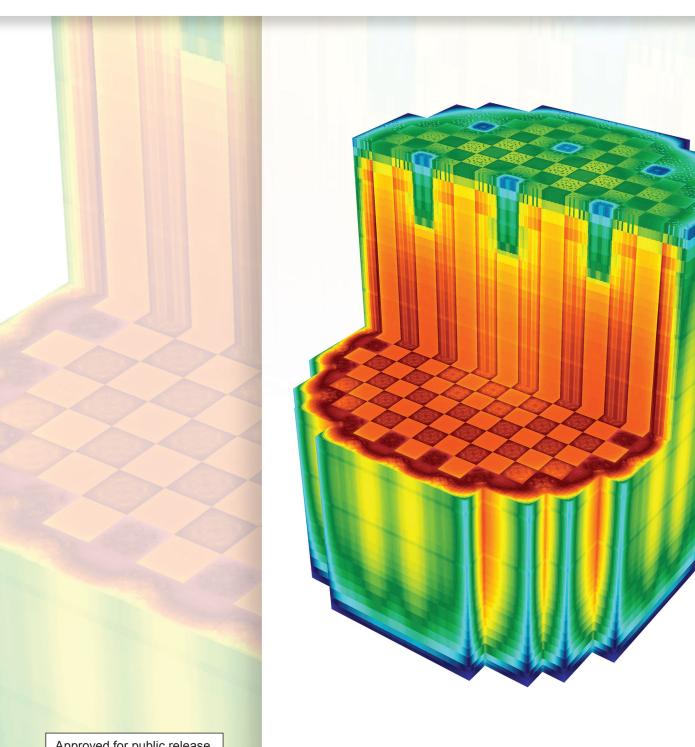
# > 1 7 < □ Annual Report

The Consortium for Advanced Simulation of Light Water Reactors — A DOE Energy Innovation Hub



Approved for public release. Distribution is unlimited.





#### **DOCUMENT AVAILABILITY**

Reports produced after January 1, 1996, are generally available free via US Department of Energy (DOE) SciTech Connect.

Website www.osti.gov

Reports produced before January 1, 1996, may be purchased by members of the public from the following source:

National Technical Information Service 5285 Port Royal Road Springfield, VA 22161 *Telephone* 703-605-6000 (1-800-553-6847) *TDD* 703-487-4639 *Fax* 703-605-6900 *E-mail* info@ntis.gov

Website http://classic.ntis.gov/

Reports are available to DOE employees, DOE contractors, Energy Technology Data Exchange representatives, and International Nuclear Information System representatives from the following source:

Office of Scientific and Technical Information PO Box 62
Oak Ridge, TN 37831 *Telephone* 865-576-8401 *Fax* 865-576-5728 *E-mail* reports@osti.gov *Website* http://www.osti.gov/contact.html

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

#### **Cover image:**

CASL Virtual Environment for Reactor Applications (VERA) predictions of transient Xenon-135 distribution during startup of Tennessee Valley Authority's Watts Bar Unit 2 Nuclear Plant at 28% of full operating power. Xenon-135 is an important radionuclide to simulate given its strong absorption of neutrons and associated impact on reactor operating behavior.

#### CASL DIRECTOR STATEMENT

On behalf of everyone at CASL, I am pleased to present this annual report for fiscal year 2017, which provides an overview of our accomplishments and highlights the impacts we are having on engineering, science, education, and workforce development. As described herein, CASL has had a very successful year making progress on our goals to develop and deliver advanced capabilities to simulate light water reactors through the development of the Virtual Environment for Reactor Applications (VERA).

The key to CASL's success is its talented and diverse team of engineers, scientists, developers, students, and operations staff. The ability of this team to seamlessly perform collaborative work across our industry, university, and national laboratory partners continues to be a strength of our organization. CASL is fortunate to receive strong input and feedback from our Board of Directors, chaired by Dr. Pete Lyons, former Deputy Assistant Secretary for Nuclear Energy and Commissioner of the US Nuclear Regulatory Commission. We are also grateful for the input from our Science Council, chaired by Dr. Bill Oberkampf, and our Industry Council, chaired by Scott Thomas of Duke Energy.

I also appreciate the leadership of Dr. Doug Burns as the CASL Deputy Director, who has moved on to other key roles at Idaho National Laboratory, and his replacement, Dr. Jim Wolf, who provides experience from his many years as manager of the RELAP5-3D program. I also recognize the exceptional support provided by our federal program leadership from the US Department of Energy's Office of Nuclear Technology Demonstration and Deployment by Tansel Selekler, Dan Funk, and Tom Miller.

CASL is making good progress in developing our capabilities to simulate challenge problems and applications, which can be seen by the active engagement of the nuclear industry. I am particularly proud that VERA has been applied to 18 commercial nuclear power plants representing nearly 100 fuel cycles of operation. The Westinghouse and AREVA fuel vendors and reactor owner/operators have generously provided data and expertise to enable our strong validation basis for VERA and challenge problem applications. A specific highlight is the use of VERA by Duke Energy, with the support of CASL staff, to evaluate the risk of crud-induced power shift (CIPS) for the Catawba Unit 2 Cycle 22 core design. This work, which is highlighted in this report, provides a good example of potential cost savings that can be realized by improved modeling and simulation.

Finally, I would like to note that we received an R&D 100 Award, an "Oscar of Innovation," as one of the top 100 innovations of 2016. This is well-deserved recognition for the many years of effort by the CASL team. Therefore, it is with great energy and enthusiasm that we complete fiscal year 2017 and move towards the future.

Sincerely,



Gen C. deli



### The Consortium for Advanced **Simulation of Light Water Reactors**

#### **Founding Partners**

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



### **Contributing Partners**

AREVA Inc. ASCOMP AG City College of New York Core Physics Inc. **Exelon Corporation** Florida State University Global Nuclear Fuel LLC Imperial College NuScale Power Pacific Northwest National Laboratory Pennsylvania State University **Purdue University** Rensselaer Polytechnic Institute Siemens Structural Integrity Associates, Inc. Texas A&M University University of California Los Angeles University of California Santa Barbara University of Florida University of Notre Dame University of Tennessee – Knoxville University of Tennessee – Chattanooga

University of Texas at Austin University of Wisconsin



### **CONTENTS**

CASL Director StatementFounding and Contributing Partners	
Contents	
Figures	
Tables	
Acronyms	v
PART 1: FY 2017 Overview	
Introduction	1
CASL Vision and Mission	
2017 Highlighted Achievements	
CASL Organization and Overall Metrics	
The Future of CASL	5
PART 2: Science and Engineering Progress and Impact	
Development and Advancement of VERA	7
Verification, Validation, and Uncertainty Quantification	
CASL Challenge Problems	
PART 3: End User Impact and Nuclear Industry Engagement	
End User Impact and Nuclear Industry Engagement	
Application of VERA to Operating Plants	
CASL Industry Council	
Test Stand Deployments	
VERA Users Group	
Engagement with the Nuclear Regulatory Commission	
CASL Strategy for Accident-Tolerant Fuels	
CASL Training CASL Institute and Education Program	
PART 4: Return on FY 2017 Taxpayer Investment	
FY17 Financial Performance	
Milestone Completion	
DOE Reportable Milestones	
POST-CASE Planning	
CONCLUSION	
	38
ACKNOWLEDGMENTS	
	29
REFERENCES	
MEI ENEIGES	

### **FIGURES**

Figure 1. High-resolution crud predictions enabled quantification of potential cost savings
(VERA left, industry methods right)
Figure 2. Improved boiling closure models leverage long-term CASL investments in high-resolution
data for development and calibration of lower resolution closure models for DNB evaluations 2
Figure 3. CASL Team celebrating the R&D100 Award
Figure 4. Impact of using CFD-informed models on crud thickness predictions
Figure 5. The CASL organization
Figure 6. The VERA code suite
Figure 7. Examples of VERA pin and assembly calculation visualization with VERAView
Figure 8. Summary of the CASL challenge problem scope
Figure 9. Neutronics (MPACT), thermal-hydraulics (CTF), and crud (MAMBA) coupling interfaces
Figure 10. Initial PWR OT∆T analysis using VERA
Figure 11. Pin power distribution for AP1000 rod ejection at HFP
Figure 12. VERA core simulator validation plan
Figure 13. NuScale and CASL staff at a project status meeting
Figure 14. Coolant temperature distribution in Cycle 8 of the NuScale SMR
Figure 15. VERA model of the NuScale Cycle 1 SMR core with steel reflector block
Figure 16. Radial vanadium current distributions compared to measured data from Watts Bar 2
Figure 17. CASL Industry Council member organizations
Figure 18. CASL Industry Council meeting in Charleston, SC, on April 4–5, 2017
Figure 19. VERA training class at Westinghouse Headquarters, on May 22, 2017
Figure 20. CASL Institute participants and faculty24
Figure 21. CASL 2017 summer students at ORNL
Figure 22. FY17 budget distribution by focus area

## **TABLES**

Table 1. CASL Focus Areas	. 6
Table 2. Summary of CASL Technical Output through FY17	. 6
Table 3. VERA Releases	. 9
Table 4. Composite PCMM Scoring for VERA	10
Table 5. FY17 Budget and Cost Summary	26
Table 6. FY17 DOE-Reportable Milestones.	27



**AFIR** autoclave fretting and impact rig

ALCC ASCR Leadership Computing Challenge

AMA advanced modeling application

American Nuclear Society ANS

**ASCR** Advanced Scientific Computing Research

ATF accident-tolerant fuel B&W **Babcock and Wilcox BWR** boiling water reactor

CASL Consortium for Advanced Simulation of Light Water Reactors

CFD computational fluid dynamics

CHF critical heat flux

CILC crud-induced localized corrosion

**CIPS** crud-induced power shift

CTF upgraded version of the COBRA-TF computer code

**DNB** departure from nucleate boiling DNS direct numerical simulation DOE **US Department of Energy** DOE-NE DOE Office of Nuclear Energy **EPRI** Electric Power Research Institute

**FMC Fuels Materials Chemistry** 

FY fiscal year

**GTRF** grid-to-rod fretting **HFP** hot full power

**HPC** high-performance computing

HZP hot zero power

INL Idaho National Laboratory

KAPI **Knolls Atomic Power Laboratory** 

LOCA loss of coolant accident LWR light water reactor

M&S modeling and simulation

M-CFD multiphase CFD

MOC method of characteristics

MOX mixed oxide fuel

NCSU North Carolina State University

**NEAMS** Nuclear Energy Advanced Modeling and Simulation

NNSA National Nuclear Security Administration

NRC **US Nuclear Regulatory Commission** 



ORNL Oak Ridge National Laboratory

OΤΔT over-temperature change in temperature

PCI pellet-clad interaction

PCMM predictive code maturity model

PHI Physics Integration

PIRT Phenomena Identification and Ranking Technique

PNNL Pacific Northwest National Laboratory

PWR pressurized water reactor
R&D research and development

REU Research Experience for Undergraduates

RIA reactivity insertion accident

RSICC Radiation Safety Information Computational Center

RTM Radiation Transport Methods

SMR small modular reactor

SPERT Special Power Excursion Reactor Test

T/H thermal hydraulics

THM thermal hydraulics methods

TMI Three Mile Island

TPBAR tritium production burnable absorber rods

TVA Tennessee Valley Authority

UIUC University of Illinois at Urbana–Champaign

UTK University of Tennessee, Knoxville

V&V verification and validation

VERA Virtual Environment for Reactor Applications

VERAIn VERA user interface VUG VERA Users Group

VVI Verification and Validation Implementation

WBN1 Watts Bar Nuclear Unit 1
WBN2 Watts Bar Nuclear Unit 2

WEC Westinghouse Electric Company

## Part 1: FY 2017 Overview

#### INTRODUCTION

The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established in July 2010 as the first US Department of Energy (DOE) Energy Innovation Hub. The consortium was initially funded for 5 years to develop advanced modeling and simulation (M&S) tools that can be used to analyze issues associated with the operation of US commercial light water reactors (LWRs). The program's focus during this period was on simulation of physical processes that affect the operation of pressurized water reactor (PWR) cores. In January 2015, the program was extended for an additional 5 years with the goal of finalizing development of the PWR analysis tools and extending the program's tools for use in the analysis of boiling water reactor (BWR) and small modular reactor (SMR) operation.

#### CASL 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 replacing design and analysis tools that are based on limited experimental data with more 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 industry professionals 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 (NRC) to help facilitate eventual industry use of the CASL tools to support licensing.

#### **2017 HIGHLIGHTED ACHIEVEMENTS**

Fiscal year (FY) 2017 was another very productive year for CASL. Some of the significant achievements completed by the program during the year are summarized in the following paragraphs:

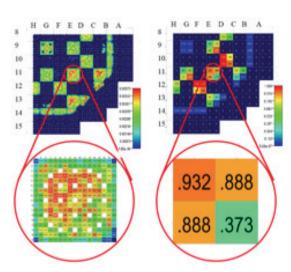
#### 1. Quantification of potential fuel cost savings to Duke Energy by comparing the risk of CIPS in core designs for Cycle 22 of Catawba Unit 2.

In a nuclear reactor, crud preferentially forms on the top half of the fuel rods in the reactor core. A significant uptake of boron into the crud causes a depression in power in the top half of the core which shifts more power to the bottom half. This phenomenon is known as crud-induced power shift (CIPS). CIPS can cause a decrease in safety and shutdown margin and limit operational flexibility, thus requiring the plant to decrease its power output to maintain sufficient shutdown margin for plant safety.

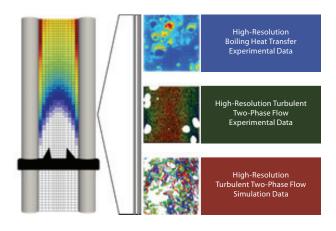
VERA simulations were performed for the Duke Energy Catawba Unit 2 reactor to assess the CIPS risk for three core designs considered low, medium, and high risk as it pertains to the impact of boron deposition on core axial power shape [1]. As illustrated in Figure 1, VERA is unique compared to existing industry design tools in that the multiphysics feedback of crud deposition and boron uptake is explicitly modeled as part of reactor operation simulation. The impact on the core power distribution for core designs with lower overall fuel costs was quantified, indicating a clear potential for VERA simulation capability. This allowed for an improved assessment of CIPS risk with a positive economic impact of approximately \$250,000 in fuel costs compared to the low-risk pattern that was actually selected.

#### 2. Demonstration of advanced computational fluid dynamics (CFD)-based capability for prediction of departure from nucleate boiling (DNB)

This activity focuses on developing, demonstrating, and assessing advanced CFDbased capability to predict DNB in pressurized water reactor (PWR) fuel. A Generation II boiling and DNB model (Figure 2) has been developed by CASL that leverages a new fundamental understanding of the partitioning of heat transfer into single and two phase boiling phenomena at the surface [2]. Improved wall heat partitioning models and closure relations were developed for dispersed vapor phase interaction with the



**Figure 1.** *High-resolution crud predictions* enabled quantification of potential cost savings (VERA left, industry methods right).



**Figure 2.** Improved boiling closure models leverage long-term CASL investments in high-resolution data for development and calibration of lower resolution closure models for DNB evaluations.

liquid carrier phase. This is based on an integrated database of direct numerical simulation (DNS) and experimental boiling studies. The resulting heat partitioning models for prediction of bubble departure frequency, growth time, and nucleation site density have been successfully validated against measurement. As implemented within the multiphase CFD (M-CFD) framework, the Generation II model is a significant improvement over earlier Generation I boiling models that were previously evaluated for prediction of DNB.

#### 3. Virtual Environment for Reactor Applications (VERA) wins R&D 100 Award

The R&D 100 awards honor innovative breakthroughs from academia, industry, and government-sponsored research agencies in materials science, biomedicine, and consumer products. In November 2016, VERA was selected for this award, also

known as the "Oscars of Invention," in recognition of its applicability to real world problems as demonstrated by its use for the startup of the Tennessee Valley Authority (TVA) Watts Bar Nuclear Plant Unit 2. The award recognizes the significant and innovative effort made by the CASL researchers in the development of this advanced nuclear M&S capability (Figure 3).

#### 4. Significant improvements in crud capabilities enable the use of the full-physics version of MAMBA in **VERA** simulations

The MAMBA code was developed during the past several years and provides a novel capability to model crud buildup on the cladding, as well as the boron uptake within the crud. In the past, a stand-alone 3D version of

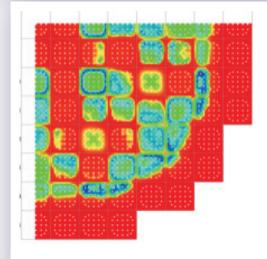
MAMBA was used to create a simplified 1D surrogate. This was incorporated into VERA to simulate CIPS as part of detailed, full-core analysis [3]. This approach successfully modeled CIPS from previous operation, but it lacked the physics necessary to fully simulate the crud deposition and boron update process. MAMBA has been rebuilt to enable coupling with the core simulator without simplified physics. Improvements to MAMBA—including optimization of memory, data structures, and time-integration schemes—have achieved substantial decreases in run time. This has enabled prediction of crud growth and erosion on all cladding surfaces to be performed in fullcore cycle depletion analyses without a simplified surrogate. In addition, models have been incorporated into VERA to account for the mass balance in the coolant of all crud source-terms. Also, a novel approach to using CFDscale flow distributions to inform the CTF subchannel thermal hydraulics (T/H) code about localized crud growth and erosion has been developed. Figure 4 shows how the error in crud thickness predictions is eliminated by using CFD-informed models with CTF. Incorporating each of these advancements provides a comprehensive crud capability which greatly enhances VERA's predictive capability for CIPS.

#### 5. Completion of the grid-to-rod fretting (GTRF) challenge problem

Coolant flow-induced vibration between structural components in LWR cores can result in progressive wear damage that may result in fuel rod failure. This GTRF phenomenon is a complex function of many variables, including reactor operating conditions, fuel clad and structural materials, and fuel oxide growth and removal rates. CASL managed development of a stage-wise GTRF engineering wear model, extensive CFD modeling of the fluid-structure interactions, structural mechanics assessments of the GTRF phenomena, and a novel autoclave fretting and impact rig to provide laboratory-scale benchmarking data



Figure 3. CASL Team celebrating the R&D 100 Award.



**Figure 4.** Impact of using CFD-informed models on crud thickness predictions.

[4]. The autoclave fretting and impact rig (AFIR) provides for a well-controlled, realistic testing of parameters (contact geometry, load, oscillation frequency and amplitude) in PWR environments. Results were used to validate the engineering wear model, allowing for a greater understanding of the materials' mechanical interactions in a reactor environment. Interactions that were analyzed include the effects of surface treatments on fuel rods and spacer grids and the role of corrosion on wear rates. The resolution of the GTRF challenge problem provides a foundation for analyzing future reactor materials such as new accident-tolerant fuel (ATF) claddings.

#### 6. CASL Summer Institute trains 27 participants

The second CASL Institute was held June 19–30, 2017 at North Carolina State University (NCSU) to provide an opportunity for education and training of students, researchers and engineers on CASL technologies. This was the first successful deployment of VERA training in a university environment, with students logging over 6,000 core-hours of HPC usage for hands-on application of VERA. Topics included the theory of reactor multiphysics and code coupling (i.e., neutronics, T/H, fuel performance, and chemistry modeling), the use of CASL codes, and the CASL challenge problems. The course was structured to provide information through lectures and application with hands-on code usage. Twenty-seven students attended the 2-week course and received certificates on successful completion. The CASL Institute serves as a model for future VERA deployments for the post-CASL user community.

#### **CASL ORGANIZATION AND OVERALL METRICS**

World-class scientists, engineers, computer scientists, and program managers from 10 CASL founding partners—in coordination with personnel from contributing partner organizations and supported by guidance from the CASL Board of Directors, the Industry Council, and the Science Council—are responsible for the continuing success of the CASL program.

These organizations have successfully demonstrated that coordination of personnel from the 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. The CASL organization is shown in Figure 5, and CASL's six technical focus areas are described in Table 1. FY17 organizational changes are listed below:

- Dr. Jim Wolf will replace Dr. Douglas Burns as the CASL Deputy Director.
- Dr. David Andersson will replace Dr. Brian Wirth as the Fuel Materials and Chemistry Focus Area lead.
- Dr. Brian Williams will serve as Acting Focus Area Lead for the Verification and Validation Focus Area due to Dr. Chris Jones' departure from the program.
- Mr. William Cramer will lead CASL program administration.

Key metrics illustrating the success of the CASL team include the number of CASL programmatic and technical reports issued, the number of distributions of VERA, and the volume of program-developed research results that have been externally published. Table 2 summarizes the program's technical output during FY17, including publications, technical reports, invited talks, and VERA licenses issued.

The total CASL program costs for FY17 were \$25 M, with \$19.5 M for technical activities, \$4.5M for program management and operations, and \$1 M for subcontracting, overhead, and taxes. Part 3 of this report provides additional cost and budget details.

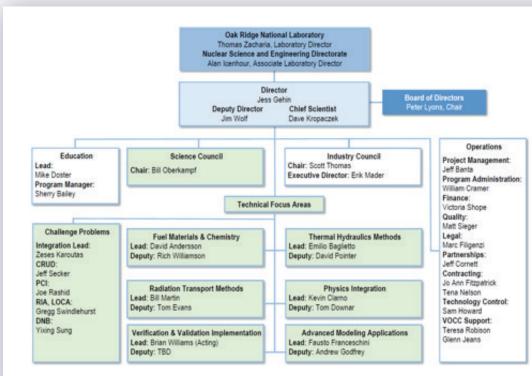
The FY17 taxpayer investment in CASL produced a wide range of M&S advances that are detailed in a comprehensive set of milestone reports. These reports document the technical progress CASL is making in the development of models and the application of VERA to the challenge problems.

#### THE FUTURE OF CASL

CASL is funded to continue research in FY18, with significant work planned on the remaining challenge problems. Guidance will be provided by CASL's Industry Council, Science Council, and Board of Directors to achieve the objectives outlined in the initial CASL proposal and renewal application, as reflected in the following end state vision for the program:

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 chalenges, emerging issues, and evolving opportunities.

Beyond FY18, a plan is being developed to establish a nuclear energy M&S program that integrates the CASL and Nuclear Energy Advanced Modeling and Simulation (NEAMS) programs. Furthermore, the VERA Users Group (VUG) continues to evolve and will represent an additional means for industry support and access to VERA.



**Figure 5.** The CASL organization.

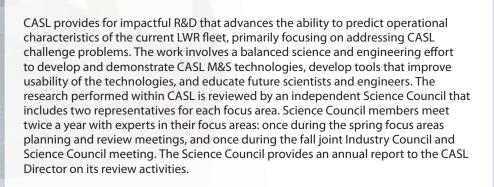
 Table 1. CASL Focus Areas.

Focus Area	Description		
Advanced Modeling Applications (AMA)	AMA is responsible for the application of VERA to industry-focused problems, including challenge problems, test stands, and other identified areas of interest. As part of this activity, AMA coordinates with the other focus areas on requirements for capabilities and to provide feedback. As a result, AMA works closely with the nuclear industry and provides compelling demonstrations of VERA capabilities and financial value.		
Physics Integration (PHI)	PHI develops VERA through multiphysics coupling and software integration of the models, methods, and data developed by other focus areas within a unified software framework. In addition, PHI has direct responsibility for developing the T/H subchannel model used in VERA. PHI collaborates with the other focus areas to deliver usable tools for performing analyses guided by the functional requirements for CASL challenge problems.		
Radiation Transport Methods (RTM)	RTM develops pin-resolved neutronics codes for VERA, which consist of a primary method based on full core, 2D method of characteristics (MOC) transport coupled with 1D transport (the 2D/1D method), and additional software for 3D full-core discrete ordinates (Sn) and hybrid Monte Carlo. RTM also supports development of nuclear data libraries and modeling of time-dependence, including delayed neutrons and isotopic depletion and decay.		
Fuels Materials and Chemistry (FMC)	FMC develops materials performance models for fuel, cladding, and fuel assembly structural materials to predict fuel and material failure. FMC also models cladding surface chemistry—particularly the deposition of species transported in the primary coolant, such as crud formation and boron precipitation. FMC provides the means to reduce reliance on empirical correlations and to enable the use of an expanded range of materials and fuel forms.		
Thermal Hydraulics Methods (THM)	THM advances existing modeling capabilities and develops new ones for T/H analysis and its integration with solver environments. The primary objective of THM is the development of single- and multiphase closure relationships for integration into existing CFD capabilities, including existing and open source codes. These models have specific application to the CIPS and crud-induced localized corrosion (CILC) CRUD challenge problems, the DNB challenge problem, and BWR modeling. THM collaborates with FMC to develop sub-grid material and chemistry models, using RTM to address coupling issues with radiation transport. THM also connects to PHI for integration and development of VERA.		
Verification and Validation Implementation (VVI)	VVI includes development, update, and execution of the VERA VVI plan. VVI includes assessments of VERA using the predictive code maturity model, in conjunction with the other focus areas. In addition, VVI also includes tools like DAKOTA, which supports verification and validation (V&V), as well as uncertainty quantification activities.		

**Table 2.** Summary of CASL Technical Output through FY17.

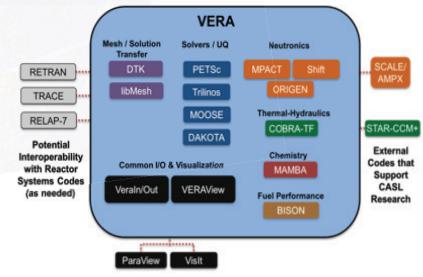
	FY17	TOTAL
VERA licenses	42	80
Journal articles	83	264
Conference papers	46	489
Invited talks	15	211
Technical reports	75	386
Milestone reports	171	846
Programmatic reports	28	303

## Part 2: SCIENCE AND **ENGINEERING PROGRESS AND IMPACT**



#### **DEVELOPMENT AND ADVANCEMENT OF VERA**

VERA is a collection of integrated simulation tools that together allow for analysis of the full range of physical processes that affect nuclear reactor operations. VERA's state-of-the-art capabilities provide unprecedented resolution for reactor analysis. 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. The VERA code suite, depicted in Figure 6, provides direct,



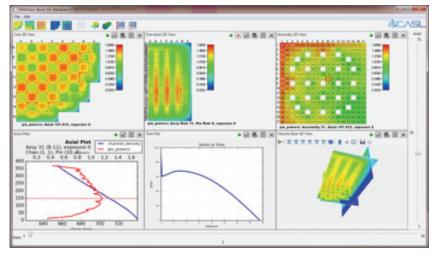
**Figure 6.** The VERA code suite.

fully coupled solutions at the fuel rod level for neutronics, T/H, fuel thermo-mechanics, and chemistry without spatial homogenization. The Monte Carlo neutronics capability in VERA's Shift can provide the neutron fluence levels on the reactor pressure vessel or at the excore detectors. The fuel performance code in VERA's BISON provides cladding integrity estimates during a fully coupled core simulation and is also extensible to allow for a highresolution prediction of pellet-cladding mechanical interaction (PCI).

The VERA user interface, VERAIn [10], provides a single common geometry model to each of the underlying physics codes, with VERA automatically managing the calculation flow, data transfer, and convergence between codes. The VERA visualization tool, VERAView [11], provides the analyst with the capability to view multiphysics simulation results such as fuel rod power and coolant channel temperature, as shown in Figure 7.

In FY17, VERA development focused on the end-user with the goal of advancing code prediction confidence, reduced computation times, and improved usability. Activities completed in FY17 associated with this goal include:

- refactoring and performance improvements in the full-physics version of MAMBA, allowing its coupling and use in VERA to replace the simplified 1D version and incorporating crud source term and mass balance models [3],
- initial demonstration of DNB capability, with continued focus on Generation II model development and validation [2],
- development of fuel fraction and contact dynamics models for PCI capability development within VERA [5],
- coupling of the Shift Monte Carlo code with MPACT in VERA to provide an initial capability for radiation transport simulations to extend beyond the core to support vessel fluence and excore detector response analyses [6],
- development of VERA transient capability with performance improvements and coupling with CTF T/H to support full 3D core reactivity insertion accident (RIA) simulations [7],



**Figure 7.** Examples of VERA pin and assembly calculation visualization with VERAView.

- continued focus on fundamental research for multiphase CFD (BWR flow regime closure relations) [8],
- development and validation of BISON fuel performance capability to support cladding deformation and fuel relocation for loss of coolant accidents (LOCAs) and to simulate transient fuel performance during rapid transients such as RIA [9], and
- improvement in usability through user friendly interface [10] and integrated visualization of simulation results [11].

Most VERA tools are designed for use on a variety of computing platforms, ranging from computing clusters available to industrial users of DOE's Leadership Computing Facilities, consisting of petascale-class platforms.

CASL's research activities are performed on computing platforms at our partner locations, including

- 75 million core hours on the Oak Ridge Leadership Computing Facility's Titan computer, resulting in a 2016 DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) award,
- 40 million core hours on Titan, resulting in a 2017 ALCC award,
- approximately 50 million corehours of usage on Idaho National Laboratory (INL) high performance computing (HPC) systems, and
- additional computers available at CASL industry partner locations, including Westinghouse, AREVA and Electric Power Research Institute (EPRI).

As VERA has matured, the software development and release process has become more stable. Every 6 months, at the start of each Plan of Record, a new candidate for release is established and is built using production computing hardware so that the newest features can be used and bugs or limitations can be identified and addressed before distribution outside of CASL. Each release includes developments from R&D milestones that were accomplished. Table 3 provides the VERA release schedule and new capabilities. Versions 3.5 and 3.6 were released and provided to users under the CASL Software Quality Assurance program [12].

#### **VERIFICATION, VALIDATION, AND UNCERTAINTY OUANTIFICATION**

V&V activities were performed in all focus areas. FMC and PHI collaborated to rebuild MAMBA with a focus on software quality assurance to enable the integration of verification tests. This resulted in a software design that includes unit testing and automated solution verification. FMC extended the validation suite of the BISON code to include additional experiments that cover a range of phenomena important to RIA and LOCA analysis. The CTF thermal fluids results were compared with experiments, CFD, and the VIPRE industry subchannel code to identify areas where the models and implementation in CTF were lacking. The new transient capability within MPACT is being evaluated using the Special Power Excursion Reactor Test (SPERT) validation, while the core simulator continues to expand the validation range through the modeling of the Babcock and Wilcox (B&W) critical experiments and additional commercial plants.

The primary findings for a first-of-a-kind V&V assessment for VERA [13] are summarized below:

- Capability gaps in the required phenomenology, defined by expert elicitation via the Phenomena Identification and Ranking Technique (PIRT) process, exist for all challenge problems considered (CIPS, PCI, DNB).
- Using a modified predictive code maturity model (PCMM) framework assessment, a nonuniform maturity is seen across various attributes; in particular, code verification, solution verification, and uncertainty quantification are scored lower for all codes and challenge problems.
- Assessment of capability and credibility must be based on evidence, yet this continues to have a large degree of subjectivity. Therefore, stakehoders must reach a consensus regarding gaps in these areas.

Table 3. VERA Releases

Version	Release date	New capabilities in release
VERA 3.5	Oct 2016	Performance improvements     VERA and VERA-EDU     versions     Demonstrated new release     process
VERA 3.6	Feb 2017	Updated cross section library Expanded release evalua- tion testing Improved robustness
VERA 3.7	Nov 2017	Shift coupling in VERA Nonsource code distribution Support for modeling combustion engineering and SMR plants
VERA 3.8	Apr 2018 (planned)	Transient VERA for RIA Inline fuel performance in VERA for PCI Updated comprehensive V&V report for VERA

PCMM scoring is shown in Table 4, with a score of 3 indicating that attributes are fully met, and 0 indicating that there is no evidence available for meeting attributes. Scoring was performed in early FY17 and is based on a preliminary version of VERA 3.6, which was released in February 2017.

The main CASL codes—CTF, BISON, and MPACT—are generally making good progress in validation. They are aligned with the challenge problems that they support. MPACT is the most mature of the three, with BISON and CTF close behind. Table 4 presents PCMM scoring for VERA. The 1D version of MAMBA results in a lower PCMM scoring than when other codes are used. The recent refactoring and integration of the full-physics version of MAMBA in FY17 will bring MAMBA up to the same level of maturity as the other codes. The V&V assessment will be updated each year to document progress in VERA development.

#### **CASL CHALLENGE PROBLEMS**

VERA is being developed to analyze real-world reactor problems. The CASL industry partners identified a set of high-priority challenge problems during formation of the consortium to help guide code development. The current set of challenge problems is summarized in Figure 8.

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

In FY17, CASL made significant improvements in CIPS simulation by extending the CIPS capability in VERA. Focus was on addressing MAMBA performance deficiencies, adding crud source and mass balance models, and providing additional model improvements to address consistency in the coupled boundary conditions of MAMBA with CTF. The most significant activity was the refactoring of MAMBA, which allows for full-physics-coupled crud simulations to be performed within VERA rather than with a simple surrogate. Work performed in FY16 identified that the 1D simplified physics version of MAMBA was not sufficient to provide the simulation fidelity needed to predict crud. However, the fullphysics version of MAMBA could not be used because of its large computing requirements.

The effort in FY17 focused on MAMBA performance, which has significantly improved and now uses only 20% of VERA CIPS simulation run time. The refactoring includes implemen-

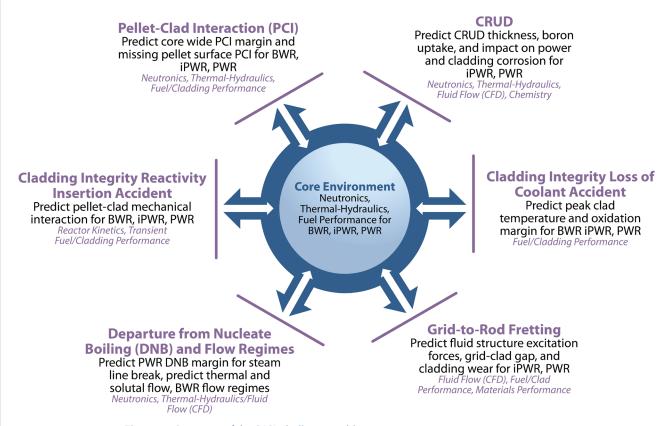
**Table 4.** Composite PCMM Scoring for VERA.

PCMM attribute	MPACT	CTF	BISON	MAMBA
Representation and geometric fidelity	3	2	2	1
Physics and material model fidelity	3	2	2	1
Predictive capability maturity model software quality assurance	2	2	2	0
Code verification	1	1	1	0
Solution verification	1	1	1	1
Separate effects validation	2	1	1	0
Integral effects validation	2	2	2	1
Uncertainty quantification	0	0	0	0
V&V Manual	Good	Good	Good	None

tation of a hierarchical class structure in MAMBA that encapsulates data and allows for localized unit testing. This allows for the same level of software quality assurance as other VERA codes.

Hi2Lo methods using CFD were also implemented to obtain greater detail in the azimuthal flow distribution and calculation of turbulent kinetic energy within CTF, thus addressing another area identified for improvement in FY16. Hi2Lo methods enable improved prediction of the threshold physics within VERA in a manner consistent with higher resolution CFD simulations.

Several major advancements were made in FY17 related to crud modeling. As noted previously, the major refactoring of MAMBA enabled a coupling of the full crud deposition/ erosion physics with the remainder of VERA. In addition, models have been defined and established to account for the release of metal ions from the primary system piping. With a global view of coolant in the system, CTF tracks the release of crud source term from corrosion on the primary system piping, as well as the deposition and erosion of ions on the cladding from every rod in the core. This will help to ensure a global balance of the mass of metals in the system. In addition, using CFD to generate high-resolution spatial maps of the heat transfer coefficient on the surface of the cladding in CTF enables a high-resolution crud solution in the full core. Figure 9 shows the updated coupling within VERA to model CIPS [3].



**Figure 8.** Summary of the CASL challenge problem scope.

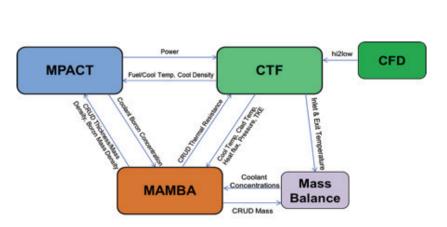


Figure 9. Neutronics (MPACT), thermal-hydraulics (CTF), and crud (MAMBA) coupling interfaces.

While several plants are not limited in their core loading by the risk of CIPS, they are limited by localized corrosion occurring behind thick layers of crud, or crud-induced localized corrosion (CILC). The prediction of CILC requires a high-resolution CFD model with resolved grid spacers, coupled with MAMBA and heat transfer in the cladding with an embedded corrosion model. This VERA capability can be embedded within a STAR-CCM+ calculation using the results of a cycle's depletion, including the crud source-terms, power distribution, and inlet flow distribution [14].

#### **Progress on the PCI Challenge Problem**

Activities in FY17 for the PCI challenge problem focused on improvements to coupling BISON within VERA and the analysis of fuel perfor-

mance for flexible power operations, also known as load following events. A new, fully coupled fuel performance and core simulation capability allows an industry user to run a standard VERA input and have the BISON fuel temperatures driving the MPACT power distributions with the CTF clad surface temperatures. This is done for every fuel rod in the core, and it results in a core-wide evaluation of cladding stresses during power maneuvers. This core-wide assessment of PCI risk was enabled by development of a 1.5D fuel performance capability in BISON that provides a fast, robust fuel solver, with all the extensibility to multidimensional options in BISON. The integrated capability also allows for one-way coupling with minimal increase in computational cost over the standard core simulator [15,21].

CASL worked with Westinghouse and Exelon through the University of Illinois Urbana-Champaign (UIUC) test stand to evaluate the integrated VERA and BISON capability to model nominal operation and flexible power operations for the Byron and AP1000 plants. With the core-wide risk assessment and a higher fidelity fuel performance calculation using BISON in 3D, a more detailed stress calculation can be performed for a select set of fuel rods to quantify the PCI risk. Additional work focused on understanding the thermomechanical-chemical state of the fuel during load following events, with the primary phenomena being pellet-clad gap closure/reopening, fission gas release as a function of power changes, and PCI stresses related to thermal expansion and swelling.

#### **Progress on the DNB Challenge Problem**

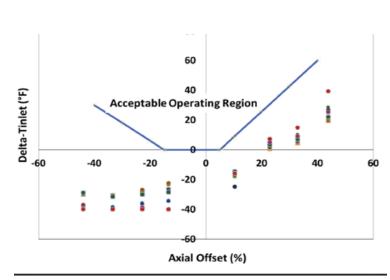
DNB activities focused on two complementary efforts: (1) development and validation of the Generation II model for prediction of heat partitioning within the STAR-CCM+ CFD simulation and (2) applications of VERA DNB margin quantification in accident analysis. Generation-II boiling model development is based on a microlayer approach, a more physical-based model that reduces the need for calibration and allows for capturing the surface characteristics of the fuel rod. Critical heat flux (CHF) is predicted based on heat partitioning. The main feature of the model is heat partitioning by wet and dry area fraction heat transfer. The model captures several effects, including bubble departure cycle (growth and wait time), bubble departure diameter relative to the underlying dry spot, and activation and interaction between nucleation sites.

The Generation-II model validation framework addresses the need for microscopic data closure development. This includes data obtained through direct numerical simulations and experiments. Results show consistent prediction of the partitioning components and include comparisons for bubble departure frequency, growth time, and nucleation site density.

The STAR-CCM+ DNB predictive capability is being used to validate and improve CTF correlations for CHF. This enables core-wide VERA simulations that will allow for prediction of DNB for postulated transients. One specific application is centered on DNB margin improvement for the over-temperature delta-temperature (OT $\Delta$ T) trip set points. This application focused on:

- using VERA to provide more realistic predictions of the core power distributions,
- the inputs to the reactor protection system OTΔT trip, and
- identification of design margins to enhance reactor safety and to reduce costs in fuel reloads and/or plant operations.

Preliminary results confirm potential benefits, as shown in Figure 10. The high-fidelity VERA simulation points show potential margin improvement when compared to the solid setpoint line, particulary for negative axial offsets representing bottom-peaked power distributions.



**Figure 10.** *Initial PWR OTΔT analysis using VERA*.

#### **Progress on the RIA Challenge Problem**

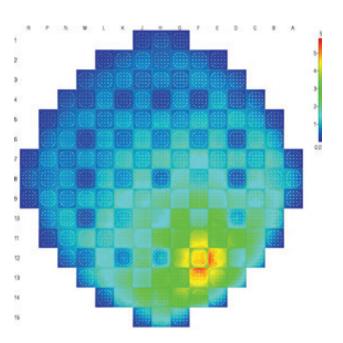
FY17 activities for the RIA challenge problem centered around three activities:

- · development of the VERA transient capability,
- · validation of VERA for transient simulations, and
- full-core PWR control rod ejection demonstration and applications.

Code development activities were focused on VERA transient improvements using MPACT and T/H feedback in CTF. Because RIA is a reactivity excursion event, numerical stability and efficient time stepping approaches are essential to computational performance. Validation activities included comparisons against the 3D RIA events in the SPERT.

Applications of RIA focused on simulation of the AP1000® hot full power (HFP) and hot zero power (HZP) rod ejection events, with a full 3D core modeling every individual rod and flow channel. The key safety parameters of importance are the peak rod enthalpy and the onset of DNB during the transient. The need for fully coupled neutronic and T/H calculations was demonstrated based on prediction of a stronger Doppler feedback within VERA than that provided by current industry methods. VERA also provides the ability to simulate reactor behavior long after an RIA. While the validation is not yet complete and there are additional user features to be incorporated, the transient VERA calculations demonstrated a robust algorithm with reasonable computational performance.

As depicted in Figure 11, the calculated rod ejection at HFP for an AP1000° shows a highly asymmetric power distribution, with the highest power near the ejected rod. The maximum power peaking factor of ~6 at the peak of the pulse ensures that this demonstration problem would stress the computational burden on VERA and the underlying material models. The RIA calculation took approximately 34 hours of wall clock time on 3,584 cores of INL's Falcon HPC system to simulate 193 state points for a 5-second rod ejection.



**Figure 11.** Pin power distribution for AP1000 rod ejection at HFP.

#### **Progress on the LOCA Challenge Problem**

FY17 LOCA challenge problem activities addressed BISON's known limitations for LOCA modeling, along with validation of the existing capability using separate effects tests. The key material and behavior models required to address transient high-temperature phenomena occurring during LOCAs in PWRs have now been implemented in BISON. Models were developed for cladding burst failure, axial fuel relocation, transient gas release, and energy deposition from rapid oxidation. These apply specifically to UO₂ fuel, Zircaloy cladding, and water coolant. During FY17, important new capabilities to address axial UO₂ fuel relocation (for 1.5D geometry) and account for oxidation energy deposition in cladding were included. Planned future development efforts include extending the axial fuel relocation model from 1.5D to 2D/3D and improving BISON's fission gas release model to include transient gas release associated with high burnup fuel structure [9].

A substantial number of separate effects validation cases (42 tests from 3 experimental series) were completed. In general, BISON predictions of cladding burst temperature, pressure, and burst time are very reasonable. However, in one experimental series involving both very high temperatures and strain rates, BISON systematically overpredicts the cladding hoop strain. BISON validation of a series of integral fuel rod experiments (6 rods) for testing fuel modeling during a LOCA has also been completed. As with the separate effects experiments, BISON predictions of burst temperature, pressure, and burst time are generally very reasonable. Comparisons to cladding peak strain and rod outer diameter axial profiles are less satisfactory, identifying material models and possibly modeling approximations (e.g., 2D-RZ vs 3D geometries), requiring additional investigation [16].

#### **Progress on the GTRF Challenge Problem**

The CASL GTRF challenge problem FY17 work scope marks the successful overall completion of the challenge problem. The completed R&D provides a comprehensive set of tools and methods for future use in the design and analysis of reactor fuel components as it relates to engineering wear and the understanding of underlying key physics phenomena [4]. The final element of the GTRF challenge problem was to procure the AFIR and associated wear rate measurements for several cladding and grid materials at different temperature, pressure, and coolant chemistry conditions. In resolving the challenge problem, the following advancements were made:

- Commercial CFD codes were demonstrated to be capable of simulating flow turbulence that induces GTRF.
- Structural mechanics modeling was shown to be capable of calculating changes in grid geometry with irradiation.
- A new material wear model was developed.
- An experimental capability was designed and applied to develop material wear data at near-reactor conditions.

Work on the GTRF challenge problem addressed the development and refinement of a predictive engineering wear model that includes (1) the role of crystallographic texture on gap openings between the spacer grid and the fuel clad, (2) the effect of creep, oxidation, and wear on fretting wear depth, and (3) multi-rod considerations that influence the locations within fuel assemblies most susceptible to GTRF. The AFIR tests provided important data for modifying the engineering wear model to account for cladding-grid material pair, cladding pre-oxidation, temperature, and coolant chemistry. The AFIR will be available for future industry testing needs in support of advanced fuel assemblies or ATF.

Key discoveries resulting from CASL's research on GTRF are described below [4].

- GTRF wear is a cumulative process, as the rate of wear can change as reactor operating conditions and surface material change. Physical changes to the contact conditions that must be modeled include oxide loss, exposure of the substrate, and hydrogen embrittlement (tribo-corrosion).
- The dissipation of frictional work during wear is affected by the partition of energy needed to generate wear particles from the surface of the cladding and grid, to form third-body debris layers, to destroy those layers, and to remove debris layer fragments. Thus, primary and secondary debris processes are envisioned.
- Structural mechanics modeling of the multiple rod and grid contact within fuel assemblies indicates that the patterns of leaking rods are concentrated along external corners and edges, in agreement with observations.
- Structural mechanics modeling has also identified the effect of crystallographic
  texture within the spacer grids, revealing that thermal-mechanical processing of
  the grids to produce basal poles aligned along the transverse or normal direction,
  as opposed to aligned along the rolling direction, will impede the development of
  fuel-grid gap that minimizes fretting wear.
- Wear and corrosion must be considered together. Fretting can dramatically promote oxidation/corrosion, and wear reduction may come at a price of oxidation/ corrosion.
- Good agreement was obtained between Oak Ridge National Laboratory (ORNL)
   AFIR and Westinghouse and the VIPER test loop on wear rate and morphology,
   thereby providing a solid foundation for correlating AFIR results with field experience and using them for training and validating GTRF models, including the
   engineering wear model.
- Surface treatment of the cladding and grid material are important. Preoxidation of ziconium alloy cladding effectively reduced the rate of cladding wear.

## PART 3: END USER IMPACT **AND NUCLEAR INDUSTRY ENGAGEMENT**

The return of the AMA focus area, along with continuing enhancements in the computational performance and accuracy of VERA, brought about a significant increase in industrial applications and user engagements in FY17. A substantial shift from R&D to application and validation was evident to stakeholders, and with increased confidence in the software came an increase in interactions and collaborations with industrial end users. This has also led to an increased number of external installations of VERA, several professional training workshops, and initial discussions of the VUG. This trajectory of success will continue through FY18 and beyond the conclusion of CASL.

The significant increase in applications and model development in FY17 was driven by the following goals.

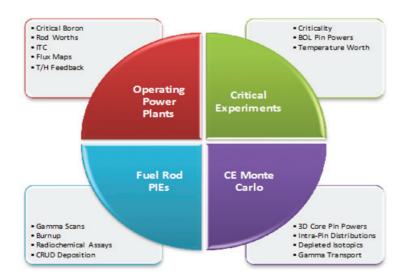
- 1. Aggressively pursue the VERA core simulator validation, including comparisons to plant data, radiochemical assays, critical experiments, high-end continuous-energy Monte Carlo results (Figure 12), and testing for a wide variety of power plants and fuel types.
- 2. Use specific real-world instances of challenge problem phenomena (CIPS, CILC, PCI, DNB, etc.) to demonstrate and validate VERA's capabilities for solving the challenge problems.
- 3. Pursue several current applications for new plants (Watts Bar Nuclear 2, AP1000® and NuScale SMR) that are particularly high in potential value due to current interest and importance to the nuclear industry.
- 4. Work directly with nuclear fuel vendors and utilities to ensure that VERA meets their needs and that it allows CASL to apply and demonstrate the software capabilities for today's most relevant applications.
- 5. Solidify CASL's end user base to ensure early adoption of VERA prior to the con-clusion of CASL.

In addition to supporting five test stands in FY17, CASL also added five new industrial collaborations to share fuel specifications, plant operating data, and commercial analysis expertise. This resulted in an increase from six reactor models in FY16 to eighteen in FY17, with plans for at least six more in FY18. At that stage, CASL will have modeled about one third of the US fleet of PWRs, providing a broad testing and validation basis for VERA and covering many power plant designs and fuel types. These models provide platforms for general software benchmarking and challenge problem applications, and in some cases, they provide new customers with validated models that can be used for analysis of currently operating plants.

- AREVA installed VERA 3.6 on their own computer to model for Cycle 12 of the Davis-Besse Nuclear Power Station, followed by core follow calculations of Cycles 12–15.
   Initial results are generally in good agreement with measured data and are very close to calculations from existing codes. Cycle 15 experienced severe CIPS, which will be simulated with the improved MAMBA in FY18.
- Arizona Public Service provided fuel and plant data for Palo Verde Unit 2 Cycles 1–9, which have now been successfully modeled with VERA. Palo Verde is currently CASL's only combustion engineering plant design and will serve as a signficant source of validation for VERA's CIPS and CILC capabilities. Palo Verde experienced mulitple CILC fuel rod failures in Cycle 9, which CASL will model in FY18.
- Duke Energy provided 65 fuel cycles of data for five units of the McGuire, Catawba, and Oconee power plants. These data include hundreds of statepoints of fine mesh in-core detector response data for validating the power distributions calculated by VERA. CIPS data and operating history are also included for the mixed oxide (MOX) lead test assemblies. Duke also provided all the core design and crud risk analysis data for the Catawba 2 CIPS risk evaluation discussed in the 2017 highlighted achievements. Currently, 15 cycles of Catawba 2 have been successfully simulated, and more Catawba, McGuire, and Oconee cycles will be modeled in FY18.
- Exelon provided fuel and cycle data and load following power histories for Byron
  Unit 1, Cycles 17–21. The data will be expanded in FY18 to include Unit 2 data and
  will be used for PCI challenge problem activities. Exelon has also provided all the
  data needed to model Three Mile Island (TMI) Unit 1 Cycles 1–10, for which Cycle 10
  had both CIPS and CILC failures, followed by postirradiation exams of the damaged
  fuel. The results of these simulations are forthcoming and will be available in FY18.
- For the NuScale test stand, NuScale has provided fuel and core design info for the
  first eight fuel cycles of their SMR. These cycles have been successfully simulated
  with VERA and compared to in-house design calculations. This application will
  continue into FY18, when crud calculations will be performed for the SMR with
  MAMBA. Figure 13 provides a photo of NuScale and CASL staff members at a recent
  test stand meeting in Charlotte, North Carolina. Figure 14 provides an example of

the coolant temperature distribution in the SMR calculated by VERA. Benchmarking of VERA against a continuousenergy Monte Carlo method of neutron transport has demonstrated that VERA is capable of accurately calculating the pin power distribution at the periphery of the SMR core, next to the solid steel reflector block that is unique to US reactors (Figure 15).

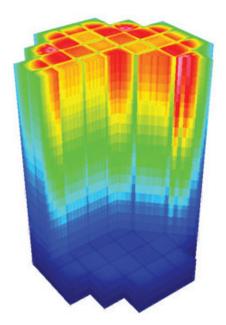
TVA, a founding partner of CASL, has increased their usage of VERA tools since the Watts Bar Unit 2 startup in FY16, when the results from VERA matched plant measurements very well. CASL completed the flux map analyses of the startup in FY17, in which the relative signal distribution in the new fixed in-core vanadium neutron detection system was very well predicted by VERA (Figure 16). In this case VERA was shown to be at least as accurate as the online core monitoring software used by TVA, which is powered by an NRC-licensed core design methodology.



**Figure 12.** VERA core simulator validation plan.



**Figure 13.** NuScale and CASL staff at a project status meeting.



**Figure 14.** Coolant temperature distribution in Cycle 8 of the NuScale SMR.

As confidence in the VERA tools has increased following the Unit 2 startup, TVA has also employed CASL tools to help answer new questions about Unit 1. In the current fuel cycle (Cycle 15), a radial power distribution anomaly exists that is larger than previous cycles. CASL has recently worked with participants of the US Tritium Technology Program (TVA, Pacific Northwest National Laboratory [PNNL], the National Nuclear Security Administration [NNSA], etc.) to simulate the tritium production burnable absorber rods (TPBARs) used in Unit 1 with the highest resolution ever performed in a whole-core simulation. Additionally, PNNL obtained VERA 3.6 and installed it on their computing resources to independently confirm CASL's results. Comparison to measurements from the Unit 1 Cycle 2 lead test assemblies demonstrates that VERA can calculate the tritium masses to within 1% of measured values. Though results from VERA appear to rule out the TPBARs as a potential cause of the power distribution anomaly, they do provide new information to TVA about other potential sources. This activity has demonstrated that other US government programs can benefit from the capabilities developed by CASL.

TVA and Westinghouse are now using VERA for confirmatory calculations of the future fuel cycles for Watts Bar Units 1 and 2. For the first time since CASL's beginning, industry core designers and operators are choosing VERA as a reliable source of alternate, high-fidelity calculations that can supplement the results of their own codes. TVA has provided CASL with 16 fuel cycles of data for validation from both Watts Bar units.

The Westinghouse test stand is being performed in conjunction with the NEAMS program and is focused on application of BISON for ATFs. In particular, Westinghouse is evaluating the code capabilities for U₃Si₂ fuel pellets, coated Zirlo<sup>TM</sup> cladding, and SiC cladding. Westinghouse has installed VERA 3.6 and 3.7 on their internal computing cluster, Binford, which can run quarter-core simulations of most US reactor designs. For AMA activities, Westinghouse has set up and built models for numerous plants, including AP1000® cycles 1–5, Seabrook cycles 1–5, Callaway cycles 1–7, Krško cycles 1–3, Farley cycles 23–28, and South Texas cycles 1–8. In FY18, VERA will be used to compare startup measurements from the Sanmen Nuclear Power Station in China—the first AP1000 reactor to startup in the world to data predicted by Westinghouse.

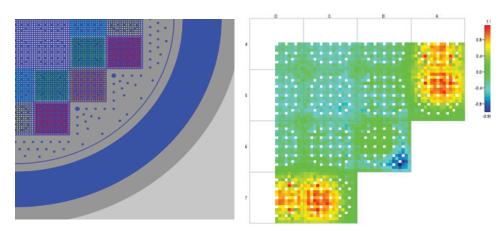


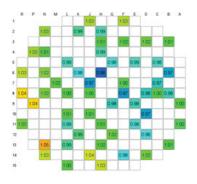
Figure 15. VERA model of the NuScale Cycle 1 SMR core with steel reflector block.

#### APPLICATION OF VERA TO OPERATING PLANTS

In FY17, VERA applications were extended to several existing plants and some new designs. These applications represent a broad spectrum of design and operating conditions for the current and future operating fleet. The analyses performed also represent a key component of the VERA V&V plan, with improved confidence in the robustness of the software's physics, geometry, and numerical solvers, especially as it relates to solving the CASL challenge problems.

Overall, CASL has expanded its applications to 18 reactors and is approaching simulation of nearly 100 operating fuel cycles. Below is a summary of the reactor applications to challenge problems and new reactor designs.

- CIPS and CILC Analyses
  - Watts Bar Unit 1 (WBN1) (Cycles 1–15) (Westinghouse Electric Company (WEC) '4-loop,  $17 \times 17$  fuel)
  - Catawba 2 (Cycles 8–21) (WEC 4-loop,  $17 \times 17$  fuel)
  - Callaway (Cycles 1–7) (WEC 4-loop,  $17 \times 17$  fuel)
  - Seabrook Unit 1 (Cycles 1–5) (WEC 4-loop,  $17 \times 17$  fuel)
  - Palo Verde 2 (Cycles 1–9) (CE System 80, 16 × 16 fuel)
  - Davis-Besse (Cycles 12–15) (B&W,  $15 \times 15$  fuel)
  - Oconee 3 (Cycle 25) (B&W, 15 × 15 fuel)
  - Three Mile Island Unit 1 (Cycles 1-10) (B&W,  $15 \times 15$  fuel)
- **PCI** Analyses
  - Byron 1 (Cycles 17–21) (WEC 4-loop, 17 × 17 fuel)
  - Braidwood (Cycles 9–10) (WEC 4-loop,  $17 \times 17$  fuel)
- Benchmarking and Validation
  - Krško (Cycles 1-3) (WEC 2-loop, 16 x 16 fuel)
  - Catawba Unit 1 (WEC 4-loop, 17 × 17 fuel)
  - McGuire Unit 1 and Unit 2 (WEC 4-loop, 17 × 17 fuel)
  - Farley 1 (Cycles 23–28) (WEC 3-loop,  $17 \times 17$  fuel)
  - South Texas 2 (Cycles 1–8) (WEC 4-loop XL,  $17 \times 17$  fuel)
- **New Plants** 
  - NuScale SMR (Cycles 1-8)
  - Watts Bar Unit 2 (Cycle 1–2) (WEC 4-loop,  $17 \times 17$  fuel)
  - AP1000® (Cycles 1–5) (WEC ATF, PCI, Startup Physics)



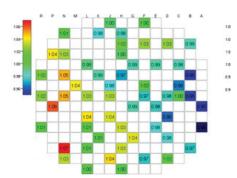


Figure 16. Radial vanadium current distributions compared to measured data from Watts Bar 2 (VERA relative errors [left] and online core monitoring software [right] in %).

#### **CASL INDUSTRY COUNCIL**

The CASL Industry Council provides programmatic oversight and review of CASL from the perspective of the nuclear power industry and ensures that CASL investments are aligned with industrial needs to obtain the maximum potential benefit. It is an important means of engaging potential end users and initiating data exchanges or collaboration on specific projects. The specific goals of the CASL Industry Council are as follows:

- early, continuous, frequent interface and engagement of end users and technology providers,
- critical review of CASL plans and products,
- optimum deployment and applications of periodic VERA releases, and
- identification of strategic collaborations between industry and CASL focus areas.

The council consists of 24 organizations and is composed of nuclear plant owner/operators, fuel and reactor vendors, engineering service providers, independent software vendors, and computer technology companies, as shown in Figure 17. In 2017, two industry council meetings were held, including a joint meeting with the CASL Science Council in October 2016 and an independent CASL Industry Council meeting in April 2017 (Figure 18). The CASL Industry Council provided clear feedback at both meetings on CASL's progress and emphasized the priorities discussed in CASL's planning meetings.

Increasingly, the CASL Industry Council meetings include presentations and feedback on VERA results from non-CASL members, demonstrating successful applications of VERA outside of CASL work scope. In FY17, the following presentations were made with very successful results and subsequent discussion:



Figure 17. CASL Industry Council member organizations.

- "Catawba CIPS Benchmarking Update" was presented by Duke Energy (jointly with Travis Lange, University of Tennessee, Knoxville [UTK]) showing the potential for significant fuel savings when performing core design with support from the VERA tools.
- "MC21 / CTF and VERA Multiphysics Solutions to VERA Core Physics Benchmark Progression Problems 6 and 7" was presented by the Naval Nuclear Laboratory (Knolls Atomic Power Laboratory [KAPL]) and showed excellent agreement between their high-fidelity code MC21 and VERA.
- "CASL-NuScale CRUD Work" was presented by NuScale and showed that VERA was successfully applied to eight cycles of their SMR, and preliminary crud results from MAMBA were promising (see test stand description).
- "Davis-Besse Cycle 15 CIPS Analysis with VERA Interim Results" was presented by AREVA (see test stand description).

#### TEST STAND DEPLOYMENTS

CASL supported five test stands in FY15, several of which are described in more detail in the previous section:

- AREVA: modeling of core follow and crud formation in Davis-Besse Cycle 15 – now underway
- University of Illinois/Exelon: evaluation of fuel duty under load follow conditions as related to PCI for Byron - completed, with followup work moved to AMA activities in FY18
- WEC: analysis of WEC SiC and U<sub>3</sub>Si<sub>2</sub> ATF concepts with BISON (joint with NEAMS) - now underway
- NuScale: analysis of crud in SMRs under natural circulation, including an investigation of integral reactor crud sources now underway
- NRC: application of CASL tools to ATFs – now underway



**Figure 18.** CASL Industry Council meeting, Charleston, SC, April 4–5, 2017.

#### **VERA USERS GROUP**

The VERA Users Group (VUG) was extensively discussed at the April 2017 CASL Industry Council meeting in Charleston, South Carolina. VUG will ensure the long-term success of CASL by sustaining the use of VERA after the program is completed. VUG will focus on practical applications to industrial problems. It will be initially composed of CASL Industry Council members interested in obtaining the CASL codes or access to those codes on a shared computer resource. Further planning will be completed in FY18, specifically with regard to license fees, deployment mechanisms, computer allocations, technical support and training.

#### **ENGAGEMENT WITH THE NUCLEAR REGULATORY** COMMISSION

Since its inception, CASL has been engaging with the NRC and has continued to meet with NRC representatives to discuss CASL code progress and to identify areas of potential collaboration. Engagements this year include participation by two NRC observers in the FY16 DOE Annual CASL Review, NRC staff members giving presentations at a CASL V&V meeting in January 2017, and meetings to discuss specific collaboration on integration of CASL and NRC computer codes.

In February 2017, the NRC Office of Regulatory Research proposed a test stand to support analysis of ATFs, and at a joint NEAMS-CASL meeting in April 2017, it was decided to pursue coupling of the NRC TRACE reactor systems code and BISON using the MOOSE infrastructure. While this will be a NEAMS-led effort, CASL will continue to engage and support the coupling activities. Plans for the first working meeting and BISON training for coupling TRACE with BISON have been developed, and BISON training has been planned for NRC staff members.

#### CASL STRATEGY FOR ACCIDENT-TOLERANT FUELS

Several US fuel vendors and utilities are planning to insert lead test rods for various ATF fuel concepts into commercial reactors during FY18 and FY19. Advanced M&S tools have the potential to accelerate the introduction of full fuel assemblies and eventual licensing of ATF reload cores for commercial reactors. Advanced M&S can be used to predict ATF fuel behavior and gain better understanding of operational performance. Such tools can also be used to expedite and guide experimental tests to gather all necessary and important test data at various conditions. These tools may be adopted by industry with eventual licensing through the NRC. Therefore, advanced M&S offers the opportunity to reduce the risk of investment, decrease capital investment, and shorten development time.

Initial CASL planning for ATF included collaboration with industry partners and other programs within DOE, including the Advanced Fuels Campaign, NEAMS, and the Light Water Reactor Sustainability Program. This resulted in a new CASL challenge problem to investigate the performance of different ATF forms and to develop the needed analysis capabilities. The ATF challenge program is based on the following:

- Analysis of ATF for normal PWR operations, including:
  - Examining the consequences for ATF introduction to operating PWRs by answering questions related to PWR physics predictions such as startup testing, core follow, and fuel burnup accumulation (fuel rod and assembly)
  - Assessing the impact of ATF introduction against core operating limits and technical specifications
  - Identifying data needs to support ATF validation
- Application of ATF to the existing scope of current challenge problems such as the RIA event
- Assessment of ATF for additional design basis accidents
- Quantifying the financial benefits that could be obtained from ATF due to increased margins, reduced fuel cycle costs, and increased operational flexibility

#### **CASL TRAINING**

In FY17, two VERA training classes were held for Westinghouse: one on March 14 in Rock Hill, South Carolina, and the other on May 22 in Cranberry Township, Pennsylvania. During these sessions, approximately 20 reactor core designers and engineers successfully completed the hands-on training using their own computing cluster, Binford. Each 1-day class provided a brief CASL overview, a description of VERA methods, and a hands-on guide to running problems with the VERA common input, progressing from small single 2D fuel lattice problems up to whole-core calculations. To ensure training success, a quick-start quide for running cases on Binford was provided in advance to all class participants, so they were able to ensure computer access and functional scripts prior to training. A photo of the Cranberry Township class is shown in Figure 19. These are the first industrial users to receive training for potential non-CASL applications.

On March 3, individual training was provided to Westinghouse and EPRI AMA staff members on the use of VERA for whole-core PCI risk screening using BISON. This training was held at ORNL and was developed and delivered by PHI staff members.

#### **CASL INSTITUTE AND 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, now in its fifth year, matches top students at NCSU with CASL faculty mentors. During the 2016–2017 academic year, six scholars engaged in projects with five students. Since the program's inception, 32 students have participated. Out of the 30 that have completed their undergraduate degrees, 15 are now attending graduate school, and 4 have completed graduate degrees. For the seventh year, the CASL Education Program participated in the American Nuclear Society (ANS) Student Conference held in Pittsburgh, Pennsylvania, in April 2017 to promote CASL research opportunities and highlight student research activities. Five CASL undergraduate research scholars presented their research at the conference.



Figure 19. VERA training class at Westinghouse Headquarters, May 22, 2017.

The CASL Education Program also supported its third Research Experience for Undergraduates (REU) in the summer of 2017. Makeiba Lewis, a student from South Carolina State University, worked with Dr. David Kropaczek at NCSU. Ms. Lewis's research focused on advanced nuclear fuel designs and the use of the CASL codes with industry codes. As a demonstration of the program's success, Bianca Cruz, CASL Education's Program REU participant in 2015, is now in the Nuclear Engineering PhD program at NCSU.

CASL currently has 101 students representing 15 universities active in CASL research. Among these students, 62% receive CASL funding, with the remaining being funded by other means. Of the 101 students, 7 are undergraduates, 12 are in graduate school at the master's level, 72 are obtaining PhDs, and 10 are postdoctoral researchers.

The CASL Institute is a 2-week education and training activity on VERA codes and methods that is open to university students and working professionals. In 2017, there were over 50 applicants, 27 of whom completed the course (Figure 20). The curriculum covered the CASL codes and challenge problems in lectures and hands-on projects. Students were certified upon successfully completing an end-of-course team project. The 2017 CASL Institute was held in June at NCSU. This represents a change from the previous year, when the first CASL Institute was held at ORNL using ORNL computing resources. The success of the 2017 CASL Institutes provides another model for access to VERA tools in a non-laboratory environment in the post-CASL phase. Holding the course offsite demonstrated the ability to address issues such as export control and access to HPC resources.

CASL also supports a suite of summer internships at ORNL and other partner organizations. In FY17, CASL hosted 10 summer students (Figure 21) at ORNL from May–August of 2017.

These students worked on a range of topics:

- Ashley Demeter (North Carolina State University) working with Mr. Andrew
- Austin Ellis (North Carolina State University) working with Dr. Stephen Hamilton
- Andrew Fitzgerald (University of Michigan) working with Dr. Shane Stimpson
- Byoung-Kyu Jeon (Purdue University) working with Dr. Kang Seog Kim
- Daniel O'Grady (University of Illinois Urbana-Champaign) working with Mr. **Andrew Godfrey**
- A. J. Pawel (University of Tennessee) working with Dr. Ben Collins
- Casey Stocking (North Carolina State University) working with Dr. Tara Pandya
- Daniell Tincher (Virginia Commonwealth University) working with Dr. Bob Salko
- Aysenur Toptan (North Carolina State University) working with Dr. Bob Salko



**Figure 20.** CASL Institute participants and faculty.



Figure 21. CASL 2017 summer students at ORNL



## PART 4: RETURN ON FY17 **TAXPAYER INVESTMENT**

The CASL leadership and operations team continued working to ensure that the program produces a strong return on taxpayer investment and that funding provided by The Department of Energy's Office of Nuclear Energy (DOE-NE) is carefully managed. The primary measure of return on investment is the successful completion of CASL's planned technical work that results in impactful outcomes for the nuclear industry. Regarding financial management, CASL's work is executed through contracts established by ORNL and is issued to CASL partner organizations. CASL's finance officer monitors the CASL contracts and tracks financial reports through monthly reports and quarterly financial teleconference calls. CASL has also continued planning for sustaining the CASL developments for the post-CASL period with a focus on defining an integrated CASL-NEAMS modeling and simulation program.

#### **FY17 FINANCIAL PERFORMANCE**

A summary of the budget and spending for the FY17 funding is presented in Table 5. The total funding includes carryover from FY16, as well as FY17 funding received from DOE. As shown, approximately 80% of the FY17 CASL costs (i.e., total costs minus subcontracting overhead and taxes) were associated with R&D work, and the remainder was associated with management, operations, and computing and collaboration infrastructure. Unspent FY17 funding will be carried over and allocated to FY18 activities. The percentage of the FY17 CASL budget by focus area is shown in Figure 22.

#### 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 222 milestones were defined for work to be performed in FY17. Of these milestones, 11 were DOE-reportable milestones, as selected in consultation with CASL's federal manager to measure CASL's performance in executing its scope.

#### **DOE REPORTABLE MILESTONES**

The FY17 DOE-reportable milestones are provided in Table 6. All milestones were completed and delivered on time.

#### POST-CASL PLANNING

In FY16, a post-CASL strategy was developed to sustain CASL activities beyond the CASL operating period. The strategy was developed with the CASL Board of Directors and presented to the CASL Industry and Science Councils. Key attributes of the strategy include:

- Industry applications will be developed by users interested in applying VERA capabilities to address issues associated with operation of the existing LWR fleet.
- Regulatory and licensing applications will be developed by organizations seeking to explore qualification of VERA tools to support submittal of license applications to the NRC.
- Education and training applications will be developed by users interested in presenting case studies using VERA tools in university classrooms and corporate training sessions.
- R&D applications will be 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. Specific activities were identified as essential elements of the post-CASL strategy:
- The VUG will be developed to provide post-CASL two-way communication between code developers and code users.
- A strategy will be developed for a DOE-NE integrated CASL and NEAMS M&S program that leverages CASL investments.

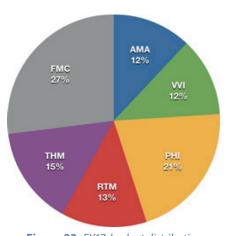


Figure 22. FY17 budget distribution by focus area.

Table 5. FY17 Budget and Cost Summary

	FY17 Budget (\$K)	FY17 Cost (\$K)
Technical Activities	22,865,361	19,506,605
Fuel Materials and Chemistry (FMC)	6,191,932	5,200,769
Thermal Hydraulics Methods (THM)	3,775,081	2,891,938
Radiation Transport Methods (RTM)	2,999,999	2,899,930
Physics Integration (PHI)	4,558,202	3,702,322
Advanced Modeling Applications	3,055,068	2,743,924
Verification & Validation Implementation (VVI)	2,285,079	2,067,722
Program Management and Operations	3,619,610	2,916,041
Management	2,190,459	1,773,017
Operations	1,429,151	1,143,024
CASL Education Program and Institute	485,930	363,780
Computing and Collaboration Infrastructure	1,379,310	1,224,043
Subcontracting Overhead and Taxes	1,316,881	1,064,564
Contingency/Reserve	649,445	-
Total	\$30,316,537	\$25,075,033

- Sustain the CASL Industry and Science Councils to continue fostering productive interactions between national laboratories, universities, and industry scientists and engineers.
- Integrate VERA into industry work processes.
- Enable industry-led regulatory licensing of the VERA tools.

FY17 activites in pursing this strategy focused on continuing development of an integrated CASL and NEAMS program and maturing the VUG.

**Table 6.** FY17 DOE-Reportable Milestones

Milestone ID	Milestone description		Deliverable references
FY17.CASL.001	Develop and deliver nuclear cross section data library supporting PWR and BWR designs	Feb-17	[17]
FY17.CASL.002	Prepare and release update to VERA to the Radiation Shielding Information Computational Center (RSICC) for distribution outside of CASL	Feb-17	[12]
FY17.CASL.003	Perform core design and CIPS analysis of a future core design and compare to industry risk analysis	Mar-17	[1]
FY17.CASL.004	Complete and document Watts Bar Nuclear Unit 2 startup analysis	Mar-17	[18]
FY17.CASL.005	Complete and demonstrate VERA with cores simulator coupled with Monte Carlo ex-core transport capability	Apr-17	[6]
FY17.CASL.006	Complete and document assessment of VERA against the Verification and Validation (V&V) Plan	Jun-17	[13]
FY17.CASL.007	Establish solution-verified CFD model of WEC $5 \times 5$ bundle for DNB validation studies	Jul-17	[19]
FY7.CASL.008	Complete and demonstrate improved VERA CIPS capabilities	Aug-17	[3]
FY17.CASL.009	Develop, demonstrate, and assess advanced CFD-based capability to predict DNB	Sep-17	[2]
FY17.CASL.010	Complete benchmarking of BISON against Loss of Coolant Accident (LOCA) experiments	Sep-17	[20]
FY17.CASL.011	Complete and document CASL research and development (R&D) on the GTRF challenge problem	Sep-17	[4]

## **CONCLUSIONS**

CASL made several significant advancements in FY17. These include key research accomplishments associated with progress on CASL's challenge problems and expansion of engagement with industry through applications to a growing number of nuclear plants. Research outcomes have added new and important capabilities to VERA that support resolution of CASL challenge problems. The CASL education program was very active, providing support to student scholars and researchers and holding the second CASL institute. A highlight of the year was receiving the R&D 100 award for development of VERA. The program remains on track to fulfill its end-state vision within the final years of CASL operations and is making strong progress toward establishing VERA as a set of tools widely used by industry, academia, and the national laboratories for advanced simulation and analysis of commercial LWRs.

For FY18, CASL is moving forward on our challenge problem development and applications. The primary focus, which is based on CASL Industry Council feedback, is on crud challenge problems (CIPS, CILC), PCI, and DNB. Work will also continue on the other challenge problems. CASL will also focus on maturing the VUG and expanding industry engagement.

## **ACKNOWLEDGMENTS**

This research was supported by the Consortium for Advanced Simulation of Light Water Reactors (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 ALCC Program. This research used resources of the Oak Ridge Leadership Computing Facility at ORNL, 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 INL, which is supported by the Office of Nuclear Energy of the US Department of Energy under Contract No. DE-AC07-05ID14517.

## REFERENCES

- 1. T. Lange, A. Godfrey, and F. Franceschini, VERA Analysis of CRUD Induced Power Shift for Catawba Unit 2 Cycle 22 Core Designs, CASL-I-2017-1301-000, March 2017.
- 2. E. Baglietto, E. Demarly, R. Kommajosyula, S. J. Kim, and R. A. Brewster, Develop, demonstrate, and assess advanced Computational Fluid Dynamics (CFD) based ca-pability for prediction of Departure from Nucleate Boiling (DNB), CASL-U-2017-1448 000, September 2017.
- 3. B.S. Collins, et al., Development of a Comprehensive CRUD-Induced Power Shift (CIPS) Capability with VERA, CASL-U-2017-1406-000, August 2017.
- 4. B. Wirth, et al., Summary report describing CASL accomplishments in support of the GTRF Challenge Problem, CASL-U-2017-1429-000, September 2017.
- 5. B. W. Spencer, J. W. Peterson, W. Jiang, Y. Liu, and A. Casagranda, BISON Contact Algorithm Improvement Support of Pellet Cladding Mechanical Interaction Modeling, CASL-U-2017-1430-000, INL/EXT-17-43399, September 2017.
- 6. T. Pandya, T. Evans, K. Clarno, and B. Collins, Excore Radiation Transport Modeling with VERA, CASL-U-2017-1311-000, April 2017.
- 7. B. Kochunas, T. Downar, Y. Liu, Q. Shen, Z. Dodson, A. Gerlach, D. Jabaay, A. Wysocki, and V. Kucukboyaci, Development of Transient MPACT-CTF Capability for RIA with DNB, CASL-U-2017-1424, September 2017.
- 8. G. Agostinelli, E. Baglietto, and S. Yoon, BWR Modeling Assessment, CASL U 2017 1472-000, September 2017.
- 9. C. P. Folsom, L. Williamson, G. Pastore, and W. Liu, Development of a RIA Experimental Benchmark for BISON, CASL-U-2017-1403-000, August 2017.
- 10. CASL VERAIn, July 2017, https://github.com/CASL/VERAin
- 11. CASL VERAView, September 2017, https://github.com/CASL/VERAview
- 12. T. Walsh, M. Sieger, M. Baird, B. Mervin, R. Bartlett, R. Lee, and K. T. Clarno, VERA-3.6 Release, CASL-U-2017-1276-000, February 2017.
- 13. C. Jones, A. Hetzler, N. Dinh, P. Athe, and M. Sieger, Verification and Validation As-sessment for VERA, CASL-U-2017-1310-000, April 2017.
- 14. S. Slattery, W. Gurecky, and N. Adamowicz, Cicada A Package for CILC Analysis, CASL-2017-1400-000, August 2017.
- 15. S. Stimpson, Demonstration of Load Follow Simulation with VERA-CS and Standalone BISON, CASL-U-1257-000, December 2016.
- 16. N. Capps, W. Liu, and J. Alvis, Evaluation of Ramp Tests for LOCA, CASL U 2017 1473 000, June 2017.
- 17. K. S. Kim, K. T. Clarno, C. Gentry, D. Wiarda, M. L. Williams, B. Kochunas, Y. Liu, and S. Palmtag, Development of the V4.2m5 and V5.0m0 Multigroup Cross Section Li-braries for MPACT for PWR and BWR, CASL-U-2017-1280-000, February 2017.
- 18. A. Godfrey, B. Collins, C. Gentry, S. Stimpson, and J. Ritchie, Watts Bar Unit 2 Startup Results with VERA, CASL-U-2017-1306-000, March 2017.
- 19. W. D. Pointer, Reference Computational Meshing Strategy for Computational Fluid Dynamics Simulation of Departure from Nucleate Boiling, CASL-U-1390, July 2017.
- 20. R. Williamson, G. Pastore, K. Gamble, R. Gardner, and W. Liu, Development of a LOCA Experimental Benchmark for BISON – Milestone L2:FMC.P15.08, CASL U 2017 1422-000, September 2017.

