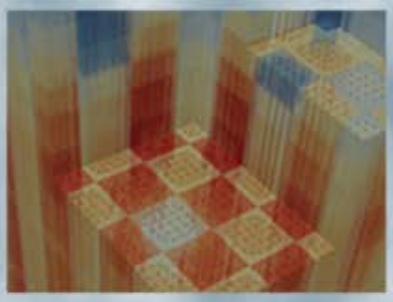
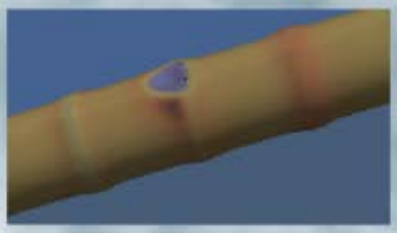
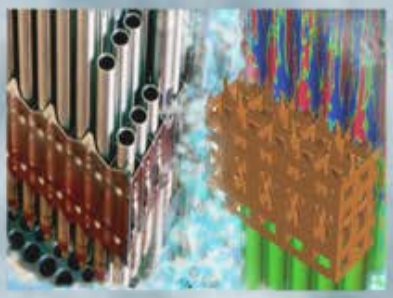
CASL-U-2015-0204-000

CASL Overview with the UK National Nuclear Computing Centre of Excellence: Experience and Lessons Learned from ORNL







Doug Kothe and Jess Gehin
Oak Ridge National Laboratory

October 10, 2014

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2015-0204-000

A DOE Energy Innovation Hub

CASL: The Consortium for Advanced Simulation of Light Water Reactors

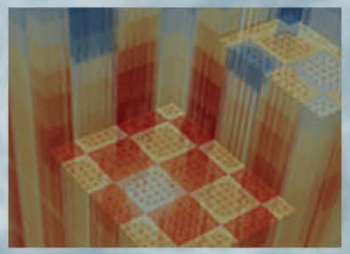
A DOE Energy Innovation Hub

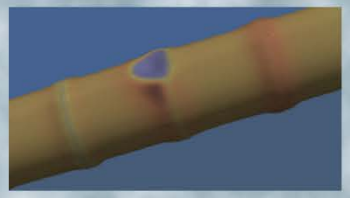
Doug Kothe (ORNL)

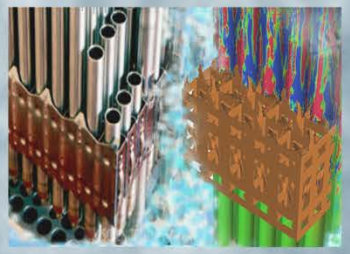
CASL Director

Jess Gehin (ORNL)

CASL Physics Integration Focus Area Lead







U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

CASL-U-2015-0204-000

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

UK National Nuclear Laboratory (NNL) Visit:

UK National Nuclear Computing Centre of Excellence: Experience and Lessons Learned from ORNL

Agenda as of October 10th, 2014

Event contact	Andrew Worrall, 865-576-9369 (office); 865-313-0177 (mobile); worralla@ornl.gov
NNL Visitors: Mark Bankhead, Robert Gregg, Daniel Mathers, Fiona McLachlan, Nick Underwood	

Time	Event	Lead	Attendees	Place
Monday, October 20th, 2014				
8:30am	1. Badging	Andy Worrall (ORNL)	NNL visitors	Badging office
9:00 am	2. Introductions	ALL	NNL visitors All ORNL participants	Building 5700, Room L204
9:30 am	3. Objective of the visit	Mark Bankhead (NNL)	NNL visitors All ORNL participants	Building 5700, Room L204
9:45 am	4. Introduction to UK Nuclear Computing Centre of Excellence	Mark Bankhead (NNL)	NNL visitors All ORNL participants	Building 5700, Room L204
10:15 am	Coffee Break			
10:30 am	5. NNL research themes related to NCCE • Reactor chemistry • Structural materials • Fuel performance • Molecular modelling	NNL	NNL visitors All ORNL participants	Building 5700, Room L204
11:30 am	6. CASL – An example at ORNL. Focus on approach to the project and high level objectives, rather than technical specifics.	Doug Kothe (ORNL)	NNL visitors	Building 5700, Room L204
12:30 pm	Lunch			ORNL cafeteria

OAK RIDGE National Laboratory

AGENDA

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Event contact	Andrew Worrall, 865-576-9369 (office); 865-313-0177 (mobile); worralla@ornl.gov

NNL Visitors: Mark Bankhead, Robert Gregg, Daniel Mathers, Fiona McLachlan, Nick Underwood

Time	Event	Lead	Attendees	Place
Monday, October 20th, 2014				
1:30 pm	7. Tour of CASL facilities (includes EVEREST, and ORNL siting study work)	Gary Mays (ORNL) Jamison Daniel (ORNL)	NNL visitors	Building 5700, CASL
3:00 pm	8. Modeling components to CASL and at ORNL • Utility view on CASL • Fuels, Materials, and Chemistry • Thermal Hydraulics Methods • Radiation Transport Methods • Validation and Modeling Applications • Physics Integration • Computational science	Rose Montgomery (TVA) TBC David Pointer (ORNL) Bob Grove (ORNL) TBC Jess Gehin (ORNL) John Turner (ORNL)	NNL visitors	Building 5700, Room L204
5:00 pm	End of Day 1			

OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Event contact	Andrew Worrall, 865-576-9369 (office); 865-313-0177 (mobile); worralla@ornl.gov			
NNL Visitors: Mark Bankhead, Robert Gregg, Daniel Mathers, Fiona McLachlan, Nick Underwood				
Time	**Event**	**Lead**	**Attendees**	**Place**
Tuesday, October 21st, 2014				
9:00 am	1. Fuel cycle modeling	Eva Sunny (ORNL) Josh Peterson (ORNL) Robert Gregg (NNL)	NNL visitors	Building 5700, Room L202
9:30 am	2. Fuel performance and related modeling	Jeff Powers (ORNL)	NNL visitors	Building 5700, Room L202
10:00 am	3. SCALE suite	Brad Rearden (ORNL)	NNL visitors	Building 5700, Room L202
10:30 am	4. Tour of ORNL computing facilities	Jim Hack (ORNL)	NNL visitors	Building 5700, Computing area
11:30 am	Lunch			ORNL cafeteria
1:30 pm	5. Tour of facilities • SNS (1:00 to 1:45 pm) • REDC (2:00 to 2:30 pm) • HFIR (2:30 to 3:30 pm) • Fuel labs (3:45 to 4:30 pm)	Nina Jalarvo (ORNL) Porter Bailey (ORNL) Chris Bryan (ORNL) Kurt Terrani (ORNL)	NNL visitors	Various
4:30 pm	6. Review of key findings and way forward	NNL (supported by Andy Worrall)	NNL visitors	Building 5700, Room L202
5:30 pm	End of Day 2			

Additional Information

It is proposed to establish a UK Nuclear Computing Centre of Excellence (NCCE) that will see industry, NNL and academia engage in national and international collaborative research in the development, validation and application of nuclear computer modeling techniques and solutions using the UK's High Performance Computing (HPC) infrastructure, particularly Science and Technology Facility Council's (STFC's) Hartree Centre. Computer modeling is an essential facet of predicting performance and lifetime of nuclear systems and underpinning their safe and economic operation. The Tildesley report (2011) commissioned by the Rt. Hon David Willetts MP, reported that for every £1 invested in E-infrastructure the output to the UK economy was £10 after two years and £25 after five years so this investment in the NCCE might be expected to yield on the order of £150 million impact on the UK economy by 2020. It is recognized in the Nuclear Industrial Strategy (NIS) as being 'fundamental to future advances in nuclear technology, including both fuel and reactors.' NCCE will provide industry with access to and the skills to exploit the hardware and software associated with HPC and big data and will conduct research in collaboration with a network of national and international research organizations on the theme of modeling, observation, validation and interpretation (MOVI) in order to support decision-making which is based on high-fidelity simulations that are validated rigorously using reliable data to achieve public credibility.

The UK NNL attendees and their specific technical area of expertise are:

- **Nuclear Computing Centre of Excellence** (M Bankhead)
  Discuss NNL plans to lead the development of model development and validation for the UK civil nuclear industry. Topics to be covered include areas for overlap with the CASL and NEAMS programmes, development of facilities to enable US-UK collaboration (including video conferencing and remote working).
- **Reactor chemistry** (Fiona McLachlan)
  NNL plans to develop reactor chemistry models (radiolysis, corrosion, cooling circuit chemistry). NNL has interests in developing advanced modelling codes (e.g. using the MOOSE frameworks) to increase fidelity of chemical models. Opportunities for sharing experience collaboration with ORNL scientists will be explored.
- **Fuel Cycle modelling** (Robert Gregg)
  The discussions will cover NNL's ORION fuel cycle modelling tool for process level assessments of fuel cycle options and links to ORNL programmes. Discussions will also cover NNL and ORNL interests in fuel performance (also linked to atomistic modelling) and neutronics modelling. These discussions could extend to plans for development of next-gen FP codes based on HPC systems.
- **Structural Materials modelling for reactor systems and components** (Nick Underwood)
  Discussions will be focused around how NNL experience in structural modelling for fuel cycle. NNL has an interest in developing its capability to provide structural modelling support to new build and advanced reactor concepts.
- **Molecular modelling of materials chemistry** (M Bankhead)
  Development of atomic and mesoscale models of materials in nuclear environments, current NNL focus is primarily aimed at waste management and reprocessing. Will discuss NNL strategic links to UK university research and plans to develop methods for fuel performance modelling on atomistic and mesoscales.

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

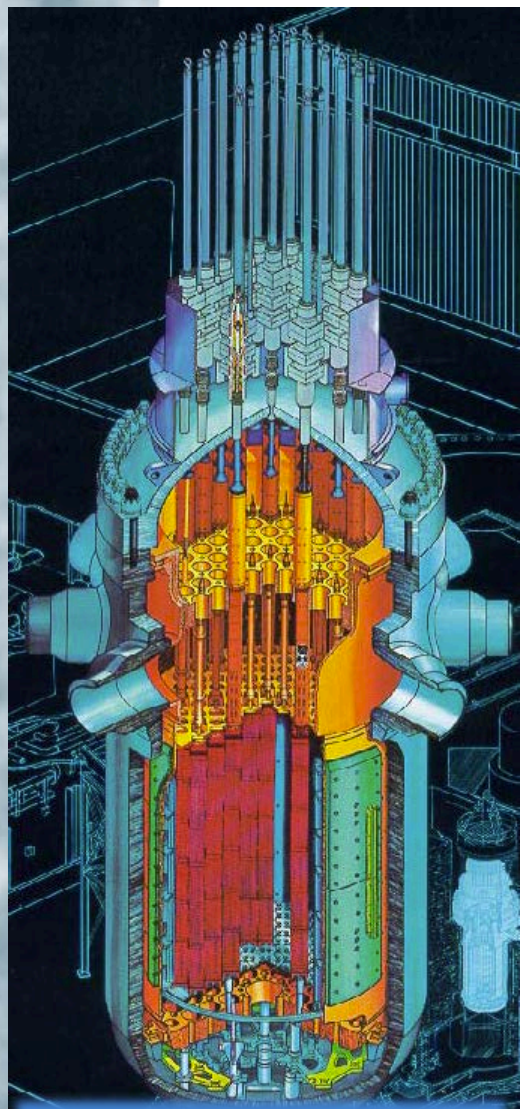
Strong Dependency on Modeling and Simulation

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]

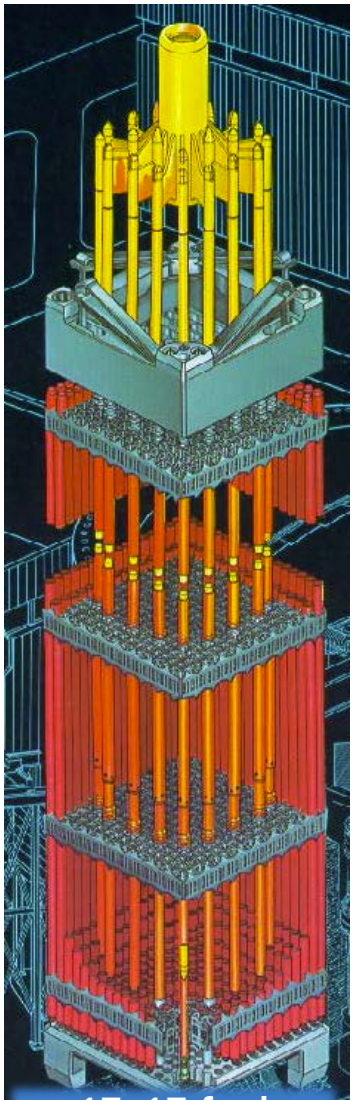
Need to minimize economic uncertainty associated with new product introduction (e.g. fuel) by employing precise predictions [1% error in core reactivity has $4M annual fuel cycle cost impact for 1 GWe unit]

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

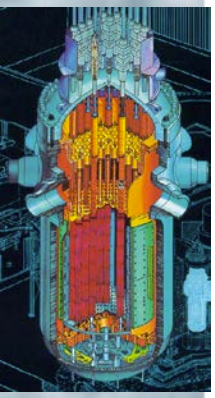
Fuel Temperatures
- 4140° F (max centerline)
- 657° F (max clad surface)

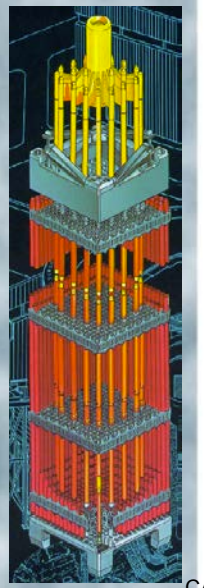
~51,000 fuel pins and over 16M fuel pellets in the core of a PWR!

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.

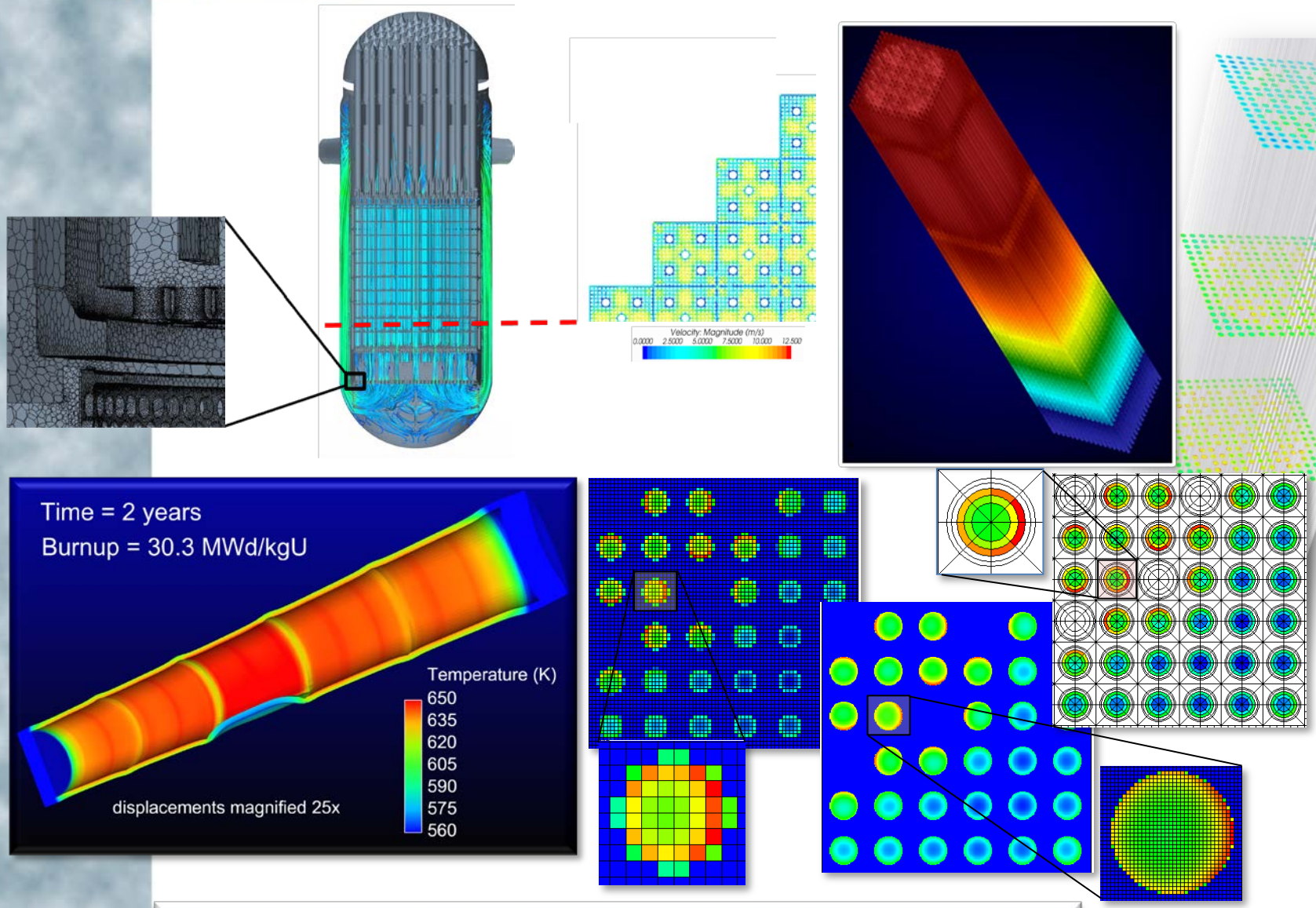
Nuclear Energy Drivers and Payoffs for M&S technology





- 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

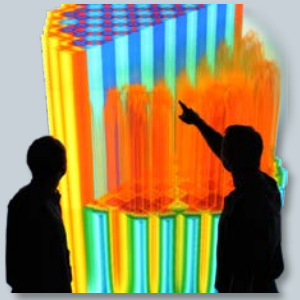


From full core to fuel assembly to fuel subassembly to fuel pin/pellet

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

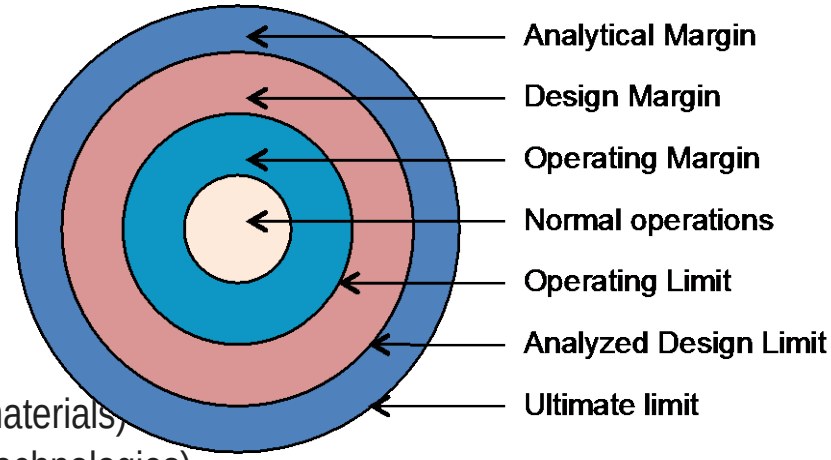
CASL Components

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)

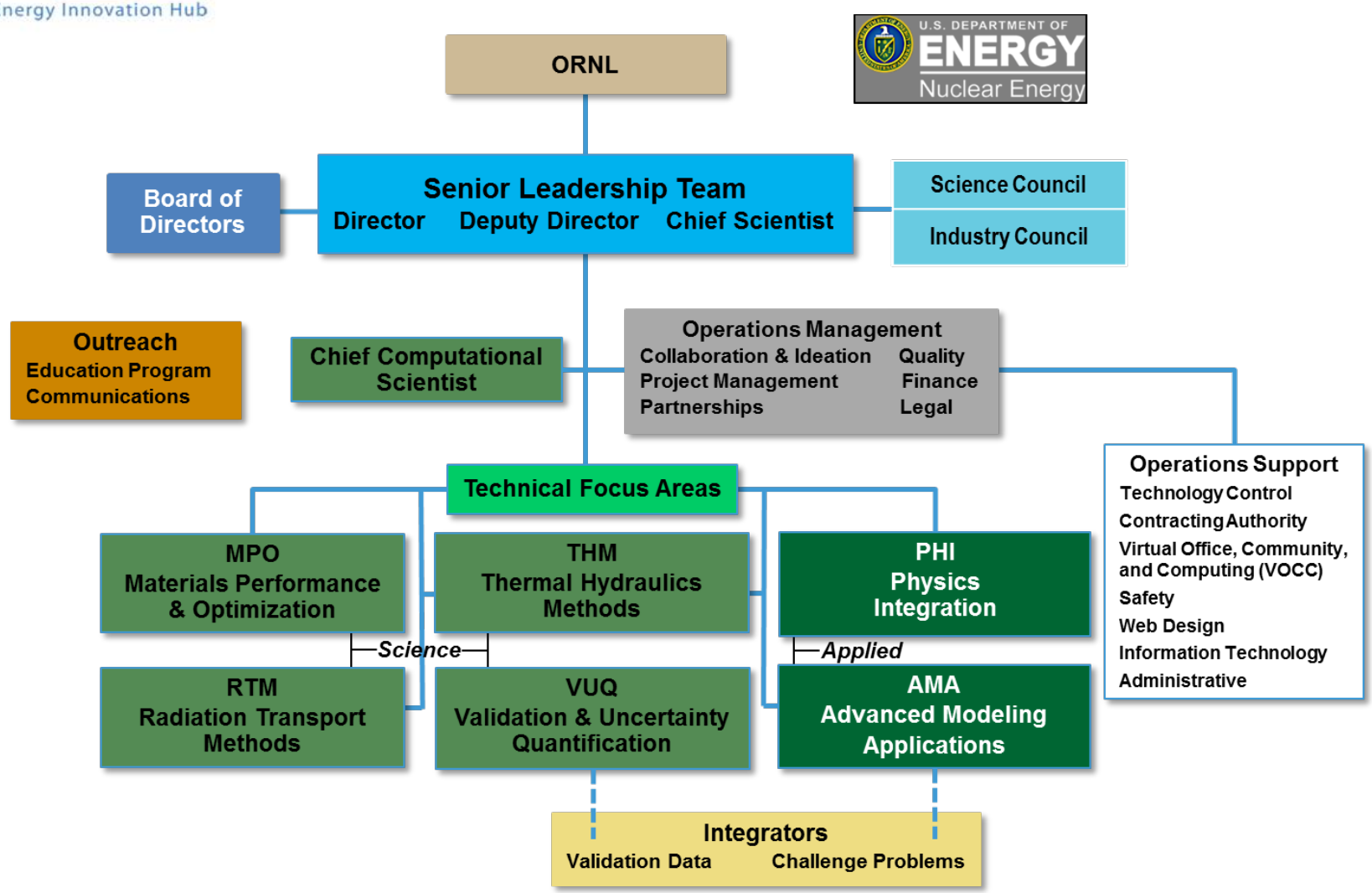


- Requires a strategic approach
  - How much is needed? How to allocate?
  - How can margin be transferred from one bucket to another?
- Key considerations
  - Plant operating parameters & assumptions (plant optimization & flexibility, load follow)
  - Fuel hardware (advanced product features & materials)
  - 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

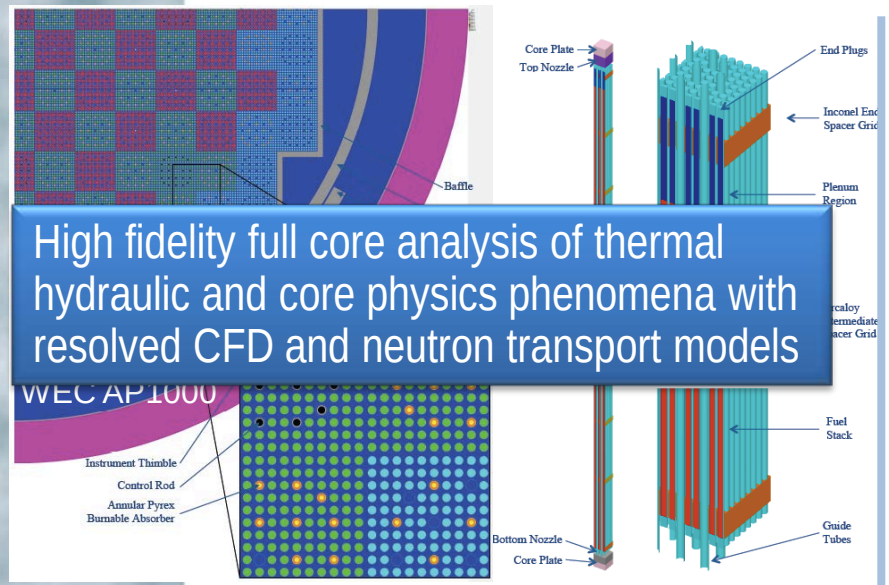
Physics Integration
Lead Jess Gehin
Deputy Scott Palmtag

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

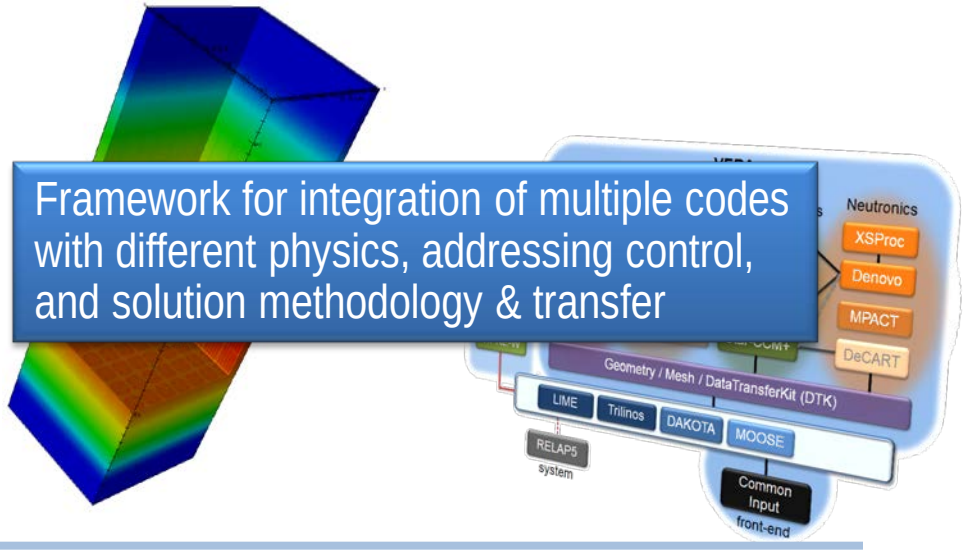
CASL Innovations

Advanced Modeling Applications



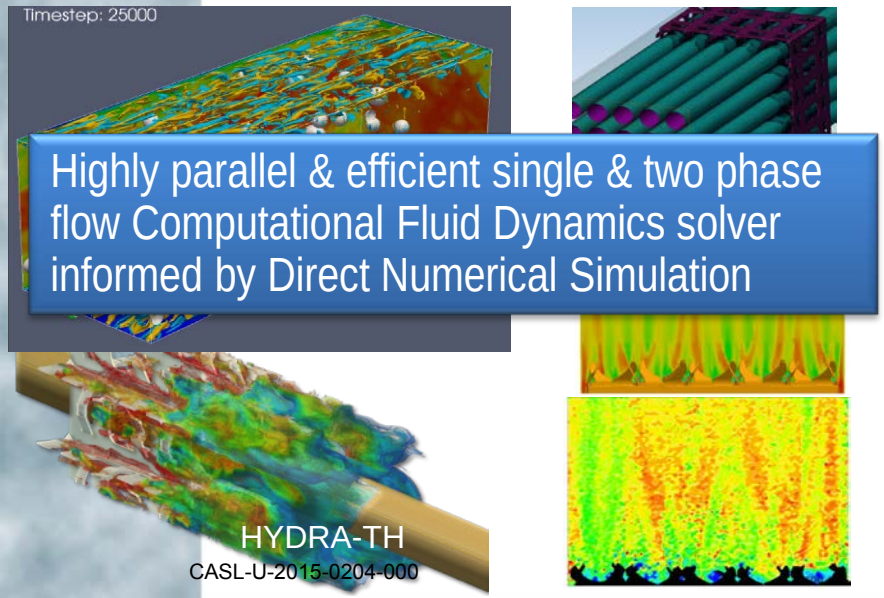
High fidelity full core analysis of thermal hydraulic and core physics phenomena with resolved CFD and neutron transport models

Physics Integration



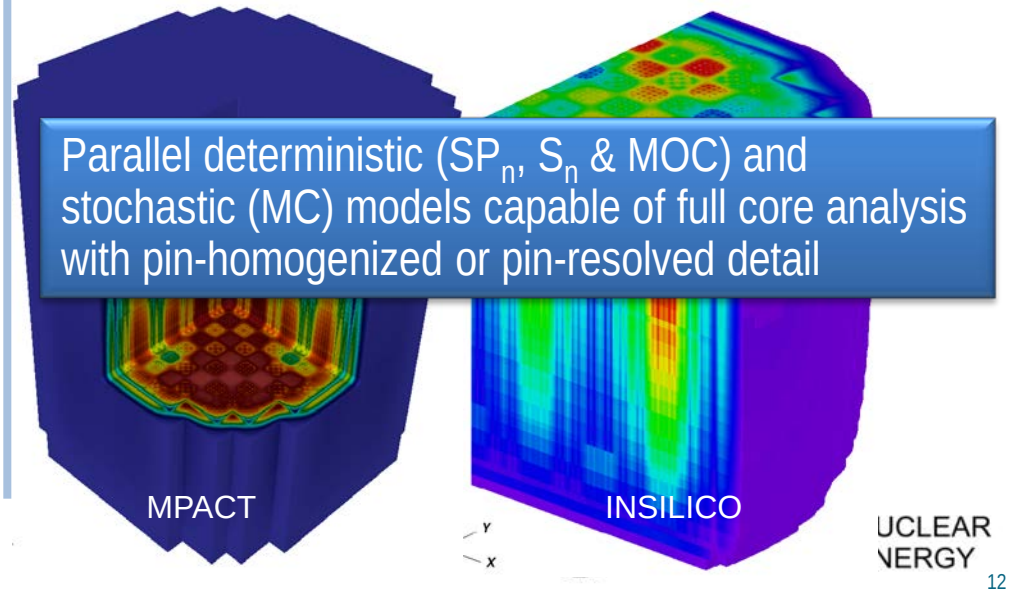
Framework for integration of multiple codes with different physics, addressing control, and solution methodology & transfer

Thermal Hydraulic Methods



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

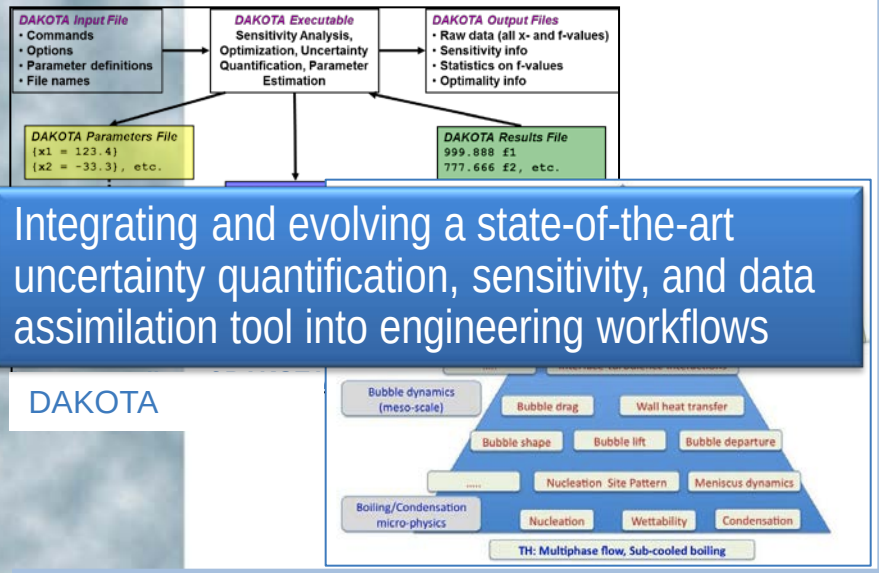
Radiation Transport Methods



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



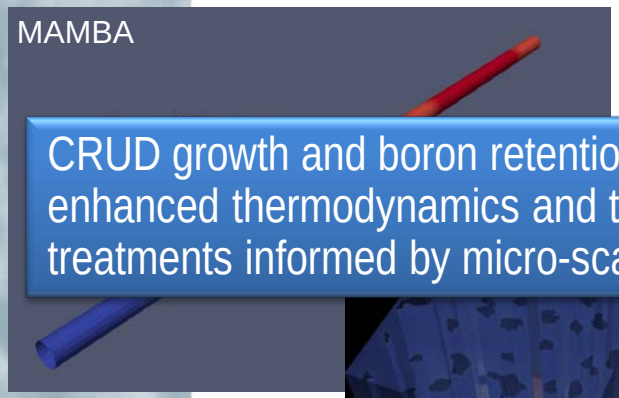
Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows

DAKOTA

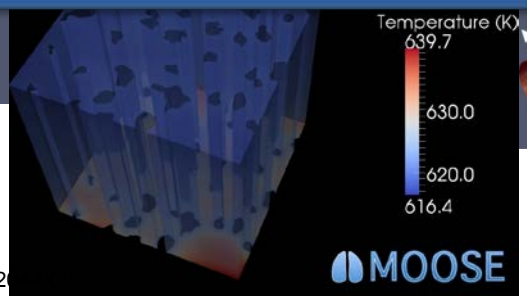
VOCC

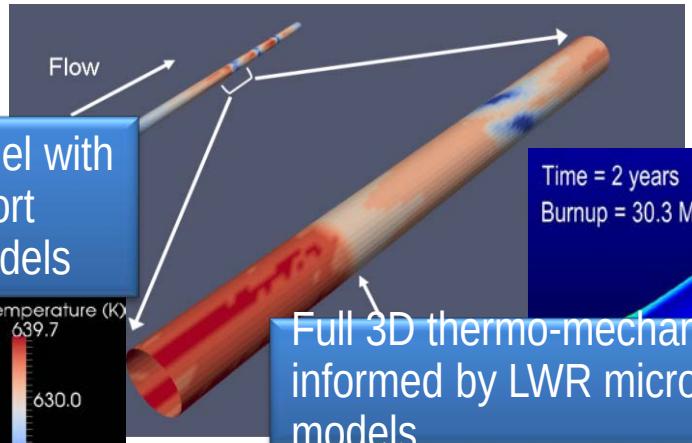
Bringing together local ("physical") and geographically distributed ("virtual") contributors in a meaningful and productive way

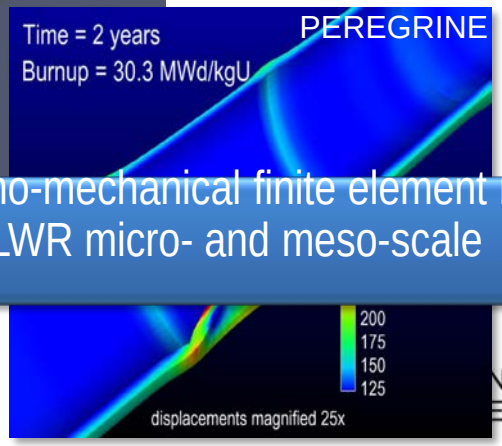
Materials Performance and Optimization



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

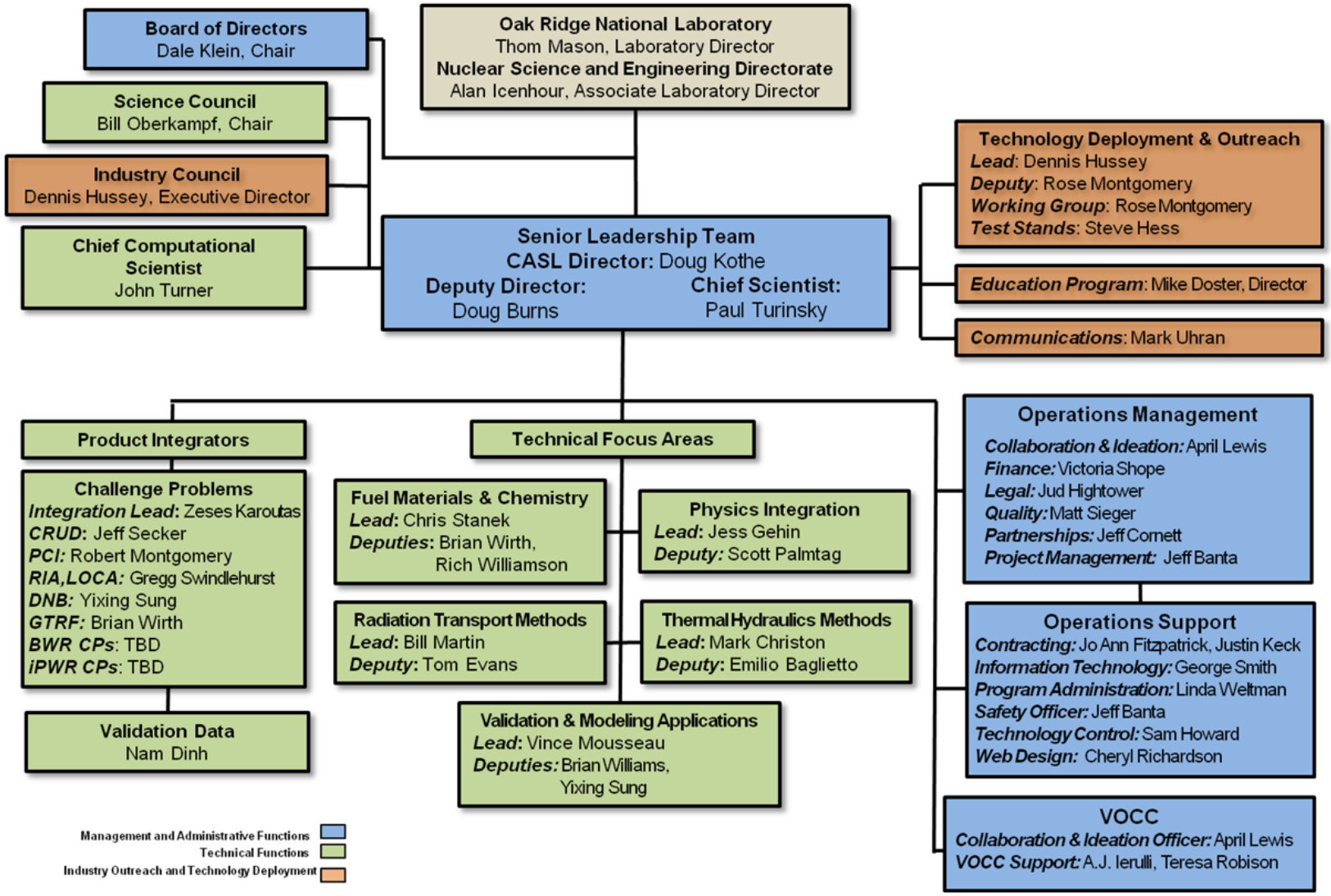






Full 3D thermo-mechanical finite element model informed by LWR micro- and meso-scale models

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)

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

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

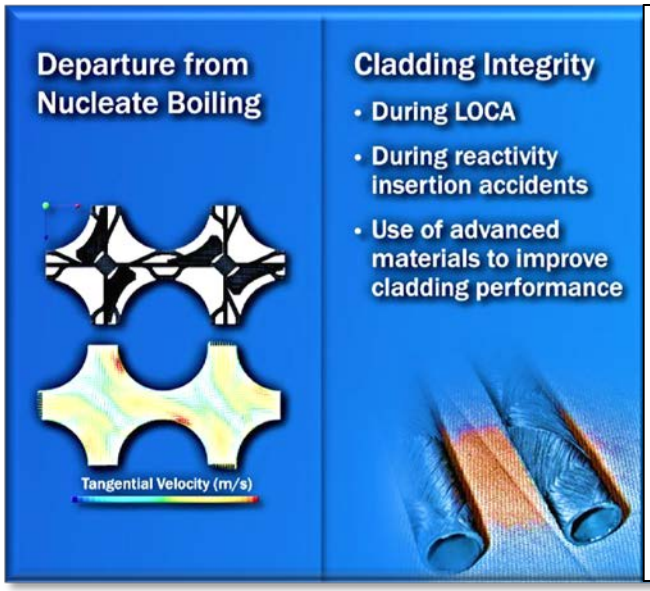
- Purpose: Independent assessment of S&T capabilities being developed and integrated into VERA

- 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

CASL Challenge Problems

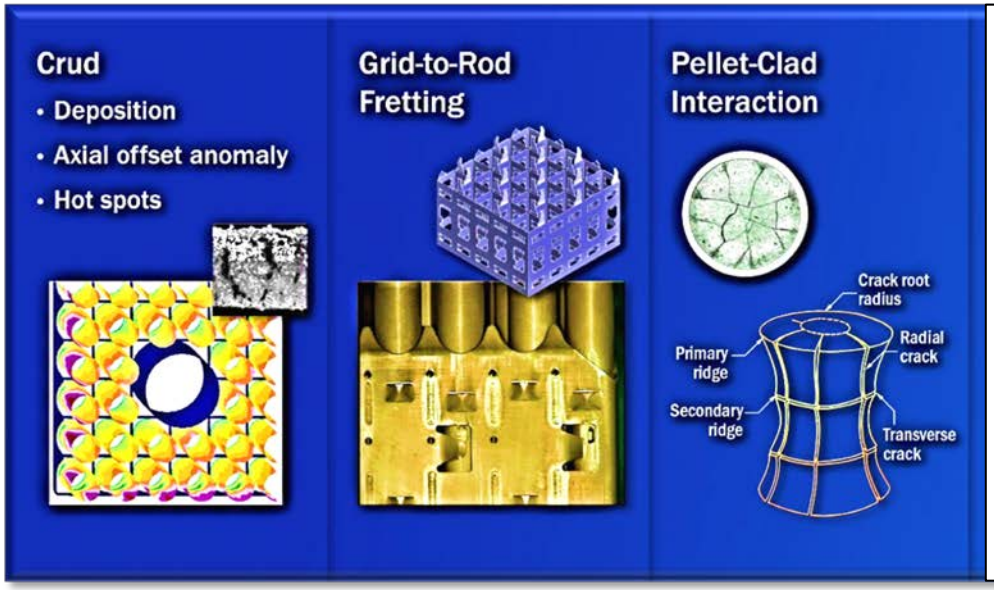
Key safety-relevant reactor phenomena that limit performance



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

VERA-CS

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

Scott Palmtag

Cladding Integrity (RIA)

- Predict PCMI Margin using MPACT and PEREGRINE2D

Gregg Swindlehurst

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

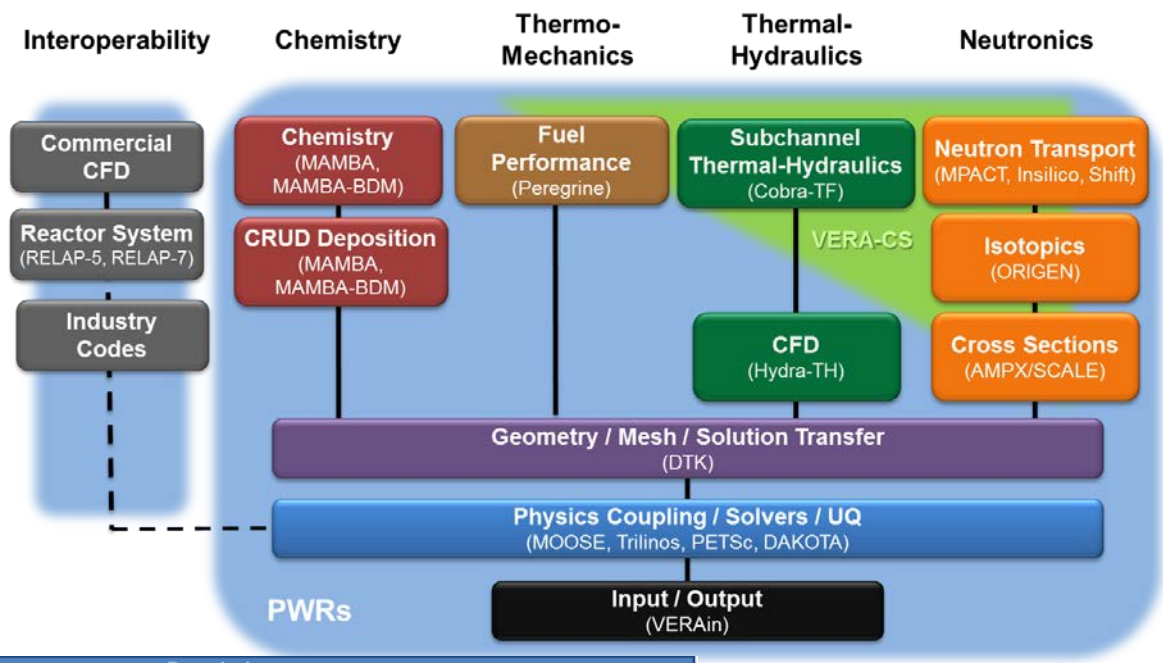
- Predict Minimum GTRF Margin in Core using PEREGRINE2D – grid to rod gap, STAR/HYDRA-TH excitation force

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)



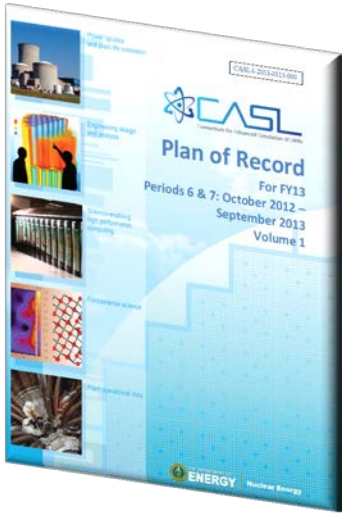
Item	Description
S/W Development Tools and Computational Infrastructure	Standardized set of compilers and configuration tools Git revision control system and S/W repository management Build & test infrastructure (TriBITS, CMake, CTest, CDash) 17 geographically dispersed code repositories, 205 TriBITS 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

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)

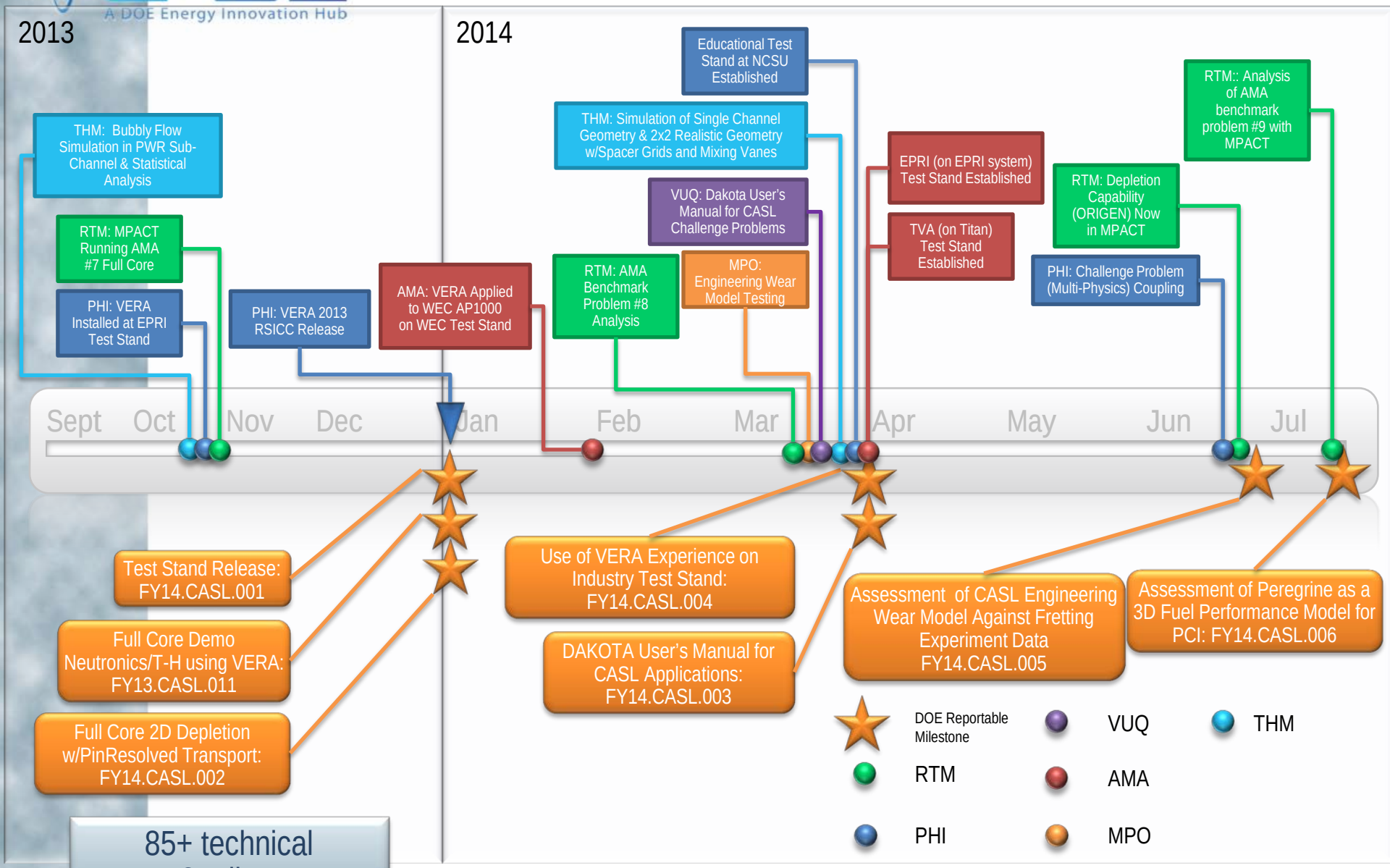
Develop and updated Tiamat coupling capability based on updated MOOSE and other VERA components (specifically those related to VERA-CS). This will provide the necessary capability to support CASL milestone L1:CASL.P9.03 "Demonstrate integrated VERA-CS for the PCI challenge problem (FY14.CASL.008)" Supported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

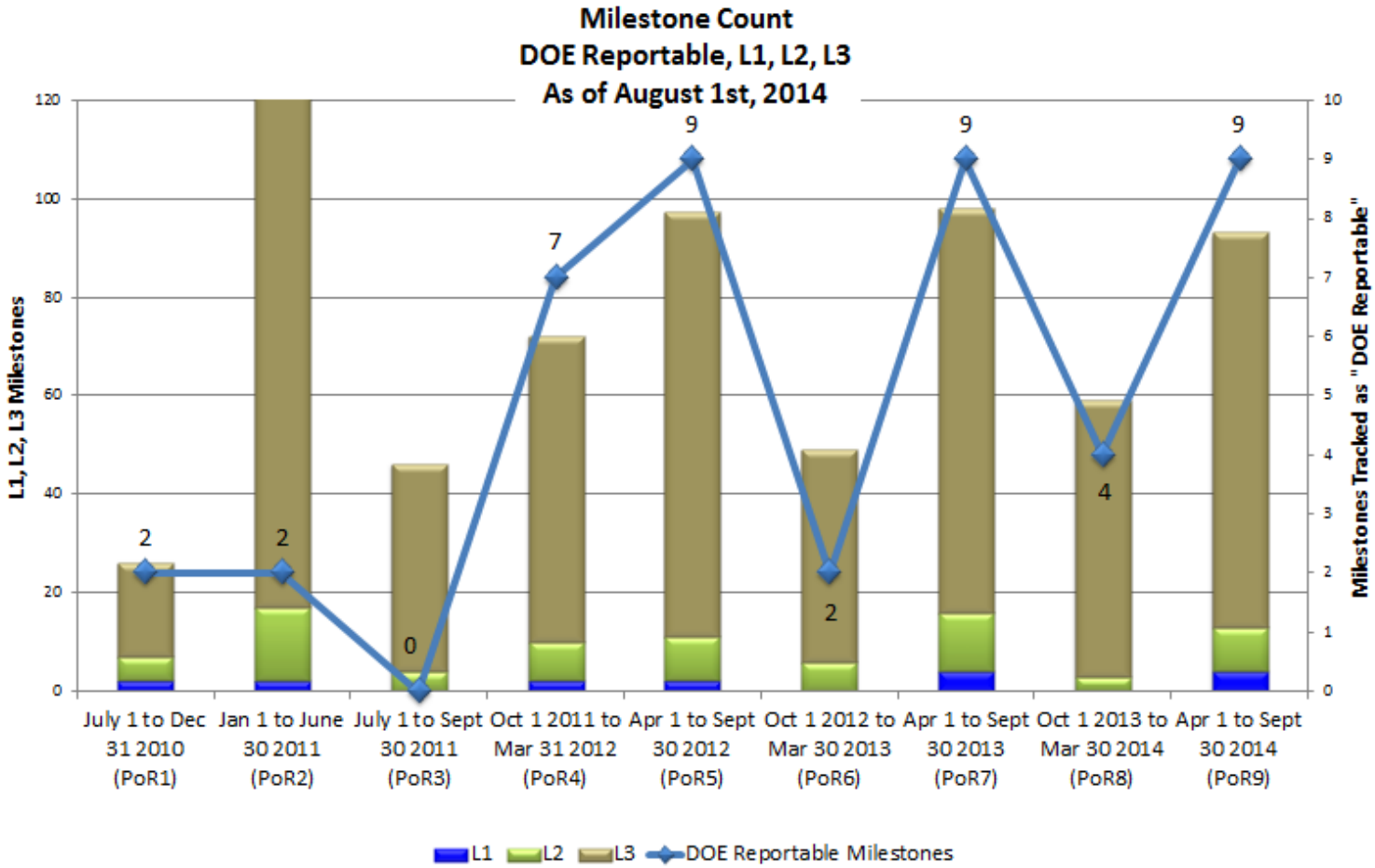
Selected Accomplishments



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

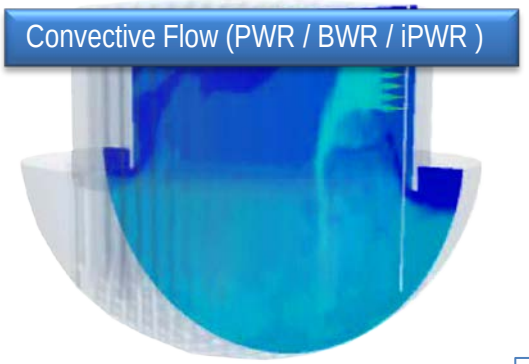
Focus Area	Documented in CASL RMS
AMA	115
VUQ	65
PHI/VRI	110
RTM	43
THM	91
MPO	67
Others	158
Total	**649**

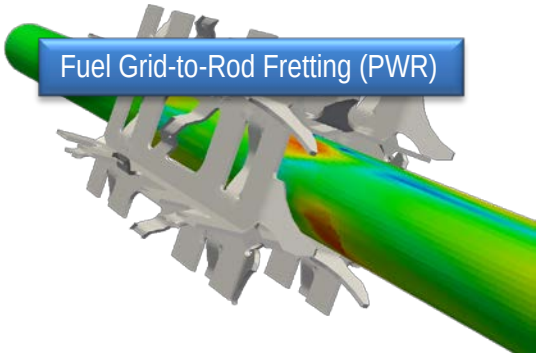
Milestone reports outside of Focus Areas

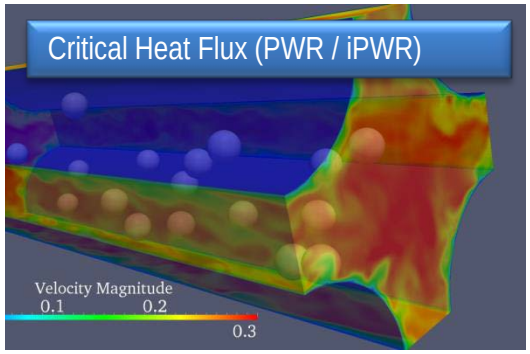
Category	Milestones Reports Maintained in CASL RMS
CASL	23
CASL internal	23
Export Control	1
Industry Council	8
Non-Focus Area	62
Production Integration	14
Project Management	5
Quality Assurance	10
Senior Leadership Team	3
Technology Control	9
Total	**158**

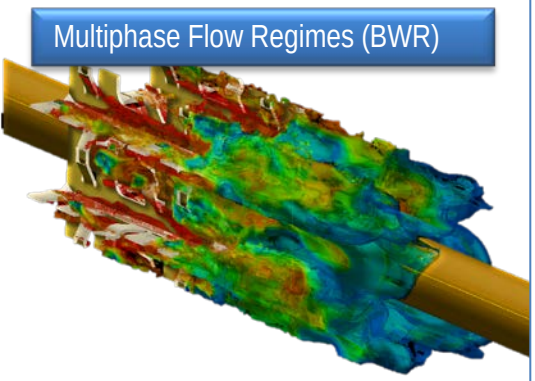
- All CASL documents are captured in the CASL Records Management System (RMS) – considered a best practice
- As many of the milestone reports as possible are being made publicly available on the CASL website (www.casl.gov)

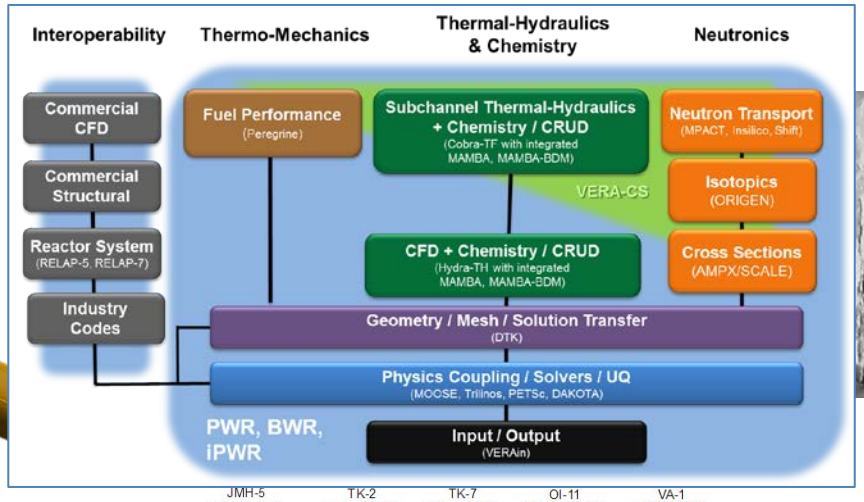
CASL Proposed Phase 2 Scope: 2015 – 2019

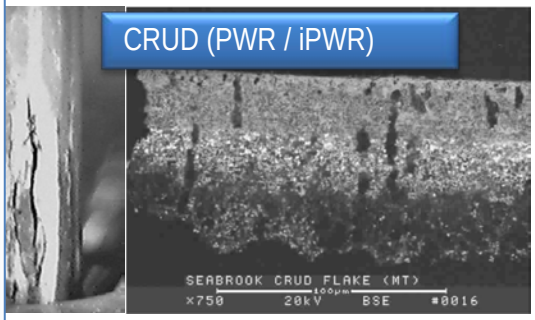


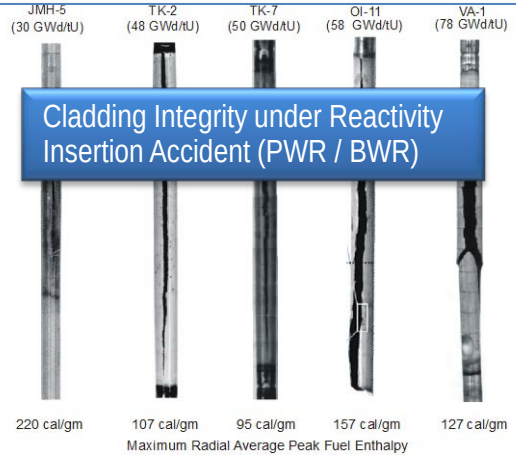


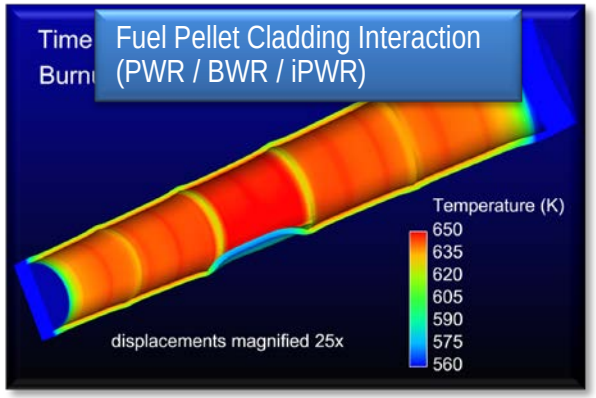




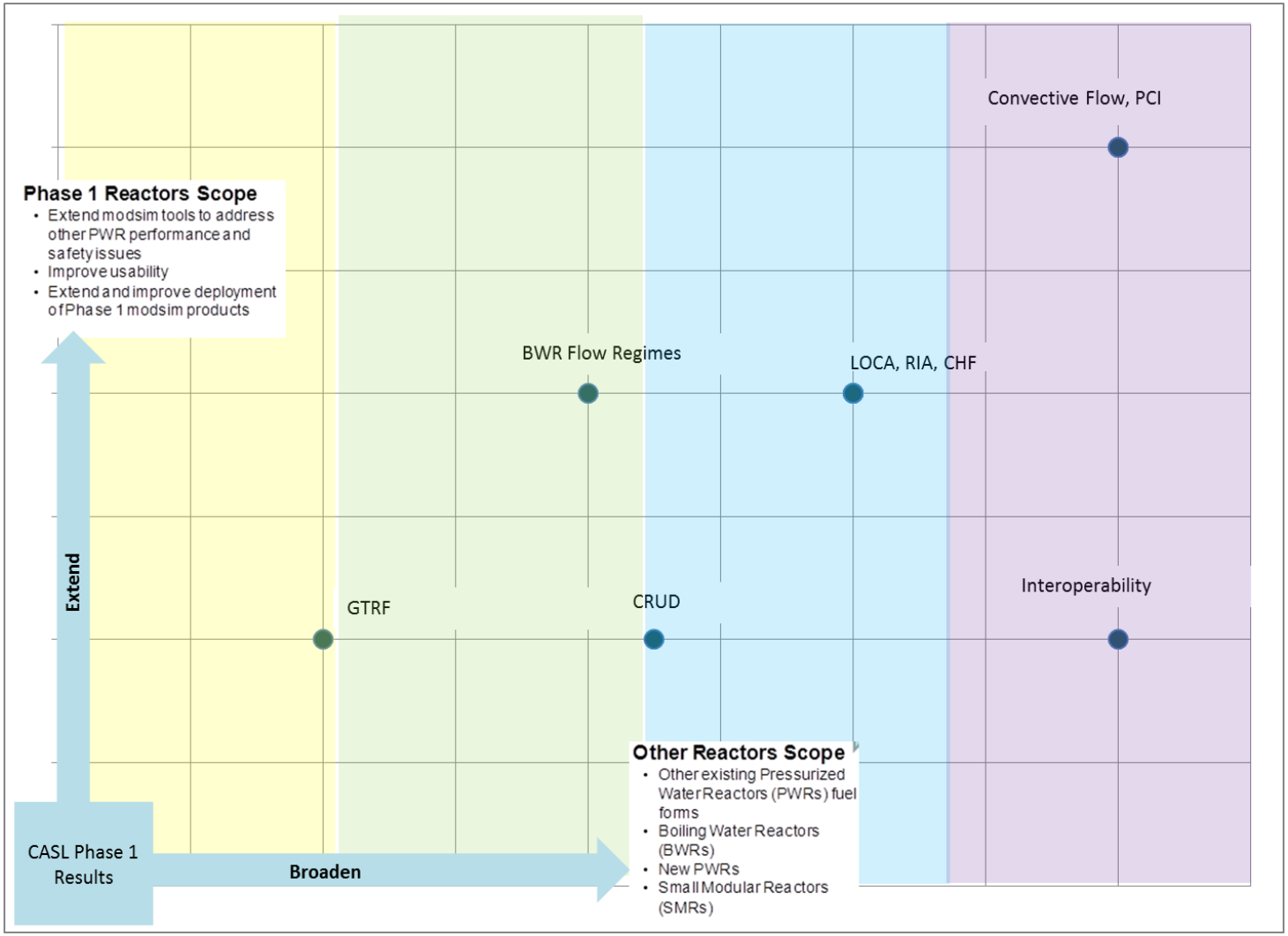








Phase 2 Scope



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

CASL Status
and looking forward

- ✓ Year 1: Build the foundation
- ✓ Year 2: Advance the science basis of the M&S technology components
  - Guided by challenge problem requirements baselined against industry capabilities
- ✓ Year 3: Assess, refine, integrate, and beta test the M&S technology components within the multi-physics Virtual Reactor environment
  - Perform initial verification and validation (V&V), sensitivity analysis (SA), and uncertainty quantification (UQ) analyses
- ✓ Year 4: Harden for robustness & efficiency and deploy & apply the coupled multi-physics Virtual Reactor technology for broader assessment and continuous improvement
  - Prepare for possible 5-year renewal that leverages development to date
- ✓ Year 5: Continue maturation of the multi-physics Virtual Reactor technology thru increased breadth and depth of testing and application offered by a general release
  - Self-sustaining technology deployment (release/support) and evolution plan in place

Document Type	Quantity (May 2014)
Journal Articles, refereed	68
Conference Papers	341
Technical Reports	37
Milestone Reports	520
Presentations	52
Workshop/Seminars	95
Reference Documents	7
Record/NR Publications	53
Management Documents	154
Awards	4
Thesis, Poster, Manual, Patent, Images	10
Total	**1,321**

Questions?

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- PUBLICATIONS
- SCIENCE AND TECHNOLOGY ARCHIVE

Publications

Journal and Conference Papers

Technical Reports

- 2014
- 2013
- 2012
- 2011

Invited Presentations

CASL scientists, engineers, and mathematicians – whether they are R&D staff, program managers, student interns, or postdoctoral associates at DOE National Laboratories; faculty, research associates, students, or postdoctoral associates at universities; or technical staff in industry – work hard to document and disseminate their R&D strategies, approach, and results in the form of journal and conference papers, technical reports, and invited presentations. They are anxious to share and discuss their results with all interested parties.

The CASL publications list continues to grow, hence this list is continuously updated, so be sure to check back here regularly. Please direct any inquiries about CASL publications or requests for electronic copies of publications to casl-info@casl.gov

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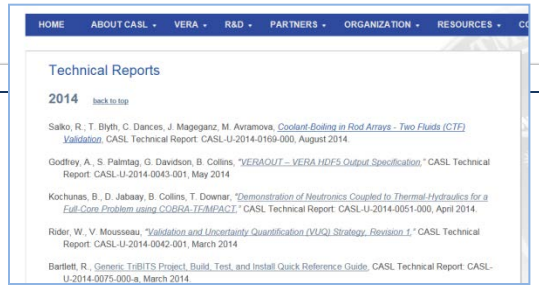

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