line authority and accountability for all aspects of CASL; Chief Scientist to drive science-based elements; Deputy Director to drive application elements; Chief Strategy Officer to drive design and regulatory elements; and experienced FA Leads and Deputies with responsibility for the core elements and integration
- Strong science, engineering, applications, and design leadership
- A commitment to one-roof approach and widespread implementation of state-of-the-art collaboration technology
- Well-informed and timely decision-making and program integration
- Independent oversight and review via an external Board of Directors, Science Council, and Industrial Council, each designed to provide the best possible independent, scientific, program management, and industrial advice. The BOD approves annual performance goals, projects, and budgets
- Integrated, professional technical Project Management across CASL for schedule and budget and an integrated operations team, providing clear leadership for ES&H, finance, program review, business management, quality, and security
• Robust technology transfer and partnerships office to ensure efficient, widespread industrial engagement and coordinated management of intellectual property, ensuring that CASL discoveries and the VR will be translated rapidly to commercial applications.

CASL Management

CASL is introducing an innovative management strategy for FAs to accelerate decision making and increase scientific understanding. To achieve that end each of the FAs has a lead and deputy lead. This leadership team was selected for their world-class accomplishments ranging from science to engineering to design. An unambiguous responsibility for management and budget lies with each FA lead. The lead and deputy jointly provide technical depth for operations and R&D that would not otherwise be possible. This innovative multidisciplinary approach enables rapid, informed decisions regarding technology or R&D.

“One-Roof” Approach

CASL implements a management strategy that imbues physical collocation; community; collaboration; central leadership; multidisciplinary teams executing a single milestones-driven plan; and integrated, co-dependent projects. The CASL-streamlined management structure includes collocation at CASL, use of technology to achieve multidiscipline collaboration, video conferencing for meetings, and a VOCC project that integrates both the latest and emerging technologies to build an extended “virtual one roof.”

CASL will be headquartered at ORNL, where the CASL leadership and a majority of the multidisciplinary, multi-institutional scientists and engineers will be located. Work performed at partner sites will be seamlessly integrated across the consortium on a real-time basis via
community and computing (VOCC) capability that integrates both the latest and emerging
technologies to build an extended “virtual one-roof” allowing multidisciplinary collaboration
among CASL staff at all sites. Many of the facilities and most of the expertise and equipment
necessary to execute CASL’s proposed research program are in place and capable of performing
substantive research almost immediately.

CASL will occupy 32,000 square feet of office space, conferencing facilities, and laboratories in the
upper two floors of an expansion of the Computational Sciences Building on the ORNL campus.

CASL Facility Siting, Acquisition, and Development

CASL will be located on the ORNL campus in the upper two floors of a $9.5M expansion of the
Computational Sciences Building. This multi-story expansion, currently under construction, is
strategically located adjacent to the DOE–sponsored Oak Ridge Leadership Computing Facility,
and is on track for occupancy in December 2010. This facility is not a new building specifically
contracted for CASL, but rather a previously planned expansion for ORNL staff in the
Computing and Computational Sciences Directorate. Office space on the 2nd floor of the Joint
Institute for Computational Sciences (JICS) Building on the ORNL campus will be the home for
the Consortium prior to occupancy in the CASL building. The space occupied by CASL staff in
the expansion will feature the following:

- 32,000 ft² of modern office space with high-speed networking and multi-media
  interconnects;
offices equipped for virtual office and telepresence technology; 
advanced, 3D, and reconfigurable scientific visualization and data analysis facility; and 
conference and meeting facilities with multi-site video conferencing and telepresence technologies.