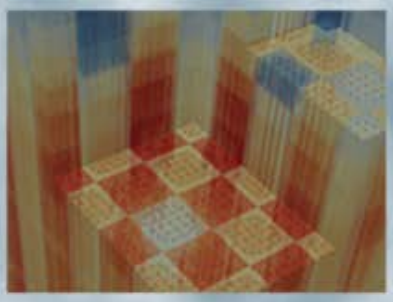
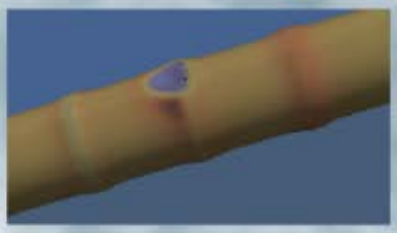
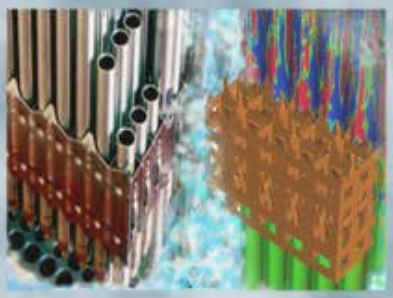
CASL Meeting with the Illinois Applied Research Institute







Douglas Kothe and Jess Gehin at the University of Illinois at Urbana-Champaign

October 6, 2014

Meeting Agenda

Visit of Dr. Douglas Kothe and Dr. Jess Gehin at the University of Illinois

Monday, October 6th, 2014
9:00 am – 4:00 pm

Discussion on a pathway to build a Test Stand in collaboration with the Oak Ridge National Laboratory and the University of Illinois.

Specific interest: *training and education, verification and validation, and plans for sustainability of the program.*

9:00 am – 10:00 am	Introduction by Dr. Jeffrey Binder, Applied Research Institute
10:15 am – 10:30 am	Meeting with Dr. Andreas Cangellaris, Dean of the College of Engineering at the University of Illinois
10:30 am – 10:45 am	Meeting with Dr. James Stubbins, Department Head of Nuclear, Plasma and Radiological Engineering
11:00 am – 12:00 pm	Seminar by Dr. Douglas Kothe on DOE Energy Innovation Hub
12:00 pm – 1:00 pm	Lunch break
1:00 pm – 4:00 pm	Technical discussion: - Dr. Jess Gehin on technical challenges of DOE Energy Innovation Hub - University of Illinois on the Test Stand, training and education, validation opportunities, and plans for sustainability of the program

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

Douglas B. Kothe
Oak Ridge National Laboratory
kothe@ornl.gov

Accelerated and translational R&D, from fundamental discovery to commercialized technology, has proven challenging for nuclear energy; innovations are challenging in an enterprise that that is inherently conservative and regulatory-driven. Translational research—a high return proposition for nuclear energy—is exactly what Energy Innovation Hubs established by the U.S. Department of Energy (DOE) strive to enable and accelerate. Hubs bring together teams of top scientists and engineers from academia, industry, and government to collaborate and overcome critical known barriers to achieving national climate and energy goals that have proven resistant to solution via the normal R&D enterprise. Hubs focus on a single topic, with the objective of rapidly bridging the gaps between basic research, engineering development, and commercialization through a close partnership with industry. To achieve this goal, the Hubs necessarily consist of large, highly integrated and collaborative creative teams working to solve priority technology challenges. For the Consortium for Advanced Simulation of Light Water Reactors (CASL), awarded as the first Hub by the DOE Office of Nuclear Energy (NE) in July 2010, the focus is on innovating commercial nuclear power generation, specifically the modeling and simulation (M&S) of nuclear reactors. CASL not only strives to bring innovation to the nuclear energy enterprise but also to help retain and strengthen U.S. leadership in two DOE mission areas: HPC-enabled M&S and nuclear energy. CASL is currently completing its fourth year of a five-year Phase 1 execution and has been granted the opportunity by DOE to submit a proposal for a second five-year Phase 2 (2015–2019) of execution.

CASL's unique partnership of government, academia, and industry possesses unparalleled collective institutional knowledge, nuclear science and engineering talent, computational science leadership, and LWR design and regulatory accomplishments. CASL has several key elements: clear deliverables and products that solve industry issues and are driven by a well-defined yet dynamic plan for executing on deliverables; a strategy of delivering prototype products early and often; defined customers and users, with "industry pull" ensured by an Industry Council with members from the nuclear energy and M&S communities; regular engagement with all levels of the U.S. Nuclear Regulatory Commission (NRC), from the research branch to the Commissioners; peer (equal) private-public partnership in management, leadership, and execution under one "virtual" roof; a lead institution (ORNL) with resource allocation authority and responsibility; an independent Science Council to review and advise on quality and relevance of its science and technology (S&T); and a Board of Directors providing oversight and advice on management, plan, and S&T strategy.

After giving a brief overview of CASL's vision, mission, strategic goals, and current status, the challenges, lessons learned, and best practices encountered during CASL's execution to date will be discussed, with illustrative examples given where possible.

CASL: The Consortium for Advanced Simulation of Light Water Reactors

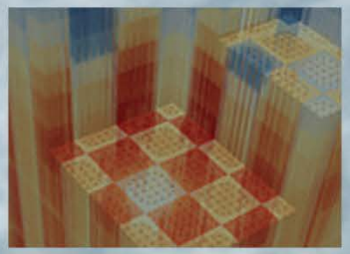
A DOE Energy Innovation Hub

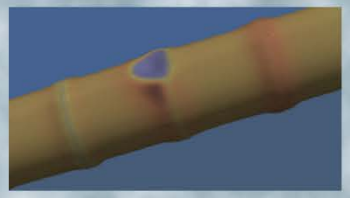
Doug Kothe (ORNL)

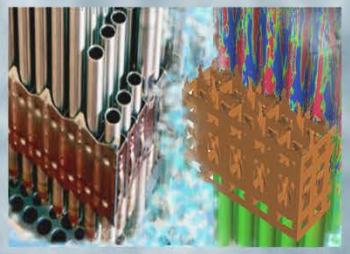
CASL Director

Jess Gehin (ORNL)

CASL Physics Integration Focus Area Lead







U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

CASL-U-2015-0199-000

CASL was the first DOE Innovation Hub

A Different Approach

- "Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges" – *Steven Chu*
- "Create a research atmosphere with a fierce sense of urgency to deliver solutions." – *Kristina Johnson*
- Characteristics
  - Leadership – Outstanding, independent, scientific leadership
  - Management – "Light" federal touch
  - Focus – Deliver technologies that can change the U.S. "energy game"

Core partners

Oak Ridge National Laboratory

Electric Power Research Institute

Idaho National Laboratory

Los Alamos National Laboratory

Massachusetts Institute of Technology

North Carolina State University

Sandia National Laboratories

Tennessee Valley Authority

University of Michigan

Westinghouse Electric Company

Contributing Partners

ASCOMP GmbH

CD-adapco

City College of New York

Florida State University

Imperial College London

Rensselaer Polytechnic Institute

Texas A&M University

Pennsylvania State University

University of Florida

University of Wisconsin

University of Notre Dame

Anatech Corporation

Core Physics Inc.

G S Nuclear Consulting, LLC

University of Texas at Austin

University of Texas at Dallas

University of Tennessee – Knoxville

Pacific Northwest National Laboratory

CASL Background

- What is CASL doing?
  - *Create* an advanced coupled multi-physics "virtual reactor" technology by adapting existing and developing new modeling and simulation (M&S) tools
  - *Effectively apply* the virtual reactor technology to provide more understanding of safety margins while addressing selected operational and design challenges of operational light water reactors
- Why?
  - Improve the performance and energy output of existing nuclear reactors by focusing on important industry defined challenge problems
  - M&S technology has long been a mainstay in the nuclear industry (vendors, owner/operators), helping to inform consequential operational and safety decisions codes daily. Current nuclear industry M&S technology, though continuously improved, has failed to capitalize on the benefits that more precise predictive capability and fundamental understanding offer (from leader to follower)
- Why do this in the Hub R&D business model?
  - Solution requires clear deliverables & products promoted by Hub R&D approach ("fierce sense of urgency")
  - Public-private partnership essential for adaptation, application, and "useful and usable" deployment of advanced M&S technologies under development at DOE national labs and universities to nuclear enterprise
- What is working?
  - Several elements have proven effective: partnerships, industry pull, technology deployment, clear deliverables and plans, effective and agile project management, 5-year time horizon, S&T guidance/review

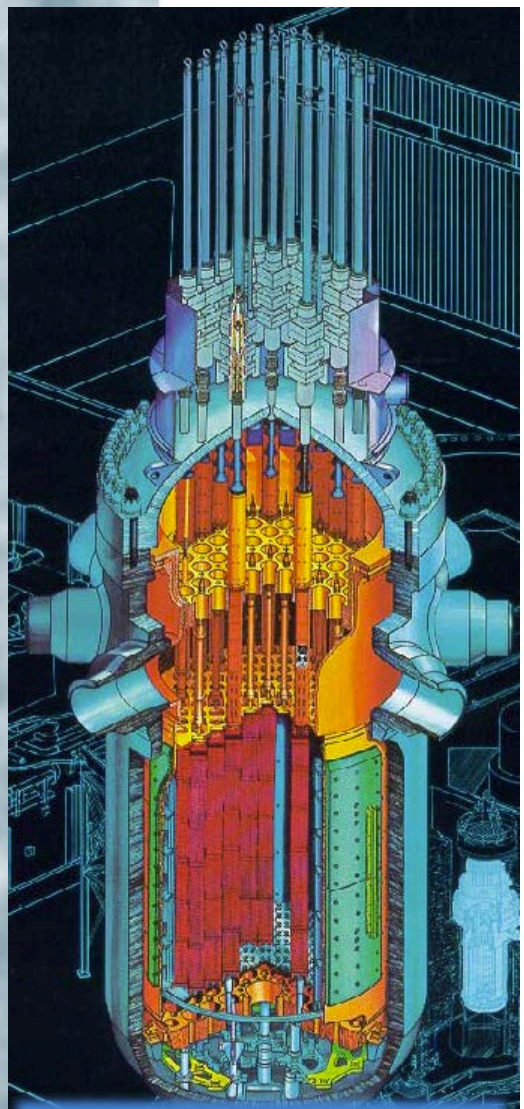
Strong Dependency on Modeling and Simulation

Need to assure nuclear safety but limited by inability to perform full-scale experimental mockups due to cost, safety & feasibility [1% power derating translates to $(5-10)M annual loss of revenue for 1 GWe unit]

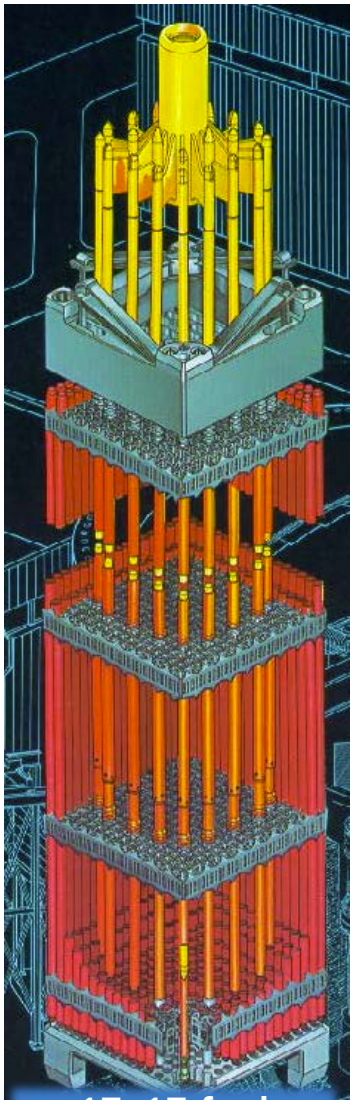
Need to minimize economic uncertainty associated with new product introduction (e.g. fuel) by employing precise predictions [1% error in core reactivity has $4M annual fuel cycle cost impact for 1 GWe unit]

Anatomy of a Nuclear Reactor

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)



reactor vessel and internals



17x17 fuel assembly

Core
- 11.1' diameter x 12' high
- 193 fuel assemblies
- 107.7 tons of UO_2 (~3-5% U_{235})

Fuel Assemblies
- 17x17 pin lattice (14.3 mm pitch)
- 204 pins per assembly

Fuel Pins
- ~300-400 pellets stacked within 12' high x 0.61 mm thick Zr-4 cladding tube

Fuel Pellets
- 9.29 mm diameter x ~10.0 mm high

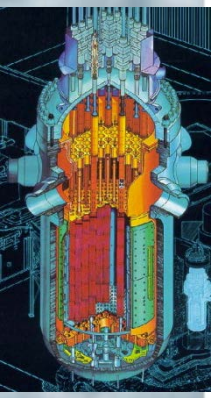
Fuel Temperatures
- 4140° F (max centerline)
- 657° F (max clad surface)

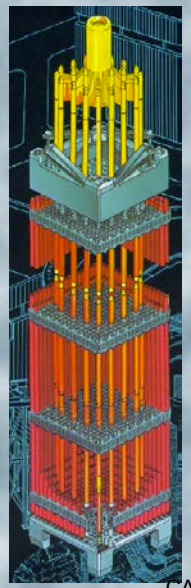
~51,000 fuel pins and over 16M fuel pellets in the core of a PWR!

Nuclear Energy Industry Dependencies and Capabilities in Modeling and Simulation (M&S)

- Why strong dependency on M&S?
  - Need to assure nuclear safety but limited by inability to perform full-scale experimental mockups due to cost, safety & feasibility [*1% power derating translates to $(5-10)M annual lose of revenue for 1,000 MWe unit*]
  - Need to minimize economic uncertainty associated with new product introduction (e.g. fuel) by employing precise predictions. [*1% error in core reactivity has $4M annual fuel cycle cost impact for 1,000 MWe unit*]
- From Leader to Follower in M&S!
  - Through *70s and 80s*, nuclear energy industry relied heavily on High Performance Computing (HPC) - such as CDCs & CRAYs - where most codes used today had their origins
  - From *90s on*, weak nuclear energy market & regulatory hurdle deterred continued investment in HPC & associated code development, so industry shifted from HPC to PC as PCs of 90s & beyond acquired computational power of earlier HPCs.
  - Industry codes used today, though continuously improved, have failed to capitalize on the benefits that more precise predictive capability & fundamental understanding offer, made possible by M&S on HPCs.

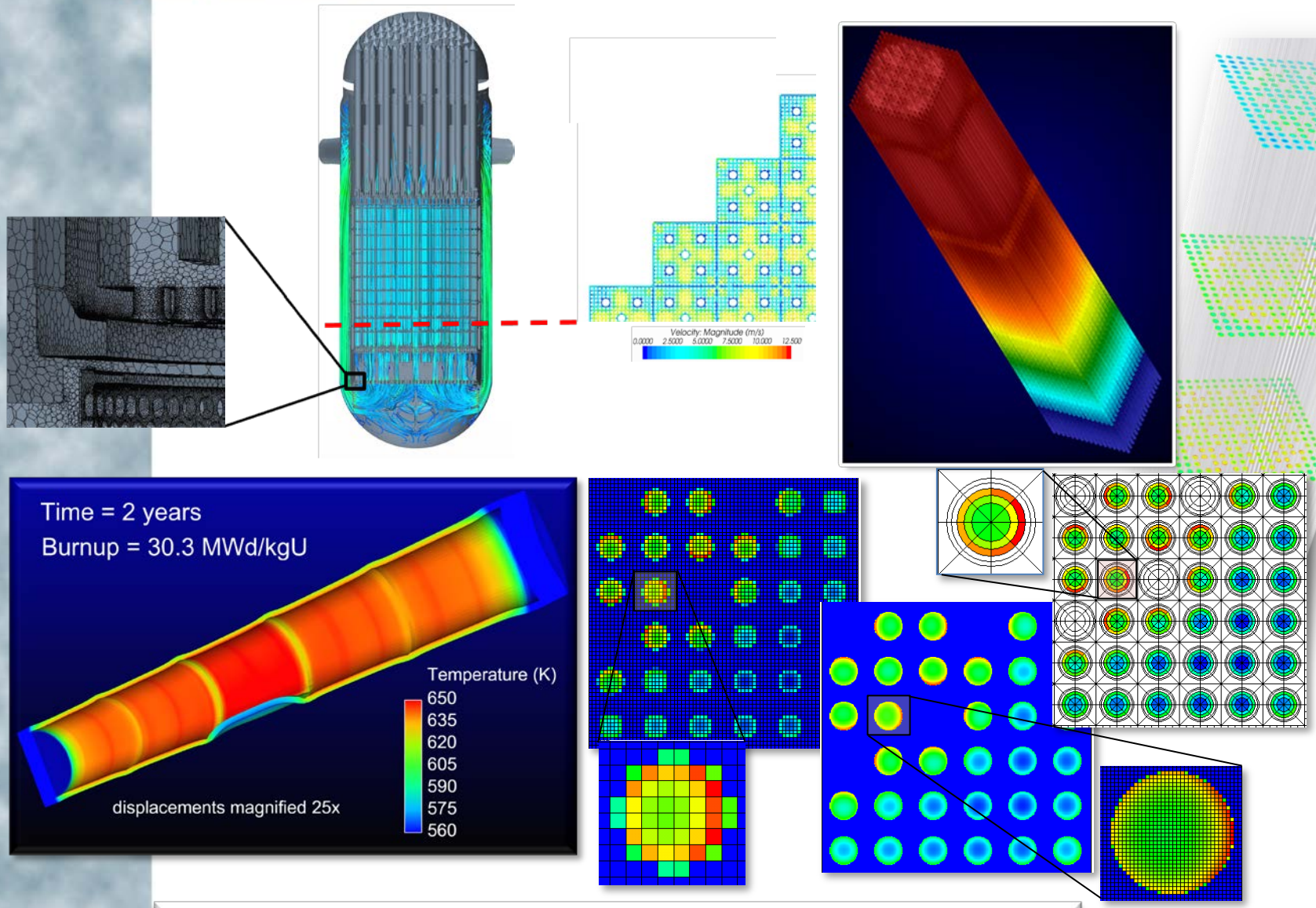
Nuclear Energy Drivers and Payoffs for M&S technology





- Extend licenses of existing fleet (to 60 years and beyond)
  - Understand material degradation to reduce inspection & replacements
- Up-rate power of existing fleet (strive for another 5-10 GWe)
  - Address power-limiting operational & design basis accident scenarios
- Inform flexible nuclear power plant operations
  - Load follow maneuvering & coolant chemistry to enhance reliability
- Design and deploy accident tolerant fuel (integrity of cladding)
  - Concept refinement, test planning, assessment of safety margins
- Margin quantification, recovery, tradeoff
  - Plant parameters, fuel hardware, reload flexibility, regulatory changes
- Resolve advanced reactor design & regulatory challenges
  - Support Gen III+ reactors under construction (AP1000), refine SMR designs
- Fuel cycle cost savings
  - More economical core loadings and fuel designs
- Used fuel disposition
  - Inform spent fuel pools, interim storage, and repository decisions

CASL Tackles the Multi-Scale Challenge of Predictively Simulating a Reactor Core

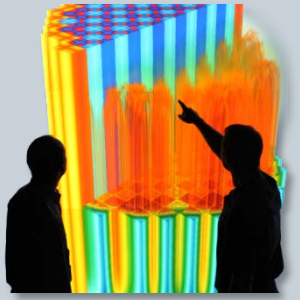


From full core to fuel assembly to fuel subassembly to fuel pin/pellet

CASL's Charter

Provide leading-edge M&S capabilities to improve the performance of operating LWRs

Vision	*Predict, with confidence, the performance and assured safety of nuclear reactors, through comprehensive, science-based M&S technology deployed and applied broadly by the U.S. nuclear energy industry*
Goals	• Develop and effectively apply modern virtual reactor technology • Provide more understanding of safety margins while addressing operational and design challenges • Engage the nuclear energy community through M&S • Deploy new partnership and collaboration paradigms
Strategies	• Virtual Environment for Reactor Applications (VERA) • Industry Challenge Problems • Technology Delivery • Targeted, Enabling R&D • Education and Training • Collaboration and Ideation



Scope

- Address, through new insights afforded by advanced M&S technology, key nuclear energy industry challenges
  - ✓ Economic operation
  - ✓ Higher fuel burnup
  - ✓ Lifetime extension

  while providing higher confidence in enhanced nuclear safety
- Focus on performance of pressurized water reactor core, vessel, and in-vessel components to provide greatest impact within 5 years

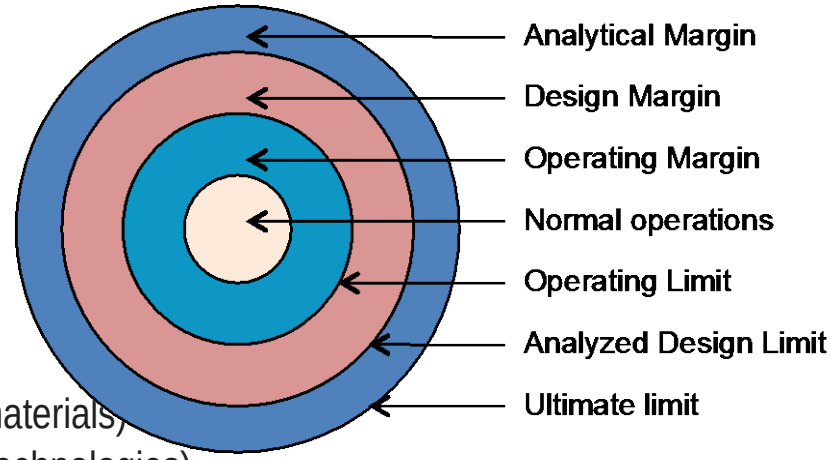
CASL Components

US team with a remarkable set of assets – Address tough industry challenges that matter – Urgent and compelling plan

Collaborate creatively – Target and foster innovation - Deliver industry solutions with predictive simulation

Margin Management

Source: Sumit Ray (Westinghouse)

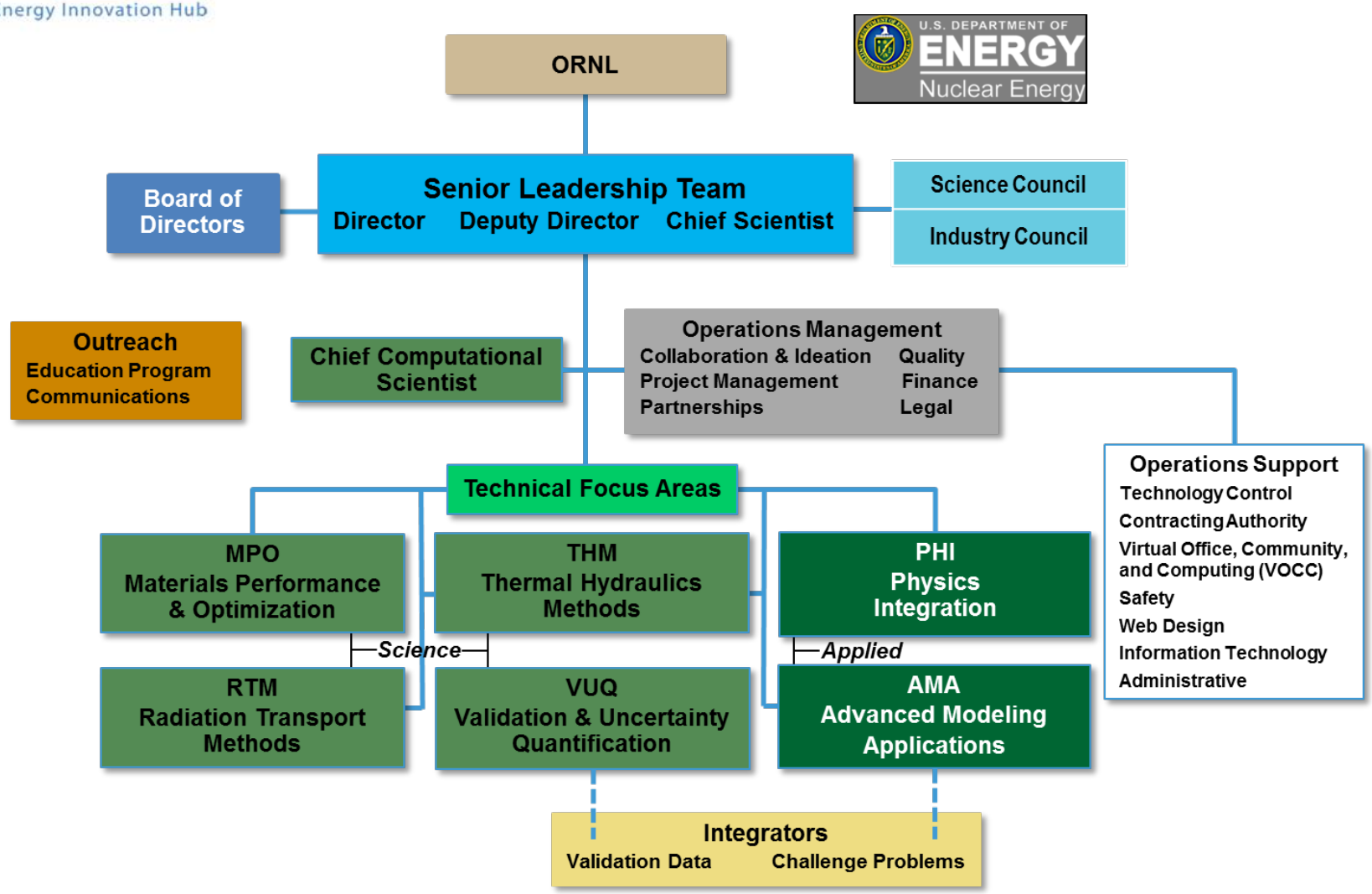


- Requires a strategic approach
  - How much is needed? How to allocate?
  - How can margin be transferred from one bucket to another?
- Key considerations
  - Plant operating parameters & assumptions (plant optimization & flexibility, load follow)
  - Fuel hardware (advanced product features & materials)
  - Design software and methodology (advanced technologies)
  - Core monitoring, In-core fuel management
  - Margins for the unknown or uncertain
  - Reload flexibility
  - Regulatory changes
- Margins can be "recovered"
  - Change in design or operation or testing, reduced safety factor
  - Reduced calculational conservatism (possibly employing advanced analytic tools)
  - Changes to design characteristics of a limiting variable
  - Decrease in the margin of one parameter to increase the margin in another
  - Modification of system or component

Margin trade-offs and evaluation of risks require involvement of many stakeholders within the Utility (Fuels and Plant Operations) and suppliers (BOP, NSSS, T/G, etc.)

One of the strategic targets for the CASL VERA toolkit is to provide enhanced insights in the area of critical reactor margins

CASL Organization



Basic structure unchanged since 2010 yet able to evolve as needed

- Addition of Product Integrators proven useful in driving critical applications, products, & outcomes that cross Focus Area boundaries

Oak Ridge National Laboratory
Thom Mason, Laboratory Director
Nuclear Science and Engineering Directorate
Alan Icenhour, Associate Laboratory Director

Science Council
Bill Oberkampf, Chair

Industry Council
Dennis Hussey, Chair

Director
Doug Kothe
Deputy Director Doug Burns
Chief Scientist Paul Turinsky

Board of Directors
Dale Klein, Chair

Outreach
Education Program Director
Mike Doster
Communications Coordinator
Mark Uhran

Chief Computational Scientist
John Turner

Operations Management

Collaboration & Ideation
April Lewis
Quality
Matt Sieger
Partnerships
Jeff Cornett
Project Management
Jeff Banta
Finance
Victoria Shope
Legal
Jud Hightower

Technical Focus Areas

Materials Performance & Optimization
Lead Chris Stanek
Deputy Brian Wirth

Validation & Uncertainty Quantification
Lead Vince Mousseau
Deputy Brian Williams

Advanced Modeling Applications
Lead Zeses Karoutas
Deputy Steve Hess
Deputy Rose Montgomery

Radiation Transport Methods
Lead Bill Martin
Deputy Tom Evans

Thermal Hydraulics Methods
Lead Mark Christon
Deputy Emilio Baglietto

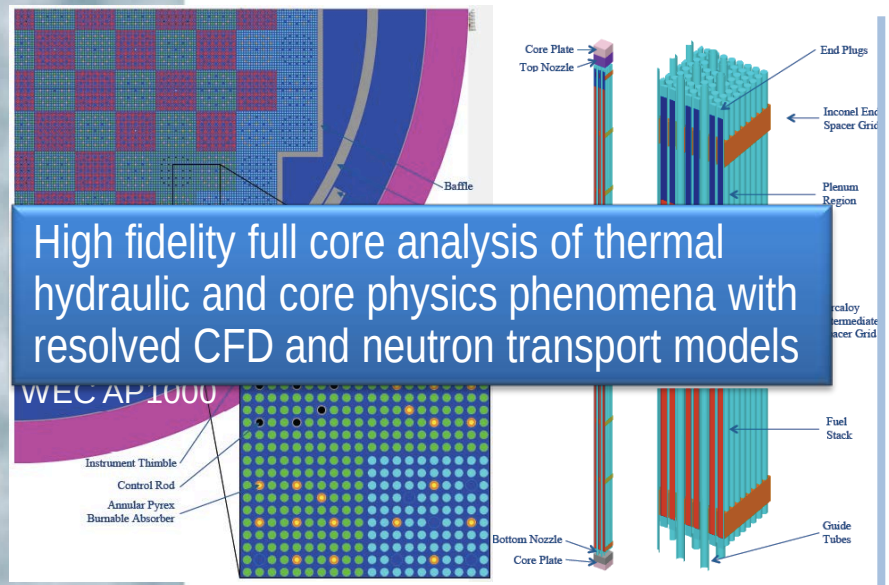
Physics Integration
Lead Jess Gehin
Deputy Scott Palmtag

Operations Support

Technology Control
Sam Howard
Contracting Authority
Jo Ann Fitzpatrick
Justin Keck
Virtual Office, Community, and Computing (VOCC)
Teresa Robison, A.J. Iurelli
Safety Officer
Jeff Banta
Web Design
Cheryl Richardson
Information Technology
Brian Zachary
Administrative
Linda Weltman

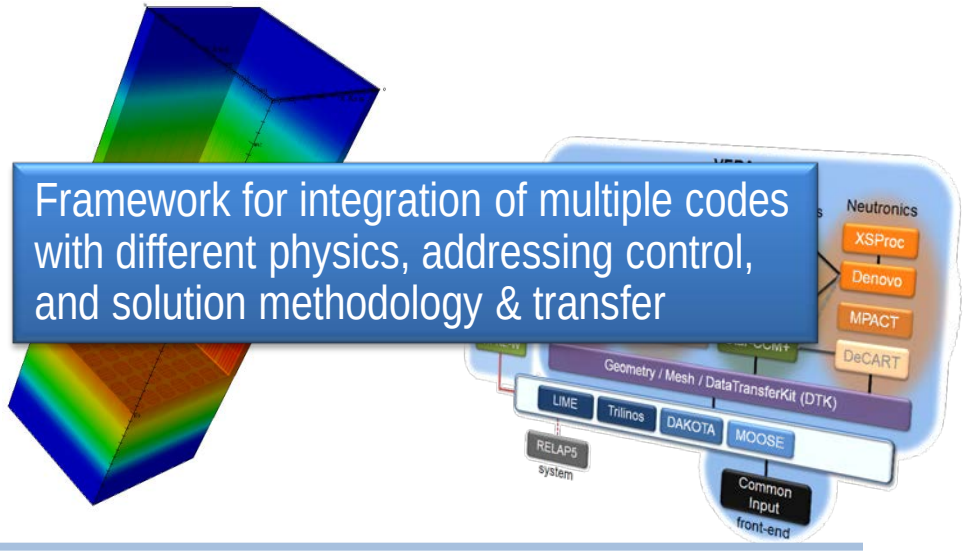
CASL Innovations

Advanced Modeling Applications



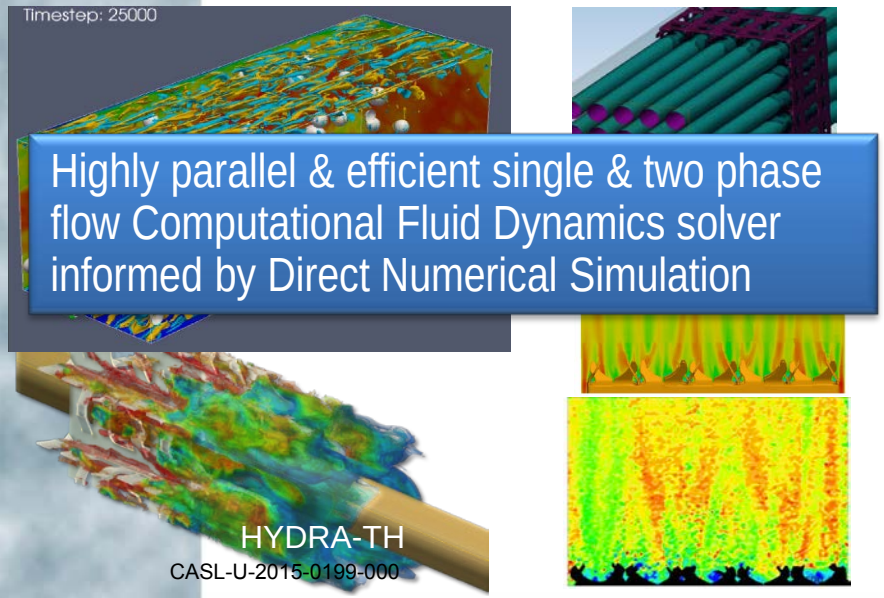
High fidelity full core analysis of thermal hydraulic and core physics phenomena with resolved CFD and neutron transport models

Physics Integration



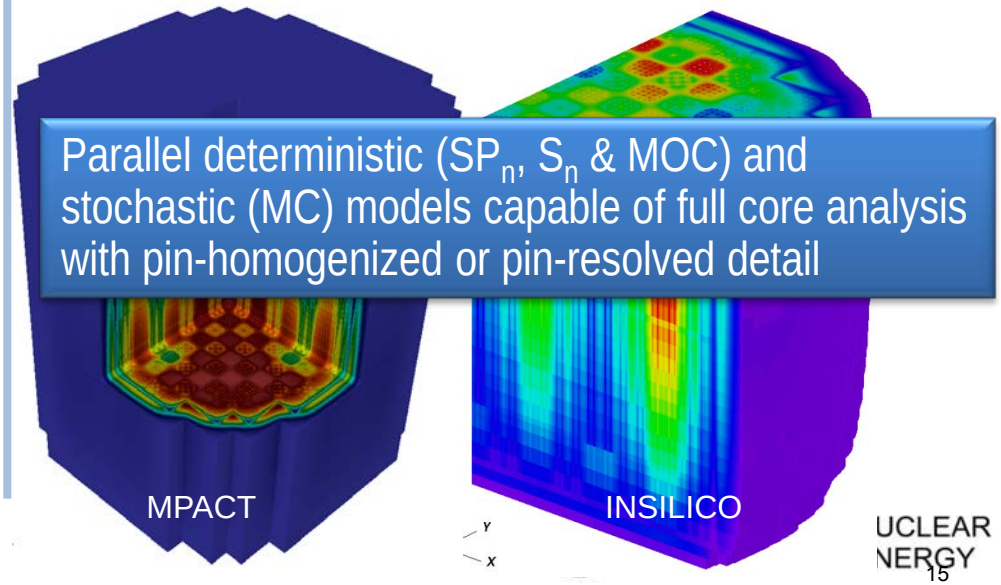
Framework for integration of multiple codes with different physics, addressing control, and solution methodology & transfer

Thermal Hydraulic Methods



Highly parallel & efficient single & two phase flow Computational Fluid Dynamics solver informed by Direct Numerical Simulation

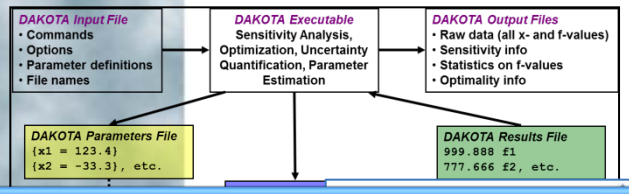
Radiation Transport Methods



Parallel deterministic (SP_n, S_n & MOC) and stochastic (MC) models capable of full core analysis with pin-homogenized or pin-resolved detail

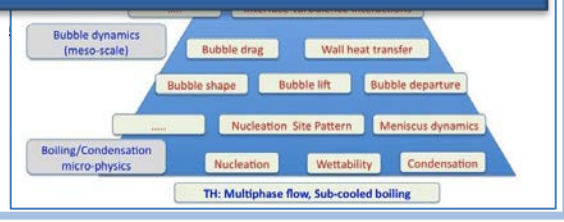
CASL Innovations

Validation & Uncertainty Quantification

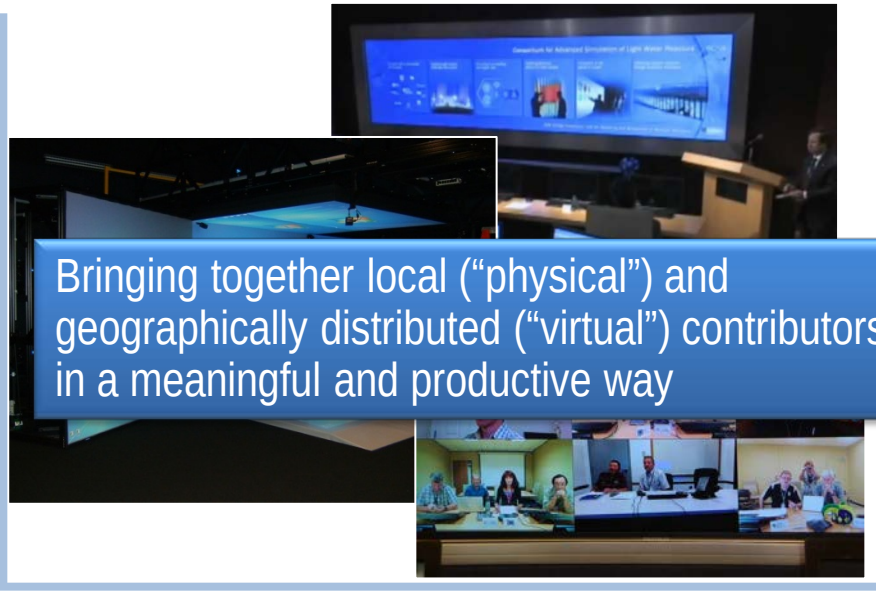


Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows

DAKOTA



VOCC

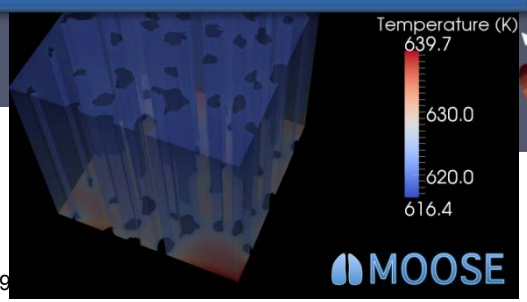


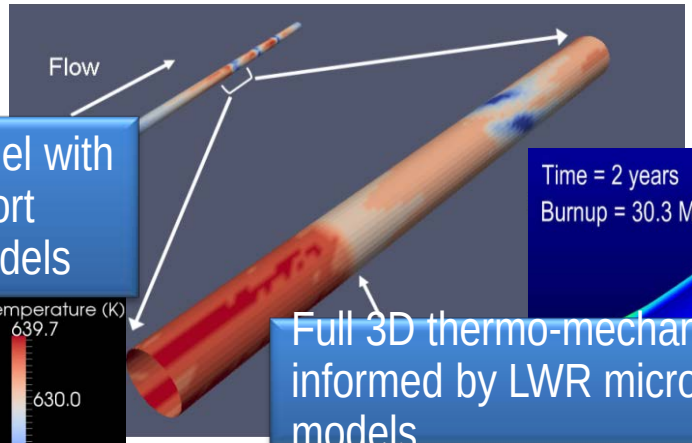
Bringing together local ("physical") and geographically distributed ("virtual") contributors in a meaningful and productive way

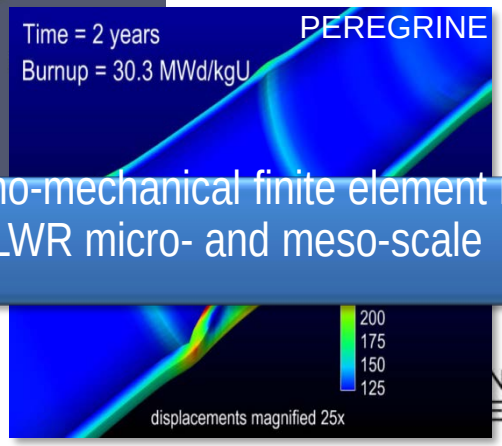
Materials Performance and Optimization

MAMBA

CRUD growth and boron retention model with enhanced thermodynamics and transport treatments informed by micro-scale models

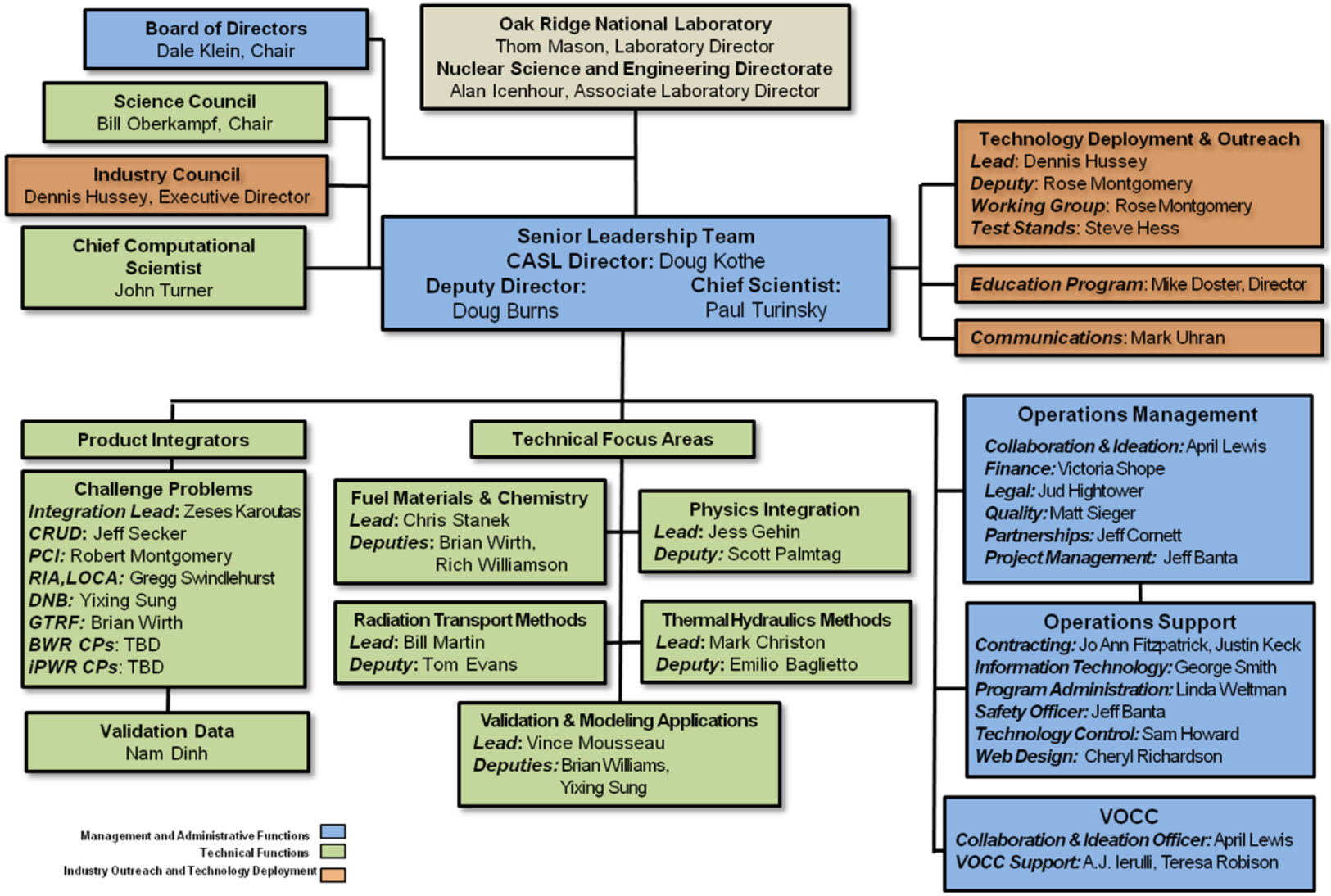






Full 3D thermo-mechanical finite element model informed by LWR micro- and meso-scale models

We Continue to Evolve our Structure



Key Elements of our Approach
Proving Effective

- ✓ *Clear deliverables that solve industry issues and are driven by a well-defined yet dynamic plan*
  - Commit to a hierarchical milestone plan with tangible deliverables; define products integrated across capabilities
- ✓ *A strategy of delivering prototype products early and often*
  - Early deployment of Hub's technology (VERA) into industrial environment for rapid and enhanced testing, use, and ultimate adoption to support real-world LWR applications
- ✓ *Defined customers and users, with "industry pull" ensured by an industry council*
  - Charter and engage Industry Council (IC) for early, continuous, and frequent interface and engagement of end-users and technology providers. Use the IC for critical review of CASL plans and products – want products to be "ours"
- ✓ *A true private-public partnership in management, leadership, and execution*
  - Engage the nuclear industry broadly (vendors, owners/operators, R&D) and at all levels of execution. Involve the best and brightest crucial for success & credibility using virtual collaboration technologies for daily interactions
- ✓ *A 5-year horizon for completion and funding with a renewal option for second 5 years*
  - 5-year period a must to attract and retain community leaders yet upon execution forces specific paths and decisions
- ✓ *Led by one institution with resource allocation authority and responsibility*
  - Not easy nor a guarantee of success but enables agility while assignment of clear authority and responsibility
  - DOE empowers lead institution and Hub leadership ("light federal touch") as long as execution and performance warrants
- ✓ *BOD providing oversight and advice on management, plan, and science & technology (S&T) strategy*
  - Not a useful body unless Hub leadership knows how to effectively utilize it; guidance of CASL BOD has been immeasurable
- ✓ *Independent councils to review and advise on quality and relevance of S&T*
  - Science Council - independent assessment of whether the scientific work planned and executed is of high quality and supports attaining CASL goals – motivates CASL leadership to more directly address problems with needed decisions

From CASL's SEAB presentation (Dec 2013)

Challenges Faced by CASL

Most overcome; some still work in progress

- Capability versus Product (balancing long- and short-term R&D)
  - Challenge Problem & Core Simulator Integrators established to drive products development
- Federal Program Integration
  - Utilizing capabilities developed elsewhere while learning how to best collaborate and leverage university supported R&D
- Program Management (planning, execution, tracking, review)
  - Virtual collaboration, S&T Councils, Board of Directors, institutionally-differing views of milestone-based program mngmt
- Metrics
  - Performance (technology-management-innovation) and outcome (strategic goal) metrics sufficient to measure performance
- Partnerships and IP Management
  - Critical work that starts pre-execution and is ongoing; includes licensing and derivative works
- Technology Deployment
  - Protecting IP and Export Controlled information, in-consortium Test Stands, external releases, CASL end state
- Supporting M&S Infrastructure
  - Ensuring adequate hardware, software, networking, visualization, data science/analytics, and IT staff is available to support R&D:
- Financial Management (budgeting, contracts, costing, etc.)
  - Resource allocation & adjustment; subcontracts (minimizing overhead); costs, invoicing, & spend projections; following formal process, satisfying partners' funding expectations (while satisfying technical development needs)
- Outreach and Communication
  - Communications planning & coordination; targeting diverse audience; publishing science output; recognizing innovative achievements

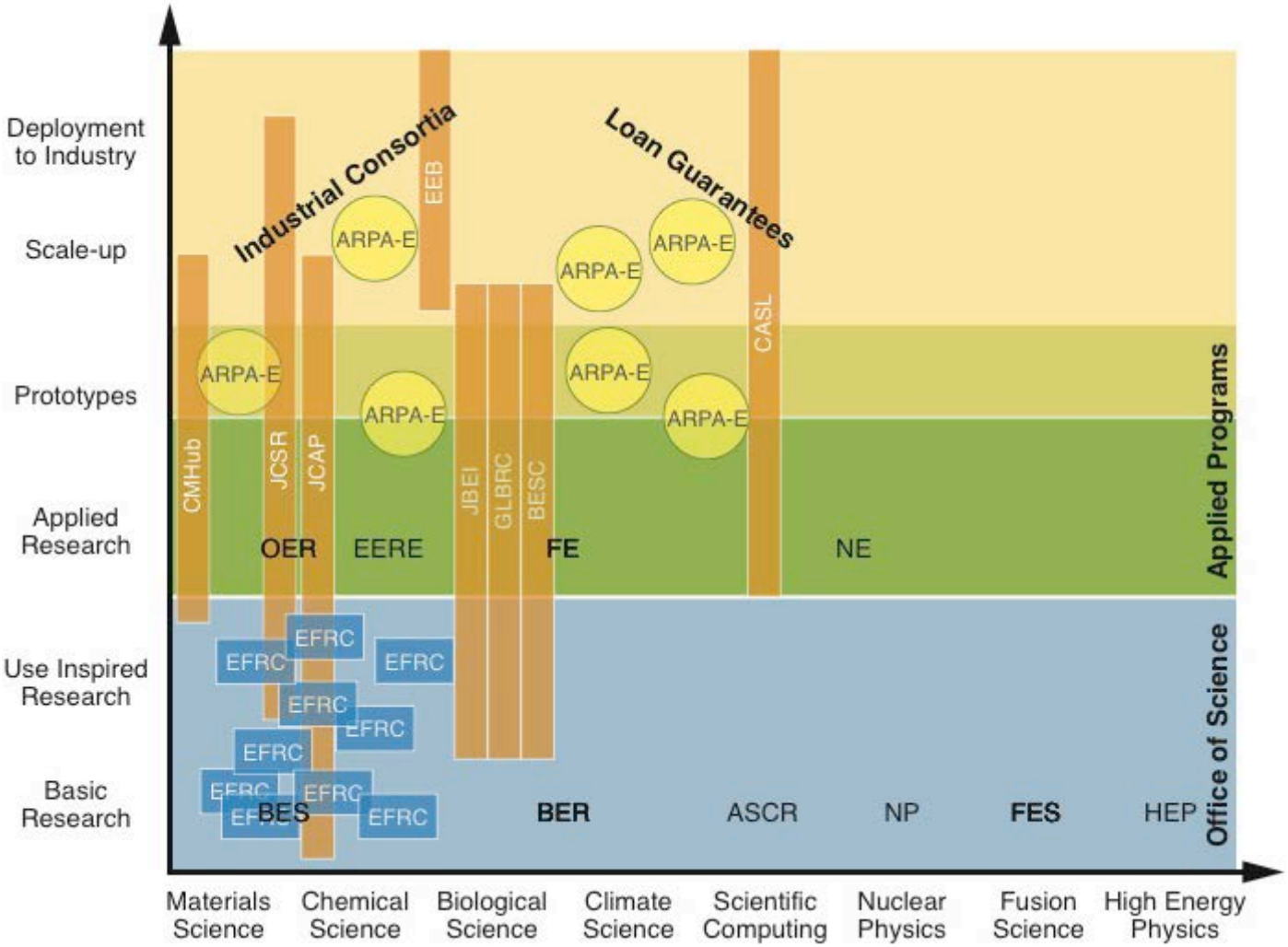
From CASL's SEAB presentation (Dec 2013)

SEAB Hubs+ Task Force Report
Selected comments, findings, recommendations

- Hubs meant to advance highly promising areas of energy science and technology from their early stages of research to the point that the risk level will be low enough for industry to commercialize the technologies. Characteristics:
  - A lead institution with strong scientific leadership;
  - A central location;
  - If geographically distributed, state-of-the-art technology for long distance collaboration;
  - A strong organization and management plan to effect goals.
- Hubs provide an excellent construct for resolving major technological and science roadblocks in order to deliver advances at the system level
- Hubs are large cross-disciplinary consortia of universities, national labs, and industry, with the objective to integrate concepts from basic science through concept prototyping or technology transfer, and to incorporate feedback from technological need and practical application to basic science
- Hubs should be accompanied by strong project management and a “stage gate” review process to ensure that the programs are making progress toward the stated goal
- For larger constructs such as Hubs, performance milestones should be established and subject to an annual review with a rebaselining procedure in close consultation between DOE and construct senior management where appropriate

Report released in Mar 2014

SEAB Hubs+ Task Force Report
Summary of Hub findings and recommendations



CASL believes it also reaches into use-inspired and basic research

Hubs+ Task Force Questions

Summary of responses from a CASL perspective

Question	CASL Perspective
What is unique about the hub funding model that has the potential to accelerate energy science and technology, and why they are important and what is necessary to make them successful?	• Clear deliverables, targeted customers/users, translational RD&D, multidisciplinary team, urgency
Interested in the hubs which have a mission and are a method of managing and funding research and development of energy technologies that span science and engineering	• CASL continues to focus and refine its charter as guided by direct input and review from DOE and its Board and Councils for Science and Industry • Five year commitment & ability to shift funding as viewed appropriate by subject matter experts assures resources allocated where needed. • See CASL Program & Management Plans, Plans of Record, Milestones
How are the participants/program/outcomes of their specific hub different from that of the regular DOE base programs? How has the whole become bigger than the sum of the parts? Is there overlap with base or ARPA-E programs and how is that managed?	• CASL has a well defined, focused mission that drives moving S&T from R&D to applications • Technical plans devised and outcomes delivered based on direct line of sight to Hub strategic goals that span multiple science & engineering domains • Impose metrics, e.g., industry pull, sense of urgency, technology deployment • Failure if outcome a collection of unrelated and independent codes & papers • Ability to build a one-team culture made up of partners from labs, industry, and universities
Is there any sharing of lessons learned between different hubs?	• A continuously updated set of CASL best practices & lessons learned can aid and apply to other R&D programs aiming to be translational and timely • Yes – regular teleconference and an annual meeting specifically chartered for sharing lessons learned and best practices between Hubs have proven useful • Hub coordination & collaboration initially organic but evolving with DOE help
How is each hub dealing with the culture change of inter-disciplinary, inter-institutional, cross fundamental-applied, cross sector collaborations?	• Culture clash a challenge to manage but critical for success – use Board! • Constant and open communication & understanding each partners goals and objectives a must. Requires daily nurturing for constructive cohesion. • Set expectations early and often. Drive culture change from leadership

Industry Role and Impact in CASL

Industry Council: Assure that CASL solutions are "used and useful" by industry and that CASL provides effective leadership advancing the M&S state-of-the-art.

Industry Council Objectives and Strategies

- Early, continuous, and frequent interface and engagement of end-users and technology providers
- Critical review of CASL plans and products
- Deployment and applications of periodic VERA releases
- Identification of strategic collaborations between industry and CASL for access to data and technical information, testing and evaluation, regulatory interface, or targeted RD&D

Outcomes and Impact

- Industrial technology-providers and end-users benefit by influencing VERA and its development process to be compatible with expected applications
- They also prepare their business and technical processes to make early use of CASL products

Industry Council Members

Owner/ Operators of Nuclear Plants	Fuel and/or SMR Vendors	Engineering Design, Service Providers, R&D	Independent Software Vendor	Computer Technology Companies	Ex-Officio
Dominion	AREVA	Battelle	ANSYS	Cray	BOD
Duke Energy	GNF	Bettis /NNPP	CD-adapco	IBM	DOE
EDF	mPower	EPRI	GSE Systems	NVIDIA	
Exelon	NuScale	Rolls Royce			
TVA	WEC	Studsvik Scandpower			

CASL Core Industry Partners Represent 3 Pillars of Nuclear Industry

- EPRI: *R&D arm* of industry as driven by near-term utility (owner/operator) needs
  - Power uprates, license extensions, new fuel designs
- TVA: *owner/operator* of 6 nuclear reactors – also brings operational reactor data for validation
  - Address power-limiting operating scenarios
- Westinghouse: *vendor* - designer and seller of commercial fuel and integrated reactor designs
  - Enhanced insights in critical reactor margins

CASL Board of Directors (BOD)
Charter

- Function
  - An advisory and oversight body for the ORNL Laboratory Director and the CASL Senior Leadership Team (SLT) on issues related to management, performance, strategic direction, and institutional interfaces within CASL; Any decisions by the BOD are made by consensus
- Charter
  - Advise the ORNL Laboratory Director on selected matters of CASL scope, schedule, budget, performance, and strategic direction
  - Advise the CASL SLT on changes to the composition of CASL partners
  - Advise the CASL SLT on strategic direction and annual performance goals; evaluate performance of the SLT on an annual or as-needed basis
  - Help the CASL SLT in participating in and overseeing the activities of the CASL Science and Industry Councils
  - Review and advise on annual project and budget plans and budget allocation changes in excess of $2M to CASL partners on an as–needed basis
  - Support the CASL and ORNL SLT in managing effective interfaces with key stakeholders, transitional and applied R&D, technology transfer, and commercialization
  - Assist in and helps foster CASL partner organization interrelationships on an as-needed basis

- CASL BOD met Sep 2013 (DC), Jan 2014 (Austin, TX), and May 2014 (virtual) and conducted 6 monthly teleconferences over past year
- CASL SLT engaged BOD members actively this past year on Phase 2 strategies and scope: set up a “Red Team” for formal review of the Renewal Proposal
- CASL Director seeks and receives 1-on-1 feedback regularly with many BOD members

CASL BOD Membership

Board Member	Affiliation	Role
Dale Klein (Chair)	University of Texas System	Chair
Alan Bishop	Los Alamos National Laboratory	Founding Partner
James J. Duderstadt	University of Michigan	At Large
Christine King	Electric Power Research Institute	Founding Partner
Phillip Finck	Idaho National Laboratory	Founding Partner
Ron Gilgenbach	University of Michigan	Founding Partner
Joseph Hoagland	Tennessee Valley Authority	Founding Partner
Hon. J. Bennett Johnston, Jr.	U. S. Senator, Louisiana (1972–1997)	At Large
Mujid Kazimi	Massachusetts Institute of Technology	Founding Partner
Terri Lomax	North Carolina State University	Founding Partner
Peter Davies	Sandia National Laboratories	Founding Partner
Sumit Ray	Westinghouse Electric Company	Founding Partner
Jim Roberto	Oak Ridge National Laboratory	Founding Partner
Tom D' Agostino	Fluor Corporation	At Large

- A diverse, distinguished, and committed group actively engaged and working to identify and address CASL challenges and issues
- Membership changes and additions this past year (since Aug 2013)
  - Christine King for Kurt Edsinger (EPRI)
  - New At-Large member Tom D'Agostino (Fluor Corporation, former head of DOE NNSA)
- BOD membership has been very stable since 2010
  - One representative per Founding Partner plus 4 At-Large (one being Chair)

BOD Strategy Subcommittee

Helped to define Phase 2 scope selection process

- Who are our customers, and what are their needs?
  - *Industry (Particularly nuclear utilities)?*
  - *Government (NRC, DOE)?*
  - *Universities?*
- What is the value proposition moving forward?
  - *Cost reduction?*
  - *Assuring continued nuclear safety?*
  - *Creation and dissemination of engineering physics and computational science understanding?*
- Should there be any change in vision or mission from the first five-year plan?
- What should be the scope, emphasis, and balance of the next five-year plan?
  - *Finish all Phase 1 goals and push for deployment?*
  - *Modest extensions (e.g., Gen III PWR, BWR)?*
  - *Stretch goals (e.g., SMRs, plant level, fuel cycles, severe accident analysis)?*
- What competency development should be stressed in Phase 2?
- What process should be used to develop the detailed proposal?
- What support does CASL need to develop a successful proposal?
- What effort should be devoted to sunset planning?

Answers documented in CASL Program Plan

Science Council
Membership

- William Oberkampf, Sandia (retired) (Chair) [Area: VUQ: FA: VUQ]
- Richard Lahey, RPI (retired) [Area: Thermal-hydraulics|FA: THM]
- Mary Wheeler, UT-Austin [Area: Applied Math|FA: VRI]
- William Weber, UT-K/ORNL [Area: Materials Science|FA: MPO]
- James Tulenko, University of Florida (retired) [Area: Materials Science|FA: MPO]
- Phillip Finck, INL (BOD Representative) [Area: Nuclear R&D|FA: VRI & AMA
- Elmer Lewis, Northwestern University (retired) [Area: Transport Theory |FA: RTM]
- Finis Southworth, Areva [Area: Nuclear R&D|FA: AMA]
- Kord Smith, Massachusetts Institute of Technology [Area: Reactor Core Simulation|FA: PHI & VRI]

Added expertise in commercial core simulator development

Science Council Overview

- Purpose: Independent assessment of S&T capabilities being developed and integrated into VERA

- Modes for Accomplishing:
  - Annual Focus Area Review and Planning Workshops (5 held in FY14)
  - Multiple teleconferences held (whole council and individual members)
  - Annual S&T Capabilities Development Review (whole council)
    - Held in September 2013
    - Next in September 2014
    - Held jointly with the Industry Council

Activities schedule to support continuity of interactions with SC members

Focus Area Review and Planning Workshops Process

- Focus Area Review & Planning Workshops range in duration from 1 to 2 days
- Leads and PIs of Focus Area make presentations (virtual or on-site)
- One or more Science Council members attend and actively participate in each workshop
- Science Council member(s) document observations and recommendations
- Focus Area leads discuss observations and recommendations with Science Council member(s)
- Focus Area leads document response to recommendations and factor into future work scope planning

Workshops have proven effective in obtaining advice from Science Council members'

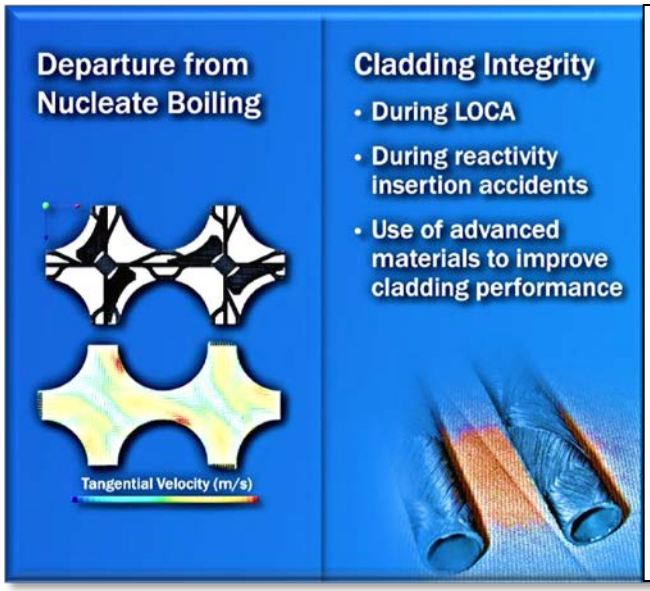
CASL Wide Preliminary Recommendations

1. SC has noted CASL's progress in addressing key issues mentioned in earlier meetings
2. Connections between CASL and industry needs should be further strengthened in Phase 2
3. Division of resources should strive for the following balance over Phase 2
   a. Model & software development (capability) 50%
   b. Demonstration & usage 20%
   c. Assessment of confidence & robustness 30%
4. Definitive agreements on intellectual property and licensing terms need to be reached
5. CASL should reexamine the balances between Focus Areas in view of the overall needs

CASL advises Point 2 will be challenging to address

CASL Challenge Problems

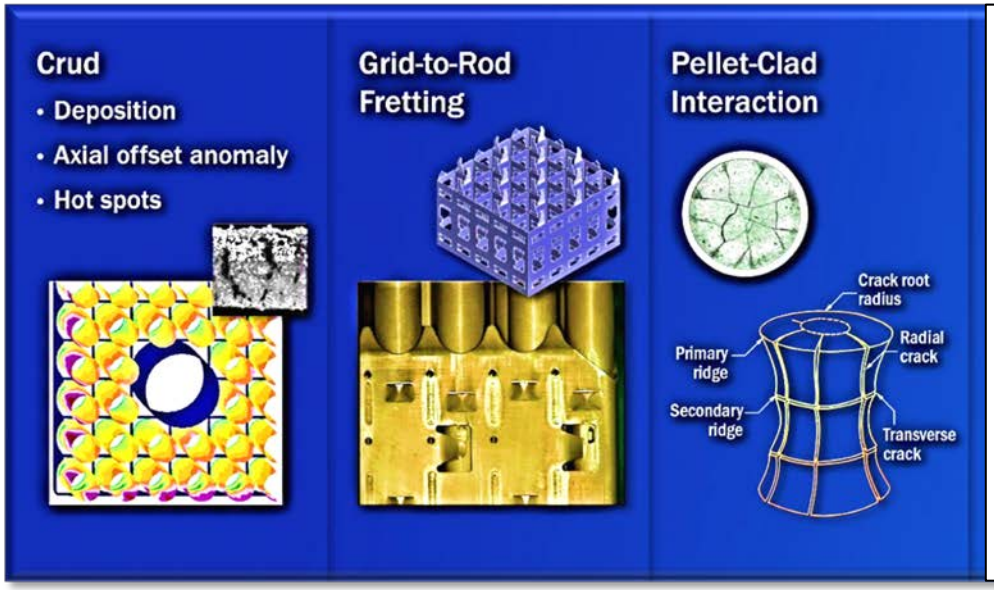
Key safety-relevant reactor phenomena that limit performance



Safety Related Challenge Problems

CASL Challenge Problems

- Are relevant industry problems whose solutions remain elusive
- Are amenable to insight afforded by advanced M&S
- Help to direct RD&D activities on CASL M&S technology
- Help to establish clear performance metrics



Operational Challenge Problems

Choosing the "Right" Challenge Problems

Category		High Rating	Medium Rating	Low Rating
Programmatic	*Leverage Phase 1*	Builds directly on current works, requires incremental R&D scope	Leverages some past work, Substantive R&D work	Start from scratch
	Feasibility	Easily accomplished within planned schedule and budget	Risk associated with schedule and/or budget	Very little assurance in delivering within 5 years & suggested budget
	DOE Synergism	Fits well with other programs without being duplicative	Works moderately well with other programs; some overlap	Does not fit well and/or is duplicative
Industry Impact	*Able to Address Existing Problems*	Provides actionable insight to a current operationally-limiting issue; cost reduction likely	Provides insight to a current industry issue or parameter that is operationally limiting, cost reduction possible	Provides info on past issue, an issue that continues to occur infrequently, or a parameter that is not operationally limiting
	Likelihood of Adoption	Highly likely – in part or as a whole by industry	Moderately likely - will require modification for adoption	Low likelihood for applicability to commercial reactors
	Applicability	Many other applications & reactor designs	Few other applications & may apply to other reactor designs	Limited application & applies to few reactor designs
	Timeliness of Technology RD&D	Leads industry need	Concurrent with industry need	Lags industry need
Science & Engineering Innovation	*Predictive Capability Maturity*	Approach leads to basic understanding with little calibration needed	Approach improves scientific understanding, but some calibration still used	Approach will continue to be highly calibrated, but with some improved methods
	Gap Between R&D & Industry Practice	Game changer relative to current industry methods	Order of magnitude higher fidelity than used by industry	Parallels current industry methods
Institutional Interest	*Alignment with Interests and Competencies*	Aligned	Somewhat Aligned	Not Aligned

Surveyed institutions ranked each proposed Challenge Problem based on specific criteria

Challenge Problem Approach

VERA products and use cases

PCI
- Predict Core Wide PCI Margin with PEREGRINE2D
- Zoom in and Predict MPS PCI leaker with PEREGRINE3D

Rob Montgomery

CRUD
- CIPS: Predict Boron Uptake with MAMBA subgrid model in COBRA-TF
- CILC: Predict Crud thk & corrosion with MAMBA subgrid model in HYDRA-TH

Jeff Secker

Cladding Integrity (RIA)
- Predict PCMI Margin using MPACT and PEREGRINE2D

Gregg Swindlehurst

VERA-CS
Insilico-MPACT/
COBRA-TF/PEREGRINE
(full depletion
for all rods in core)

Scott Palmtag

Cladding Integrity (LOCA)
- Predict PCT – Oxidation Margin using PEREGRINE2D & System Code RELAP5 or W COBRA-TRAC

Gregg Swindlehurst

DNB
- Predict DNB Margin for RIA with MPACT and COBRA-TF
- Predict Mixing & DNB with CFD using STAR/HYDRA-TH

Yixing Sung

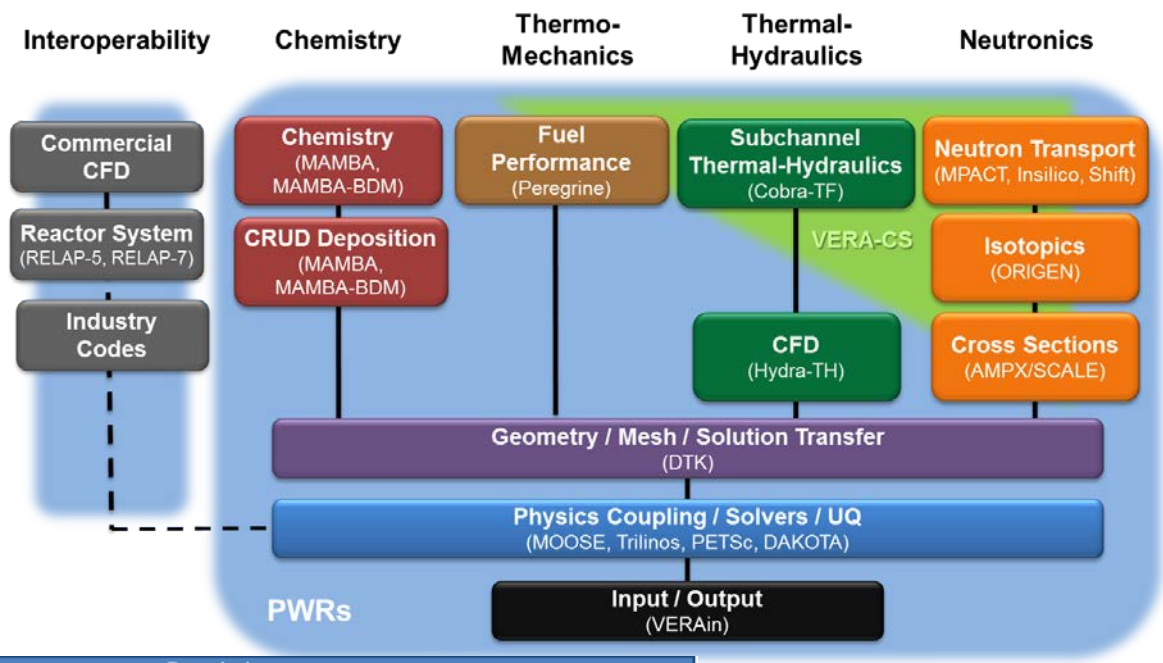
GTRF
- Predict Minimum GTRF Margin in Core using PEREGRINE2D – grid to rod gap, STAR/HYDRA-TH excitation force

Brian Wirth

For each Challenge Problem apply DAKOTA using coupled tools for UQ

CASL's Virtual Environment for Reactor Applications (VERA)

VERA capabilities expected at Phase 1 conclusion (Apr 2015)

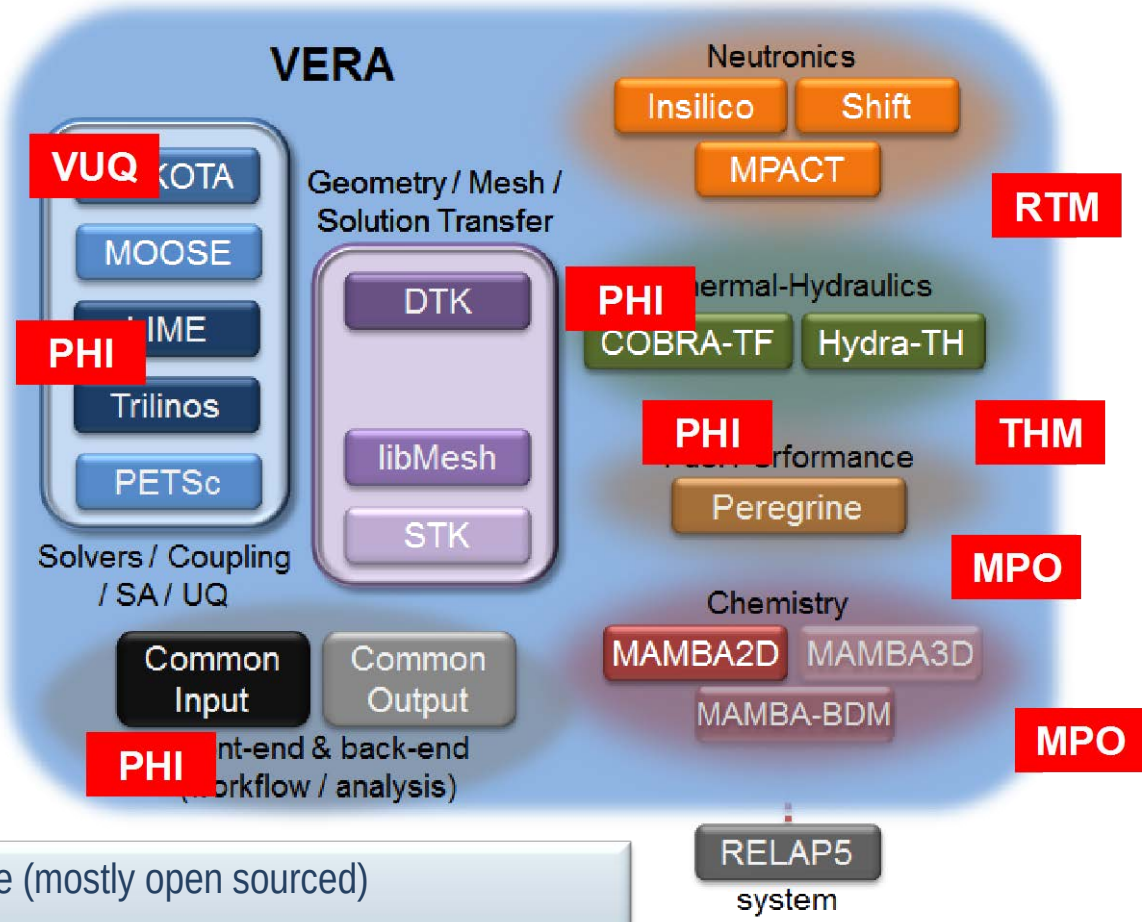


Item	Description
S/W Development Tools and Computational Infrastructure	Standardized set of compilers and configuration tools Git revision control system and S/W repository management Build & test infrastructure (TriBITS, CMake, CTest, CDash) 17 geographically dispersed code repositories, 205 TriBITS packages, 26k files, 8M lines of source code
Infrastructure Components	Trilinos, VERAIn, Common Output, DTK, LIME, DAKOTA, MOOSE, libMesh, PETSc, STK, MOAB, NiCE
Core Simulator Components	COBRA-TF (CTF), SCALE/XSProc, Insilico, MPACT
Other Physics Components	Hydra-TH, Shift, Mamba2D/3D, Peregrine, Drekar
Integrated Industry Components	ANC, VIPRE-W, BOA, VABOC
Interoperable Components	DeCART, Star-CCM+, RELAP5-3D
Coupled Components	ANC+VIPRE-W, ANC+VIPRE-W+BOA, DAKOTA+VIPRE-W, DAKOTA+VIPRE-W+BOA, DAKOTA+CTF, CTF+MAMBA2D, CTF+Insilico, CTF+Insilico+Peregrine (Tiamat), CTF+MPACT
Testing	Continuous Integration (CI), Unit, Regression - 648 tests executed nightly, additional weekly tests
Workflow and Analysis Tools	Paraview, VisIt, EnSight
Active Developers and Users	Approximately 95 developers, geographically dispersed at CASL partner institutions. Approximately 34,000 total commits (modifications) to all source repositories. Over 100 active users of VERA capabilities.

VERA current technology portfolio

VERA Status

Integrates physics components from focus areas



- Mature infrastructure (mostly open sourced)
- Automated testing and growing test base
- Many new coupling developments and implementations
- Rapidly-evolving Core Simulator (VERA-CS)
- 2014 RSICC release (later this CY) will have major functionality upgrades relative to 2013 release

VERA-CS

Painfully easy to measure progress with our "AMA Benchmark Progression Problems"

FY11

- SCALE cross-section processing for DENOVO in VERA ✓
- DENOVO pin cell capability with SCALE in VERA ✓

FY12

- #1 2D HZP Pin Cell ✓
- #2 2D HZP Lattice ✓
- #3 3D HZP Assembly ✓

FY13

- #4 HZP 3x3 Assembly CRD Worth ✓
- **#5 Physical Reactor Zero Power Physics Tests (ZPPT)** ✓
- #6 HFP BOL Assembly (begin Challenge Problem coupling) ✓
- #7 HFP BOC Physical Reactor ✓

FY14

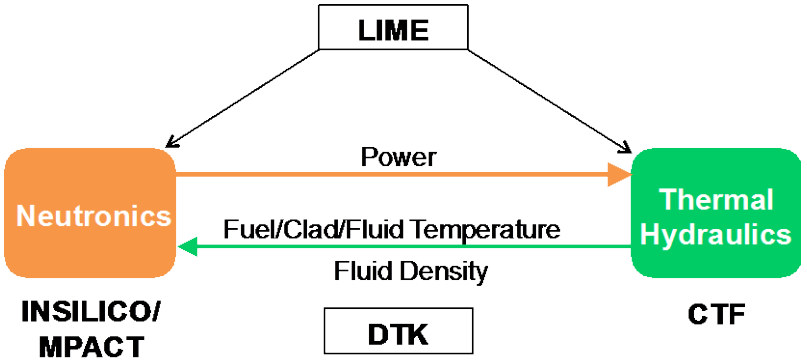
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical Reactor Refueling

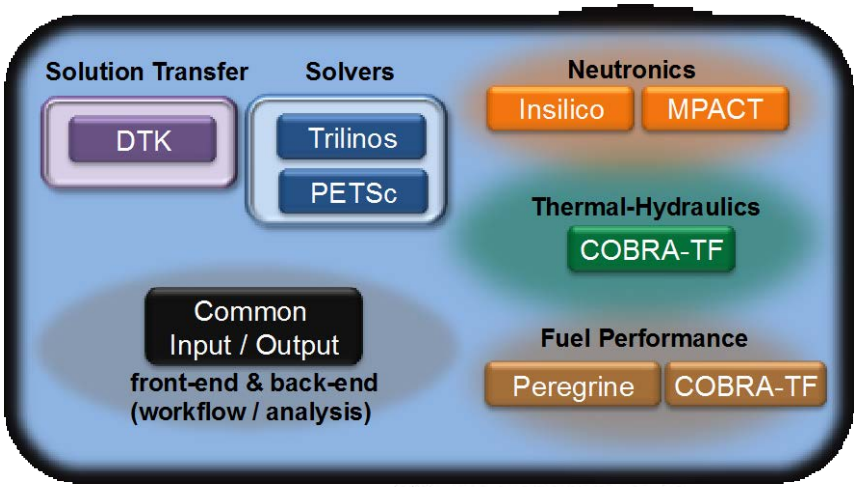
demonstrable progress

DOE reportable L1 milestone (*Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback*) recently completed in Sep 30 2014

VERA Coupled Capability
The Core Simulator (VERA-CS)

- VERA-CS is a subset of VERA components that are used to model the steady-state operation of the reactor and depletion
- Contains neutronics, thermal-hydraulics and fuel rod temperature components
- Key Achievements/Applications:
  - Insilico/CTF full-core hot-full power capability
  - MPACT/CTF full-core hot-full power capability
  - Initial depletion capability applied to 2D and 3D problems
  - Applied to AP1000 in Westinghouse Test Stand
  - Applied to SMR by TVA/UTK

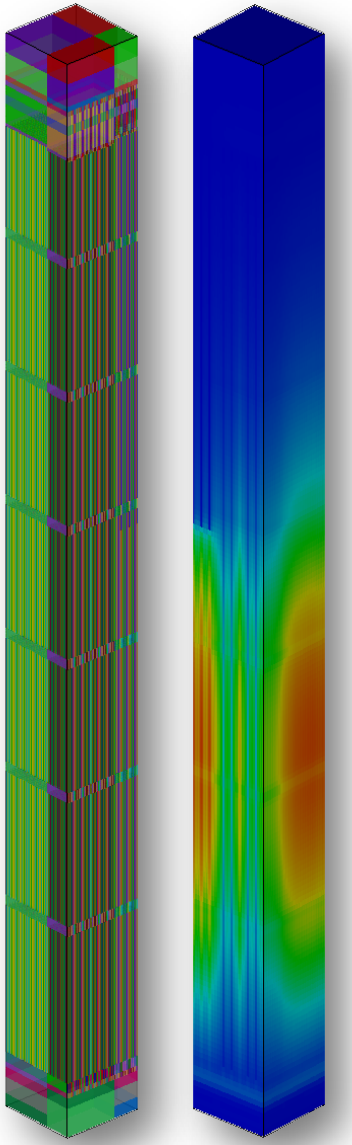




CASL Innovations

CASL vs. Industry Core Simulators

Physics Model	Industry Practice	CASL (VERA-CS)
Neutron Transport	3-D diffusion (core) 2 energy groups (core) 2-D transport on single assy	3-D transport 23+ energy groups
Power Distribution	nodal average with pin-power reconstruction methods	explicit pin-by-pin
Thermal-Hydraulics	1-D assembly-averaged	subchannel (w/crossflow)
Fuel Temperatures	nodal average	pin-by-pin 2-D or 3-D
Xenon/Samarium	nodal average w/correction	pin-by-pin
Depletion	infinite-medium cross sections quadratic burnup correction history corrections spectral corrections reconstructed pin exposures	pin-by-pin with actual core conditions
Reflector Models	1-D cross section models	actual 3-D geometry
Target Platforms	workstation (single-core)	1,000 – 300,000 cores

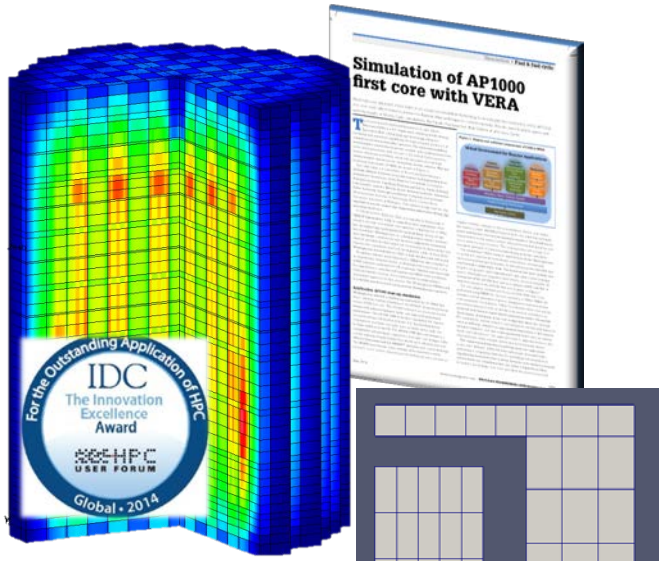


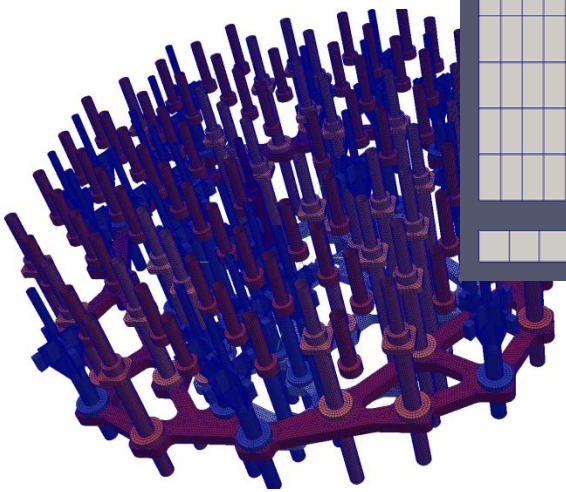
CASL current and planned capabilities will leapfrog calibrated industry core simulators that use lumped homogenization and correlation-based closures

Technology Deployment

We have now deployed 3 Test Stands

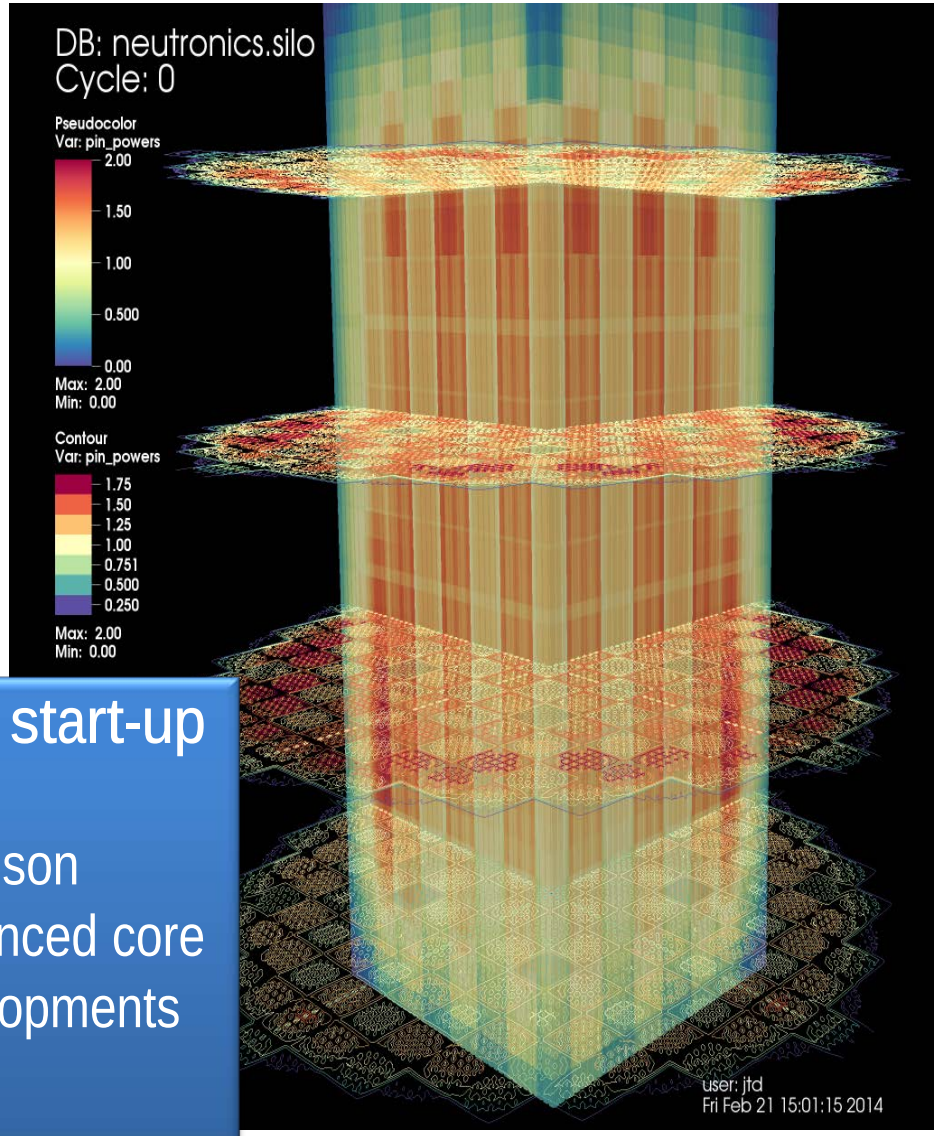
- Early deployment to industry for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
  - Westinghouse (Mar 2013): Test VERA core simulator's ability to analyze AP1000 first core startup
  - EPRI (Nov 2013): Benchmark VERA fuel performance (Peregrine) on PCI applications utilizing new EPRI's computing platform
  - TVA (Mar 2014): Test VERA CFD capability (Hydra-TH) on lower plenum flow anomaly observed in operational reactors
- CASL Test Stands have exposed technology gaps, deployment needs, and driven continuous improvement
  - Have become a best practice for us
- More Test Stands on the horizon





Timeline for CASL Westinghouse (WEC) Test Stand

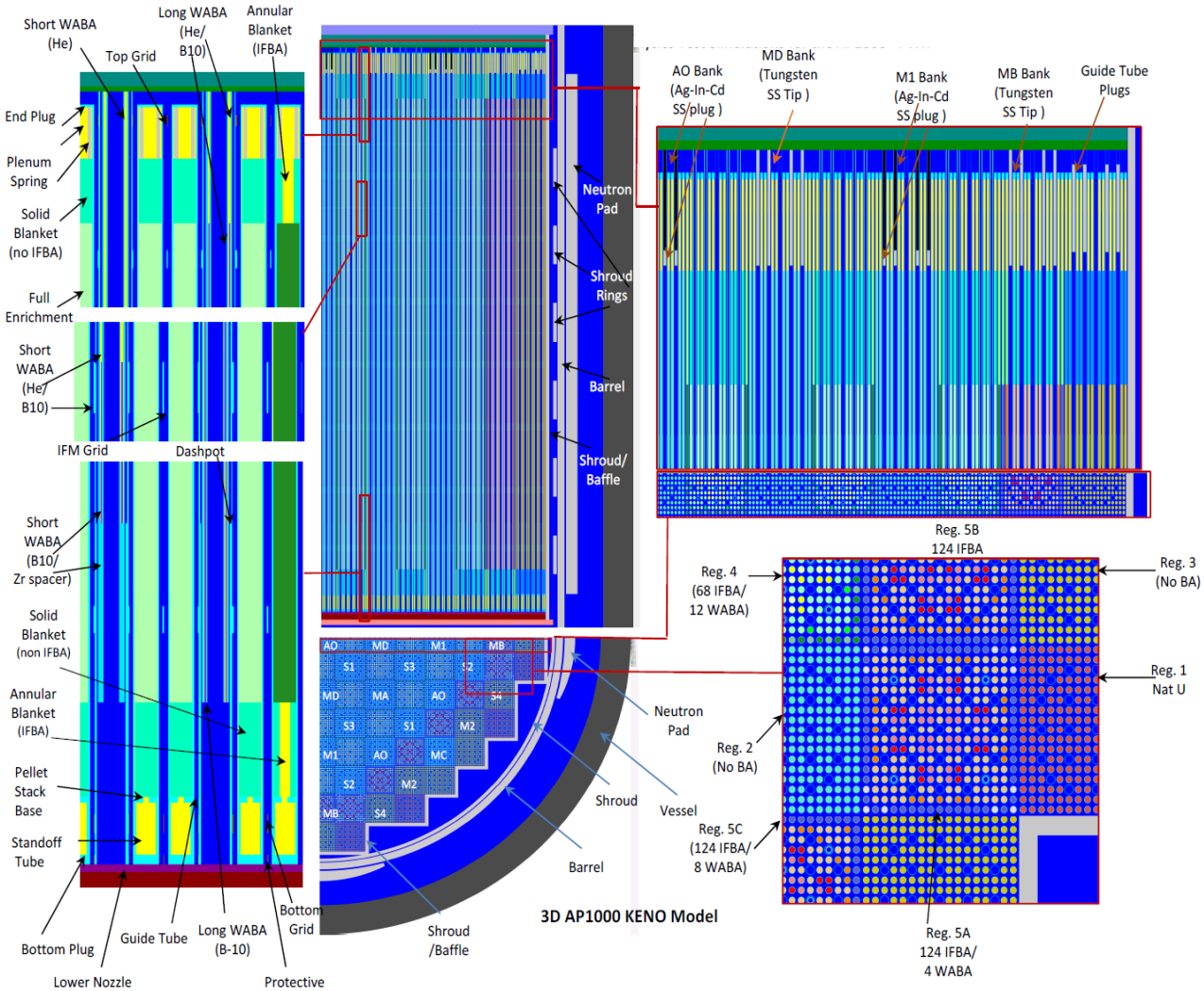
- early 2013: Test Stand discussion
- April 2013: Scope proposed by WEC
- June 2013: VERA deployment at WEC
- July-Nov 2013: Technical analysis
- Jan 2014: Analysis completed and documented (Mar 2014)



Enhanced confidence in AP1000 PWR start-up predictions

- High-quality benchmarks for code comparison
- Expanded application of VERA to an advanced core
- Feedback from WEC to guide future developments
- Framework for VERA build and update

AP1000 Advanced First Core Model



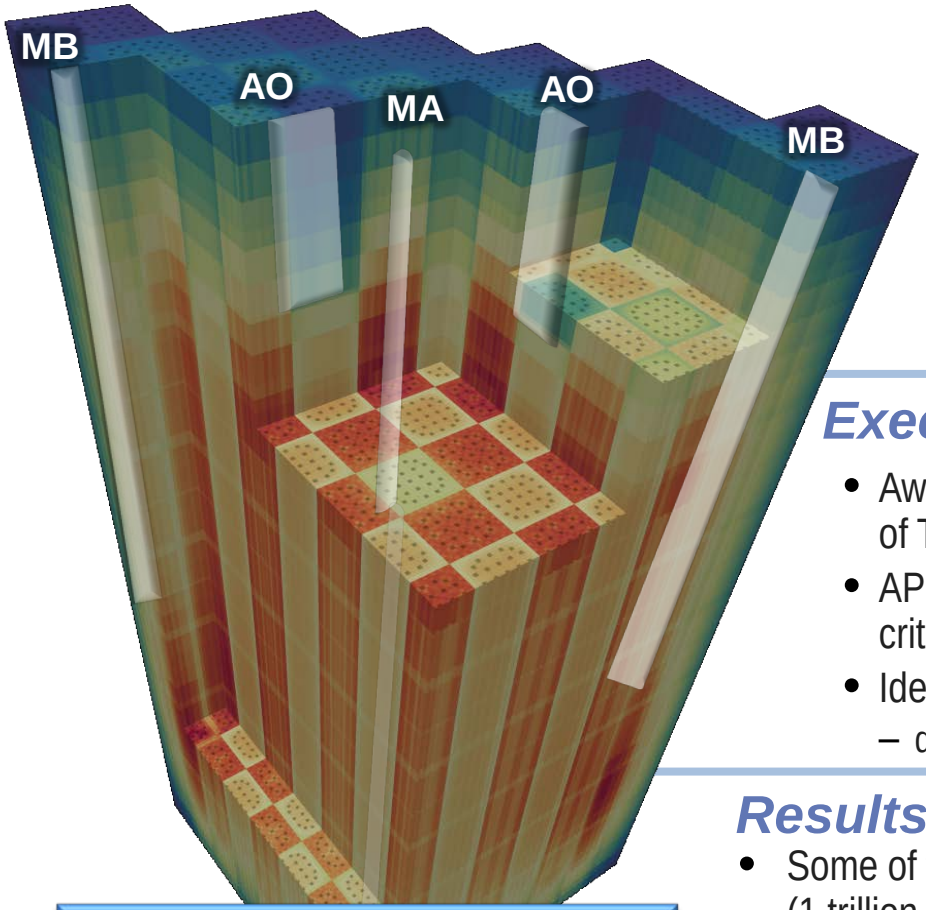
AP1000 Monte Carlo model shown. *Thanks to VERA common input, it has been possible to generate a complete AP1000 core model within a compact and intuitive input.*

The AP 1000 features an advanced first core with several enrichments and fuel heterogeneities which allows to quickly achieve equilibrium cycle after fuel shuffle and reload.

The advanced first core is a major economic advantage since it reduces the number of transition cycles before equilibrium but it also poses challenges to the simulation.

VERA high-fidelity physics provided an ideal match for simulating this challenging core and gain confidence in the start-up predictions

Evaluation of Shift: VERA Continuous-Energy Monte Carlo Quarter-Core Zero Power Physics Test



Monte Carlo prediction of power distribution for an AP1000 with multiple control rod banks inserted (AO, MA, and MB).

Goals

- Compare fidelity and performance of Shift against Keno, SP_N, and S_N (Denovo)
- Generate high-fidelity neutronics solution for code comparison of solutions for predicting reactor startup and physics testing

Execution

- Awarded 60 million core-hours on Titan (worth >$2M) as part of Titan Early Science program
- AP1000 model created and results generated for reactor criticality, rod worth, and reactivity coefficients
- Identical VERA Input models used for Shift, SP_N, and S_N
  - dramatically simpler than KENO-VI input model

Results

- Some of the largest Monte Carlo calculations ever performed (1 trillion particles) have been completed
  - runs used 230,000 cores of Titan or more
- Excellent agreement with KENO-VI
- Extremely fine-mesh S_N calculations, which leverage Titan's GPU accelerators, are under way

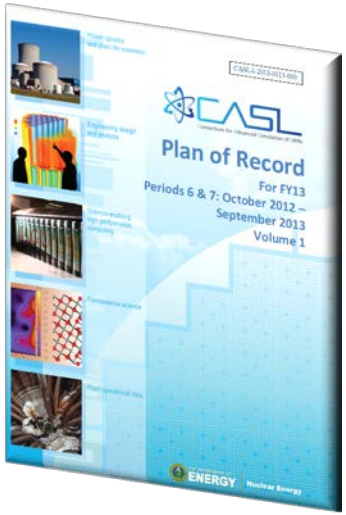
How are we Reviewed Annually?

1. Is CASL managing the Energy Innovation Hub in accordance with the plans provided in the proposal and summarized in the NE Hub Oversight Plan?
2. Have the management plans changed and if so are the justifications for those changes sufficient?
3. Is CASL receiving feedback and direction from its Board of Directors and Councils? What actions are being taken in response to that feedback?
4. Are the CASL financials being adequately managed and appropriately adjusted given the available funds?
5. Given the available funds, is CASL achieving its planned technical milestones? Are those milestones being reviewed and accepted as being met by adequate technical experts?
6. What metrics are being used to guide the management of CASL and are they sufficient to assess the performance of the Hub?
7. Has the CASL adequately responded to the findings of the previous DOE review report?

CASL Continues to Plan and Execute With our Evolving Plan of Record (PoR) Process

We have finished PoR-1 thru PoR-9 . . .

- CASL is planned and executed in a series of 6-month periods known as the *Plan of Record* (PoR)
- PoR is a documented implementation plan of L1-L3 milestones, tasks, and risks ("who does what when")
- Each PoR is a living document describing expectations for the next six months
  - Senior Leadership Team (SLT) defines/refines L1 milestones with DOE concurrence
  - Extended Leadership Team (ELT) [Focus Area Leads + Challenge Problem Integrators] meets to discuss L1 and proposed supporting L2 and L3 milestones
  - Focus Area (FA) Leads work with staff and enter milestone information into project management database (Trac)
  - SLT iterates with FA Leads on milestones to finalize
  - Trac and PoR document finalized; baseline established and under change control



A structured continuously improving process to plan, execute and deliver results

Phase 1 Milestone Progress

Using lessons learned moving forward

- Have a defined and documented milestone life cycle process
- Pay attention to getting the “right” milestone completion criteria
- Formal milestone change control helps to prevent chaos (no attention to milestones) and death marches (undue focus)
- Milestone performance, if the milestones are “right”, are good indicators of other performance (staff, leaders, partners)
- Milestone importance is relative (hence the hierarchy)
- Implement and use an open tool (e.g., TRAC) for milestone progress –a PM-accessible-only tool (e.g., P3E) erects collaboration & communication barriers
- Milestones also help communicate work challenges and interdependencies
- Identifying and implementing milestone-based risk trigger points and mitigation actions are doable
- Take care to “right-size” the process and procedures and continuously improve

While we our milestone-based process has been effective, it can be improved upon. It also cannot be replicated in its entirety as we move to new scope. We believe, especially for early-career staff, that the best-practice PM approaches in CASL can be carried over and implemented in future DOE projects and programs.

Our Milestone Database
For Planning, Tracking, Reviewing

L2:PHI.P9.01

Opened 10 months ago
Last modified 4 weeks ago

Reported by:	j9i	Owned by:	Pawlowski
PoR	PoR-9	Keywords:	PHI
Cc:	p8d, gnv, pmy, uy7, kto	DOE Reportable Milestone?:	FALSE
Primary Owner:	gnv		
Short Description:	Challenge Problem Coupling		
Start Date:	2013-10-01	End Date:	2014-06-30
Actual End Date:	2014-06-30	Completion Status:	Deliver (100% complete)
Parent Tickets:		Blocked By:	
Blocking:			
Execution Responsibility:	Lead: Pawlowski Supporting: INL MOOSE developers, Scott Palmtag, Stuart Slattery		
AMA Benchmark Progression Problem:	-	Challenge Problem Supported:	PCI
Execution Plan:	1) Modify Tiamat driver to support updated components. This includes the ability to resolve the same time step in MOOSE, developing a more stable ramping procedure for Peregrine, integrating the vera input parser for all aspects of the solve, merging the cobra_denovo coupled problem inot he main driver (ability to disable Peregrine) (5/1/2014) 2) Execute problem 6 couplings with Tiamat (6/1/2014) 3) Execute VERA-CS + Peregrine coupling on single assembly case (6/15/2014) 4) Document results (6/30/2014)		
Export Control:	No	Proprietary Information:	No
Links to Supporting Work:	• CASL PHI Kanban Tickets • Changes to PHI Kanban Tickets		
Completion Evidence Location:	https://portal12.ornl.gov/sites/casl/Shared%20Documents/Forms/AllItems.aspx?RootFolder=%2Fsites%2Fcasl%2FShared%20Documents%2FProgram%20Mana		
Completion Criteria:	Updated Tiamat coupler demonstrated on problems 6 and neutonics-subchannel-fuel performance single assembly problem. Document development and results in report.		
Reviewers:	Gehin		
Reviewers Comments:	Document has been reviewed and comments provided and addressed in an updated version of the milestone deliverable report. The milestone work was also presented in the PHI session at the CASL round table on July 14, 2014.		
Baseline Change:	-	Scope Change:	no
Schedule Change:	no	Budget Change:	no
New End Date:		New Budget Request:	
Baseline Change Comments:			
Issue:	Describe the issue		
Issue Corrective Action:	Describe the corrective action related to the associated issue.		

Description (last modified by p8d) (diff)

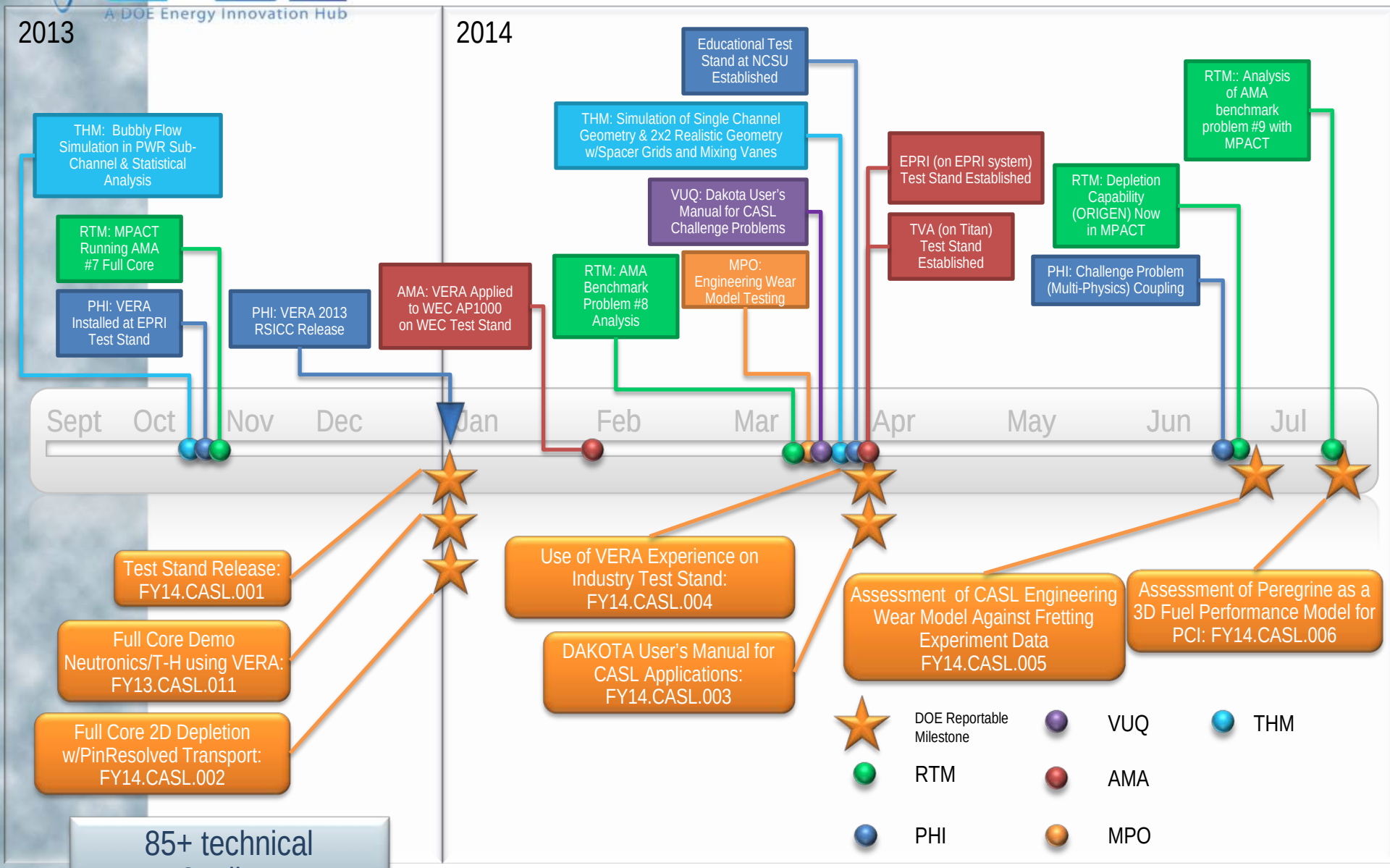
Develop and updated Tiamat coupling capability based on updated MOOSE and other VERA components (specifically those related to VERA-CS). This will provide the necessary capability to support CASL milestone L1:CASL.P9.03 "Demonstrate integrated VERA-CS for the PCI challenge problem (FY14.CASL.008)" Supported capabilities include neutronics-subchannel coupling, support for depletion, and neutronics-subchannel-fuel performance coupling.

This milestone relies on significant changes to the MOOSE/Peregrine multiapp infrastructure and will not be completed until these changes are made.

Subtickets (add)

We continue to tailor and refine the Trac Open Source package – "for enhanced wiki and issue tracking system for software development projects" – for our own purposes

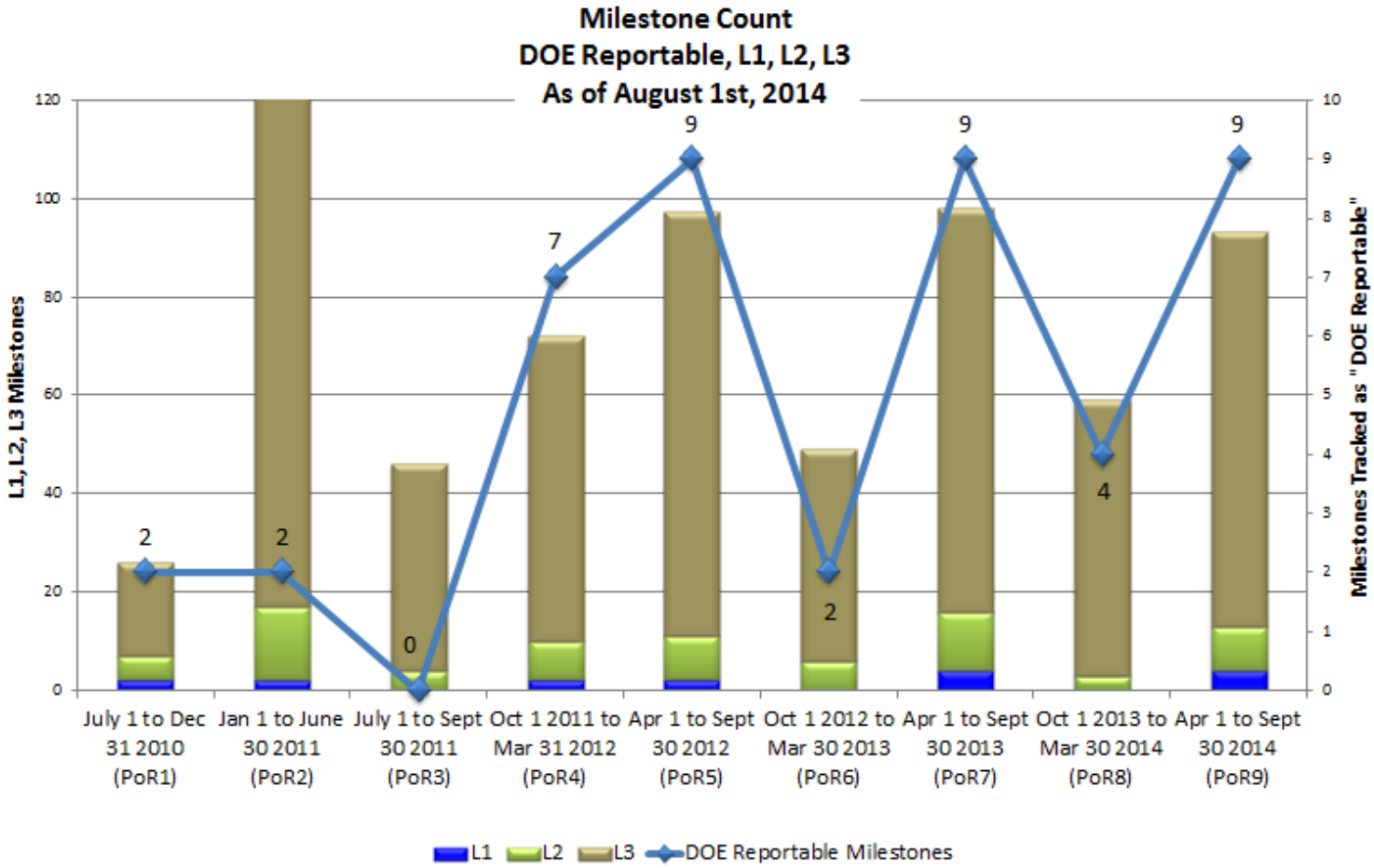
Selected Accomplishments



85+ technical L1–L3 milestones

CASL Milestone Statistics

Milestones delivered since CASL start (Jul 2010)



Milestone count: 13 L1s, 62 L2s, 474 L3s

1887 milestone documents in the CASL records management system

Phase 1 Milestone Progress

Milestone delivery has led to *many* technical reports

Period	L1 Milestones			L2 Milestones			L3 Milestones		
	Milestones Delivered	Milestones Reports	Records Delivered	Milestones Delivered	Milestone Reports	Records Delivered	Milestones Delivered	Milestone Reports	Records Delivered
PoR-1	2	3	7	5	4	8	19	28	40
PoR-2	2	7	11	15	33	46	110	128	166
PoR-3	0	0	0	4	9	11	42	57	85
PoR-4	2	3	5	8	10	16	62	79	107
PoR-5	2	3	5	9	16	21	82	82	136
PoR-6	0	0	0	6	13	15	43	66	95
PoR-7	4	6	9	9	13	20	74	51	79
PoR-8	0	0	0	3	6	6	35	31	47
PoR-9	0	1	2	0	0	0	3	0	0
Total	**12**	**23**	**39**	**59**	**104**	**143**	**476**	**522**	**755**

Milestone reports by Focus Area

Focus Area	Documented in CASL RMS
AMA	115
VUQ	65
PHI/VRI	110
RTM	43
THM	91
MPO	67
Others	158
Total	**649**

Milestone reports outside of Focus Areas

Category	Milestones Reports Maintained in CASL RMS
CASL	23
CASL internal	23
Export Control	1
Industry Council	8
Non-Focus Area	62
Production Integration	14
Project Management	5
Quality Assurance	10
Senior Leadership Team	3
Technology Control	9
Total	**158**

- All CASL documents are captured in the CASL Records Management System (RMS) – considered a best practice
- As many of the milestone reports as possible are being made publicly available on the CASL website (www.casl.gov)

Phase 1 Milestone Progress

Risks encountered and mitigated or being managed

Category	Risk Description	Risk Mitigation
Technical	Unclear path for robust, efficient, and accurate pin-resolved and pin-homogenized transport capabilities	Provide combination of RTM-developed Insilico, MPACT, and Shift capabilities to cover all neutronics use cases
Programmatic*	M&S product definitions do not explicitly and adequately match industry requirements	Focused efforts and resources on core simulator (VERA-CS) product and recognition that all CPs map to VERA products
Technical	Inadequate nuclear data and cross section processing technology	Initially underestimated effort and resources for nuclear data and cross sections now receiving adequate focus and attention
Technical*	Inability to deliver required multiphase CFD capabilities in a timely fashion	Evolving and maturing Hydra-TH effort now the singular focus of THM with adequate resources
Technical	Existing core-wide thermal hydraulics (subchannel) capabilities inadequate	Imported and integrated community-wide CTF subchannel capability with support for needed physics and algorithm development
Technical	Baseline (industry) CRUD deposition and growth models cannot be directly adopted to achieve CP fidelity targets	New MAMBA and MAMBA-BDM CRUD evolution codes initiated with development focused on advanced capabilities that fill industry gaps
Technical*	Uncertain fuel performance modeling starting point and path forward	Existing and evolving NEAMS-based INL MOOSE/BISON M&S framework chosen for base Peregrine technology starting point
Technical*	Challenges in integrating VUQ into development and ultimately into designer workflows	Forced cross-fertilization of industry/DOE/academia by combining industry-led AMA and DOE-led VUQ focus areas into new VMA
Technical*	Difficulty in evolving a heterogeneous, coupled multi-physics software integration environment	Ensure that PHI (previously VRI) has adequate scope, resources, and staff to cover broad computer and computational science needs
Technical	Existing partner structural mechanics/dynamics technologies do not match requirements for simulating in-reactor scenarios	De-scope structural mechanics/dynamics code development activities in favor of leveraging industry and ISV capabilities
Resource*	Applicable experimental data for validation of physics-based capabilities not available or accessible	Influence other programs, institutions, and vendors/utilities to fill data gaps; define and resource-load validation data needs and priorities; quantify M&S uncertainties resulting from current data gaps
Programmatic*	Maintaining consortium chemistry and cohesion	Open, team-based and bottom-up planning; open decisions informed by founding partner input; open, constant communication among founding partners
Programmatic	Inability to easily and effectively deploy CASL-developed technologies	Implement software license agreements for VERA and its components; useful and actionable IP Management Plan; work proactively with BOD
Resource	M&S infrastructure needs outstrips unsupported supply	Work to better leverage founding partner capabilities; use reserve funds to purchase/upgrade compute platforms; work with DOE NE in laying out a plan to o expand and upgrade its computing resources; work proactively with BOD

*** Denotes risks identified in the CASL Phase 1 proposal.**

7 of 14 top risks were anticipated in the Phase 1 proposal

Charge 4: Financial Management

Are the CASL financials being adequately managed and appropriately adjusted given the available funds?

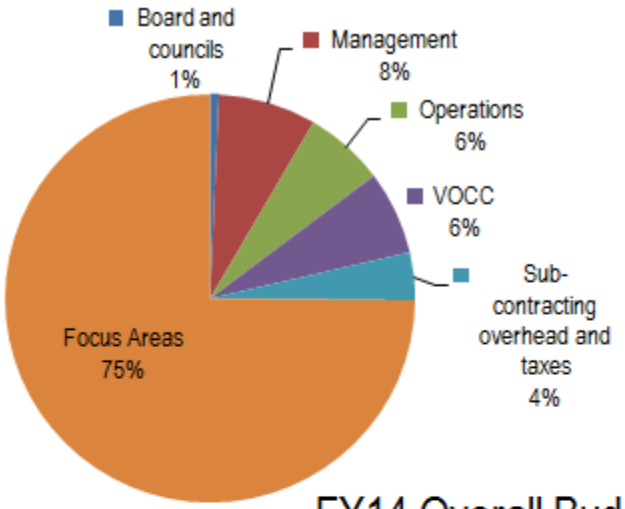
2014 review: Yes – During the review and in the material provided to the Review Team, CASL was able to provide a very clear picture of its financial situation. The challenges of monthly funding from DOE beginning in January , 2014 were handled while keeping the partners working without significant stop work actions.

Financial management improvements in FY14

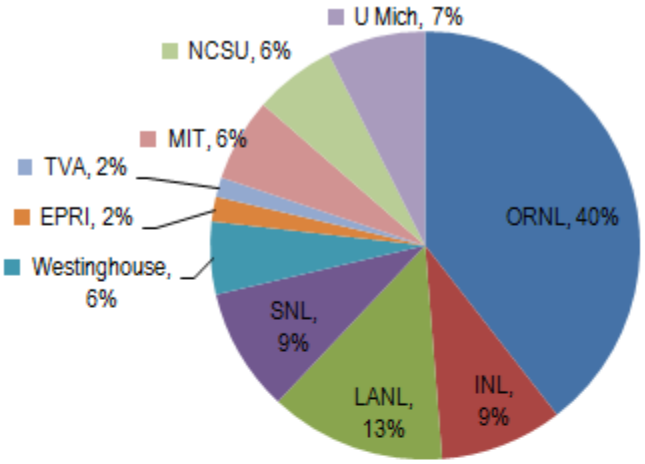
- Improved communication with DOE regarding monthly cash flow and continual improvement of cash flow planning for subcontracts during very challenging financial cash flow situations
  - 26 subcontracts and 7 Memorandum Purchase Orders (MPOs for DOE labs) executed this year.
  - Partners stayed funded despite near misses in Feb on multiple subcontracts/MPOs when funding was not received in January as expected. Adjustments made to keep the partners funded even if required to do greater than 30 monthly funding modifications to subcontracts and MPOs.
  - Worked closely with DOE to help on future funding planned
- Improved cost reporting to DOE every month
  - Partners began providing their own current month cost estimates by contract prior to month end to ORNL.
  - Results were more accurate and timely partner cost being reported to DOE each month regardless of invoicing.
  - Results were more capability of projecting funding needs.
- Improved reports to CASL management
  - Partners were asked to provide faster cost detail financial reporting through the current month prior to actual invoicing to know what work was being done by budget category.
  - Results were more accurate and timely reports by budget category for CASL management. This is especially helpful as year end approaches for FA leaders to determine future year funding.
  - Also even though invoices may be going through the normal delays, the CASL reports can reflect the true partner costs expected in invoices. Note: Results can be seen in less projected payable costs on next slide than previous years meaning the cost is allocated to correct budget categories through May or June.
  - Formal process for baseline budget change (BCC) helping to enforce openness and upstream approvals

- Cash flow interrupts have dire consequences; this concern remains upon a Phase 2 go-ahead in FY15
- Current resource allocation and financial management processes not expected to change significantly
- Plan for 5-year modifications to existing founding partner subcontracts should a Phase 2 term be awarded

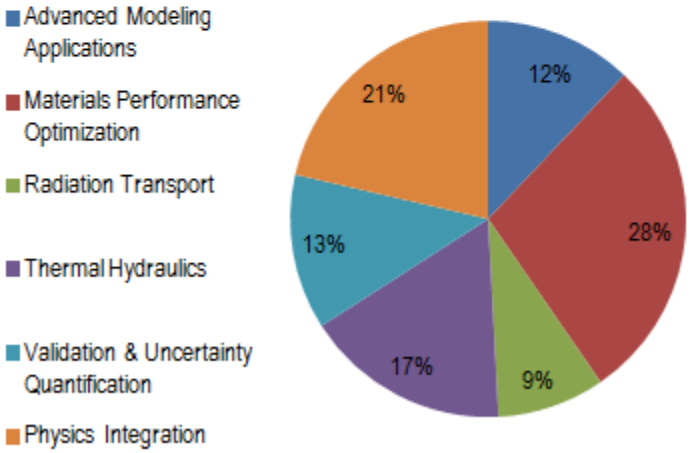
FY14 budget distribution



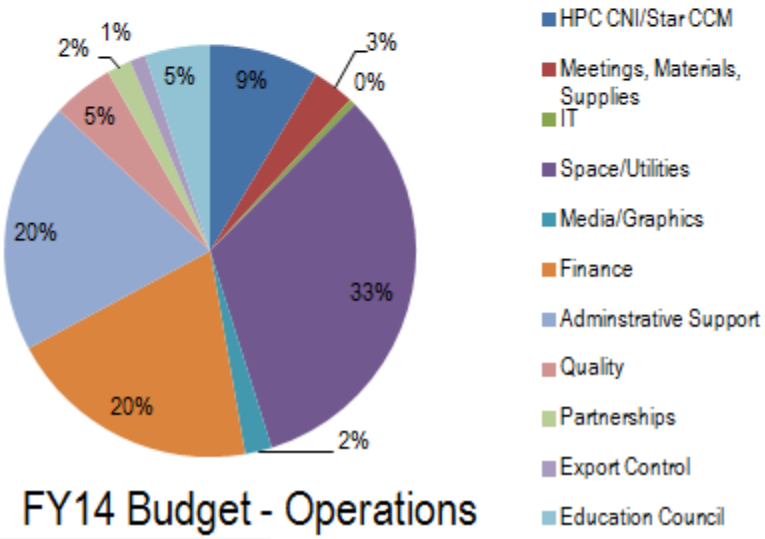
FY14 Overall Budget



FY14 actual core partner distribution



FY14 Budget - Focus Area



FY14 Budget - Operations

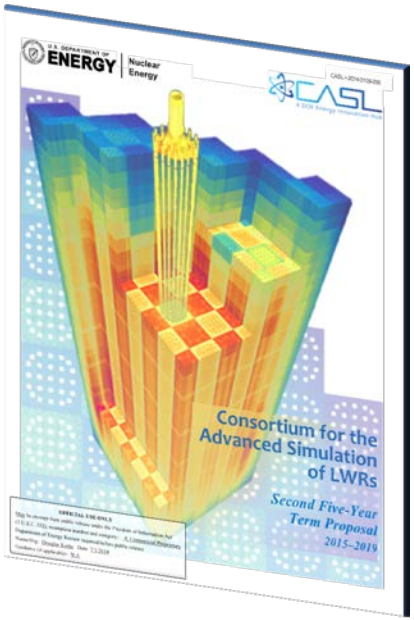
We have set aggressive (~15%) reduction targets for FY15 in management, operations, and contracting overhead

Phase 2 Renewal Proposal

Document Structure

TABLE OF CONTENTS

EXECUTIVE SUMMARY III
TABLE OF CONTENTS VI
LIST OF TABLES VIII
LIST OF FIGURES X
ACRONYMS XII
1 INTRODUCTION 1
2 PHASE 1 PROGRESS 1
2.1 MILESTONE AND PROJECT PERFORMANCE 2
2.2 SUCCESSFUL COMPLETION OF DOE ANNUAL REVIEWS 6
2.3 PUBLICATIONS AND INNOVATIONS 7
2.4 TECHNOLOGY DEPLOYMENT AND OUTREACH 8
2.4.1 VERA Releases 9
2.4.2 Test Stands 10
2.4.3 Education Program 11
2.4.4 IP Management and Technology Licensing 12
2.5 CASL'S ONE-ROOF: VIRTUAL OFFICE COMMUNITY AND COMPUTING 12
3 PHASE 2 OBJECTIVES AND STRATEGY 13
3.1 BROADENING AND DEEPENING CASL'S PHASE 1 TECHNOLOGY 14
3.1.1 PWR / BWR / iPWR Convective Flow Challenge Problems 16
3.1.2 PWR / iPWR CHF (DNB) Challenge Problems 16
3.1.3 BWR Flow Regimes Challenge Problem 17
3.1.4 PWR / BWR / iPWR PCI Challenge Problems 17
3.1.5 PWR / BWR RIA Challenge Problems 18
3.1.6 PWR / BWR LOCA Challenge Problems 19
3.1.7 PWR / iPWR CRUD (CIPS and CILC) Challenge Problems 19
3.1.8 PWR GTRF Challenge Problem 20
3.1.9 Interoperability 20
3.2 EXTENSIONS AND ADDITIONS TO VERA 20
3.2.1 VERA Extensions 21
3.2.2 VERA Additions 22
3.2.3 Middleware/Infrastructure 22
3.2.4 Validation and Uncertainty Quantification Activities 23
3.3 PHASE 2 LEVEL 1 MILESTONES 24
3.4 TECHNICAL FOCUS AREA ROADMAPS 24
3.4.1 Fuel Materials and Chemistry 26
3.4.2 Physics Integration 27
3.4.3 Radiation Transport Methods 28
3.4.4 Thermal-Hydraulics Methods 29
3.4.5 Validation and Modeling Applications 30
3.5 TECHNOLOGY DEPLOYMENT AND OUTREACH 31
3.5.1 Sustainability of CASL Technology 31
3.5.2 Outreach Activities 31
3.5.3 Test Stand Deployments 32
3.5.4 VERA Release and Support 32
3.6 EDUCATION PROGRAM 33
3.7 PROGRAM INTEGRATION 33
4 TEAM CAPABILITIES AND PROJECT MANAGEMENT STRATEGY 34
4.1 ORGANIZATIONAL STRUCTURE AND TEAM CAPABILITIES 35
4.2 EVOLUTION OF THE CASL ONE-ROOF APPROACH 36
4.3 RESOURCE ALLOCATION 36
4.4 RISK MANAGEMENT 38
5 SUMMARY 40



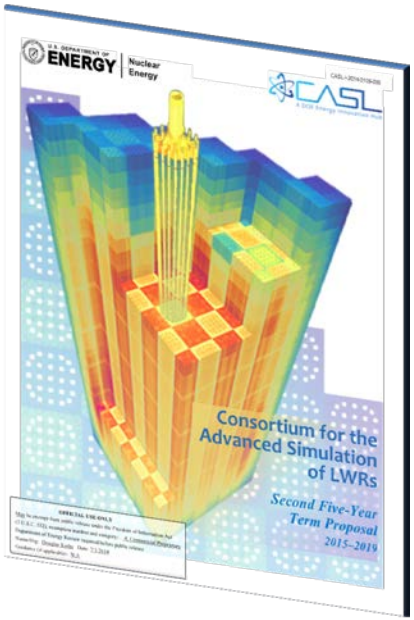
CASL-I-2014-0109-000

Phase 2 Renewal Proposal

Document Structure

TABLE OF CONTENTS, CONTINUED

APPENDIX A. PHASE 1 PERFORMANCE **A-1**
A.1. SCIENCE AND TECHNOLOGY PROGRESS A-1
A.2. TECHNOLOGY DEPLOYMENT A-22
A.3. PRODUCTIVITY METRICS A-31
A.4. PLAN OF RECORD AND MILESTONE PERFORMANCE A-49
A.5. BUDGET AND COST SUMMARY A-58
A.6. DOE ANNUAL REVIEWS A-63
APPENDIX B. PHASE 2 IMPLEMENTATION **B-1**
B.1. CHALLENGE PROBLEM DESCRIPTIONS B-1
B.2. PHASE 2 SCOPE SELECTION PROCESS B-9
B.3. DETAILED TECHNICAL FOCUS AREA ROADMAPS B-13
B.4. TECHNOLOGY DEPLOYMENT VEHICLES B-22
B.5. VIRTUAL ONE-ROOF EVOLUTION DETAILS B-36
B.6. PROGRAM INTEGRATION DETAILS B-39
APPENDIX C. TEAM AND MANAGEMENT ST RUCTURE **C-1**
C.1. CONSORTIUM PARTNERSHIP C-1
C.2. CHANGES TO THE ORGANIZATIONAL STRUCTURE FOR PHASE 2 ..... C-4
C.3. BIOGRAPHICAL SKETCHES C-18
APPENDIX D. KEY PROJECT MANAGEMENT INITIATIVES **D-1**
D.1. FINANCIAL MANAGEMENT D-1
D.2. PROJECT MANAGEMENT D-3
D.3. SOFTWARE ENGINEERING AND QUALITY ASSURANCE D-8
D.4. RISK MANAGEMENT D-12
D.5. TECHNOLOGY CONTROL PLAN D-19
D.6. RECORDS MANAGEMENT D-23
D.7. TRAINING PROGRAM D-24
APPENDIX E. LETTERS OF SUPPORT **E-1**
APPENDIX F. REFERENCES **F-1**



CASL-I-2014-0109-000

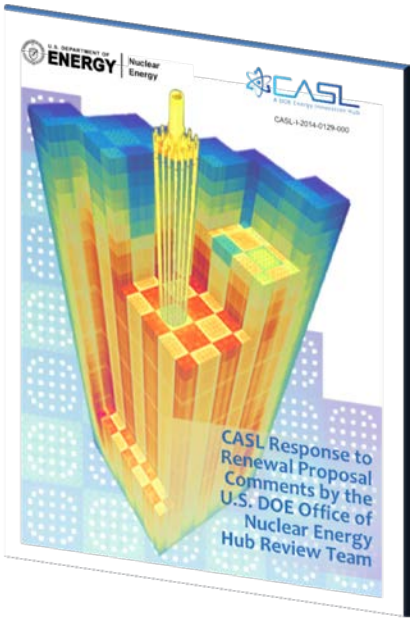
Phase 2 Renewal Proposal

Response to Review Comments

TABLE OF CONTENTS

EXECUTIVE SUMMARY III
TABLE OF CONTENTS IV
1 INTRODUCTION 1
2 PHASE 1 – CREATING THE FOUNDATION 1
2.1 NRC INTERACTIONS 1
2.2 TECHNOLOGY ADJUSTMENTS 2
2.3 USE AND EXTENSION OF EDUCATIONAL PROGRAM ACTIVITIES 3
2.4 LESSONS LEARNED FROM THE DOE OFFICE OF INSPECTOR GENERAL AUDIT 4
3 PHASE 2 – PLANS FOR VERA SIMULATION CAPABILITIES 5
3.1 SCOPE DEEPENING AND BROADENING 5
3.2 VERA EXTENSION PLANS FOR ACCIDENT TRANSIENTS 6
3.3 VERA EXTENSION PLANS FOR OUT-OF-CORE PHENOMENA 6
3.4 PLANS FOR MULTI-PHASE FLOW AND RELEVANCE TO BWRS 6
3.5 VERA PLANS FOR STRUCTURAL MECHANICS CAPABILITIES 7
3.6 PLANS FOR FACING TECHNICAL CHALLENGES 7
4 PHASE 2 – CASL CODE VALIDATION PLANS 8
4.1 LEVEL OF VALIDATION PLANNED FOR VERA 9
4.2 EXPERIMENTAL DATA NEEDED FOR THE VERA VALIDATION PLAN 9
4.3 ACQUIRING THE NEEDED VALIDATION DATA 9
4.4 VALIDATION METHODS USED 10
5 PHASE 2 – CASL TEAM 10
5.1 TEAM MEMBER ROLES 10
5.2 TEAM MEMBER CAPABILITIES 11
5.3 SENIOR LEADERSHIP TRANSITION 11
5.4 REINVIGORATION OF CASL ACTIVITIES 12
6 BEYOND PHASE 2 – CASL CODE SUSTAINMENT PLANS 12
6.1 ADVANCED MODELING WORKING GROUP 12
6.2 STRATEGY AND PLAN FOR CODE LICENSING 13
6.3 VERA SUPPORT OF CURRENT AND FUTURE NUCLEAR FLEET 14

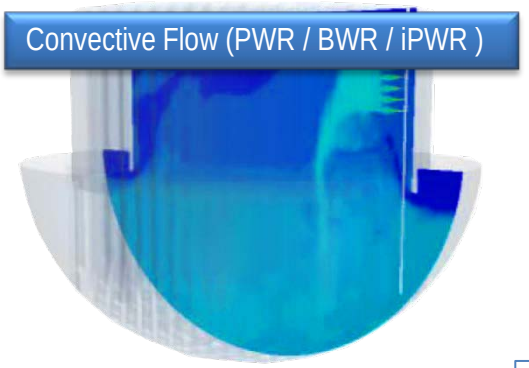
CASL Response to Renewal Proposal Comments by U.S.DOE-NE Hub Review Team iv CASL-I-2014-0129-000

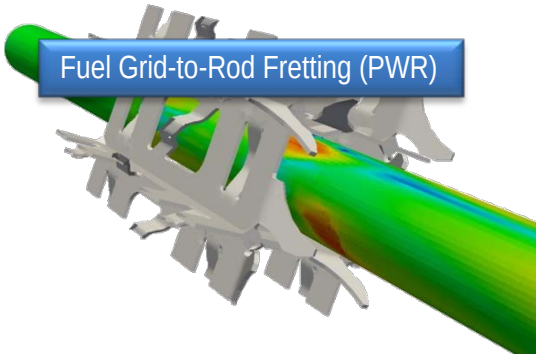


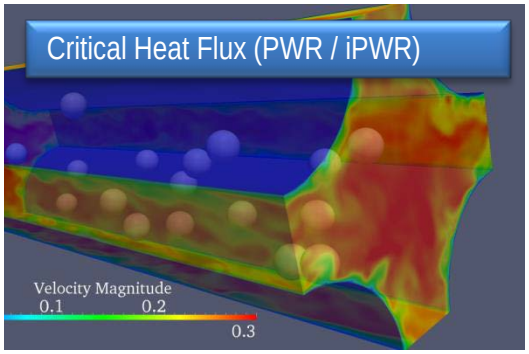
We appreciate the detailed and helpful comments received by the Review Team. Our responses in some cases reflect assumptions and best estimates by the CASL leadership at the present time, which may change as further knowledge and experience is gained

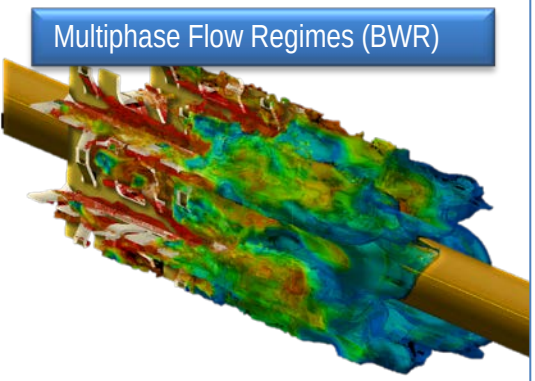
CASL-I-2014-0129-000

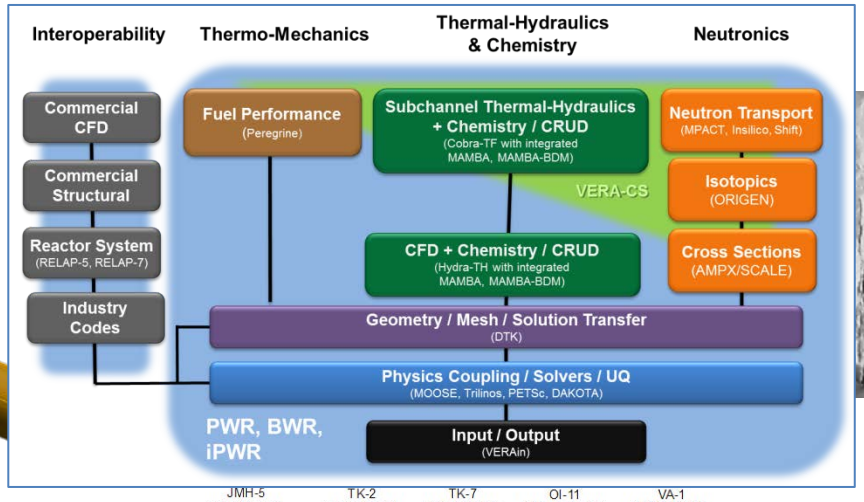
CASL Proposed Phase 2 Scope: 2015 – 2019

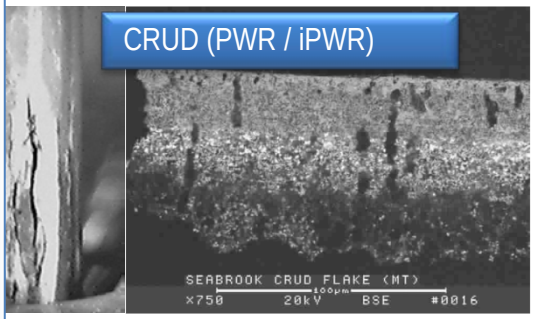


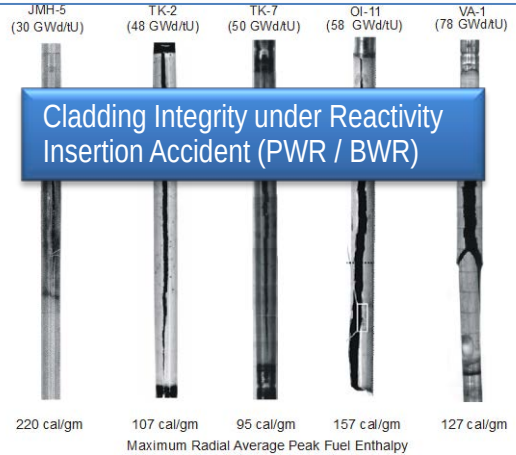


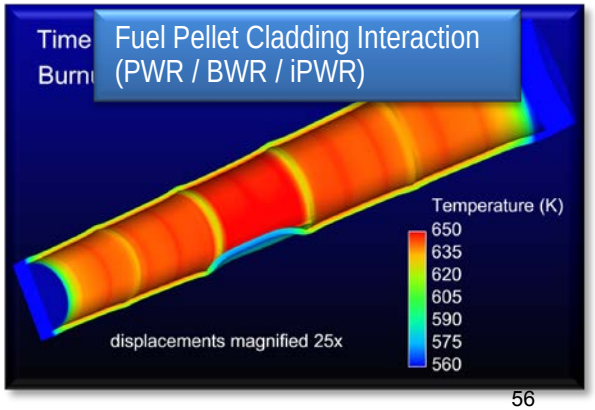




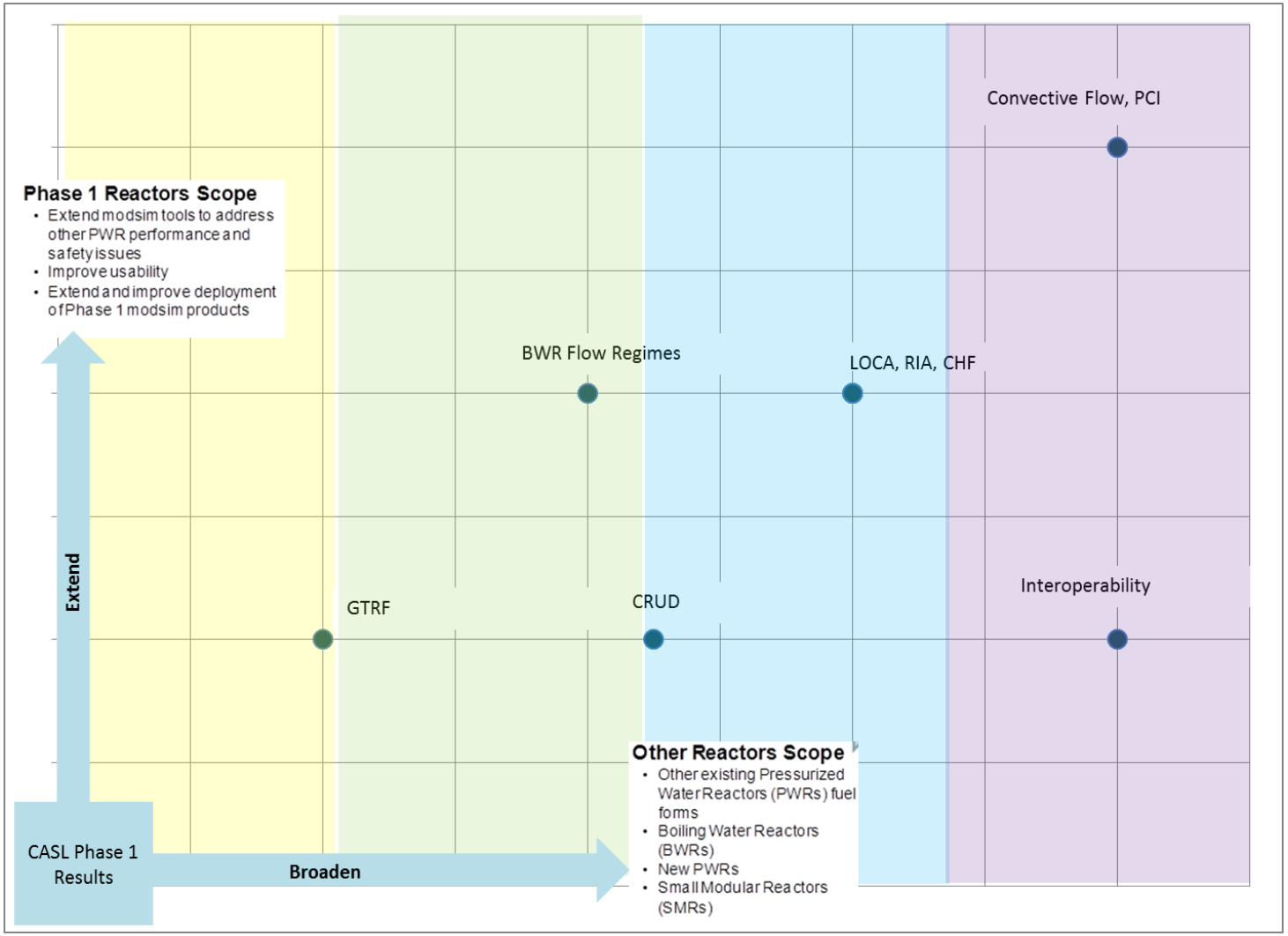








Phase 2 Scope



Target End State Capabilities

- VERA-CS
  - PWR & iPWR full-core, pin resolved, depletion & transient capability
  - BWR sub-core (stretch full-core), pin resolved, depletion capability
- PCI: PWR, iPWR and BWR capability
- CRUD: PWR & iPWR capability
- GTRF: PWR & iPWR pin behavior (stretch gap opening), wear, fluid forces & interoperability (structural mechanics)
- DNB: PWR & iPWR core-wide (subchannel) & M-CFD
- LOCA: PWR, iPWR & BWR fuel response (IC, corrosion and balloning)
- RIA:
  - PWR & iPWR full-core, pin resolved, transient neutronics, subchannel, fuel performance capability
  - BWR sub-core (stretch full-core), pin resolved, transient (stretch neutronics), subchannel, fuel performance capability
- Other Thermal-Hydraulics (M-CFD): Thermal & solutal driven flows (single phase) & BWR nominal operating conditions flow regimes
- Interoperability: Structural mechanics, systems simulation & core simulator

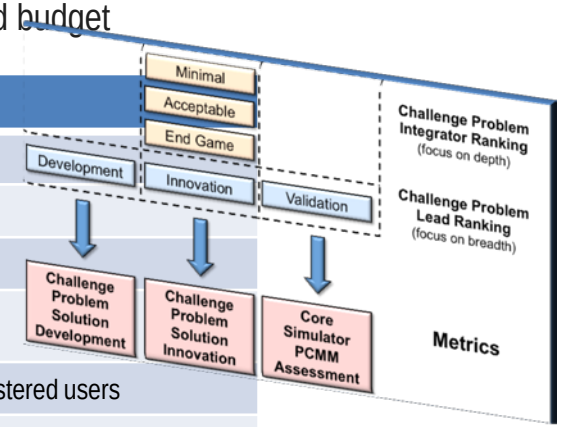
Supplemental Material

Metrics

Used to guide and assess its performance

- CASL has defined Outcome and Performance Metrics (measured every Plan of Record)
  - *Outcome Metrics* that represent higher level metrics spanning organizational groups and lower lever performance measures (key performance indicators – map to strategic goals)
  - *Performance Metrics* that measure specific areas of performance and act as early indicators
    - Project management, student/university/industry engagement, infrastructure uptime, VERA development
- CASL also appeals to its Board and Council structure for measuring performance
  - *Industry Council* assesses CASL's technology (VERA) usefulness and usability
  - *Science Council* assesses CASL's quality of science and engineering and its ability to identify and adjust to new circumstances and effectively communicate with the technical community
  - *Board of Directors* assesses CASL's management performance – its ability to manage a vastly diverse team to deliver the planned technical scope on target, schedule and budget

Strategic Outcome	Metric
Address design, operational, and safety challenges for LWRs	Challenge Problem Solution Development
	Challenge Problem Solution Innovation
Develop and effectively apply modern virtual reactor technology	Challenge Problem PCMM Assessment
	Core Simulator PCMM Assessment
Engage nuclear community through modeling and simulation	Number of VERA licenses granted, open source downloads, & registered users
	Industry Council & User Group activity / membership
	Faculty, graduate and/or postdoctoral researchers utilizing and/or evolving VERA
Deploy new partnership and collaboration paradigms	VOCC Laboratory and technology availability/utilization
	Virtual collaboration endeavors leveraging or attributable to CASL VOCC technology



VERA Analysis of Watts Bar 1 Hot Full Power

Milestone L2:AMA.P7.02 delivered Dec 2013

Purpose

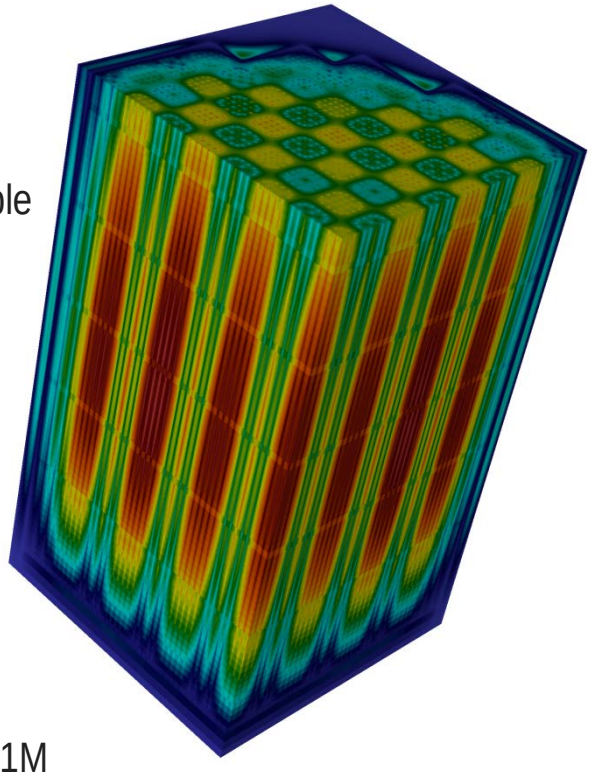
- First large-scale coupled multi-physics model of operating PWR reactor using Components of CASL's Virtual Environment for Reactor Applications (VERA)
- Features resolved are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1: geometry for fuel, burnable absorbers, spacer grids, nozzles, and core baffle

Execution

- Common input used to drive all physics codes
- Multigroup neutron cross sections calculated as function of temperature and density (SCALE/XSPROC)
- SPN neutron transport used to calculate power distribution (DENOVO)
- Subchannel thermal-hydraulics in coolant (COBRA-TF)
- Rod-by-Rod heat conduction in fuel rods (COBRA-TF)
- Simulation ran in 14.5 hours on Titan using 18,769 cores – over 1M unique material (fuel/coolant/internals) regions resolved

Next Steps

- Add fuel depletion and core shuffling
- Compare results to plant measured data



Thermal Flux Profile in Reactor Core

Remarkable resolution of physics and geometry

What enhanced capabilities over current practices will CASL provide?

Predictive capabilities

- Utilization of more science based models
- Utilization of micro and mesa scale models to increase understanding and provide closure relationships

Phase-space resolution

- Space, time, energy and angle
- Pin-resolved detail

VUQ practices

- Verification & validation
- Data assimilation
- Uncertainty quantification

Computational resource utilization

- Hardware: multiprocessor, multicore & GPUs
- Software: object oriented, I/O standards, third-party software (modern solvers)

What enhanced capabilities over current practices will CASL provide?

Fluids (HYDRA-TH)

- Current Practices: Closed channel HEM, limited sub-channel &limited CFD
- CASL Practices: Sub-channel, CFD & MCFD
- Why not utilize commercial CFD/MCFD code?
  - Need to access source code to enable advanced solution algorithms
  - Desired high utilization of evolving HPC architectures

Radiation Transport (MPACT & INSILICO)

- Current Practice: MG Lattice Physics (2D MOC Transport)=>FG Core-wide Physics (3D Nodal Diffusion)=>Pin-wise power/flux (reconstruction)
- CASL Practice: MG Core-wide Physics (2D MOC Transport)/Axial Leakage (1D or 3D SPN)
- Why not Sn or Monte Carlo?
  - Computational burden *currently* to great

High level differences of current versus CASL capabilities

Fuel Performance (PEREGRINE)

- Current Practice: 2D with experimentally derived closure models
- CASL Practice: 2D and 3D with experimentally derived and micro/meso scale modeling derived closure models

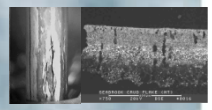
Crud Chemistry (MAMBA & MAMBA-BDM)

- Current Practice: 2D with limited chemical species & experimentally derived models' parameters
- CASL Practice: 1D, 2D and 3D with expanded chemical species, experimentally & micro modeling derived models' parameters, and new cladding corrosion model

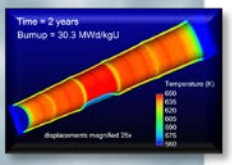
Multiphysics (VERA)

- Current Practice: Lower fidelity single-physics modeling coupling via one-way sweep or iterative sweep
- CASL Practice: Appropriate fidelity single-physics modeling coupling via appropriate loose to tight (e.g. JFNK) or total removal of required coupling (e.g. no lattice physics)

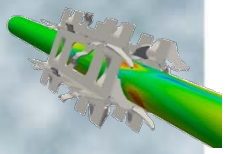
Challenge Problem Updates



- CRUD
  - ✓ Continued evolution of advanced crud capabilities (MAMBA, MAMBA-BDM)
  - ✓ Coupled CTF / MAMBA for CIPS (5x5 Seabrook Cycle 5 rod array
  - ✓ Improved STAR-CCM+ / MAMBA coupling (5x5 Seabrook Cycle 5 rod array)
  - ✓ WEC updated ANC/VIPRE/BOA linkage with new EPRI BOA 3.1
  - ✓ HYDRA / MAMBA and CTF / MAMBA linkage underway (MAMBA embedded)



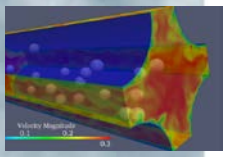
- PCI
  - ✓ Peregrine 2D/3D development for modeling full-rod and local geometries
  - ✓ Lower-length scale material modeling of cladding (VPSC)
  - ✓ Peregrine integration into VERA-CS for multi-rod/multi-assembly simulations
  - ✓ EPRI Test Stand PCI testing and benchmarking of Peregrine



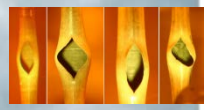
- GTRF
  - ✓ Engineering wear model development and experimental fretting wear tests
  - ✓ Parametric study of influences of key GTRF phenomena

Overall CP Product Integrator Zeses Karoutas (now Chief Engineer @ WEC) has done a great job in coordinating this effort

Challenge Problem Updates



- DNB
  - ✓ CTF rod bundle mixing and DNB test simulations, RIA experimental simulation, reactor core modeling under DNB limiting conditions
  - ✓ Hydra-TH rod bundle model and execution on industry computer, rod bundle single-phase mixing initial study
  - ✓ VUQ study initiated on rod bundle turbulent mixing model calibration



- Cladding Integrity (RIA and LOCA)
  - ✓ Charters and Implementation Plans completed
  - ✓ Peregrine dev (cladding corrosion/H pickup, matl props, RIA transient test)
  - ✓ COBRA-TF subchannel T/H development (whole core models, RIA demo)
  - ✓ MPACT transient neutronics development (capability demonstrated)
  - ✓ MPACT coupled to COBRA-TF completed (next step – Peregrine)

Good overall progress since last year

VERA Usage for Challenge Problems

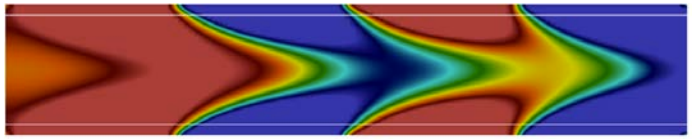
Challenge Problem	Time Scale (Seconds, Minutes, Hours, Days, Years)	Spatial Scale of Phenomena	Code Coupling Required
Crud-CIPS	Y (*always implies VERA-CS depletion*)	Core-wide	VERA-CS – MAMBA
Crud-CILC	Y	Core-wide to Few pin-wide	VERA-CS + Hydra – Peregrine – MAMBA
GTRF	Y + 50 Hz	Core-wide to Few pin-wide	VERA-CS - Peregrine + Hydra
PCI	Y + M to H	Core-wide to Few pin-wide	VERA-CS – Peregrine + Hydra – Peregrine
DNB	Y + S to M	System-wide to assembly-wide	VERA-CS - RELAP + Hydra – Peregrine
LOCA	Y + S to M	Pin-wide	Peregrine (B.C. from WEC)
RIA	Y + S	Few pin-wide	VERA-CS – Peregrine

S&T Program: FY14 Highlighted Accomplishments (to date)

- Thermal-Hydraulic Methods (THM)

❖ Hydra-TH Capabilities Enhancements

- Incorporation of porous drag, CHT, Hydra-Mamba coupling, and performance enhancements
- Addition of additional turbulence models: Spalart-Allmaras Rotation and Curvature Correction, k-e models (Standard, RNG model, non-linear model (anisotropic viscosity model)
- Continuing verification and validation activities
- Integration of MAMBA as subgrid model (in progress)



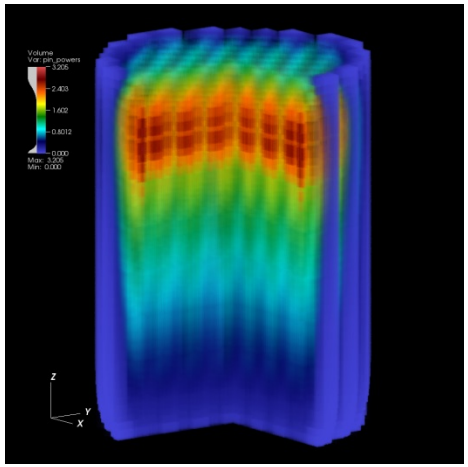
❖ Closure Relationships Development

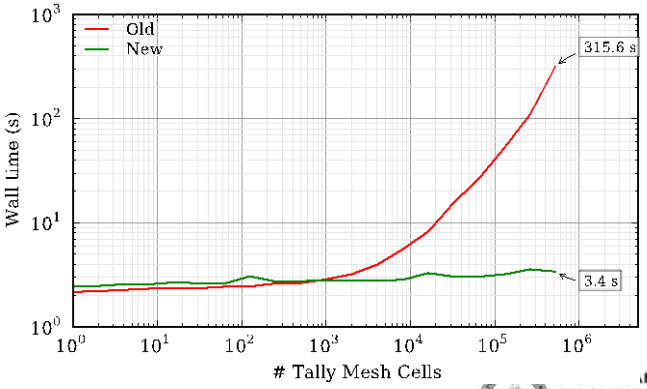
- Experimental work: Subcooled flow boiling database, gas-liquid two-phase flow experiments, effects of CRUD on boiling
- Interface tracking / DNS: Lift force on a single bubble, phase change
- Large scale ITM / data analysis: Transient motion of large number of bubbles, simulations and analysis of two-phase flow in a subchannel, DNS of single-phase flow through 2x2 mixing vanes / spacer grid geometry

S&T Program: FY14 Highlighted Accomplishments (to date)

- Radiation Transport Methods (RTM)
  - Support for integrated x-section generation/transport solver capability (Insilico), using Sn or SPn
  - Refactored 2D MOC/1D diffusion code (MPACT) with additions of depletion, thermal-hydraulic feedback, and transient capabilities, with improved resonance treatment (ESSM); and, examination of transport vs diffusion axial treatment.
  - Improvements for continuous energy Monte Carlo code (Shift) in computational efficiency using hybrid methods, low overhead tallying, & domain decomposition, along with improved treatment of Doppler broadening

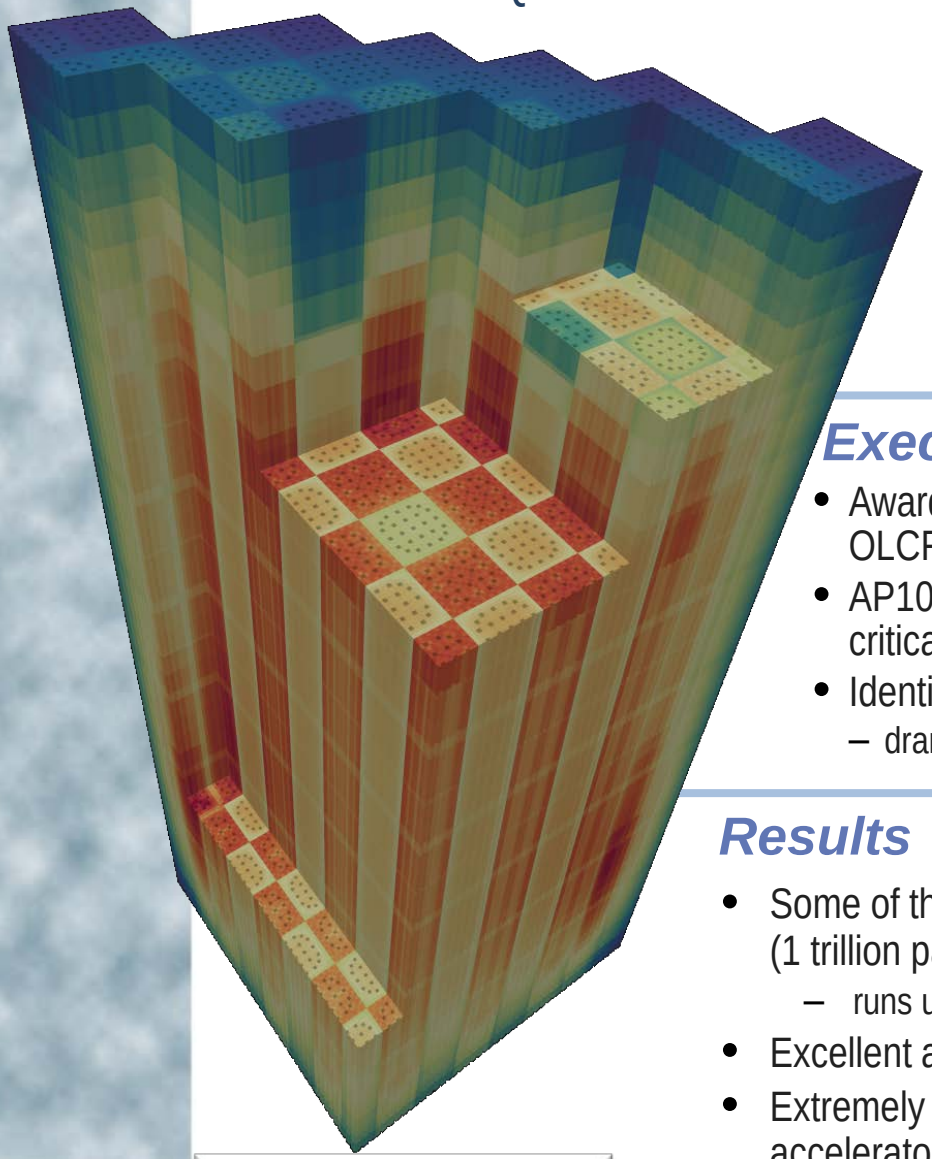
Bringing together Insilico (ORNL) & MPACT (UM) teams has proven effective





Evaluation of Shift: VERA Continuous-Energy Monte Carlo Capability

Quarter-Core Zero Power Physics Test



AP1000 pin powers

Goals

- Compare fidelity and performanc of Shift against Keno, SP_N, and S_N (Denovo)
- Generate high-fidelity neutronics solution for code comparison of solutions for predicting reactor startup and physics testing

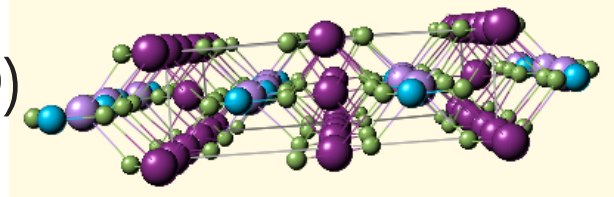
Execution

- Awarded 60 million core-hours on Titan (worth >$2M) as part of OLCF-3 Early Science program
- AP1000 model created and results generated for reactor criticality, rod worth, and reactivity coefficients
- Identical VERA Input models used for Shift, SP_N, and S_N
  - dramatically simpler than KENO-VI input model

Results

- Some of the largest Monte Carlo calculations ever performed (1 trillion particles) have been completed
  - runs used 230,000 cores of Titan or more
- Excellent agreement with KENO-VI
- Extremely fine-mesh S_N calculations, which leverage Titan's GPU accelerators, are under way

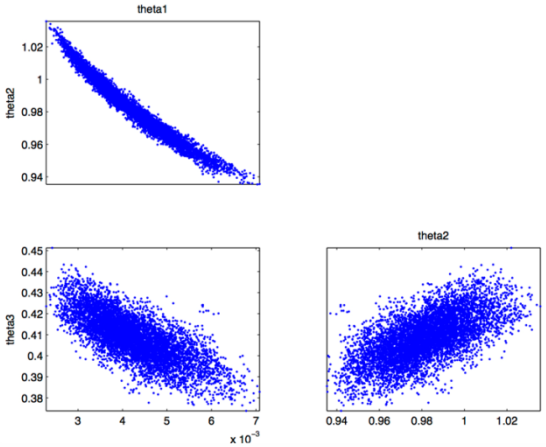
S&T Program: FY14 Highlighted Accomplishments (to date)



- Materials Performance & Optimization (MPO)
  - Crud:
    - MAMBA-BDM - Addition of Darcy two-phase flow & cladding oxidation model
    - MAMBA
      - Development of 1D version for integration into Hydra-TH as subgrid model
      - MAMBA-STAR CCM+prediction of Seabrook Station CRUD deposits
      - Improved thermodynamic models for Bonaccordite [$Ni_2Fe^{3+}(BO_3)O_2$] Nickel Ferrite Clusters
  - PCI:
    - Lower-length scale material modeling of cladding
      - Visco-plastic self consistent model (VPSC) for thermal and irradiation creep and growth
      - Dislocation density crystal plasticity model for Zr-cladding fracture
      - Corrosion and hydriding behavior of Zr-alloys
    - EPRI Test Stand support
    - Pellet-Clad interaction contact model and pellet crack models
    - Study of clad stresses via 2D vs 3D models, effect of pellet crack length
    - Peregrine-VERA-CS coupling and application to PCI
  - GTRF:
    - Cladding wear test & usage in 3-stage wear model validation

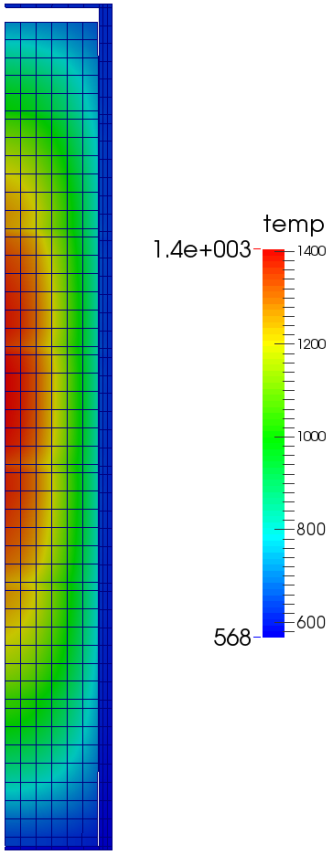
S&T Program: FY14 Highlighted Accomplishments (to date)

- Validation & Uncertainty Quantification (VUQ)
  - Development and application of rigorous solution verification methodology, including evaluating numerical discretization introduced error
  - PCMM assessment of Insilico
  - Verification, validation and UQ of VERA-CS for Progression Problem 6 (single fuel assembly with T-H feedback)
  - Reduced-order methods development using a gradient free dimension reduction for multi-physics coupled code
  - Update of Dakota Baysian Inference capability
  - Development of a generic VUQ plan
  - Authoring of a “Best Practice” guide for CASL usage of Dakota



S&T Program: FY14 Highlighted Accomplishments (to date)

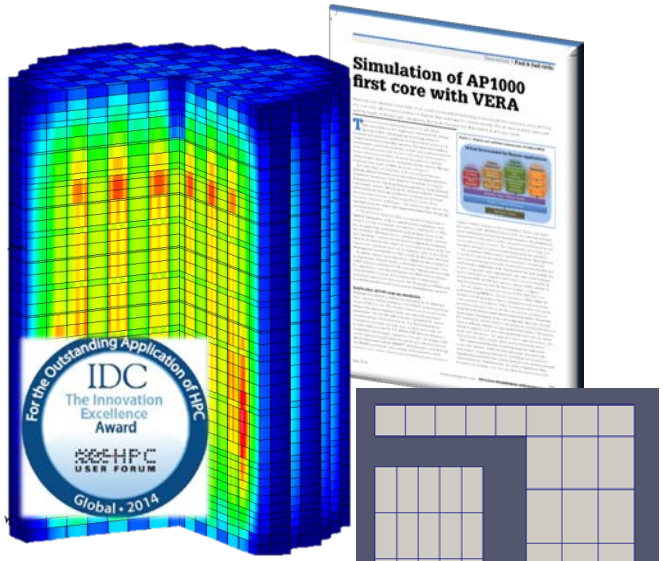
- Physics Integration (PHI)
  - Advancement of VERA-CS to Progression Problem 9 using MPACT-CTF (addition of depletion (Origen API), transient fission products, incore detector response).
  - Coupling of VERA-CS to Peregrine using improved coupling infrastructure using Tiamat (then PIKE) and DTK conserving energy.
  - Assessment of mutiphysics solution acceleration methods.
  - Continued development of parallel data transfer capability for multi-processor/multi-core architectures (DTK) improving computational efficiency and adding surface transfer capability.
  - Parallelization, closure relationships improvements and validation of CTF.
  - Support for WEC Test Stand on analyzing AP1000 Cycle 1 BOC.

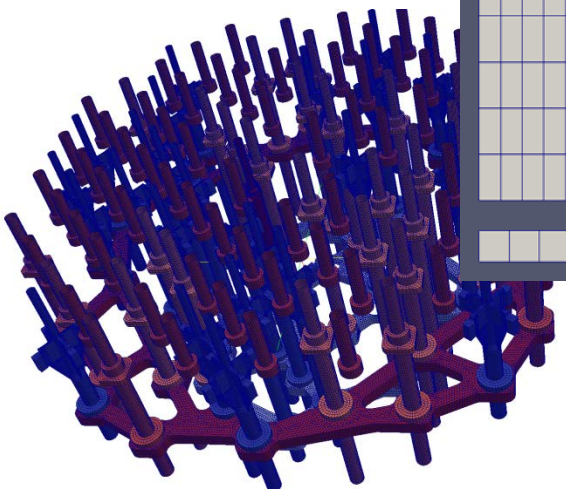


Technology Deployment

We have now deployed 3 Test Stands

- Early deployment to industry for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
  - Westinghouse (Mar 2013): Test VERA core simulator's ability to analyze AP1000 first core startup
  - EPRI (Nov 2013): Benchmark VERA fuel performance (Peregrine) on PCI applications utilizing new EPRI's computing platform
  - TVA (Mar 2014): Test VERA CFD capability (Hydra-TH) on lower plenum flow anomaly observed in operational reactors
- CASL Test Stands have exposed technology gaps, deployment needs, and driven continuous improvement
  - Have become a best practice for us
- More Test Stands on the horizon



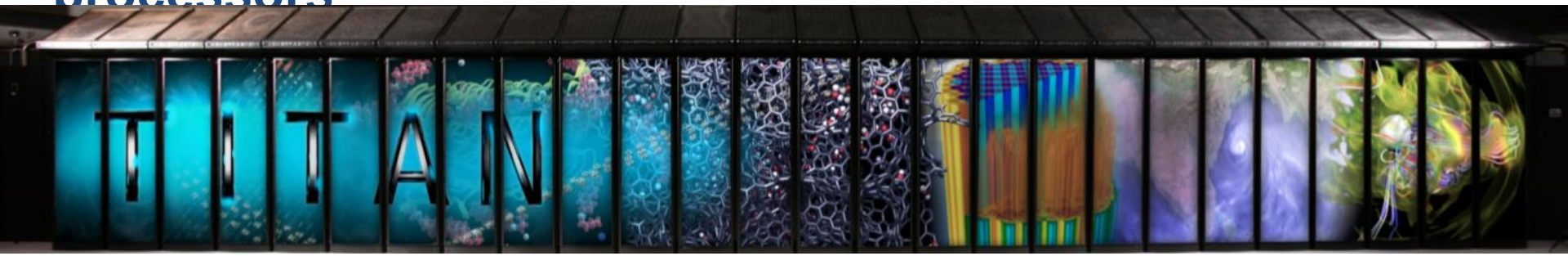


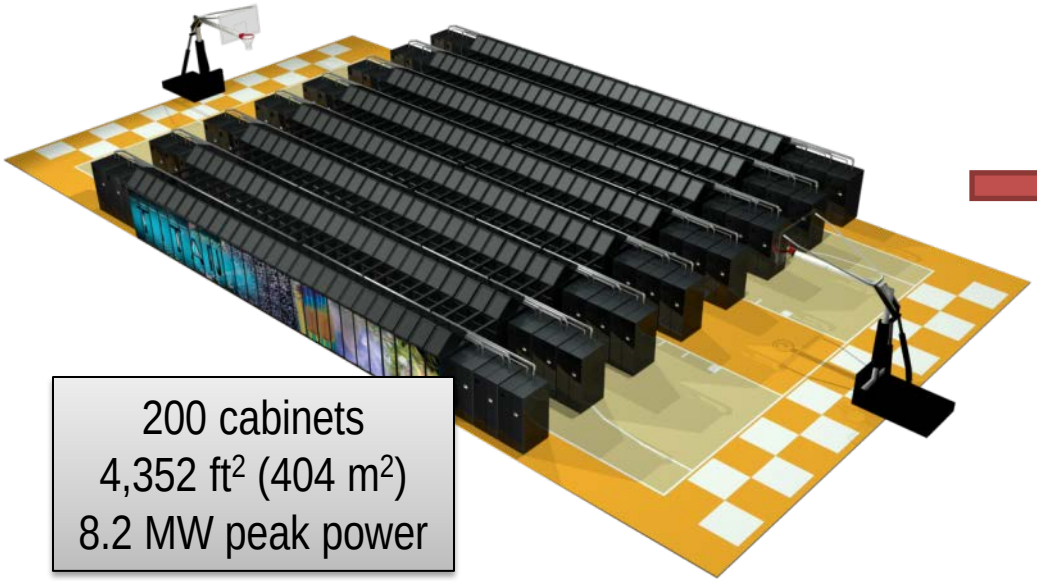
Validation Accomplishments

- There is a large amount of validation work being performed for the CASL codes:
  - CTF: PSBT, BFBT, FRIGG, Harwell, GE3x3, CE 5x5, PNNL 2x6, and Westinghouse Mixing Tests
  - Peregrine: Halden, Studvik SuperRamp & RIS0
  - Peregrine,Bison: GTRF wear model data from ORNL & AECL.
  - Hydra Validation: TAMU 5x5, MIT subcooled boiling data, Westinghouse Mixing Tests, closure relationships using single effect tests.
  - Hydra Benchmarks: Erturk, Moser, Prasad, Elmadi, de vahl Davis & Ghia
  - Insilico ÷ Validation: Watts Bar; Benchmarks SHIFT, KENO
  - MPACT Validation: Watts Bar, B&W 1484, 1810, SPERT & Takahama
  - MPACT Benchmarks: KENO, Insilico & Shift.
  - Shift: Watts Bar, B&W 1484 & B&W 1810
  - Mamba: WALT loop data & CRUD pictures & scrapings from Seabrook

CPIs & FAs will give more details during their presentations

ORNL's "Titan" Hybrid System:
Cray XK7 with AMD Opteron + NVIDIA Tesla processors





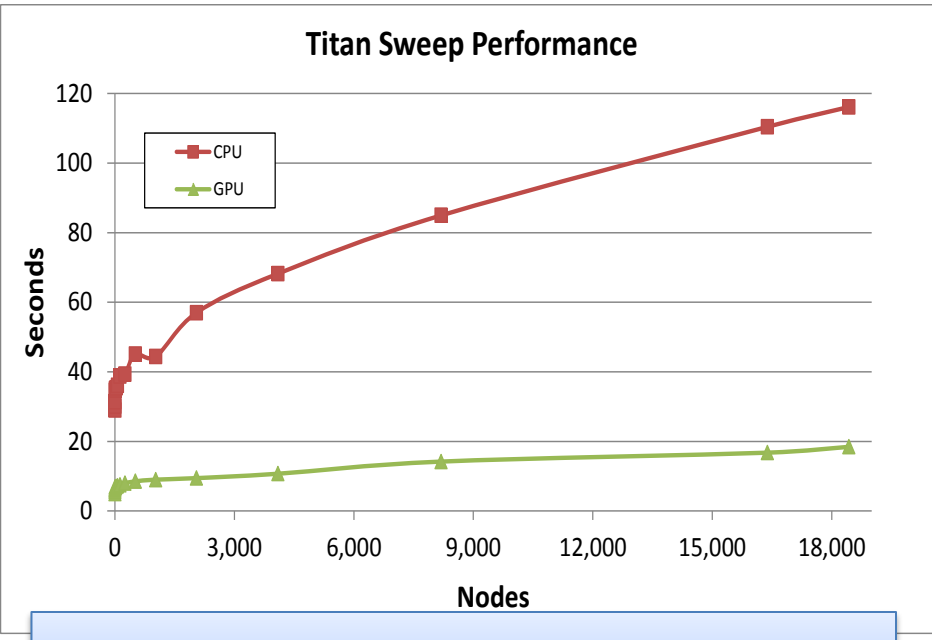
200 cabinets
4,352 ft^2 (404 m^2)
8.2 MW peak power

SYSTEM SPECIFICATIONS:

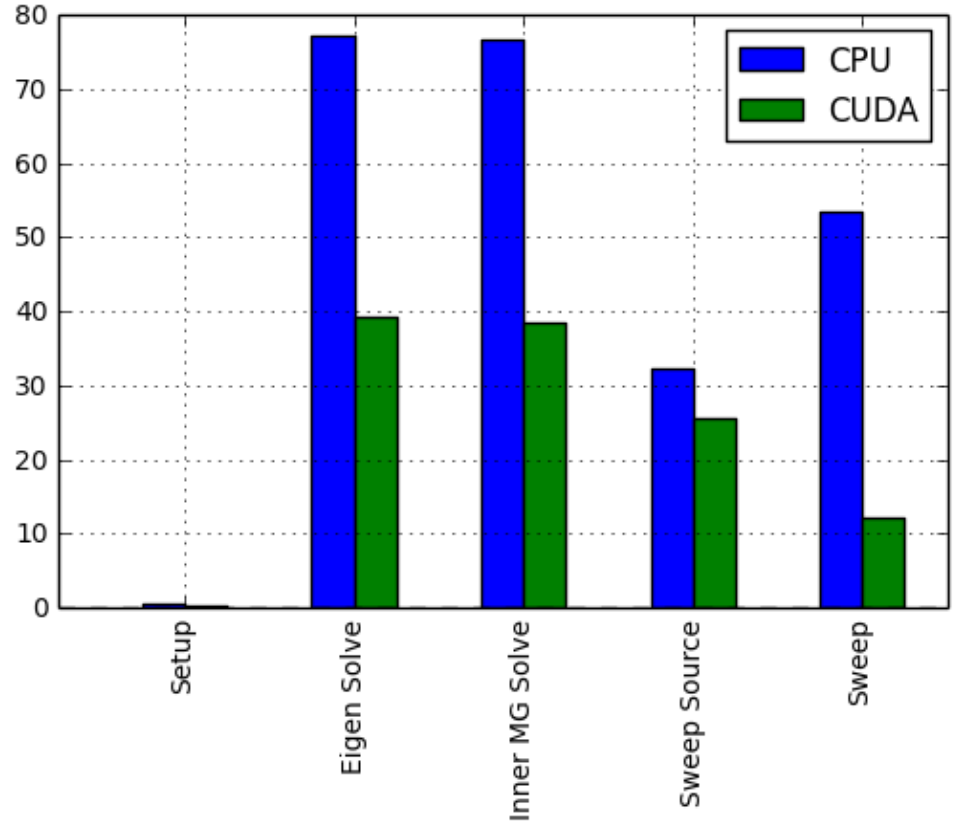
- 27.1 PF/s peak performance
  - 24.5 GPU + 2.6 CPU
- 17.59 PF/s sustained perf. (LINPACK)
- 18,688 compute nodes, each with:
  - 16-Core 2.2 GHz AMD Opteron 6200 CPU
  - NVIDIA Tesla K20x GPU (2688 "cores")
  - 32 GB DDR3 + 6 GB DDR5 memory
- 710 TB total system memory
- 32 PB parallel filesystem (Lustre)
- Cray Gemini 3D Torus Interconnect
- 512 Service and I/O nodes

Throwing away 90% of available performance if not using GPUs

Denovo S_N Acceleration



CPU vs. GPU sweeper, Titan, Kepler K20x



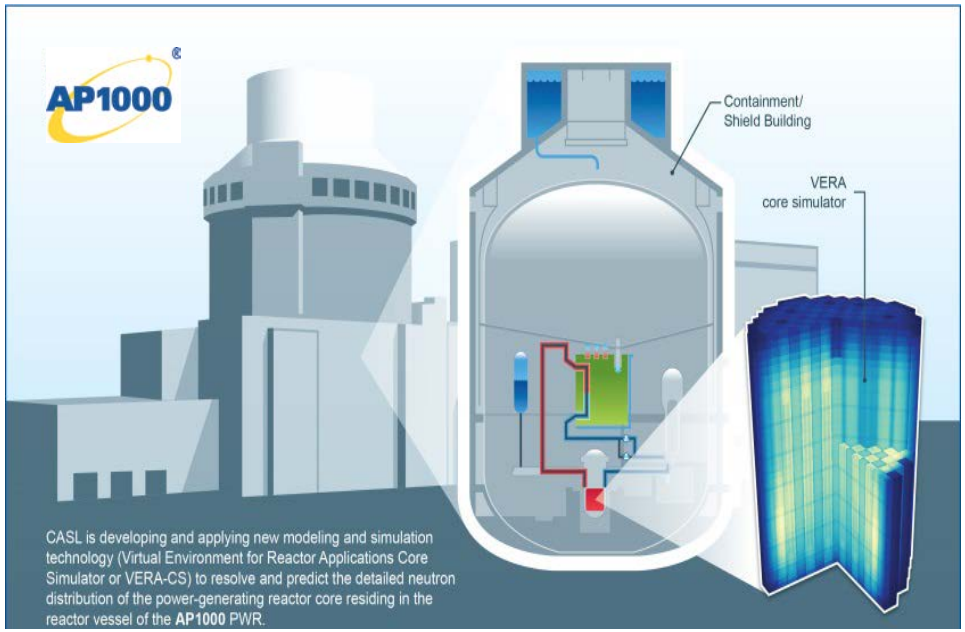
Full Denovo run, CPU vs. GPU sweeper, CPU+GPU vs. CPU only

- SWEEP kernel re-written in C++ & CUDA, runs on CPU or GPU
- Refactored SWEEP is in mainline code
- Titan: SWEEP speedup of 6-7x, Denovo speedup ~3.8x
- Scaling to over 200K cores with opportunities for increased parallelism on GPUs
- Refactored code 2x faster on Cray XT5 (CPU only)

Westinghouse VERA Test Stand

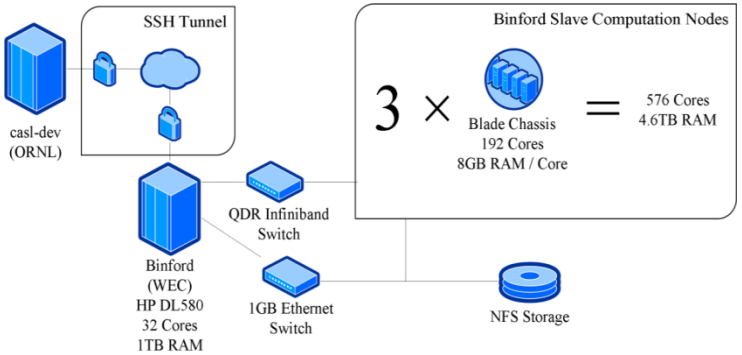
VERA deployed on Westinghouse computer cluster and employed for a high-impact industrial application:

- AP1000 PWR start-up core physics tests simulation



Pictorial of the AP1000 plant with the fission rate distribution predicted by VERA during one of the startup physics tests measurements. It will be possible to compare the VERA predictions against measured data when the first AP1000 unit will come on line in 2015 (Sanmen, China). All the AP1000 units under construction will feature the same startup core modeled by VERA.

VERA-CS simulations performed on a dedicated Westinghouse computer cluster where VERA has been deployed by a CASL-Westinghouse team.
The graphic below shows the computer arrangement and communication to automate VERA updates from the ORNL central repository as new capabilities are being added.



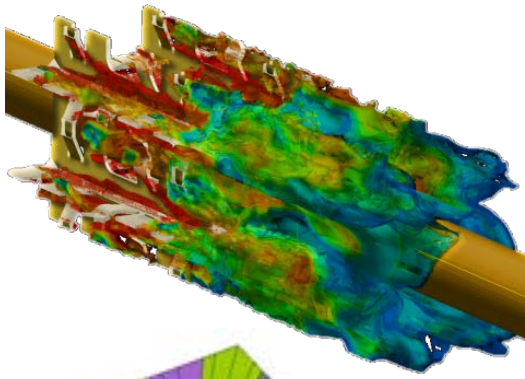
The Westinghouse VERA build is operational and exercised by Westinghouse personnel.

Approaches to neutronics balance accuracy and computational requirements. As part of Titan Early Science, we compared 3 methods (blue rows below).

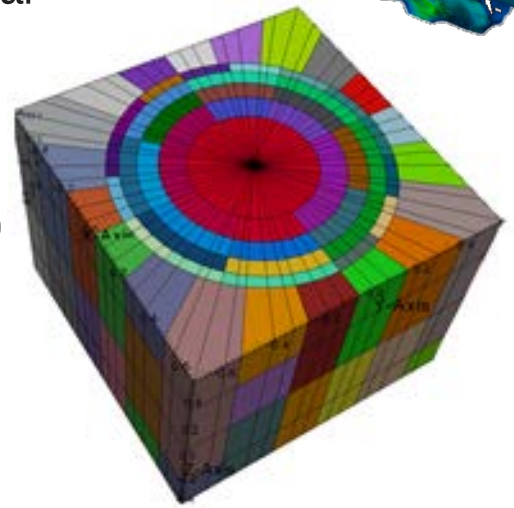
Method	Attributes	Code	Cross Sections	Energy	Scat-tering	Lang., cost	Scalability
Simplified P_N (SP_N)	Cartesian mesh, Lin. Syst.	Insilico	pin-homogen-ized	multigroup	P_N	C++, low	linear solver-dependent
Discrete Ordinates (S_N)	Cartesian mesh, Wavefront	Denovo	self-shielded by region	multigroup	P_N	C++, high	>200,000
Method of Characteristics (MOC)	unstruct. mesh, Ray tracking	MPACT	subgroup	multigroup	P_N	Fortran, medium	in testing
Monte Carlo	CAD, particle tracking	Keno-IV	evaluated	continuous	continuous	Fortran, very high	few hundred
M							

As part of the OLCF CAAR effort, Denovo was GPU-accelerated via CUDA.

Acceleration efforts are underway or in initial phases for other VERA components

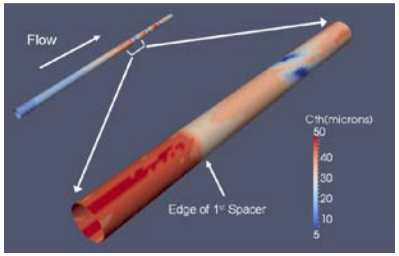


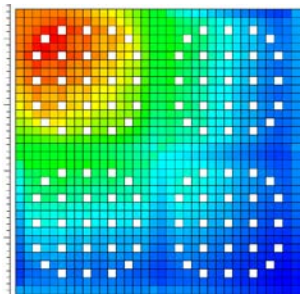
- Hydra-TH (CFD, unstructured finite volume)
  - Performance analysis, code optimization and scaling efforts have improved performance and scaling for both single phase and multiphase (MPI only)
  - Collaboration with NVIDIA has been under way for over a year to exploit hybrid parallelism (MPI + threads)
    - Incorporating NVIDIA's AMG GPU lib, AmgX, into Hydra (https://developer.nvidia.com/amgx)
  - Thread other parts of the code (OpenMP, OpenACC, CUDA)
- MPACT (neutronics, Method of Characteristics)
  - Fortran, so OpenACC is most appropriate path forward
  - NVIDIA staff stationed full-time at ORNL identified to assist team
- Shift (neutronics, Monte Carlo)
  - Core Exnihilo kernels, including Shift, have been extracted and are being released as an open-source mini-app (Profugus)
  - NVIDIA staff have been identified to assist in Shift acceleration
  - Currently awaiting export control ruling for release

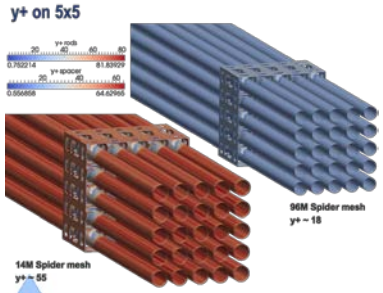


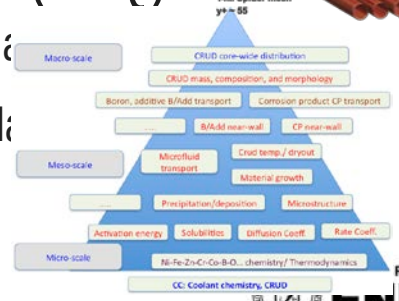
Enabling R&D CASL Objectives

- Fuel Materials and Chemistry (FMC)
  - Mature 3D fuel performance capability with full assessment against CRUD/PCI/GTRF problems. Validated fuel performance models inform assessments of safety margin (PCI) and best operational practices (CRUD, GTRF). Functional capability and partial assessment for RIA- and LOCA-based transient problems.
- Radiation Transport Methods (RTM)
  - Robust 3D pin-resolved transport and prototype hybrid Monte Carlo transport with modern cross section/shielding treatments and coupling to T-H, fuel, and corrosion chemistry capabilities
- Thermal Hydraulics Methods (THM)
  - Robust 3D steady-state/transient turbulent multi-phase capability with subcooled boiling models, an initial assessment of DNB, and complementary with a modern subchannel capability
- Validation and Uncertainty Quantification (VUQ)
  - Mathematical tools and methodologies integrated a accessible to enable quantifying sensitivities and uncertainties in full-scale multi physics PWR simula









By 2015

Industry Council

Assure that CASL solutions are "used and useful" by industry and that CASL provides effective leadership advancing the M&S state-of-the-art.

Objectives and Strategies

- Early, continuous, and 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
- Identification of strategic collaborations between industry and CASL Focus Areas

Outcomes and Impact

- CASL benefits from advice on technical requirements, schedules, commercialization strategies, and computer requirements
- Industry Council can influence the CASL product to be compatible with expected applications and can better prepare internal technical and business processes

Industry Council Membership

Owner/ Operators of Nuclear Plants	Fuel and/or NSSS Vendors	Engineering Design, Service Providers, R&D	Independent Software Vendor	Computer Technology Companies	Ex-Officio
Dominion	AREVA	Battelle	ANSYS	Cray	BOD
Duke Energy	GNF	Bettis /NNPP	CD-adapco	IBM	DOE
EDF	B&W Power Generation	EPRI	Dassault Systemes	NVIDIA	
Exelon	NuScale	Rolls Royce	GSE Systems		
TVA	WEC	Studsvik Scandpower			

Activities since August 2013

Value Proposition

- CASL Development
- Use Case Value

Test Stands

- Westinghouse
- EPRI
- TVA

VERA Interoperability

- CFD tools
- Neutronics
- Sub-channel TH

Utility/Vendor Interactions

- Duke
- AREVA
- GNF

FY14 Budget
Costs through Jun 2014

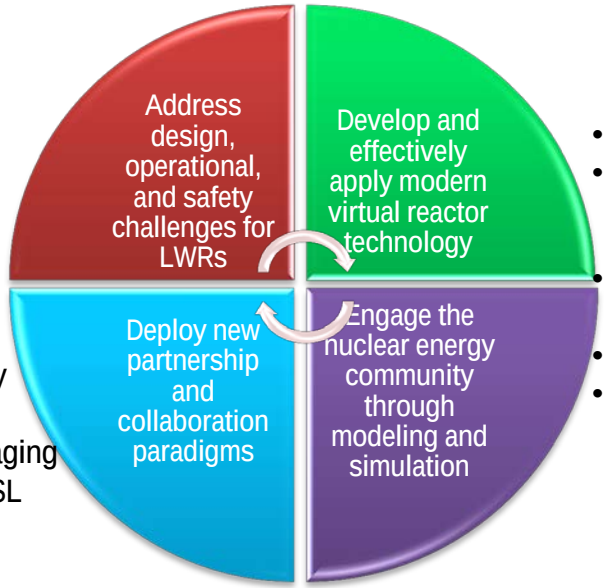
CASL element	FY13 baseline carryover after reallocation	FY14 budget	Total FY14 budget	FY14 cost (June 2014)
DOE Hub FY14 budget		$ 23,124,866		
Management	$ 179,846	$ 2,002,211	$ 2,182,057	$ 1,544,280
Operations	$ 200,338	$ 1,576,810	$ 1,777,148	$ 1,143,241
VOCC infrastructure	$ 358,304	$ 1,500,000	$ 1,858,304	$ 859,862
Board and councils	$ 3,936	$ 192,355	$ 196,291	$ 65,283
Focus areas	$ 3,808,447	$ 17,260,173	$ 21,068,620	$ 12,467,907
Advanced Modeling Applications	$ 561,199	$ 1,979,106	$ 2,540,304	$ 1,278,702
Materials Performance Optimization	$ 1,668,599	$ 4,300,000	$ 5,968,599	$ 2,803,256
Radiation Transport	$ (100,781)	$ 1,950,790	$ 1,850,010	$ 1,430,172
Thermal Hydraulics	$ 307,639	$ 3,225,000	$ 3,532,639	$ 2,192,592
Validation & Uncertainty Quantification	$ 818,635	$ 1,850,000	$ 2,668,635	$ 1,602,675
Physics Integration	$ 553,156	$ 3,955,277	$ 4,508,433	$ 3,160,511
Projected payable invoices	$ -	$ -	$ -	$ 114,314
Sub-contracting overhead and taxes	$ 193,392	$ 865,934	$ 1,059,326	$ 629,907
Contingency/reserve	$ 533,360	$ (272,617)	$ 260,743	$ -
Total	$ 5,277,623	$ 23,124,866	$ 28,402,489	$ 16,824,793

Charge 6: Metrics

What metrics are being used to guide the management of CASL and are they sufficient to assess the performance of the Hub?

- *2013 Review findings*: The Review Team found that CASL has made progress in defining it performance metrics. This includes developing a methodology for how CASL performance metrics are tied to achieving particular outcomes important to meeting the objectives of the Hub. The Review Team also found that CASL is doing a good job of defining how performance will be ranked for the various measures so they can be accumulated to provide a higher level view of the overall performance of the Hub.
- We continue to use our Outcome and Performance Metrics (measured every PoR) to measure progress (see Doug Burns talk)
  - Outcome Metrics for higher level metrics spanning organizational groups and lower lever performance measures
  - Performance Metrics that measure specific areas of performance and act as early indicators

- Challenge Problem Development
- Challenge Problem Innovation



- Challenge Problem PCMM Assessment
- Core Simulator PCMM Assessment

- Number of VERA licenses granted, open source downloads, & registered users
- Industry Council & User Group activity
- Faculty, graduate and/or postdoctoral researchers utilizing or evolving VERA

- VOCC Lab availability and utilization
- Collaborations leveraging or attributable to CASL

Phase 2
Expected Accomplishments

- Established BWR and iPWR core simulator capabilities within VERA, and qualification of the Phase1 PWR capabilities;
- Qualified core-wide CIPS prediction capabilities, including qualified CFD-based subregion simulation, with corrosion product treatments applicable to PWRs and iPWRs;
- Demonstrated GTRF analysis methodology components including an advanced wear model;
- Demonstrated capabilities for PWR fuel performance and PCI predictions using both subgrid and full core geometry, established fuel performance capabilities for BWRs and iPWRs for normal operating conditions, and demonstrated capability to predict BWR fuel performance during LOCA and RIA events;
- Qualified multi-phase CFD capabilities for bubbly flow regimes and prediction of onset of DNB using M-CFD for PWRs and iPWRs, qualified capabilities for thermal/solutal convective fluid flow with boron solution/dissolution chemistry models, demonstrated capability for prediction of onset of DNB during low flow conditions such as post-trip loss of offsite power events for iPWRs and PWRs, and demonstrated M-CFD capability for the flow regimes that exist during normal operations of a BWR;
- Enhanced verification, validation, and documentation of VERA components;
- Established of a self-sustaining post-CASL entity with an active advanced M&S working group and transition of the CASL processes to that entity.

Meeting Agenda

Visit of Dr. Douglas Kothe and Dr. Jess Gehin at the University of Illinois

Monday, October 6th, 2014
9:00 am – 4:00 pm

Discussion on a pathway to build a Test Stand in collaboration with the Oak Ridge National Laboratory and the University of Illinois.

Specific interest: *training and education, verification and validation, and plans for sustainability of the program.*

9:00 am – 10:00 am	Introduction by Dr. Jeffrey Binder, Applied Research Institute
10:15 am – 10:30 am	Meeting with Dr. Andreas Cangellaris, Dean of the College of Engineering at the University of Illinois
10:30 am – 10:45 am	Meeting with Dr. James Stubbins, Department Head of Nuclear, Plasma and Radiological Engineering
11:00 am – 12:00 pm	Seminar by Dr. Douglas Kothe on DOE Energy Innovation Hub
12:00 pm – 1:00 pm	Lunch break
1:00 pm – 4:00 pm	Technical discussion: - Dr. Jess Gehin on technical challenges of DOE Energy Innovation Hub - University of Illinois on the Test Stand, training and education, validation opportunities, and plans for sustainability of the program

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

Douglas B. Kothe
Oak Ridge National Laboratory
kothe@ornl.gov

Accelerated and translational R&D, from fundamental discovery to commercialized technology, has proven challenging for nuclear energy; innovations are challenging in an enterprise that that is inherently conservative and regulatory-driven. Translational research—a high return proposition for nuclear energy—is exactly what Energy Innovation Hubs established by the U.S. Department of Energy (DOE) strive to enable and accelerate. Hubs bring together teams of top scientists and engineers from academia, industry, and government to collaborate and overcome critical known barriers to achieving national climate and energy goals that have proven resistant to solution via the normal R&D enterprise. Hubs focus on a single topic, with the objective of rapidly bridging the gaps between basic research, engineering development, and commercialization through a close partnership with industry. To achieve this goal, the Hubs necessarily consist of large, highly integrated and collaborative creative teams working to solve priority technology challenges. For the Consortium for Advanced Simulation of Light Water Reactors (CASL), awarded as the first Hub by the DOE Office of Nuclear Energy (NE) in July 2010, the focus is on innovating commercial nuclear power generation, specifically the modeling and simulation (M&S) of nuclear reactors. CASL not only strives to bring innovation to the nuclear energy enterprise but also to help retain and strengthen U.S. leadership in two DOE mission areas: HPC-enabled M&S and nuclear energy. CASL is currently completing its fourth year of a five-year Phase 1 execution and has been granted the opportunity by DOE to submit a proposal for a second five-year Phase 2 (2015–2019) of execution.

CASL's unique partnership of government, academia, and industry possesses unparalleled collective institutional knowledge, nuclear science and engineering talent, computational science leadership, and LWR design and regulatory accomplishments. CASL has several key elements: clear deliverables and products that solve industry issues and are driven by a well-defined yet dynamic plan for executing on deliverables; a strategy of delivering prototype products early and often; defined customers and users, with "industry pull" ensured by an Industry Council with members from the nuclear energy and M&S communities; regular engagement with all levels of the U.S. Nuclear Regulatory Commission (NRC), from the research branch to the Commissioners; peer (equal) private-public partnership in management, leadership, and execution under one "virtual" roof; a lead institution (ORNL) with resource allocation authority and responsibility; an independent Science Council to review and advise on quality and relevance of its science and technology (S&T); and a Board of Directors providing oversight and advice on management, plan, and S&T strategy.

After giving a brief overview of CASL's vision, mission, strategic goals, and current status, the challenges, lessons learned, and best practices encountered during CASL's execution to date will be discussed, with illustrative examples given where possible.