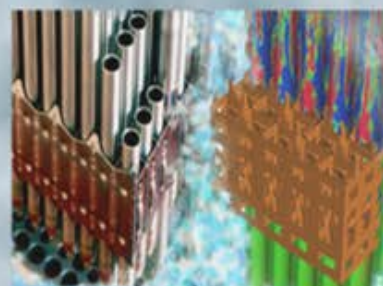
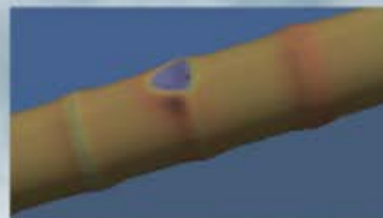
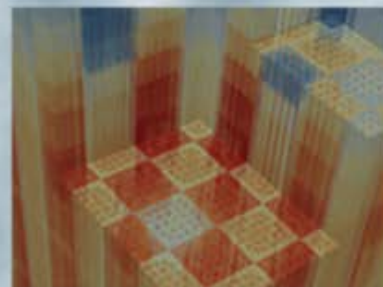


# CASL Annual Report Fiscal Year 2016

October 2016



## REVISION LOG

| Revision | Date       | Affected Pages | Revision Description |
|----------|------------|----------------|----------------------|
| 0        | 10/28/2016 | All            | Original             |
|          |            |                |                      |
|          |            |                |                      |
|          |            |                |                      |

**Document pages that are:**

Export Controlled: None

IP/Proprietary/NDA Controlled: None

Sensitive Controlled: None

**Distribution:**

To: Tansel Selekler, DOE-NE

Pete Lyons, Chair, CASL Board of Directors

Members, CASL Board of Directors

William Oberkamp, Chair, CASL Science Council

Scott Thomas, Chair, CASL Industry Council

Thom Mason, Director, ORNL

Alan Icenhour, Associate Laboratory Director, Nuclear Science and Engineering Directorate, ORNL

Copy: NA

## MESSAGE FROM THE CASL DIRECTOR

On behalf of everyone at CASL, I am pleased to provide this annual report for fiscal year 2016 that provides an overview of our work and accomplishments and highlights the impacts that we are having on engineering, science, education, and workforce development. As you will find in its contents, CASL has had a very successful year making progress on our goals to develop and deliver advanced modeling and simulation capabilities to simulate light water reactors. We are now fully in our second phase that is emphasizing maturity of our Virtual Environment for Reactor Applications (VERA) that is demonstrated through a growing number of applications to operating reactors.

The key to CASL's success is its talented and diverse team of engineers, scientists, developers, students and operations staff. The ability of the work to be performed seamlessly across our industry, university and national laboratory partners continues to be a strength of our organization. In addition, CASL continues to get strong input and feedback from our Board of Directors with Dr. Pete Lyons, former Deputy Assistant Secretary for Nuclear Energy and Commissioner of the Nuclear Regulatory Commission taking on the Chair position from the Dr. Jim Duderstadt, who we are indebted to for sound advice and direction. We are also grateful for the feedback from our Science Council, chaired by Bill Oberkampf and our Industry Council, chaired by Scott Thomas of Duke Energy. We also appreciate the technical leadership of long-serving Chief Scientist, Prof. Paul Turinsky, who has stepped down this year. This role has been taken over by Prof. Dave Kropaczek, who comes to us with two decades of experience in modeling and simulation tools in the nuclear industry.

CASL is making good progress on our capabilities to simulate our Challenge Problems, specifically CRUD induced power shift, CRUD induced localized corrosion, and pellet-clad-interaction, with these areas being the focus of our industry engagement efforts. In addition to this work, an outstanding opportunity for us this year was modeling the startup of Tennessee Valley Authority's Watts Bar Unit 2, which is now in full commercial operation. This was a team effort with staff across the CASL partnership working together to achieve excellent results in demonstrating the usefulness of VERA. Further, we are engaging broadly with the nuclear industry with projects with Westinghouse, Electric Power Research Institute, AREVA, Duke Energy, University of Illinois/Exelon, Arizona Public Service and NuScale in progress.

We have also been looking to the future of CASL with the development of a strategy for CASL beyond its 10-year operation period. A cornerstone of this strategy includes a closer alignment with DOE-NE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program that would lead to an integrated modeling and simulation program in 2020. There are also numerous opportunities to support DOE and industry initiatives in collaborations with the Light Water Reactor Sustainability Program, the use of CASL capabilities to support the development and deployment of accident tolerant fuels, and support for used fuel storage and transportation.

Sincerely,

Dr. Jess C. Gehin, Director

## BOARD OF DIRECTORS STATEMENT

The Board of Directors for the Consortium for Advanced Simulation of Light Water Reactors (CASL) serves as an advisory and oversight body for the Oak Ridge National Laboratory Director and the CASL Senior Leadership Team. In this role, the Board interacts on a frequent basis with the CASL leadership team and regularly reviews CASL progress toward achieving its goal of delivering advanced modeling and simulation technologies that will improve the safety and operational performance of the country's commercial nuclear reactor fleet.

The Board believes that CASL is continuing to deliver innovation and technical leadership in the development of advanced modeling and simulation tools that will help industry improve the safety and performance of the country's nuclear reactor fleet. The CASL tools have now reached a point where they can simulate highly complex operations, such as startup and testing of new reactor systems, and provide nearly real-time insights to plant operations staff as reactor conditions change. The tools have been steadily streamlined so that they can run on computer systems that are widely available to nuclear utilities, vendors, and researchers, and a range of support tools have been developed that let users quickly visualize simulation results at a level of detail that has never before been available.

The consensus of the Board is that CASL is a highly valuable research and development program that is well on its way toward producing a strong return on its taxpayer investment. The program has effectively combined individual strengths of the country's nuclear industry, universities, and national laboratories to create tools that have the potential to revolutionize many of the ways that nuclear reactor operations and safety are analyzed. The Board strongly supports continued funding for development of the tools during the remaining three years of CASL operations, and encourages DOE-NE to develop and implement a strategy that will allow the CASL tools to be maintained and improved beyond the end of the program's operational period, consistent with the post-CASL plan that was developed during FY 2016. The country's nuclear energy industry is already benefiting from CASL's work, and there is a strong need to continue development of modeling and simulation capabilities that will help industry achieve new insights and create new technical breakthroughs in the future. The Board believes that CASL is one of the tools that the country can use to fill that need.

CASL Board of Directors

## SCIENCE COUNCIL STATEMENT

The CASL Science Council provides independent assessment of the CASL scientific work plans and execution to ensure that it is of high quality and supports attaining the CASL goals. Science Council members represent the diverse set of technical fields that are required to perform these assessments. The Science Council fulfills this purpose by participating in the Focus Areas' Annual Review and Planning Meetings, the Joint Industry Council/Science Council Annual Review Meeting, teleconferences, and reviews of selective milestones and reports.

The Science Council believes that CASL is performing superb applied research with this past year seeing the most progress of all years since the beginning of CASL. The change in direction last year on thermal-hydraulics to shift from the development of new computational fluid dynamics software to the improvement of two-phase flow models in existing software has resulted in an improved capability for modeling departure from nucleate boiling. CASL continues to make good progress on neutronics and core simulation with good results demonstrated in applications to operating reactors and comparisons to plant data, including transient capabilities. It is noted that impressive run-time efficiency improvements have been achieved which have allowed the VERA codes to be deployed in an industry partner computing environment. The fuel performance and CRUD simulation capabilities are advancing as well, with increasing benefits being demonstrated through coupling of these physics with the core simulation capabilities. Increased effort is needed to achieve the verification and validation required to support industry applications of the CASL tools. This increased effort in V&V and applications over the development of software and fundamental models should be achieved partially in FY17, but more aggressively in the upcoming years. Overall, the Science Council believes that CASL is making very good progress on their goals and in the process is having a strong impact on the technical community.

On Behalf of the CASL Science Council,

Dr. William L. Oberkampf  
Science Council Chair

## INDUSTRY COUNCIL STATEMENT (PRELIMINARY)

The CASL Industry Council represents the end users of the CASL products and provides periodic feedback to the CASL Program. The Industry Council gives the CASL Program guidance on functional requirements that support development of the CASL software and provides input on the program's software deployment strategies. The Industry Council held two information exchange meetings with the CASL Program during FY 2016. The meetings focused on discussion of how the CASL software can be used to evaluate reactor operational and licensing issues, the status of the program's software development efforts, and strategies for increasing industry use of the CASL tools.

The Industry Council believes CASL is continuing to make steady progress toward developing advanced simulation tools that will help improve reactor operations and safety. The coupled, high fidelity software that CASL is developing, and its efforts to make the tools useful and accessible to industry analysts, have the potential to significantly improve reactor operations and safety analyses. Of particular interest is CASL's work on developing tools that address the program's challenge problems, including the CRUD and pellet clad interaction related challenges that may improve core reload pattern efficiencies.

Additional work is needed to fully define important inputs to the modeling and simulation tools, such as CRUD source terms and thermal-hydraulic parameters. Additional verification and validation of the tools will be needed before they will be ready for use in application. However, CASL's recent demonstrations, including work on simulating the Watts Bar Unit 2 and Westinghouse AP1000® reactor startups using computing resources that may soon be accessible to industry, indicate the software tools are reaching a level of maturity that should allow them to provide increasingly useful analyses.

The Industry Council believes the tools will continue to improve over the remaining three years of the CASL operational period, and that the program is expected to deliver high quality simulations tools that are valuable to the nuclear industry.

On Behalf of the CASL Industry Council,

Scott B. Thomas  
Industry Council Chair



## The Consortium for Advanced Simulation of Light Water Reactors

### Founding Partners

Oak Ridge National Laboratory  
 Idaho National Laboratory  
 Los Alamos National Laboratory  
 Sandia National Laboratory  
 University of Michigan  
 North Carolina State University  
 Massachusetts Institute of Technology  
 Electric Power Research Institute  
 Tennessee Valley Authority  
 Westinghouse Electric Company



### Contributing Partners

Anatech Corp.  
 AREVA Inc.  
 ASCOMP AG  
 CD-adapco  
 City College of New York  
 Core Physics Inc.  
 Florida State University  
 Global Nuclear Fuel LLC  
 Imperial College  
 Pacific Northwest National Laboratory  
 Pennsylvania State University  
 Rensselaer Polytechnic Institute  
 Seoul National University  
 Southern States Energy Board  
 Texas A&M University  
 Ulsan National Institute of Science and Technology  
 University of Florida  
 University of Notre Dame  
 University of Tennessee  
 University of Tennessee–Chattanooga  
 University of Texas at Austin  
 University of Wisconsin





## CONTENTS

|                                                                       |        |
|-----------------------------------------------------------------------|--------|
| Message from the CASL Director .....                                  | iii    |
| Board of Directors Statement.....                                     | iv     |
| Science Council Statement.....                                        | v      |
| Industry Council Statement (preliminary) .....                        | vi     |
| Figures .....                                                         | x      |
| Tables .....                                                          | x      |
| Acronyms .....                                                        | xi     |
| <br>Part 1: FY 2016 CASL Overview .....                               | <br>1  |
| CASL's Vision and Mission.....                                        | 1      |
| 2016 Highlighted Achievements .....                                   | 2      |
| Summary of Funding and Investments.....                               | 4      |
| The Future of CASL.....                                               | 4      |
| <br>Part 2: Science and Engineering Progress and Impact .....         | <br>5  |
| Status of the Virtual Environment for Reactor Applications.....       | 5      |
| VERA Performance Improvements .....                                   | 6      |
| Extension of VERA to Additional Reactor Types.....                    | 7      |
| Interoperability with Commercial Modeling Tools .....                 | 8      |
| Verification, Validation, and Uncertainty Quantification.....         | 8      |
| Progress on CASL Challenge Problems .....                             | 8      |
| <br>Part 3: End User Impact and Education/Workforce Development ..... | <br>16 |
| Engaging VERA End Users.....                                          | 16     |
| CASL Industry Council .....                                           | 16     |
| Education Support and Training.....                                   | 20     |
| <br>Part 4: Return on FY 2016 Taxpayer Investment .....               | <br>24 |
| FY 2016 Financial Performance .....                                   | 24     |
| Milestone Completion .....                                            | 25     |
| Post-CASL Planning.....                                               | 26     |
| Conclusion .....                                                      | 28     |
| Acknowledgments .....                                                 | 28     |
| References.....                                                       | 29     |

## FIGURES

|                                                                                                                                                                                         |    |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Figure 1. Hot zero power beginning of cycle fission rate distribution in WBN-2 (quarter-core). .....                                                                                    | 2  |
| Figure 2. Summary of M&S tools included in VERA. ....                                                                                                                                   | 5  |
| Figure 3. Summary of VERA-CS performance improvements on a quarter-core 3D hot full power simulation achieved during FY 2016. ....                                                      | 7  |
| Figure 4. Summary of CASL challenge problem scope. ....                                                                                                                                 | 9  |
| Figure 5. Simulation results for CRUD and oxide layers on Seabrook fuel rods [4]. ....                                                                                                  | 10 |
| Figure 6. Calculated cladding hoop stress for each fuel rod and assemblies selected for further analysis from WBN-1 cycle 6 (top) and cycle 7 (bottom) [5]. ....                        | 11 |
| Figure 7. Calculated CHF compared to measured CHF at the corresponding test conditions [6]. ....                                                                                        | 13 |
| Figure 8. SPERT III E core cross section at midplane and corresponding MPACT model [7]. ....                                                                                            | 14 |
| Figure 9. Texture and grain interaction modeling (left) is being used to inform gap opening in grid spacer elements (right). ....                                                       | 15 |
| Figure 10. CASL Industry Council member organizations. ....                                                                                                                             | 16 |
| Figure 11. Example VERAView widgets showing rod ejection simulation results. ....                                                                                                       | 18 |
| Figure 12. Comparison of VERA results to WBN-2 control bank worths. ....                                                                                                                | 20 |
| Figure 13. Kayla Coleman received 3rd place for her CASL-supported research at an ORNL poster session. (Also shown are CASL director Jess Gehin and research mentor Kevin Clarno). .... | 22 |
| Figure 14. Participants in the first CASL Summer Institute at ORNL in June 2016. ....                                                                                                   | 23 |
| Figure 14. Post CASL strategy use-cases [13]. ....                                                                                                                                      | 27 |

## TABLES

|                                                                                    |    |
|------------------------------------------------------------------------------------|----|
| Table 1. Summary of CASL Technical Output through FY 2016. ....                    | 4  |
| Table 2. Comparison of MPACT and SHIFT Results with WBN-2 Startup Measurements* 19 |    |
| Table 3. FY 2016 Funding—Budget and Cost Summary .....                             | 24 |
| Table 4. FY 2016 CASL DOE-Reportable Milestones. ....                              | 25 |

## ACRONYMS

|         |                                                            |
|---------|------------------------------------------------------------|
| BWR     | boiling water reactor                                      |
| CASL    | Consortium for Advanced Simulation of Light Water Reactors |
| CFD     | computational fluid dynamics                               |
| CILC    | CRUD-induced localized corrosion                           |
| CIPS    | CRUD-induced power shift                                   |
| CRUD    | Chalk River unidentified deposits                          |
| CTF     | upgraded version of COBRA-TF computer code                 |
| DNB     | departure from nucleate boiling                            |
| DOE     | US Department of Energy                                    |
| DOE-NE  | DOE Office of Nuclear Energy                               |
| FY      | fiscal year                                                |
| INL     | Idaho National Laboratory                                  |
| LWR     | light water reactor                                        |
| M&S     | modeling and simulation                                    |
| MWth    | megawatt thermal                                           |
| ORNL    | Oak Ridge National Laboratory                              |
| PCI     | pellet-clad interaction                                    |
| PWR     | pressurized water reactor                                  |
| R&D     | research and development                                   |
| RIA     | reactivity insertion accident                              |
| SMR     | small modular reactor                                      |
| TML     | transient multi-level                                      |
| TVA     | Tennessee Valley Authority                                 |
| VERA    | Virtual Environment for Reactor Applications               |
| VERA-CS | VERA Core Simulation                                       |
| VWG     | VERA Working Group                                         |
| WBN-1   | Watts Bar Nuclear Unit 1                                   |
| WBN-2   | Watts Bar Nuclear Unit 2                                   |
| XFEM    | extended finite element method                             |



## PART 1: FY 2016 CASL OVERVIEW

The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established in July 2010 as the first Department of Energy (DOE) Energy Innovation Hub. The consortium was initially funded for five years to develop advanced modeling and simulation (M&S) tools that can be used to analyze issues associated with operation of US commercial light water reactors (LWRs). The program's focus during this period was on modeling and simulation of physical processes that affect operation of pressurized water reactor (PWR) cores. In January 2015, the program was extended for an additional five years with the goal of finalizing development of the PWR analysis tools and extending the program's tools for use in analysis of boiling water reactor (BWR) and small modular reactor (SMR) operations.

The world-class scientists, engineers, computer scientists, students, and program managers from the 10 CASL founding partners and contributing partners, supported by guidance from the CASL Board of Directors, Industry Council, and Science Council, are responsible for the continuing success of the program. In 2016, this represents nearly 350 people across these organizations who are associated with CASL. These organizations have successfully demonstrated that coordination of personnel from nuclear industry, universities, and national laboratories who have access to world-class computing and research facilities can drive the development of innovative M&S products and allow for successful transfer of new technologies to the private sector.

### CASL's Vision and Mission

The CASL program's vision statement has remained constant over its period of operations:

***To predict with confidence, the performance and assured safety of nuclear reactors, through comprehensive, science-based M&S technology deployed and applied broadly by the US nuclear energy industry.***

To achieve this vision, CASL must

- promote an enhanced scientific basis and understanding of reactor operations by developing robust science-based predictive capabilities;
- develop a highly integrated multiphysics M&S environment based on high-fidelity tools;
- incorporate uncertainty quantification into the M&S environment development process;
- educate today's reactor engineers in the use of advanced M&S tools through direct engagement in CASL activities, and develop the next generation of engineers through use of appropriate curricula at partner universities; and
- engage the US Nuclear Regulatory Commission to help facilitate eventual industry use of CASL tools to support licensing of advanced reactor applications.

## 2016 Highlighted Achievements

FY 2016 was a very productive year for CASL with excellent progress across CASL work areas. Significant achievements this year include:

1. **The Virtual Environment for Reactor Applications (VERA) suite of high-fidelity M&S tools was used to follow the startup and power ascension of the Watts Bar Nuclear Power Plant Unit 2 (WBN-2) with outstanding accuracy in comparisons with plant measurements (Figure 1).**

WBN-2 is the first commercial nuclear reactor to come online in the United States in two decades. In partnership with the Tennessee Valley Authority (TVA) and Westinghouse Electric Corporation, CASL performed high-fidelity physics calculations before startup and ongoing simulations as the plant moved toward commercial operations. Modeling the startup and following the entire reactor power ascension process was the largest simulation performed by CASL to date, and it demonstrated VERA's ability to provide close to real-time insight into complex reactor operations.

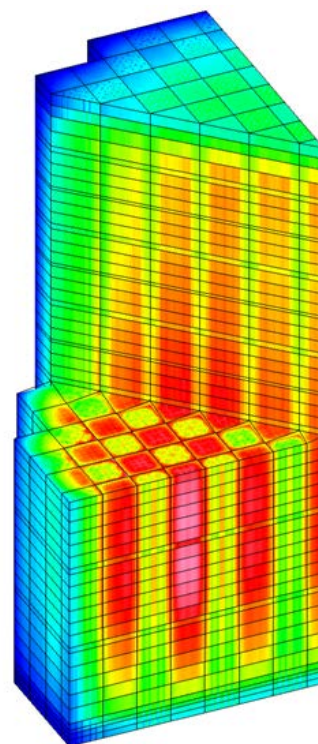


Figure 1. Hot zero power beginning of cycle fission rate distribution in WBN-2 (quarter-core).

2. **Detailed analyses of Pellet-Clad Interaction (PCI) was performed for cycles 6 and 7 of Watts Bar Unit 1 (WBN-1) demonstrating use of BISON to perform fuel performance calculations for quarter-core and more detailed single fuel pin simulations including assessment of missing pellet surfaces.**

An analysis of WBN-1 was performed to investigate PCI fuel cladding failures that occurred in cycles 6 and 7 involving quarter-core simulations of all fuel rods with BISON to identify areas of interest followed by detailed three-dimensional simulations to analyze key indicators for PCI. The demonstration represents a culmination of effort in fuel performance simulation development and integration with core simulation capabilities and provides the ability to screen all fuel rods in the core along with localized three-dimensional analysis for selected rods.

3. **Computer resource requirements for the VERA core simulator (VERA-CS) were significantly reduced to achieve the goal of a cycle depletion on 1,000 cores overnight to allow its use on industry computing clusters.**

Significant improvements in the computational performance of the MPACT neutronics capability and the CTF thermal-hydraulics parallelism have reduced computational requirements by a factor of five. Quarter-core cycle depletions can now be simulated overnight on 1,000 computer cores, which is a performance rate

that will allow industry to run significant problems on widely available computing clusters. This will greatly expand the ability to apply VERA through industry on their own computer systems.

**4. Research and development was performed to extend VERA to BWRs with improvements in CTF subchannel thermal hydraulics and continued development of second generation two-phase closure models for computational fluid dynamics (CFD).**

In the second five-year phase of CASL, research is being performed to extend the applicability of VERA to BWRs. The primary development has focused on improving models for two-phase (liquid and steam) water in both the COBRA-TF subchannel thermal-hydraulics code, which is the primary tool used for core-wide thermal-hydraulics in VERA and in the development of improved second generation closure models for use in CFD.

**5. CASL held its first Summer Institute with 24 participants from universities, industry, and national laboratories.**

The CASL Summer Institute was a two-week course held in June at Oak Ridge National Laboratory that included lectures and hands on experience with VERA. The lectures covered both the methods and details of the VERA computational tools and overviews of the CASL Challenge Problems. The participants used VERA on practical problems that were presented at the end of the institute.

**6. VERA was selected by *R&D Magazine* as a finalist for an R&D 100 Award.**

The R&D 100 awards are known as the “Oscars of invention” and honor products that have brought innovation and top technology to industry over the past year. This award recognizes the technology developed by CASL as well as its use by industry on real-world problems. The winners of the 2016 R&D 100 Awards will be announced on November 3, 2016.

The R&D performed by CASL is well documented in a range of publications including journal articles, technical reports, and conference papers, which are summarized in Table 1. Journal articles were published in a number of leading technical journals, including those submitted for a special issue of the *Journal of Computational Physics*. CASL staff also widely publish and present papers at relevant conferences. Milestone deliverables are documented in periodic reports, and other technical and programmatic information appears in various reports. Most of these reports are available on the CASL website at [www.casl.gov](http://www.casl.gov).

More details associated with the full range of FY 2016 CASL accomplishments are provided in Parts 2, 3 and 4 of this report and describe the impact and return on taxpayer investment of the investment in CASL.



## Summary of Funding and Investments

The total CASL FY 2016 funding provided by the DOE Office of Nuclear Energy (DOE-NE) was \$24.3M, with \$23M being available to the program after DOE holdbacks for small business and other initiatives. When combined with the \$7.3M in carry over from FY 2015, the total funding available for FY 2016 was \$30.3M. The total costs for the program were \$23M, with \$5M for program management, operations, infrastructure, contract overhead, and taxes, and \$18M to support technical work (see Part 3 for additional details).

Table 1. Summary of CASL Technical Output through FY 2016

|                             | FY 2016 | Total |
|-----------------------------|---------|-------|
| <b>Journal articles</b>     | 56      | 181   |
| <b>Conference papers</b>    | 54      | 443   |
| <b>Invited talks</b>        | 20      | 196   |
| <b>Technical reports</b>    | 83      | 311   |
| <b>Milestone reports</b>    | 128     | 675   |
| <b>Programmatic reports</b> | 40      | 275   |

The FY 2016 taxpayer investment in CASL produced a wide range of M&S advances that are detailed in the 128 milestone reports that are mostly available for unlimited distribution through the CASL website. This includes the successful completion of all 11 of the milestones provided to DOE as a metric for CASL's FY 2016 performance evaluation. The accomplishments detailed in the reports are producing positive effects in nuclear science and engineering, nuclear energy industry work practices, and nuclear energy education and workforce development that are summarized in Parts 2 and 3 of this report. Part 4 of the report presents a more detailed summary of how the FY 2016 CASL funding was spent and describes work that is being performed to preserve taxpayer investment in CASL.

## The Future of CASL

CASL is currently expecting to receive its last year of government funding in FY 2019, so preparations for transitioning the program's R&D into the post-CASL period have begun. The following end state vision for the program has been established to help guide these preparations:

***By the end of the CASL operational period, CASL will have successfully developed and deployed advanced M&S technologies that can be used with confidence to solve the CASL challenge problems and address future nuclear energy industry challenges, emerging issues, and evolving opportunities.***

CASL leadership, working with the Board of Directors, have prepared a post-CASL strategy for the period beyond 2019. Part 4 of this report also includes a discussion of the post-CASL strategy.

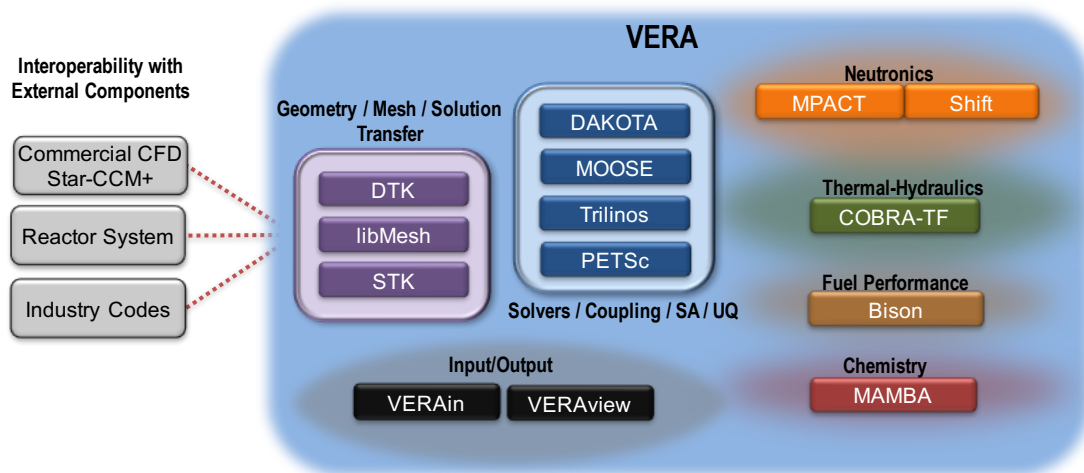
## PART 2: SCIENCE AND ENGINEERING PROGRESS AND IMPACT

The funding provided by DOE and investments from CASL partners were used to perform impactful R&D that advances the ability to predict operational characteristics of the current LWR fleet. The work involved a balanced science and engineering effort, including development and demonstrations of CASL M&S technologies, development of tools that improve usability of the technologies, and education of future scientists and engineers.

### Status of the Virtual Environment for Reactor Applications

VERA is a collection of simulation tools that can be coupled together to allow for analysis of the full range of physical processes that affect nuclear reactor operations. The state-of-the-art capabilities within VERA provide unprecedented resolution for reactor analysis through high-fidelity multiphysics couplings. The components for steady-state reactor core simulation were selected to eliminate the barriers facing modern industrial methods for improved accuracy on smaller spatial scales. VERA provides direct fully coupled solutions at the fuel rod level for neutronics and thermal-hydraulics without any spatial homogenization. Isotopic depletion and transmutations occur locally within single three-dimensional calculations, avoiding the need for macroscopic spectral corrections to simplified history models. The user interface is designed to be easy to use by engineers and provides a single common geometry model for each of the underlying physics codes. VERA also automatically manages the calculation flow, data transfer, and convergence among VERA codes.

The current configuration of the simulation environment is shown in Figure 2. The environment includes a subset of capabilities known as the VERA core simulator (VERA-CS) that can be grouped together to provide functionality similar to current industry tools but with considerably more fidelity and resolution.



**Figure 2. Summary of M&S tools included in VERA.**

The latest release of VERA, version 3.5, includes selected computational tools and supporting infrastructure that solve neutronics, thermal-hydraulics, fuel performance, and coupled physics problems. The tools included in the release are still under active

development and are subject to modifications, so they have not been fully validated and are being released for test, evaluation, and research purposes.

The infrastructure components included in VERA 3.5 provide a simplified common user input capability and provide for physics integration with supporting data transfer and iterative solution algorithms. The release includes two neutronics modeling capabilities: MPACT supports deterministic analysis methods and SHIFT supports stochastic analysis. A thermal-hydraulics capability provided by the CTF subchannel code allows for thermal-hydraulics analyses of single and multiple fuel assemblies. The distribution also includes a coupled neutronics/thermal-hydraulics capability and the nuclide transformation analysis code ORIGEN, which together form VERA-CS. Recently MAMBA, the VERA chemistry component, has been integrated into VERA-CS to support analysis of Chalk River unidentified deposits (CRUD) growth and boron deposition in CRUD.

BISON is a modern finite-element-based nuclear fuel performance code that has been under development at the INL since 2009 that can be used to calculate fuel rod temperatures, fuel rod internal pressures, fission gas volumes and release, cladding integrity characteristics, and changes in fuel rod dimensions during reactor operation. These capabilities allow for simulation of power cycling, fuel conditioning and deconditioning, and high-burnup fuel performance; support for power uprate scoping studies; and support for identification of initial conditions for accident analyses. BISON has been integrated into VERA-CS by using the code to replace the fuel rod model in CTF, and linkage to other physics using the CASL data transfer kit has been demonstrated.

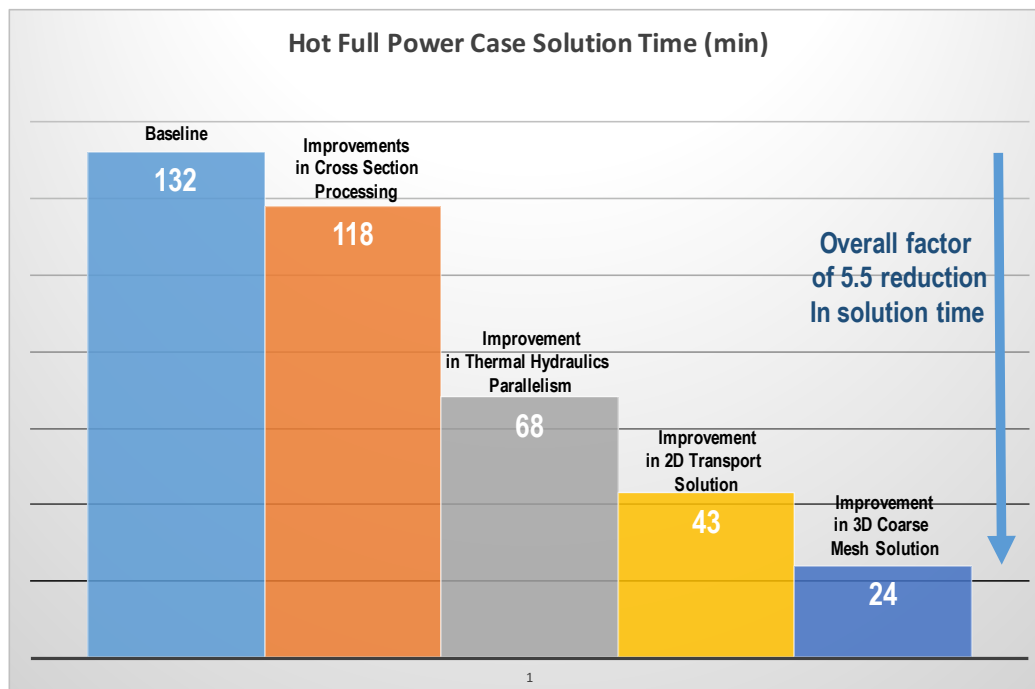
Most of the VERA tools are being designed for use on a variety of computing platforms, ranging from computing clusters that are available to industrial users to DOE's Leadership Computing Facilities, which consist of petascale-class (and eventually exascale-class) platforms. CASL's research activities are performed on computing platforms at our partner locations including two 75 million core-hour allocations through the DOE Office of Science ASCR Leadership Computing Challenge on the Oak Ridge Leadership Computing Facility's Titan supercomputer, which is provided by an award from the DOE Advanced Scientific Computing Research Leadership Computing Challenge. CASL activities also used approximately 50 million core-hours on Idaho National Laboratory (INL) high performance computing systems and extensive time on the Lonestar 4 computer at the Texas Advanced Computing Center.

## **VERA Performance Improvements**

The amount of time required to complete large analyses using the VERA tools was significantly improved during FY 2016 [1]. The improvements were demonstrated using the results of two analyses. The first was simulation of a quarter-core hot full-power case using WBN-1 geometry and the second was simulation of the first five states of WBN-1 cycle 1 with depletion. Both cases were run using 870 processors on the Oak Ridge National Lab (ORNL) Nuclear Science and Engineering Directorate cluster.

Figure 3 illustrates the run-time improvements that were achieved for the quarter-core hot full-power case. The figure shows the results of improvements that were completed in six key aspects of the simulation. The improvements are shown in the order in which they were completed and, for each improvement, the run time is plotted by component so that the run-time changes can be seen from left to right. The final run time for the hot full-power case

was 24 minutes and 5 seconds on 870 cores, which was an improvement of five and a half times compared with the 2015 baseline. Similar results were achieved for the cycle depletion case with five depletion points.



**Figure 3. Summary of VERA-CS performance improvements on a quarter-core 3D hot full power simulation achieved during FY 2016.**

## Extension of VERA to Additional Reactor Types

BWR capability development during FY 2016 focused on addition of three features in CTF [2]. First, a new preprocessor utility was developed that is capable of handling BWR-specific design elements (e.g., channel boxes and large water rods). An FY 2015 milestone led to the development of this preprocessor capability for single-assembly models, and the FY 2016 work expanded the utility to make it applicable to serial and parallel modeling of multiple BWR assemblies. The preprocessor is extensible to PWR models to allow for simulation of new PWR designs and may be applicable to analysis of SMR natural circulation operations.

Second, an outer iteration loop capability was added to CTF to allow the code to use the new preprocessor. The iteration loop allows for adjustment of inlet mass flow rates to equalize pressure loss over all assemblies that are not connected to channel boxes. The feature was tested on a full-core, mock BWR/4 model with nonuniform power distribution, and individual assembly pressure drops converged to within 0.05 psi of the core average in five outer iterations.

The third feature added during FY 2016 provides the capability to assess the standard convergence metrics that are used by CTF to determine when a simulation has reached steady state. An order of convergence study was performed for a model representative of a BWR 8 × 8 fuel bundle with nonuniform power distribution, and the study demonstrated that convergence of solved bundle pressure drops and exit flow quality was consistent with the

theoretical first-order convergence of CTF.

### **Interoperability with Commercial Modeling Tools**

Compatibility of VERA with industry software tools continues to be a part of the CASL implementation strategy. The most important interoperability accomplishment during FY 2016 was development of an interface between the VERA chemistry code MAMBA-1D and the commercial code STAR-CCM+®. STAR-CCM+® is a commercial, closed-source CFD code developed by CD-adapco that can be operated through a graphical user interface or a JAVA application programming interface. A library referred to as SUMAC (STAR-CCM+® user code and MAMBA-1D cycle simulator) was developed at the University of Michigan to enable computationally efficient multistate cycle simulations and STAR-CCM+®/MAMBA-1D coupling. The coupling library allows for state-of-the-art high-resolution CRUD simulations made possible through the use of high-fidelity thermal-hydraulic boundary conditions provided by CFD [3].

CASL also made extensive use of the ABAQUS finite-element structural mechanics code, developed by Dassault Systems, to perform structural mechanics analysis in support of the GTRF challenge problem including the simulation of the fuel rod gap development and wear over the course of operation.

### **Verification, Validation, and Uncertainty Quantification**

An efficient surrogate-based data assimilation method was also demonstrated using a quarter-core three-dimensional model representative of WBN-1 cycle 1. [3] The data assimilation results were used to requantify the uncertainty for simulation and to investigate the effect of calibrating parameters on uncertainties associated with quantities of interest. The study found that data assimilation can be performed using high-fidelity core simulations with reasonable computational costs and that the analysis method significantly reduces uncertainties by up to 75% for maximum fuel pin power, 82% for maximum fuel pin temperature, and 55% for the multiplication factors. The ROMUSE software used to perform the analysis is now being incorporated into the DAKOTA tools that are used to perform VERA uncertainty quantification.

### **Progress on CASL Challenge Problems**

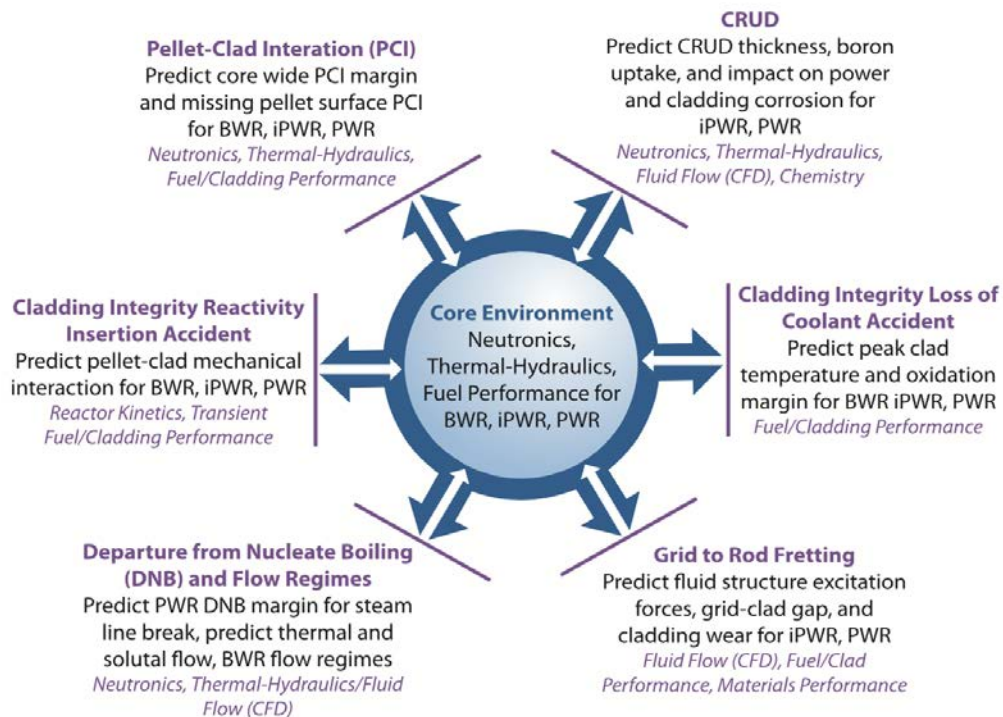
VERA is being developed to analyze real-world reactor problems. Consequently, CASL industry partners identified a set of high-priority challenge problems during formation of the consortium to guide code development. The challenge problems were updated in FY 2015 to reflect the current state of VERA development and to incorporate challenges associated with BWRs and SMRs. The current set of challenge problems is summarized in Figure 4.

### ***Progress on CRUD Challenge Problems***

The CASL FY 2016 CRUD challenge problem work continued to focus on analysis of CRUD-induced power shift (CIPS) and CRUD-induced localized corrosion (CILC).

In combination with MAMBA, VERA-CS has been shown to produce accurate CIPS modeling for the Seabrook and Watts Bar nuclear reactors using plant data for the nickel and iron source terms that influence CRUD formation. Not all CIPS modeling will have access to similar plant data, so work on a MAMBA source term model was initiated during FY 2016.





**Figure 4. Summary of CASL challenge problem scope.**

The primary CRUD source in PWRs is corrosion in steam generator tubing. This corrosion develops as oxygen diffuses into the base metal and transforms alloy elements from the metallic state to the oxide state. Divalent metal ions are then released into the water as soluble metal ions. The metal ion release rate is dependent on the diffusion coefficient of oxygen, oxide layer thickness and composition, and coolant conditions. Three coolant chemistry conditions promote corrosion and release of corrosion products: high oxygen content, low pH, and high temperatures. Work has begun to incorporate all of these factors into a MAMBA mass balance and soluble/insoluble species transport model following the systems level analysis capability included in the Westinghouse BOA code.

A full core simulation of the Seabrook reactor core was performed with the VERA-CS neutronics code MPACT coupled to the subchannel code CTF, and the power distribution obtained with MPACT/CTF was used as input for the MAMBA-3D chemistry code coupled to STARCCM+. [4] The STAR-CCM+®/MAMBA-3D codes were used to simulate a  $5 \times 5$  subregion of Seabrook cycle 5 fuel assembly G70 that contained a fuel rod that failed as a result of CILC (rod G70G09), and the CRUD and oxide distributions in the subregion were compared with measured plant data as shown in Figure 5. The simulation results agreed well with all visual observations, including:

- Buildup of CRUD and thick oxide was mostly confined to the upper part of the fuel rods.
- Oxide levels generally showed a step increase in spans 5 and 6, while oxide levels in the remaining spans were significantly lower.

- No strong trend was found for preferred CRUD orientation in water rods (thimbles).
- CRUD was mostly patterned in vertical stripes, with the stripes maintaining the same orientation over multiple grid spans. In a few cases, a gradual spiral pattern of CRUD deposits within a grid span was observed.

The simulations also strongly agreed with measured data. In particular, the axial and azimuthal location of the maximum combined CRUD and oxide thickness in the failed rod was accurately predicted, as was the thickness of CRUD and oxide at the location of pin failure.

Overall, very promising results were obtained from this work, which suggests the CASL VERA tools are able to contribute to the understanding of CILC and are able to support identification of high-risk fuel rods.

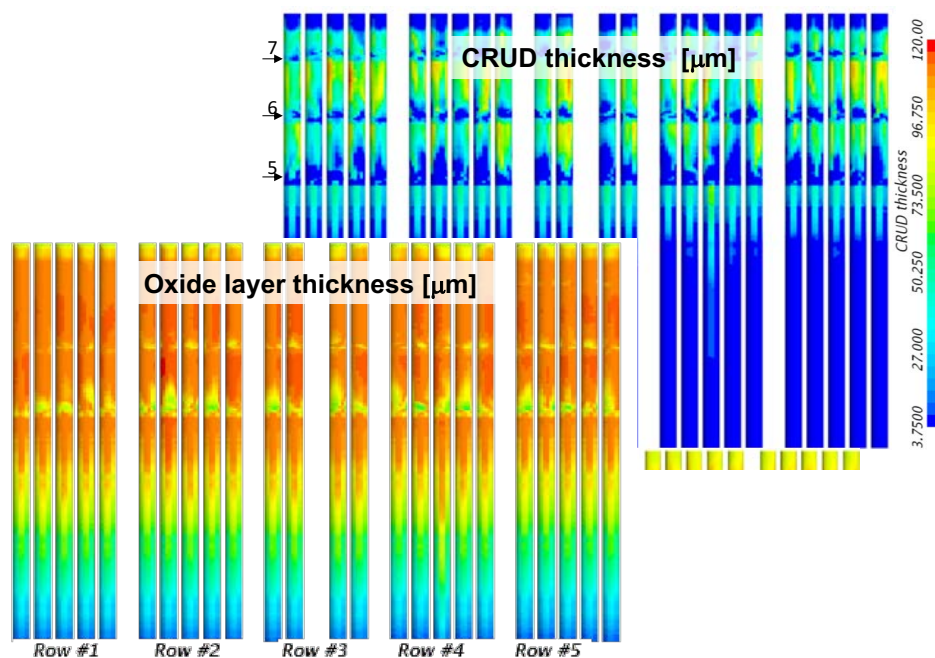


Figure 5. Simulation results for CRUD and oxide layers on Seabrook fuel rods [4].

### ***Progress on the Pellet-Clad Interface Challenge Problem***

Demonstration of the VERA pellet-clad interaction (PCI) analysis capabilities continued during FY 2016 with quarter-core modeling of WBN-1 cycles 6 and 7 [5] using the BISON fuel performance code.

WBN-1 cycles 6 and 7 included cladding failures that, at the time, were believed to have been caused by PCI. The quarter-core analysis was used to calculate maximum, minimum, average, and integral quantities of interest across each fuel rod, and clearly showed that hoop stress levels in the fuel were significantly lower than the stress that would be required to cause PCI failure. As a result, the analysis indicated the failures were likely caused by an external factor, such as missing pellet surfaces, rather than by classical PCI. The analyses were also able to distinguish between the behavior of cycle 6, which had a relatively simple power history, and the cycle 7 history where the presence of CIPS drove rapid changes in fuel temperature and stress distributions. The cycle 6 analyses were completed using



roughly 39,500 core-hours on the INL Falcon computing system, and the cycle 7 analyses used approximately 37,500 core-hours.

The minimum gap thickness distributions calculated in the analyses identified rods that likely experienced early fuel-cladding contact, which is a precursor for high cladding-hoop stresses that can lead to cladding failure. Changes in peak centerline fuel temperature, which can drive swelling and subsequent fuel-cladding contact and stress, also helped identify rods that were candidates for more detailed analysis. The assemblies selected for analysis based on fuel rod stress states are outlined in black in Figure 6. Twenty-six rods from cycle 6 and 25 rods from cycle 7 were selected.

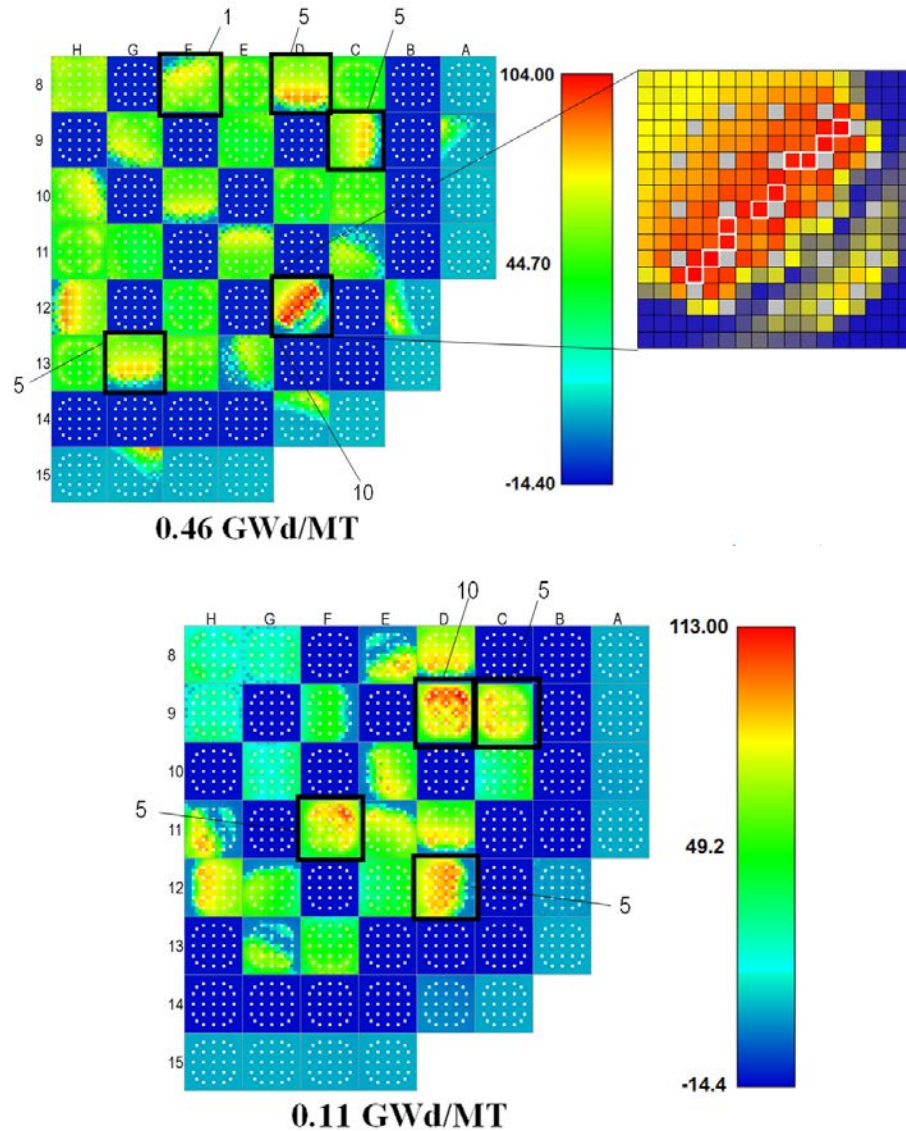


Figure 6. Calculated cladding hoop stress for each fuel rod and assemblies selected for further analysis from WBN-1 cycle 6 (top) and cycle 7 (bottom) [5].

The BISON PCI analysis capability was further enhanced during FY 2016 by addition of frictional contact algorithms to the BISON two-dimensional and three-dimensional fuel simulation packages. Before these additions, the majority of BISON simulations used either frictionless or glued contact representations. The FY 2016 work demonstrated that frictional

effects could have significant impact on cladding mechanical response to elongation. The work also added three new features to BISON, including a newly implemented hybrid formulation for enforcing contact, improvements to the contact slip damper, and new contact test problems.

Another feature that was added to BISON is the capability to represent discrete cracks in cladding and fuel using the extended finite element method (XFEM). Because XFEM cracks do not have to be embedded in a model's mesh, XFEM improves modeling of fractures in nuclear fuel because it can represent discrete fractures in a mesh-independent manner, it allows for realistic modeling of crack propagation, and it can simplify the creation of models where the effects of discrete fuel fractures are of interest. Constraint enforcement across XFEM interfaces can currently be used to model heat transfer across crack interfaces, and contact capabilities have been successfully demonstrated on a PCI model. Future work related to XFEM modeling will include expanding constraint enforcement capabilities to permit modeling mechanical interactions, such as contact, cohesive behavior, and crack healing across XFEM interfaces. Techniques for enforcing contact on the sides of cut elements will also be refined to enforce contact at the edge of cut domains rather than at phantom nodes.

### ***Progress on the Departure from Nucleate Boiling Challenge Problem***

Two departure from nucleate boiling (DNB) modeling approaches are being developed by CASL [6]. The first approach leverages the robustness of first generation boiling closures and extends them to DNB, including a macrolayer-based triggering technique that relies on local void fraction distributions on heated rods. The first assessment of this approach was completed during FY 2016 and reasonably good predictions were achieved, particularly for high- and low-flow subcooling conditions. The assessment involved a qualitative and quantitative comparison of simulated DNB results with existing experimental DNB datasets, and the validated simulation approach led to the development of best practice guidelines for DNB modeling in nuclear thermal-hydraulic applications.

The main results and key findings of the FY 2016 DNB model development work included:

- Development and testing of a subcooled flow boiling DNB calculation using a multiphase CFD approach.
- Calculation of full history-of-boiling curves and the DNB points for each test condition and comparison of the calculation results with corresponding experimental DNB datasets.
- The trend behavior of the calculated DNB followed general observations from experimental DNB literature.
- The DNB simulations based on the proposed CFD methodology strongly agrees (i.e., less than 20% deviation) with independent experimental datasets over the range of the test conditions (Figure 7).

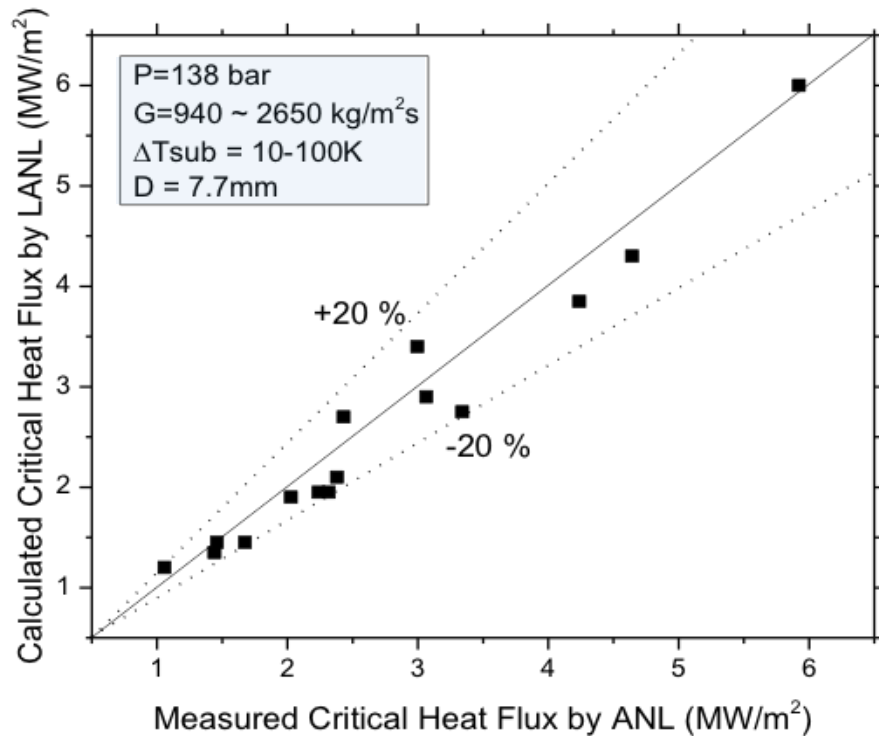


Figure 7. Calculated CHF compared to measured CHF at the corresponding test conditions [6].

### ***Progress on the Reactivity Insertion Accident Challenge Problem***

A significant FY 2016 achievement related to the reactivity insertion accident (RIA) simulation was the development, implementation, verification, and validation of methods in MPACT that are needed to solve whole-core, time-dependent neutron transport problems with pin-resolved detail using internal thermal-hydraulic feedback [7]. The work included development and implementation of an innovative transient multilevel (TML) method that reduces the computational burden for full core transient simulations. In this method longer time steps are used for the slowly varying and computationally expensive method of characteristics angular flux solutions, and smaller time steps are used to capture the more rapidly varying spatial and amplitude flux variations using computationally efficient coarse mesh finite difference and point kinetics equation time-dependent solutions. The TML method is particularly important for transients, such as super-prompt RIAs in which power changes very rapidly within the first second of a transient, especially for events that begin from the zero power condition.

The new MPACT method uses a backward Euler discretization in time, which does not require storage of angular fluxes. However, using large time steps in the backward Euler discretization for the method of characteristics solution has the potential to introduce numerical instabilities that would then impose time step size limitations and limit the performance of the TML method. This limitation was an important numerical challenge, and overcoming it required development of an innovative exponential transformation method that could be used for practical RIA calculations.

Finally, a detailed convergence analysis was performed on the time-dependent neutron

transport equation using the Fourier analysis technique. A thorough understanding of the transport equation's convergence properties provided confidence for applying the TML method for all anticipated transient applications in an operating LWR.

Verification of the MPACT transient capability was performed using a series of regression problems based on the VERA benchmark suite, the two-dimensional TWIGL, and three-dimensional OECD C5G7-TD transient benchmarks. Code validation was performed using selected tests from the SPERT-III E-Core experiments (Figure 8). MPACT results for the SPERT-III test 86 and test 60 cases agreed with the experimental data. Finally, hypothetical three-dimensional hot full power super-prompt and sub-prompt transients were designed and simulated for the Watts Bar reactor. The results confirmed the feasibility of performing VERA-CS transients for practical large-scale LWR problems.

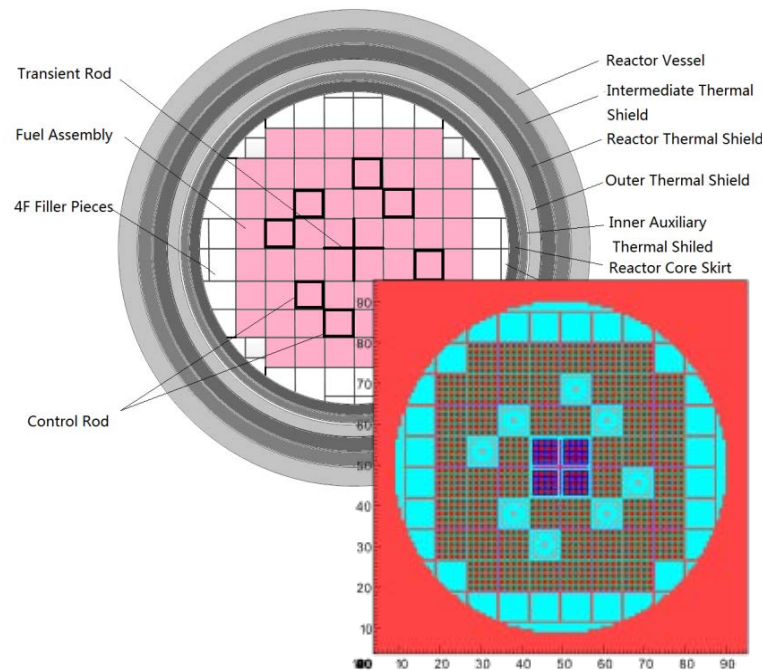


Figure 8. SPERT III E core cross section at midplane and corresponding MPACT model [7].

The BISON development team also made progress in RIA analysis by participating in the second Organization for Economic Cooperation and Development benchmark focused on simulating RIA behavior using fuel performance codes [8]. Results from an earlier first benchmark demonstrated a large amount of scatter in predictions from various codes, so a second benchmark that includes simpler cases was designed to clarify differences in modeled results. The second benchmark includes ten cases that initially isolate transient thermal behavior and gradually increase in complexity by including mechanical effects and thermal-hydraulic behavior. BISON has been run on most of the cases and compared with several other fuel performance codes. Specific comparisons between BISON and FRAPTRAN show a reasonable comparison between the codes, particularly in the area of transient thermal behavior. A second phase of the benchmark that is planned for next fiscal year will include RIA sensitivity and uncertainty analysis.

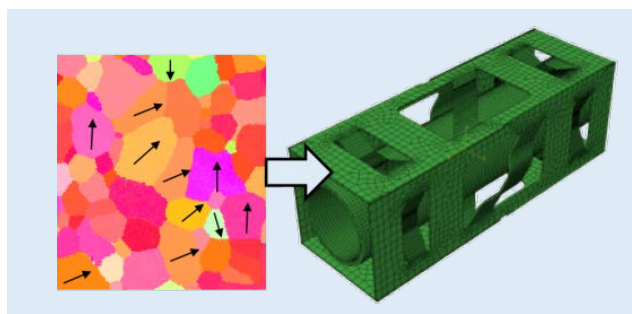
### ***Progress on the Grid to Rod Fretting Challenge Problem***

FY 2016 work on the grid to rod fretting (GTRF) challenge problem focused on coupling creep and wear effects, and examining the regimes in which creep and wear control stress relaxation. The two mechanisms were coupled in simulations that assumed different friction coefficients, excitation pressures, and wear coefficients, and initial misfits were run to explore how different parameters affect the wear profile and the time at which the grid and cladding lose contact. The simulations indicated that two stages exist during the relaxation of the contact force: partial slip and full slip. When partial slip occurs, the dominant relaxation mechanism is creep. During this regime, the wear scar propagates across the contact, and there is a transition to full slip. Once full slip occurs across the entire interface, and the contact forces are relatively low, the creation of a wear scar becomes the dominant relaxation mechanism. In this regime, reducing the wear coefficient and the amplitude of excitation force delays the formation of a gap between the grid and cladding.

The wear profile developed during full slip occurs homogeneously, so for a given initial interference, there is a master curve for the wear scar that does not depend on the friction coefficient, the amplitude of the excitation pressure, or the wear coefficient. Therefore, the wear profile is defined by the maximum wear depth, which in turn depends on the number of wear cycles and the product of the square of the excitation pressure times the wear coefficient. This relationship allows for modeling to be used to estimate the effects of parameters that are often poorly defined for the GTRF problem.

In order to develop data to inform new wear model, a new autoclave fretting-impact wear has been designed and is currently being fabricated. This experimental rig can provide data for a range of materials at conditions higher temperature and pressure conditions – water temperatures of 220°C and 24 bar.

Research was also performed to develop a physics-based crystal plasticity framework for modeling irradiation growth and creep to interface with the finite element code ABAQUS to study the contact forces and the gap evolution between the spacer grid and the cladding tube as a function of irradiation in a fuel rod assembly. Deformation mechanisms governing the gap opening have been identified and correlated to the texture-dependent material response (Figure 9). These simulations predict the contribution of irradiation growth and creep to the gap opening between the cladding tube and the springs and dimples on the spacer grid. Loading conditions representative of fuel rods at the periphery show larger gap opening, which is in agreement with in-reactor data.



**Figure 9. Texture and grain interaction modeling (left) is being used to inform gap opening in grid spacer elements (right).**

Current plans call for the work on the GTRF challenge problem to be finalized in FY17.



## PART 3: END USER IMPACT AND EDUCATION/WORKFORCE DEVELOPMENT

An increasing amount of CASL's activity is focusing on the expanding set of VERA end users who are looking to apply VERA to their own problems of interest. Additionally, CASL is also focused on educating the current and future workforce on the use of advanced computing tools and capabilities.

### Engaging VERA End Users

Several specific activities were targeted in FY 2016 to support engagement with VERA's end users, ranging from Industry Council meetings and engagements, VERA Working Group meetings, continuing VERA releases, expanding Test Stand deployments, and improving usability.

### CASL Industry Council

An important means of engaging the CASL end users and stakeholders is through the CASL Industry Council. The council consists of 24 organizations and is comprised of nuclear plant owner/operators, fuel and reactor vendors, engineering service providers, independent software vendors, and computer technology companies (Figure 10). In 2016, two meetings of the Industry Council were held including a joint meeting with the CASL Science Council in November and an independent Industry Council meeting in April. The Industry Council provided solid feedback at both meetings on CASL's progress and emphasized their priorities, which were taken into account in CASL's planning meetings.

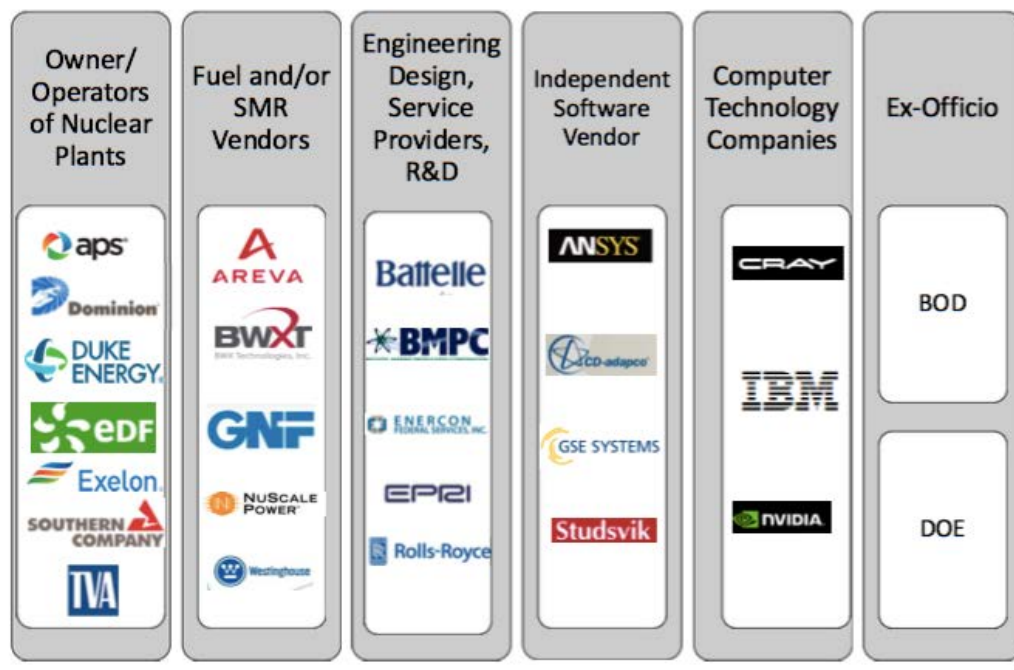


Figure 10. CASL Industry Council member organizations.



### ***VERA Working Group***

The concept of the VERA Working Group (VWG) was established during FY 2015, and the group's first meeting was held during April 2016 after the spring 2016 CASL Industry Council meeting. The VWG is an administrative body that enables the sustained use and development of VERA; finds and supports users; and facilitates VERA R&D, code upgrades, and distribution through funding provided by users of the CASL codes. As evidenced by the active participation of a large number of Industry Council members in the Working Group meeting, there appears to be Industry Council support for starting up the VWG. Actions identified during the meeting included distribution of the draft group charter that was included in the CASL phase 2 renewal proposal. Future meetings of the group will likely be scheduled in coordination with Industry Council meetings until the VWG charter is approved and the community of VERA users begins to expand.

### ***VERA Releases***

During FY 2016, there were two major releases of the VERA environment to users outside of CASL and several distributions to Test Stands. In the VERA 3.4 package [9], CASL condensed the supported set tools and capabilities, removing components that are obsolete and are no longer under development. VERA 3.5 [10] represents an incremental release, with improvements to core component capabilities, significant performance improvements, the addition of VERAView, and updated documentation.

VERA 3.4 was the first CASL release to see broad distribution to academia, national laboratories, and industry. The Radiation Safety Information Computational Center distribution process was finalized in FY 2016, with test and evaluation licensing and online registration. Thirty-four VERA test and evaluation licenses were executed in FY 2016 to a variety of users in academia, industry, and national laboratories, including the University of California at Berkeley, the University of Illinois at Urbana-Champaign, AREVA, Exelon, Southern Co., Pacific Northwest National Laboratory, and Argonne National Laboratory.

The CASL Support, Improvement, and Corrective Action Tracking system also operated without issue during FY 2016. Forty-seven support tickets were opened during the year, and 39 were closed. CASL only received four user support requests through the user support tracking system despite the relatively high number of distributions to new users.

### ***Test Stand Deployments***

Two CASL Test Stand applications were initiated during FY 2016. The first was with AREVA NP to perform comparisons of VERA predictions for CRUD presence and severity with CRUD deposit data obtained via visual inspections at the Davis-Besse Nuclear Power Station. AREVA and the CASL leadership team reached an agreement on the Test Stand scope of work, and AREVA will be using their own computing resources as well as developing a proposal to obtain access to the ORNL Titan leadership-class computer to support completion of the Test Stand scope.

The second Test Stand application was with the University of Illinois at Urbana-Champaign to apply VERA to analyze fuel duty related to the PCI. As part of the Test Stand, a mini-PWR model was developed to test MPACT/CTF capability with reduced computational burden and a two-dimensional full core model was developed to test parallel MPACT/CTF capabilities for PWR depletion.

Planning for several new Test Stand applications was also started during FY 2016. Potential future Test Stands include:

- NuScale Power™ plans to use VERA to assess CRUD risks for SMR applications.
- A Westinghouse multiyear effort to model accident-tolerant fuel—a joint CASL/NEAMS Test Stand—is planned.
- Rolls-Royce Ltd. plans to use VERA-CS to analyze a new SMR design the company is developing.

### ***Improvements in Usability—VERAView Development***

VERAView has been developed as an interactive graphical interface that supports visualization and engineering analyses of VERA output data [11]. The Python-based software is easy to install, intuitive to use, and rapidly produces plots and data drawn from VERA simulations. It directly reads the VERAOut HDF5 file format and interprets reactor data based on dataset size and shape. As a result, VERAView is able to display almost any HDF5 data and is not limited to VERA codes. For instance, CASL has used VERAView to compare processed results from non-CASL codes such as KENO-VI and MCNP, as well as industry design and analysis codes.

VERAView incorporates a modular widget design, and the code's event sequences allow for unlimited expansion of tools, data views, and calculations. The selection of Python as the source language also gives VERAView instant access to thousands of libraries and add-ons, and provides an easy-to-use platform for future developers to create custom widgets as new needs arise. An example of VERAView output is shown in Figure 11.

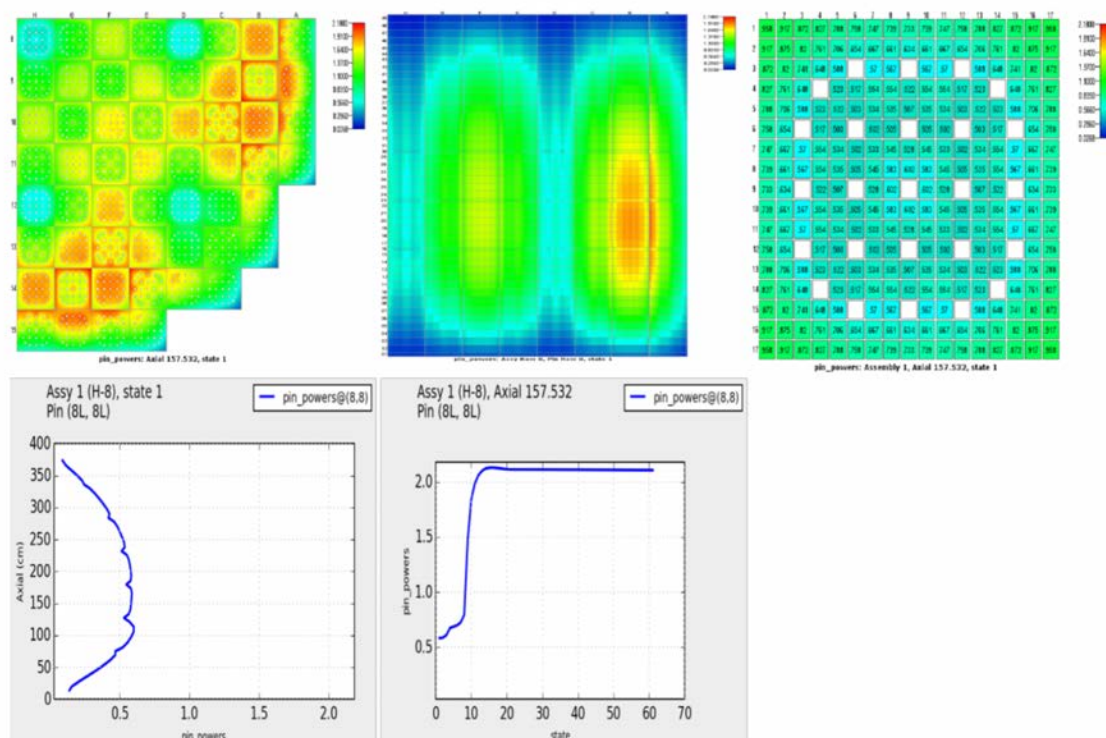


Figure 11. Example VERAView widgets showing rod ejection simulation results.

## ***Demonstration and Applications of CASL Tools***

CASL is actively applying and demonstrating VERA to operating plans and industry-driven analysis through our challenge problems and through specialized analyses motivated by CASL industry partners and Test Stands. Two applications demonstrating industry impact are highlighted below.

### ***Application of VERA to Watts Bar Nuclear Unit 2 Startup***

A very important demonstration of the VERA suite was completed in 2016 when the software tools were used to simulate startup and power escalation for the WBN-2 reactor. TVA's WBN-2 is the first new reactor to come online in the United States in nearly two decades, and it presented a perfect opportunity to test VERA capabilities on a modern reactor design. The reactor achieved initial criticality and began power ascension on May 23, 2016. CASL analysts used VERA tools and the INL Falcon computing platform to perform high-fidelity physics calculations before startup and ongoing simulations as the plant increased power toward commercial operations.

WBN-2 is a traditional Westinghouse four-loop PWR with an ice condenser containment design, much like its sister WBN-1. Its reactor core consists of 193 nuclear fuel assemblies of the Westinghouse 17 × 17 design placed in a cylindrical arrangement. Cycle 1 is loaded in three enrichment regions to optimize the fuel costs and fuel rod power distribution. The fuel-loading pattern is similar to other first cycle designs like WBN-1, but this is the first time that integral fuel burnable absorber and wet annular burnable absorber have been used in an initial startup. Another new feature included in WBN-2 is the use of fixed vanadium in-core detectors, rather than the moveable fission chambers used in most previous Westinghouse plants of this type. The reactor is rated at 3,411 MWth, and the fuel assembly, control rod bank positions, and in-core detector locations are the same as WBN-1.

Table 2 and Figure 12 summarize results from the WBN-2 analyses. The results show that VERA was able to predict important startup parameters and follow control rod bank positioning during power ascension with a very high degree of accuracy. Additionally, the power ascension calculations were performed at close to real time, demonstrating VERA's ability to produce results that can be used to quickly analyze emerging issues that might arise during normal plant operations.

***Table 2. Comparison of MPACT and SHIFT Results with WBN-2 Startup Measurements\****

|                                                 | Measured | MPACT<br>Difference | SHIFT<br>Difference |
|-------------------------------------------------|----------|---------------------|---------------------|
| Initial Critical Boron Concentration (ppmB)     | 1,089    | -14                 | -2                  |
| 2nd Critical Boron after First Shutdown (ppmB)  | 1,051    | -16                 | -6                  |
| 3rd Critical Boron after Second Shutdown (ppmB) | 1,036    | -17                 | -7                  |
| 4th Critical Boron after Third Shutdown (ppmB)  | 1,017    | -17                 | -6                  |
| Isothermal Temperature Coefficient (pcm/°F)     | -5.31    | -0.15               | —                   |

\*Measurements courtesy of TVA

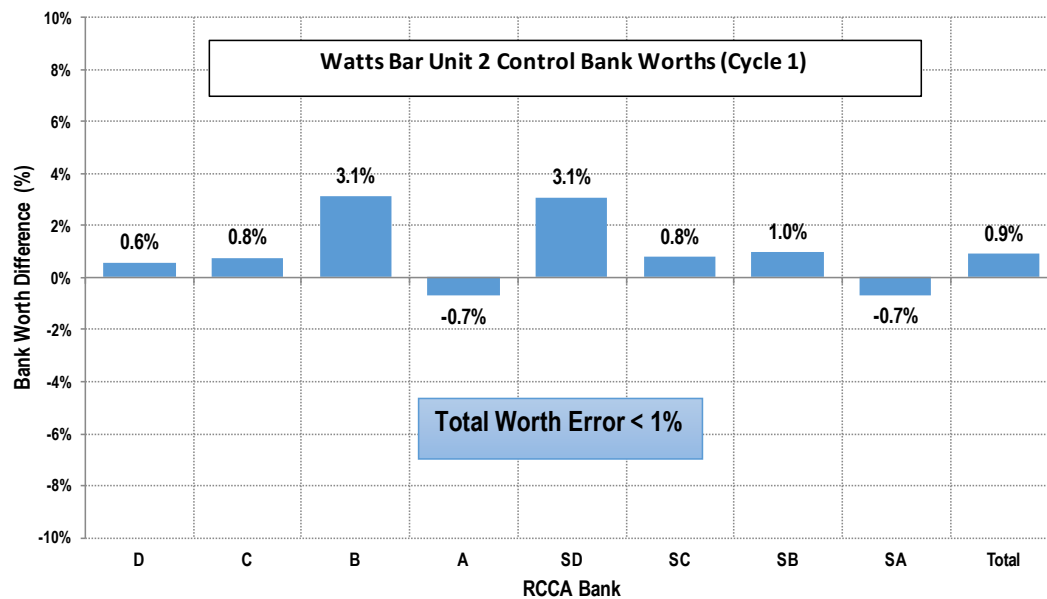


Figure 12. Comparison of VERA results to WBN-2 control bank worths.

### ***Assessing DNB for High-Flow vs Low-Flow Steamline Break***

A Westinghouse-led study of the DNB limiting case analysis for a postulated PWR main steam line break event initiated at hot zero power was also completed during FY 2016 [12]. The work focused on analyzing event coolant flow using the latest versions of MPACT and CTF. The new calculations of high flow with offsite power and low flow without offsite power cases were based on revised core boundary conditions from RETRAN and inlet flow and temperature distributions from STAR-CCM+. Parametric sensitivity studies and uncertainty quantification analyses were performed using the Wilks nonparametric approach to determine the DNB limiting case. The results of the study confirmed that the high flow case with offsite power is more limiting than the low flow case without offsite power for the cycle 1 core of a four-loop PWR, which supports the conclusion of the current plant safety analysis. The evaluation process established by the study is applicable to other reload cores and other plant types.

### **Education Support and Training**

CASL is committed to the development of future scientists and engineers and engages students at all levels in CASL research. There are currently 104 students actively participating in CASL research. Fourteen active students are currently undergraduates, 12 are in graduate school at the masters level, 68 are pursuing a PhD, and 10 are postdoctoral trainees. Nearly two-thirds of the active students have received CASL funding, and the others are sponsored by fellowships and other programs. In addition, CASL has provided training and engagement opportunities to support workforce development for career staff and engineers.

### ***CASL Education Program***

The goals of the CASL Education Program are to ensure that CASL results and technology are integrated into university undergraduate and graduate course curricula and to encourage the transfer of CASL technologies to industry users. Programs that support these goals include undergraduate research opportunities, summer internships, development of new courses at participating universities, and the CASL Institute.

The CASL Undergraduate Research Scholars Program is in its fourth year of matching top students at North Carolina State University with CASL faculty mentors. Each undergraduate participating in the program receives research experience as well as monetary compensation. Since the program's inception, 27 students have participated. Of the 23 who have completed their undergraduate degree, 11 are currently attending graduate school, and three have completed graduate degrees.

To support its diversity mission, the CASL Education Program funded its second summer undergraduate researcher in 2016. Jamell Walls Paschal, a student from South Carolina State University, worked under the guidance of J. Michael Doster and was granted a personal stipend plus an allowance for housing and food to support his work at North Carolina State. Paschal's project compared experimental data provided by the Nuclear Power Engineering Corporation of Japan to model predictions of two-phase flow behavior in BWR fuel bundles.

The CASL Education Program continued to support the development of course modules at partner universities. Instructional material development focused on fuel performance, core thermal-hydraulics, and radiation transport using the VERA framework. The course modules and supporting sample problems were made available for use in university classrooms and were used at the CASL Institute.

### ***Summer Internships***

CASL supports summer internships primarily at the national laboratory partners with a majority of the students working at ORNL. In FY 2016, ORNL hosted 11 students, who worked on a range on of topics with ORNL mentors. Examples of projects include:

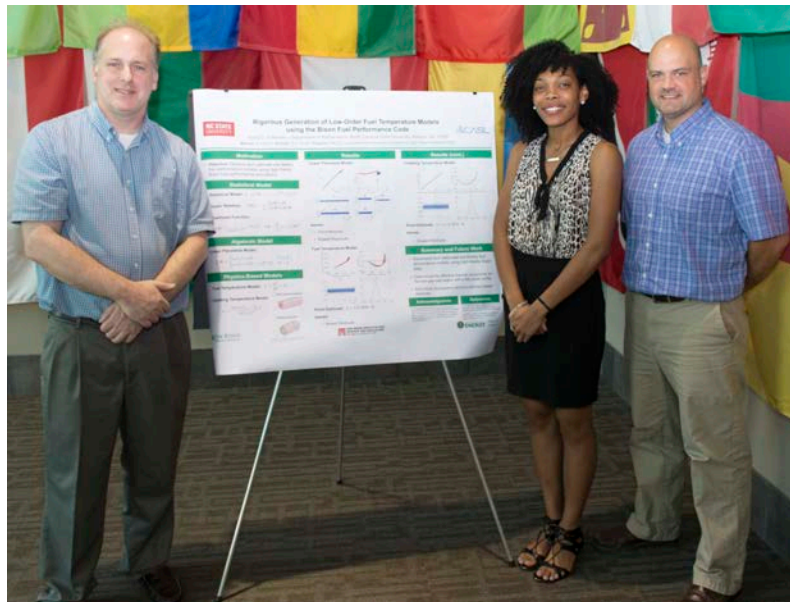
- Xingang Zhao, MIT – Worked with PHI and assisted in further developing and assessing COBRA TF for Boiling Water Reactor (BWR) applications. Specific tasks included expanding on the CTF validation matrix to include tests from the BWR Full-Size Fine-mesh Bundle Tests (BFBT) and making source code modifications to extend the CTF HDF5 output capability to multi-assembly BWR models.
- Kayla Coleman & Aysenur Toptan, NCSU – Participated in improving the fuel performance models in CTF using experimental data and the higher fidelity code, Bison. Specifically, the CTF gap model was targeted for optimization initially, which included open and closed gap conduction. Students began by extracting experimental data from the literature and used this to calibrate existing CTF model coefficients. The data will be used to create a test-suite that will be run in Bison.
- Austin Ellis, NCSU – Worked with Tom Evans of RTM on hybrid fission source acceleration techniques for Monte Carlo convergence.
- Taylor Blyth, Penn State – Participated in CTF modeling of grid effects on heat transfer and turbulence using a higher-fidelity CFD code to inform the lower-fidelity models. Participation involved the actual development of the downstream heat transfer enhancement model and the spacer grid loss coefficients.
- Aaron Graham, University of Michigan - goal is to modify how the subplane mesh is determined to align partially inserted control rods and burnable poisons with the subplane mesh. Once this is done, the method for calculating homogenized cross-sections for CMFD should be updated to use the explicit cross sections rather than mixed ones (i.e., use the control rod cross-sections in the upper subplanes and



moderator cross-sections in the lower subplanes). The hope is that doing this will preserve the overall reaction rates in the MOC plane but provide improved axial profiles for the scalar fluxes and surface currents calculated by the CMFD system.

- Han Li, Texas A & M and Mengnan Li, NCSU worked with THM contributed to the validation of the Computational Fluid Dynamics code STAR-CCM+® for application to two phase boiling flows in Boiling Water Reactor (BWR) primary coolant loops or Pressurized Water Reactor (PWR) secondary loops.

As part of the internship experience, students prepare posters to present at the ORNL summer research poster session. North Carolina State University student Kayla Coleman was recognized with a third place poster award for her outstanding project titled “Rigorous Generation of Low-Order Fuel Temperature Models Using the BISON Fuel Performance Code”. CASL will continue this program of encouraging students to participate in internships with CASL partners (Figure 13).



**Figure 13. Kayla Coleman received 3rd place for her CASL-supported research at an ORNL poster session. (Also shown are CASL director Jess Gehin and research mentor Kevin Clarno).**

### **CASL Institute**

The first CASL Institute was held at ORNL during the summer of 2016. The institute was a two-week workshop designed to educate faculty, undergraduate and graduate students, and engineering professionals with an interest in CASL research. The workshop introduced participants to CASL, the VERA framework, and VERA’s component physics packages, and included presentations on the CASL challenge problems, data needs for code validation, and developments in high performance computing. Twenty-seven students and one faculty member representing 12 universities earned the CASL-VERA Certificate upon completion of the Institute. An industry representative from NuScale Power™ participated in the institute with the prospect of future involvement in the program (Figure 14).





Figure 14. Participants in the first CASL Summer Institute at ORNL in June 2016.

### ***VERA Training***

CASL also provided training to Test Stand teams at their home locations. In December 2015, VERA training was held in Lynchburg, Virginia, for AREVA and specifically focused on the use of VERA-CS for CIPS analysis. Hands-on training was provided, and a range of training exercises were performed on AREVA's computer system. In May 2016, a training session was held at the University of Illinois Urbana–Champaign to support their Test Stand application of PCI performance under load follow conditions involving faculty, students, and staff from the University of Illinois and Exelon. Training was provided on the core simulator and BISON using the University of Illinois iForge computer system. In addition, through a combined CASL-NEAMS initiative, BISON-specific training was provided to Westinghouse in September 2016 at their location in Columbia, South Carolina, to support analysis of accident tolerant fuels.

## PART 4: RETURN ON FY 2016 TAXPAYER INVESTMENT

The CASL leadership team continued working to ensure the program produces a strong return on taxpayer investment and that funding provided by DOE-NE is carefully managed. CASL work is executed through contracts established by ORNL and issued to the CASL partner organizations. These contracts were streamlined during FY 2016 and, in most cases, extended to cover the remaining CASL operational period to minimize the effort required for annual contract updates. Partner financial reporting requirements were also streamlined, and quarterly financial reviews were established to help ensure reporting consistency. A significant amount of work was also completed during the year to define activities for the next three years in preparation for post-CASL sustainment of CASL modeling tools.

### FY 2016 Financial Performance

A summary of the budget and spending for the FY 2016 funding is presented in Table 3. As shown, approximately 80% of the FY 2016 CASL operational costs (i.e., total costs minus subcontracting overhead and taxes) were directly associated with R&D, and the remainder was associated with management, operations, and infrastructure. Unspent FY 2016 funding is carried over and allocated to FY 2017 activities.

**Table 3. FY 2016 Funding—Budget and Cost Summary**

|                                          | FY 2016 Budget<br>(\$K) | FY 2016 Cost<br>(\$K)* |
|------------------------------------------|-------------------------|------------------------|
| <b>Technical Activities</b>              |                         |                        |
| Fuels, Materials, and Chemistry          | \$6,218,644             | \$4,111,963            |
| Radiation Transport Methods              | \$2,723,918             | \$2,342,697            |
| Thermal-Hydraulics Methods               | \$3,464,408             | \$2,643,445            |
| Physics Integration                      | \$4,651,524             | \$4,150,529            |
| Validation and Modeling Applications     | \$4,081,118             | \$3,259,301            |
| Technology Deployment and Outreach       | \$2,274,073             | \$1,160,660            |
| <b>Total Technical Activities</b>        | <b>\$23,413,685</b>     | <b>\$17,668,596</b>    |
| <b>Program Management and Operations</b> |                         |                        |
| Management                               | \$2,448,512             | \$2,014,237            |
| Operations                               | \$1,295,837             | \$1,076,004            |
| Infrastructure                           | \$1,320,506             | \$1,141,183            |
| <b>Total Management and Operations</b>   | <b>\$5,064,855</b>      | <b>\$4,231,424</b>     |
| Subcontracting Overhead and Taxes        | \$1,287,152             | \$1,058,573            |
| Contingency/Reserve                      | \$479,950               | —                      |
| <b>Total</b>                             | <b>\$30,245,642</b>     | <b>\$22,958,594</b>    |

\*Estimated September 2016 cost

## Milestone Completion

CASL's R&D activities are organized through an annual planning process into a set of milestones and an execution plan. A total of 153 level 1, 2, and 3 milestones were defined for work to be performed in FY 2016. Of these milestones, 11 are DOE-reportable milestones are selected in consultation with CASL's Federal Manager as a means to measure CASL's performance in executing its scope. The FY 2016 DOE-reportable milestones are provided in Table 4. CASL completed 100% of these on time.

**Table 4. FY 2016 CASL DOE-Reportable Milestones**

| Milestone ID         | Milestone Description                                                                                                                      | Completion Date |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| <b>FY16.CASL.001</b> | Develop and test subchannel thermal hydraulics to support modeling of BWR operations                                                       | January 2016    |
| <b>FY16.CASL.002</b> | Demonstrate Uncertainty Quantification and Data Assimilation for Watts Bar Unit 1 Cycle 1                                                  | March 2016      |
| <b>FY16.CASL.003</b> | Identify fuel performance capabilities needed for analysis of Reactivity Insertion Accidents (RIA) and complete Initial Implementation     | May 2016        |
| <b>FY16.CASL.004</b> | Initiate VERA working group by holding first meeting                                                                                       | April 2016      |
| <b>FY16.CASL.005</b> | Complete VERA integrated Verification and Validation (V&V) requirements and planning and update V&V manuals for individual codes           | June 2016       |
| <b>FY16.CASL.006</b> | Define post CASL sustainability strategy                                                                                                   | July 2016       |
| <b>FY16.CASL.007</b> | Demonstrate VERA Core Simulator performance improvements                                                                                   | August 2016     |
| <b>FY16.CASL.008</b> | Implement VERA transient capability with internal heat conduction feedback for PWRs for analysis of Reactivity Insertion Accidents (RIA)   | September 2016  |
| <b>FY16.CASL.009</b> | Demonstrate DNB analysis methods using CFD for Non-Mixing Vane and V5H grid spacers                                                        | September 2016  |
| <b>FY16.CASL.010</b> | Assess the analysis capability for core-wide PWR Pellet-Clad Interaction (PCI) screening and demonstrate detailed 3-D analysis on selected | September 2016  |
| <b>FY16.CASL.011</b> | Qualify CFD-based PWR CRUD Induced Localized Corrosion (CILC) capability to identify high-risk fuel rods                                   | September 2016  |

## Post-CASL Planning

A post-CASL strategy was developed and delivered to DOE-NE in July 2016 [13]. The purpose of the document is to describe the CASL strategy for sustaining the VERA software tools after the operational period is complete. CASL is currently expected to receive its last year of DOE-NE funding in FY 2019, so the post-CASL planning activity was started during FY 2016 to identify steps that need to be taken during the next three years to prepare for the transition to the post-CASL period. The post-CASL planning activity was completed with strong support from the CASL Board of Directors.

The following four post-CASL use cases were identified during the strategy development activity. These use cases describe important applications of VERA tools that are likely to emerge in the post-CASL period (Figure 14):

- **Industry applications** developed by users who are interested in applying VERA capabilities to address issues associated with operation of the existing LWR fleet.
- **Regulatory and licensing applications** developed by organizations that would like to explore qualification of the VERA tools to support submittal of license applications to the US Nuclear Regulatory Commission.
- **Education and training applications** developed by users interested in presenting case studies using the VERA tools in university classrooms and corporate training sessions.
- **Research and development applications** developed by users interested in applying VERA to new R&D applications and modifying the VERA source code to experiment with new and existing modeling capabilities.

The primary deployment strategy for the CASL tools was also identified. The strategy will involve issuing a series of exclusive and/or nonexclusive licenses through ORNL that will allow users to access the VERA software package for commercial and noncommercial purposes. The primary deployment strategy may also be supplemented by substrategies that open additional distribution pathways, depending on the post-CASL demand for the VERA tools.

Finally, the following five activities were identified as essential elements of the post-CASL strategy:

- Develop the VERA Working Group to provide post-CASL two-way communication between code developers and code users
- Develop a strategy for an integrated DOE-NE M&S program that leverages CASL investments
- Sustain the CASL Industry and Science Councils to continue fostering productive interactions between national laboratory, university, and industry scientists and engineers
- Integrate VERA into industry work processes

- Enable industry-led regulatory licensing of VERA tools

A draft roadmap that identifies specific activities that support the essential post-CASL elements was developed. Activities identified in the roadmap will be incorporated into the program's annual planning process over the next three years.

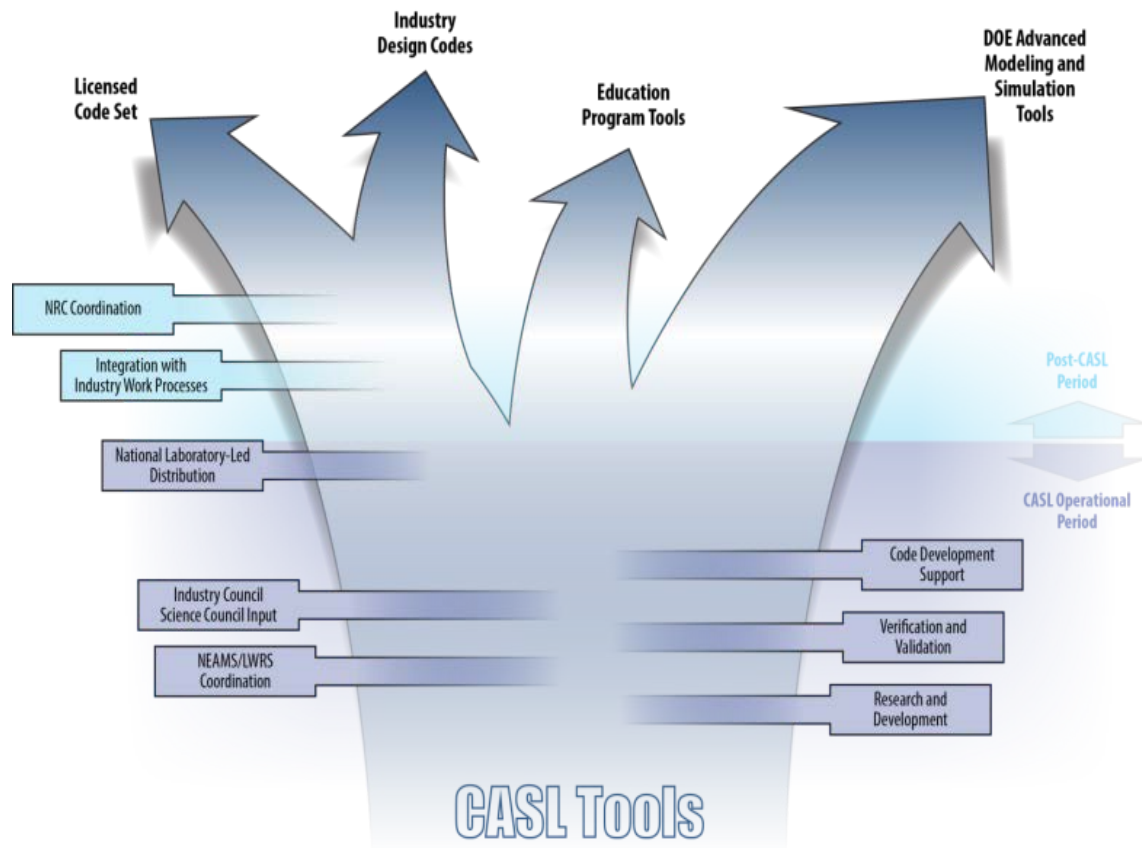


Figure 14. Post CASL strategy use-cases [13].

## CONCLUSION

FY 2016 marked another productive year for CASL. It included a range of important achievements including highly accurate modeling of the WBN-2 reactor startup, implementation of a transient operation capability that will support further challenge problem progress, and dramatic improvements in the speed and efficiency of VERA analysis tools. The program remains on track to fulfill its end state vision within the final three years of CASL operations, and it is making strong progress toward establishing VERA as a set of tools that are widely used by industry, academia, and the national laboratories for analysis of LWR operations.

## ACKNOWLEDGMENTS

This research was supported by the Consortium for Advanced Simulation of Light Water Reactors ([www.casl.gov](http://www.casl.gov)), an Energy Innovation Hub (<http://www.energy.gov/hubs>) for Modeling and Simulation of Nuclear Reactors under US Department of Energy Contract No. DE-AC05-00OR22725.

An award of computer time was provided by the ASCR Leadership Computing Challenge (ALCC) Program. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the US Department of Energy under Contract No. DE-AC05-00OR22725.

This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory (INL), which is supported by the Office of Nuclear Energy of the US Department of Energy under Contract No. DE-AC07-05ID14517.



## References

1. Collins, B., S. Hamilton, M. Jarrett, K. S. Kim, B. Kochunas, Y. Liu, S. Palmtag, R. Salko, S. Stimpson, A. Toth, and B. Yee. 2016. *Summary of VERA-CS Performance Improvements*, CASL-U-2016-1171-000 (August 2016)
2. Salko, R., A. Wysocki, B. Collins, A. Godfrey, C. Gosdin, and M. Avramova, *Development and Testing of CTF to Support Modeling of BWR Operating Conditions*, CASL-U-2016-1030-000 (January 2016).
3. Khuwaileh, B., and P. Turinsky, *Data Assimilation and Uncertainty Quantification Using VERA-CS for a Core-Wide LWR Problem with Depletion*, CASL-U-2016-1054-000 (March 2016).
4. Manera, A., D. Walter, V. Petrov, B. Kendrick, B. Wirth, R. Sweet, J. Rizk, V. Kucukboyaci, J. Secker, *Qualification of CFD-based PWR CILC Capabilities for the Identification of High-Risk Fuel Rods*, CASL-U-2016-1195-000 (September 2016).
5. Capps, N., J. Rashid, S. Stimpson, K. Clarno, and B. Wirth, *Assessment of the Analysis Capability for Core-Wide PWR Pellet-Clad Interaction (PCI) Screening*, CASL-U-2016-1200-000 (September 2016).
6. Downar, T., Y. Xu, A. Zhu, B. Kochunas, and D. Jabaay, *Transient Capability in MPACT with Internal Heat Conduction Feedback for Analysis of PWR Reactivity Insertion Accidents*, CASL-U-2016-1188-000 (September 2016).
7. Baglietto, E., E. Demarly, S. J. Kim, *Demonstration of DNB Analysis Methods using CFD*, CASL-U-2016-1197-000 (September 2016).
8. Williamson, R., C. Folsom, G. Pastore, S. Veeraraghavan, *Reactivity Insertion Accident (RIA) Capability Status in the BISON Fuel Performance Code*, CASL-U-2016-1104-000 (May 2016).
9. Sieger, M., Mervin, B., Baird, M., Bartlett, R., *VERA and VERA-EDU 3.4 Release Notes*, CASL-U-2015-1007-000 (November 2015).
10. Sieger, M., Mervin, B., Baird, M., Bartlett, R., *VERA and VERA-EDU 3.5 Release Notes*, CASL-U-2016-1114-000 (July 2016).
11. Godfrey, A., and R. Lee, *VERAView User's Guide*, CASL-U-2016-1058-000 (March 2016).
12. Sung, Y., V Kucukboyaci, X. Yiban, L. Cao, R. Salko, H. Zhang, C. Brown, *VERA-CS Evaluation of PWR MSLB DNB Limiting Case with Respect to Coolant Flow*, CASL-U-2016-1161-000 (August 2016).
13. Burns, D. E., J. Gehin, and D. Kropaczek, *Post-CASL Strategy*, CASL-U-2016-1103-000 (July 2016).