CASL: Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub

Progress and Future Plans

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Presentation to the

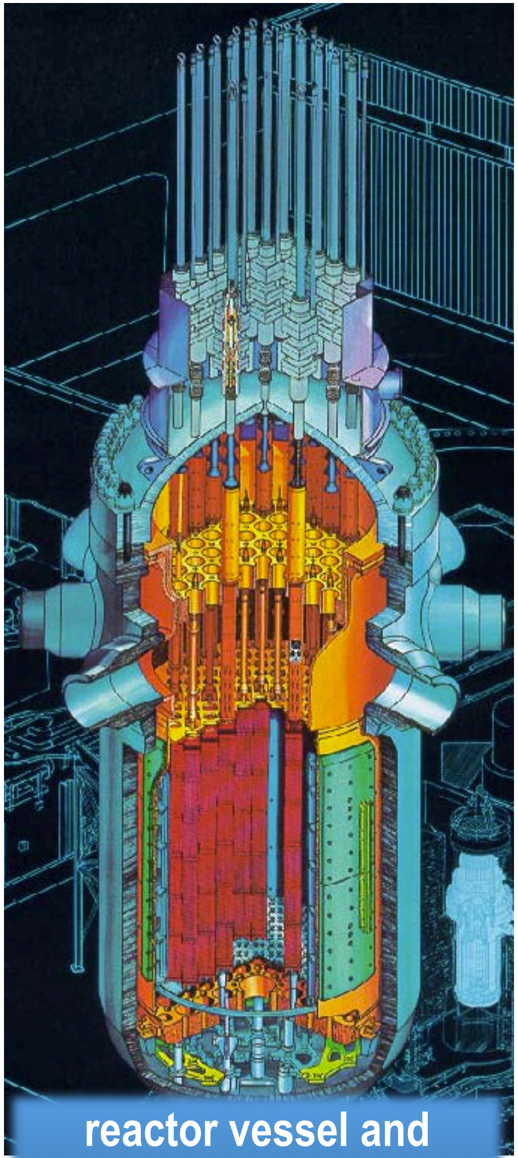
Oak Ridge National Laboratory

Science Advisory Board

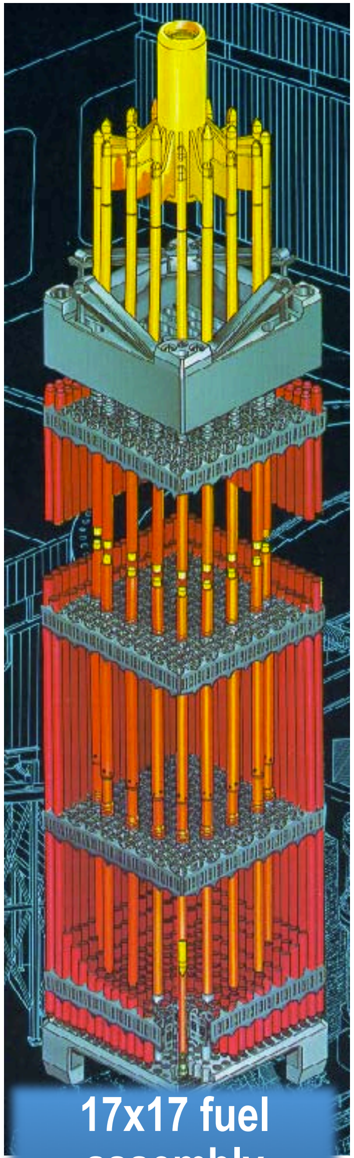
July 17, 2014

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!

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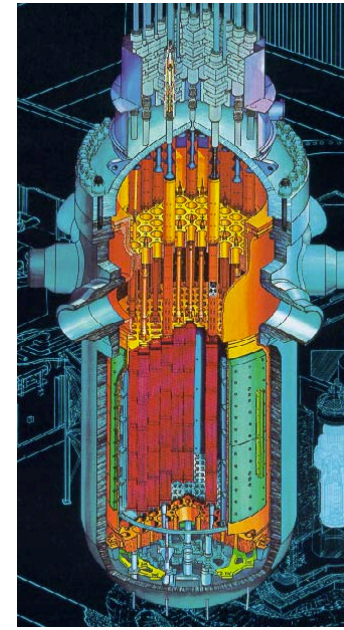
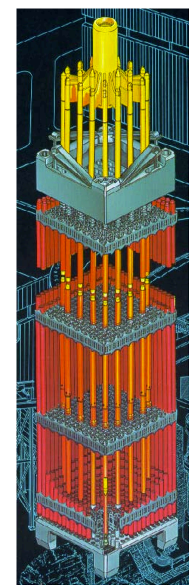
Nuclear Energy Drivers and Payoffs for M&S technology

- **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





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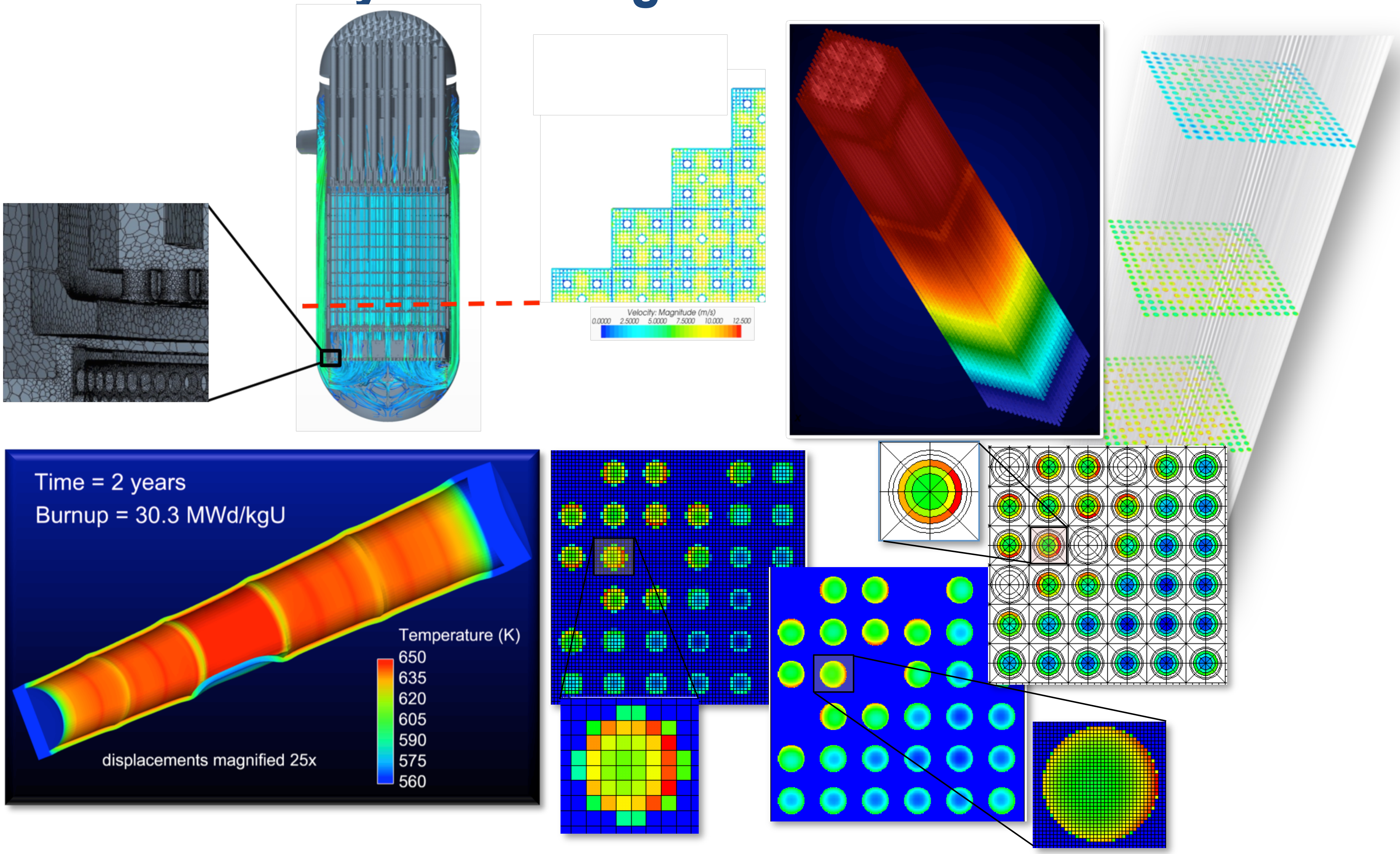
CASL Targets the Multi-Scale Challenge of Predictively Simulating a Reactor Core



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

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
- **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

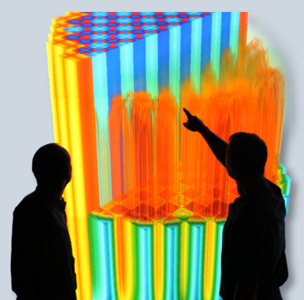
Need to assure nuclear safety but limited by inability to perform full-scale experimental mockups due to cost, safety & feasibility [1% power derating translates to $(5-10)M annual loss of revenue for 1 GWe unit]

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]

CASL's Charter

Mission is to provide leading-edge modeling and simulation capabilities to improve the performance of currently operating light water reactors

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
  - ✓ furthering power uprates
  - ✓ 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

Elements of CASL's Approach That are Proving Effective

With continuous improvement drawing on feedback from customers/clients/users

- ✓ ***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

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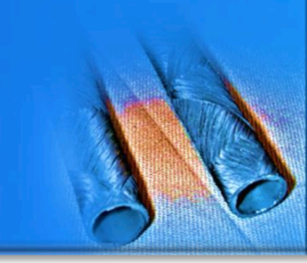
CASL Challenge Problems

Key safety-relevant reactor phenomena that limit performance

Departure from Nucleate Boiling

Cladding Integrity

- During LOCA
- During reactivity insertion accidents
- Use of advanced materials to improve cladding performance



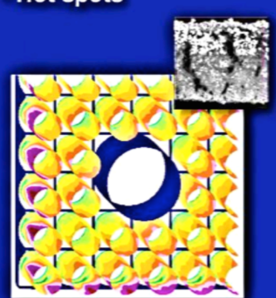
Safety Related Challenge Problems

CASL is committed to delivering simulation capabilities for

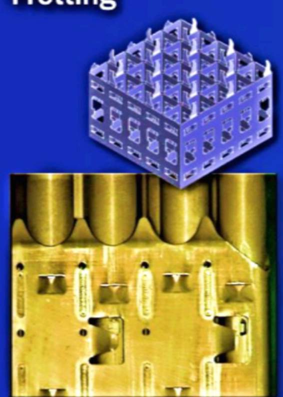
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

Crud

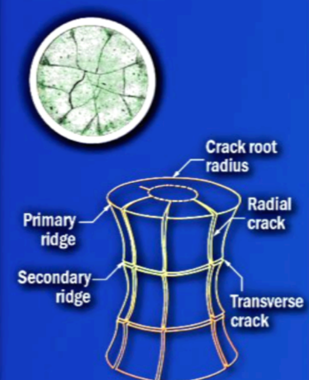
- Deposition
- Axial offset anomaly
- Hot spots



Grid-to-Rod Fretting



Pellet-Clad Interaction



Operational Challenge Problems

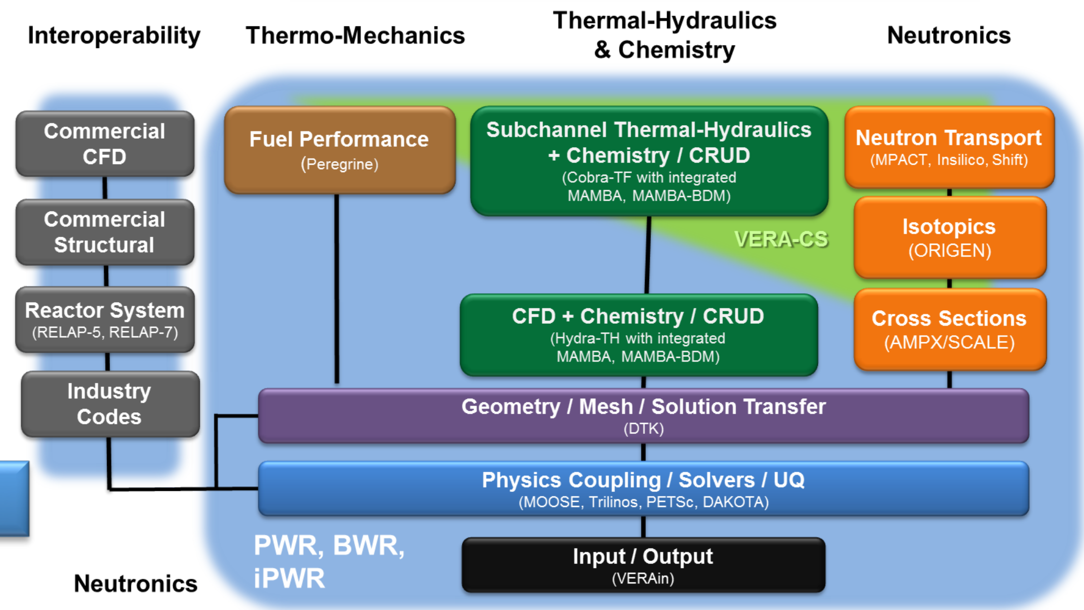
VERA: Virtual Environment for Reactor Applications

CASL's evolving virtual reactor for in-vessel LWR phenomena

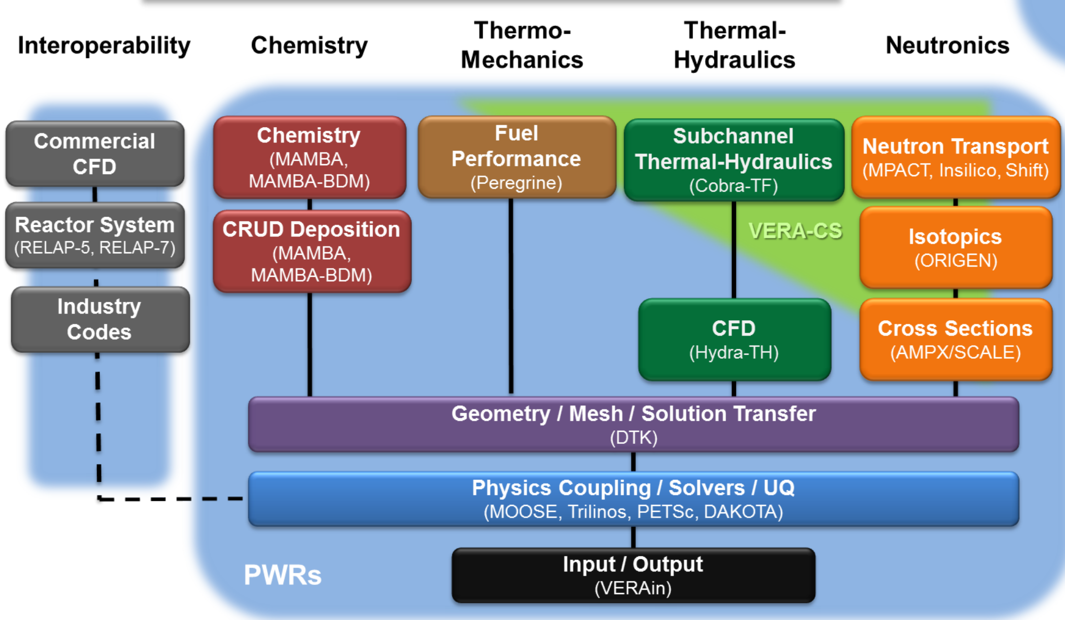
CASL has 3 M&S technology products

1. VERA-CS as the fast running core simulator, which has value both standalone and for providing power histories, etc for more detailed codes
2. Engineering suite of standalone codes with ability to couple 2 or more within VERA or in other environments
3. Leadership suite of high fidelity codes used to drive improvements in 1 and 2

VERA in 2019 (Phase 2 conclusion)



VERA in 2015 (Phase 1 conclusion)

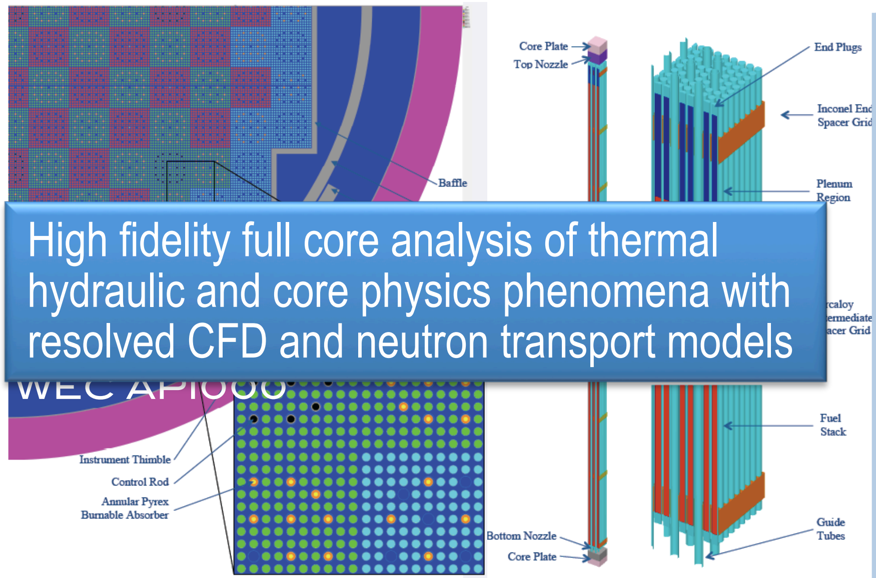


Current Technology Portfolio

Item	Description
S/W Development Tools and Computational Infra-structure	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 Compo-nents	COBRA-TF (CTF), SCALE/XSProc, Insilico, MPACT
Other Physics Components	Hydra-TH, Shift, Mamba2D/3D, Peregrine, Drekar
Integrated Industry Compo-nents	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.

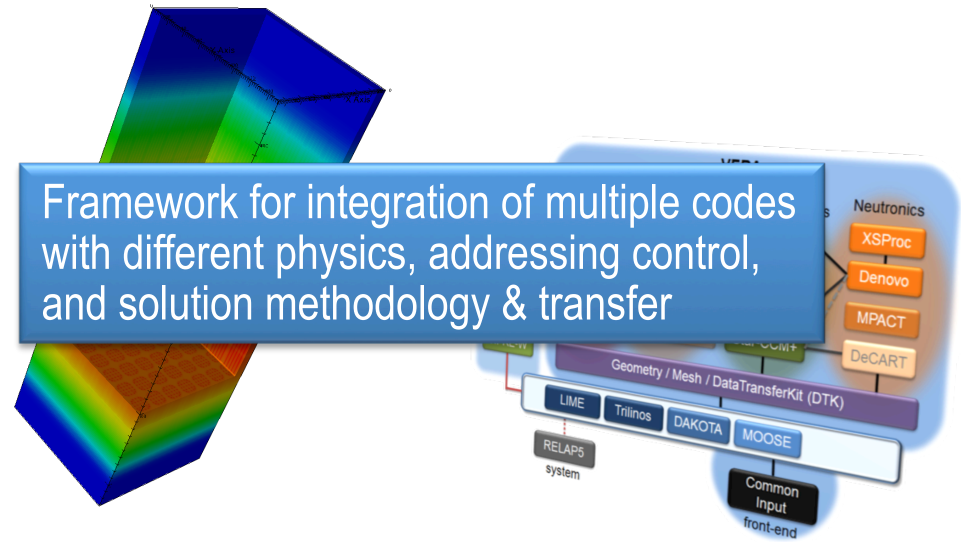
CASL Innovations

Advanced Modeling Applications



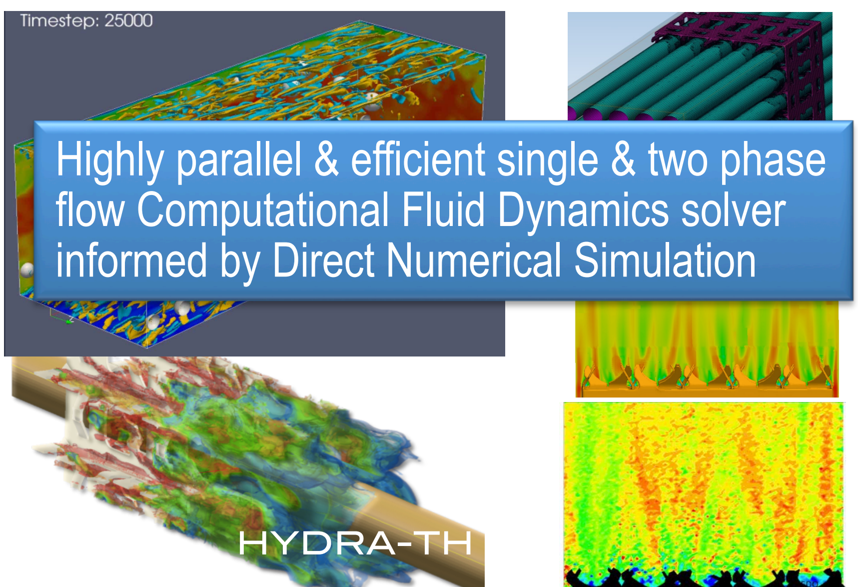
High fidelity full core analysis of thermal hydraulic and core physics phenomena with resolved CFD and neutron transport models

Physics Integration



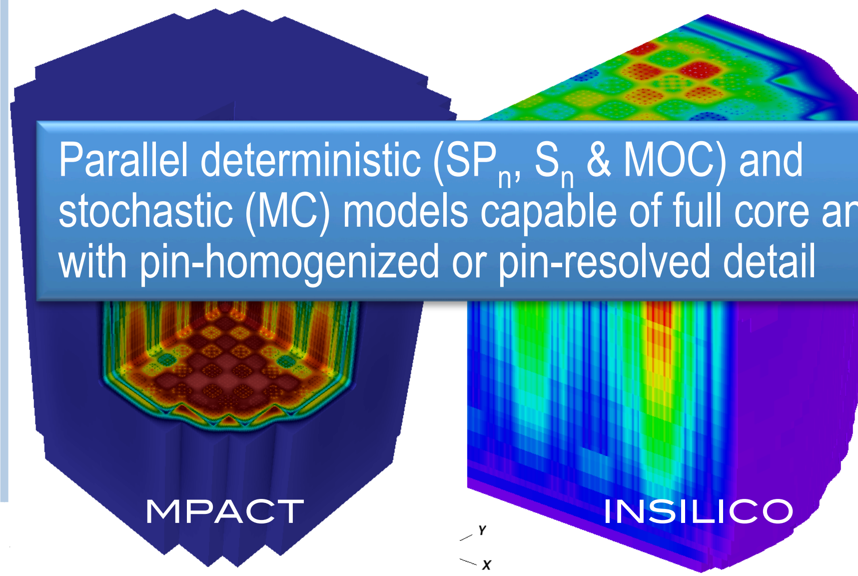
Framework for integration of multiple codes with different physics, addressing control, and solution methodology & transfer

Thermal Hydraulic Methods



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

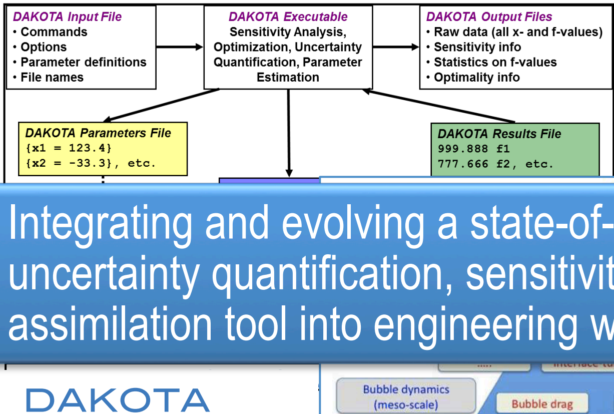
Radiation Transport Methods

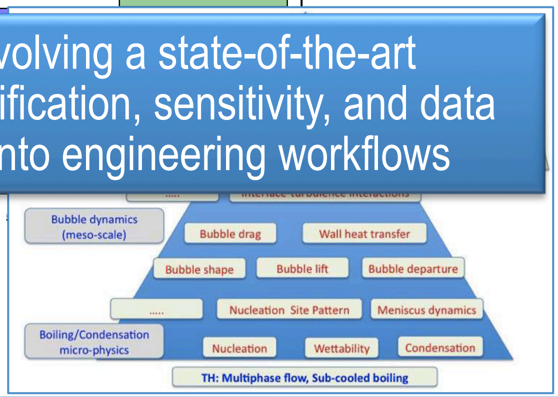


Parallel deterministic (SP_n, S_n & MOC) and stochastic (MC) models capable of full core analysis with pin-homogenized or pin-resolved detail

CASL Innovations

Validation & Uncertainty Quantification



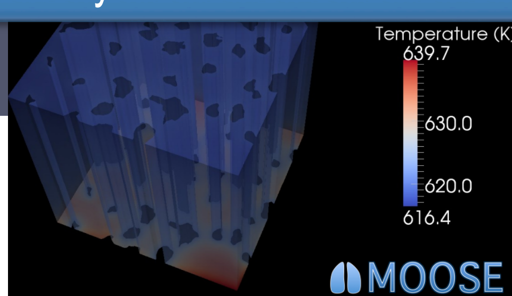


Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows

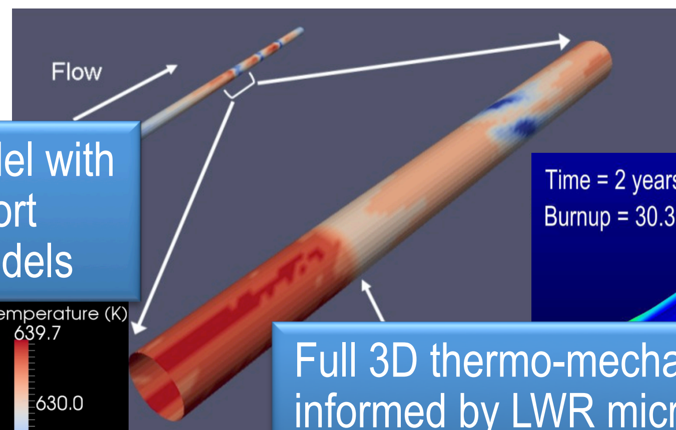
VOCC

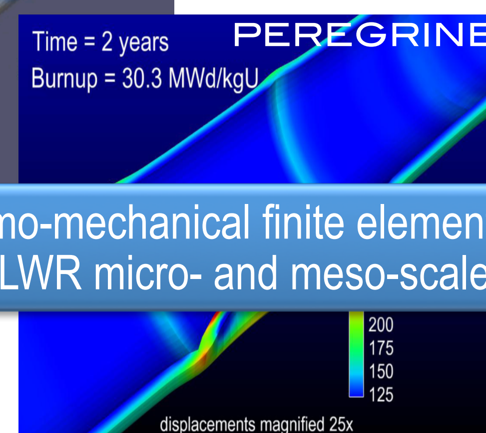
Bringing together local (“physical”) and geographically distributed (“virtual”) contributors in a meaningful and productive way

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

Reactor Core Physics Benchmarking

Outstanding operational reactor results with the new and evolving neutronics capability

Purpose

- Document performance for CASL Core Physics Progression Problems 1-5
- Benchmark results vs. measured Watts Bar Unit 1 Cycle 1 zero power physics testing data
- Document independent user experience and computational resources required

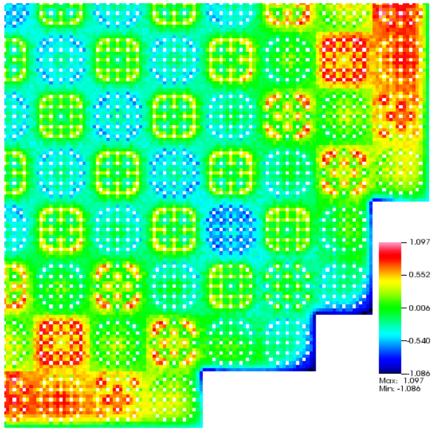
Summary Results

Prob. #	Typical Eigenvalue Difference (pcm)	Typical Pin Power RMS (%)	Number Compute Cores	Typical Runtime
1	-211	--	8	~3 secs
2	-126	0.12%	8	~1 min
3	-116	0.27%	464	~2 min
4	-113	0.95%	464	~33 min
5	-88	0.74%	2784	~75 min

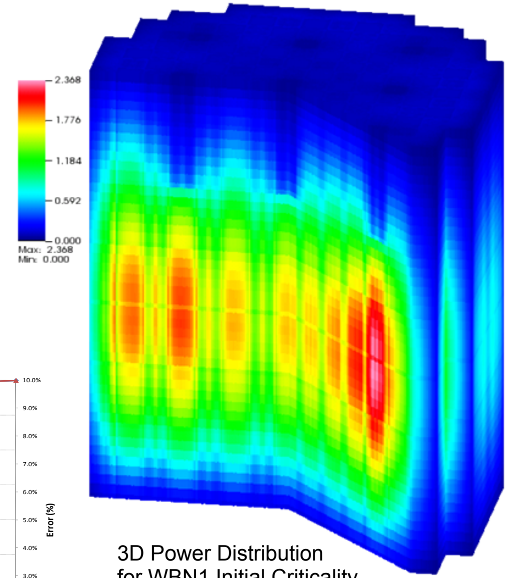
Watts Bar Unit 1 Initial Startup Results

Item	Measured Difference	CE KENO-VI Difference
Criticality†	-225 ± 57 pcm	-96 ± 13 pcm
Control Rod Worths†	3.3 ± 1.5%	0.8 ± 0.3%
Differential Boron Worth	0.61 pcm/ppm	-0.05 pcm/ppm
Isothermal Temperature Coefficient	-1.55 pcm/F	-0.54 pcm/F

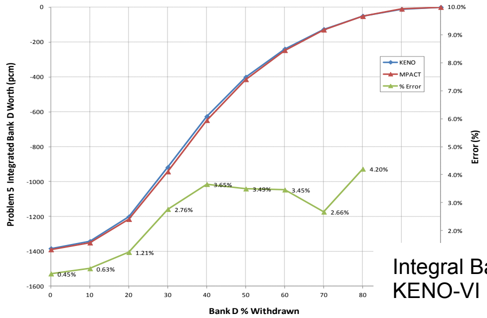
†mean ± standard deviation



Radial Power Comparison to CE KENO-VI



3D Power Distribution for WBN1 Initial Criticality



Integral Bank D Worth Comparison to CE KENO-VI

Conclusions and Feedback

- Good accuracy and stability with reasonable runtimes
- Small radial and axial power tilts for whole core models
- Needs IFBA treatment (5x slower)
- Needs control rod tip treatment (<80 pcm)
- Needs thermal expansion & rotational symmetry
- Needs faster runtime for T/H coupling

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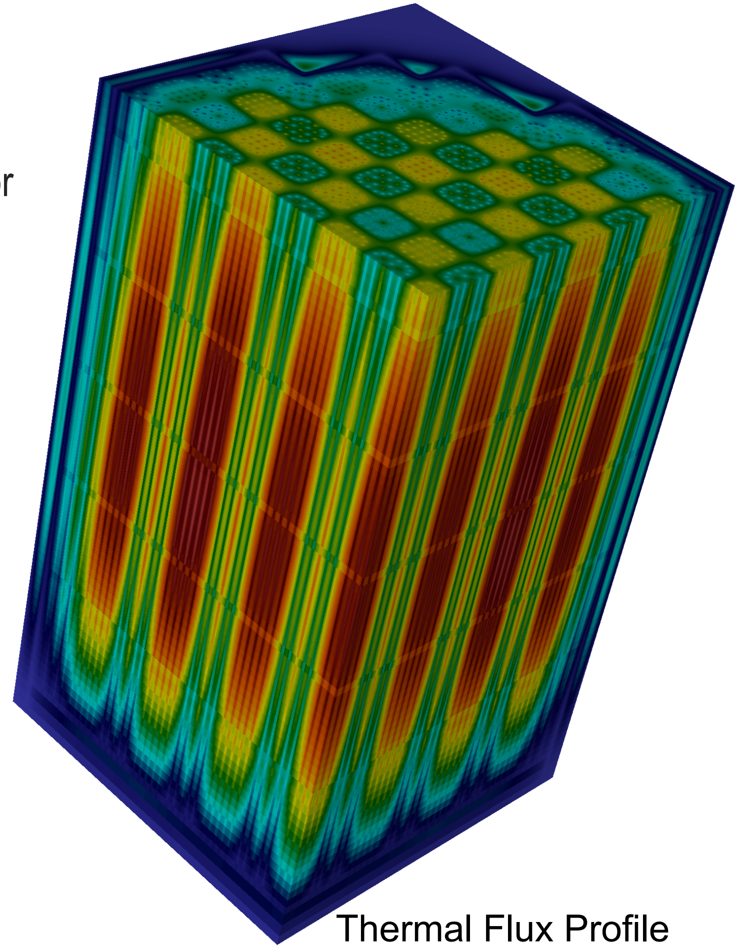
VERA Analysis of Watts Bar 1 Hot Full Power

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



Thermal Flux Profile in Reactor Core

Next Steps

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

Remarkable resolution of physics and geometry

New VERA Continuous-Energy Monte Carlo Capability (Shift) – Quarter-Core Zero Power Physics Test

Goals

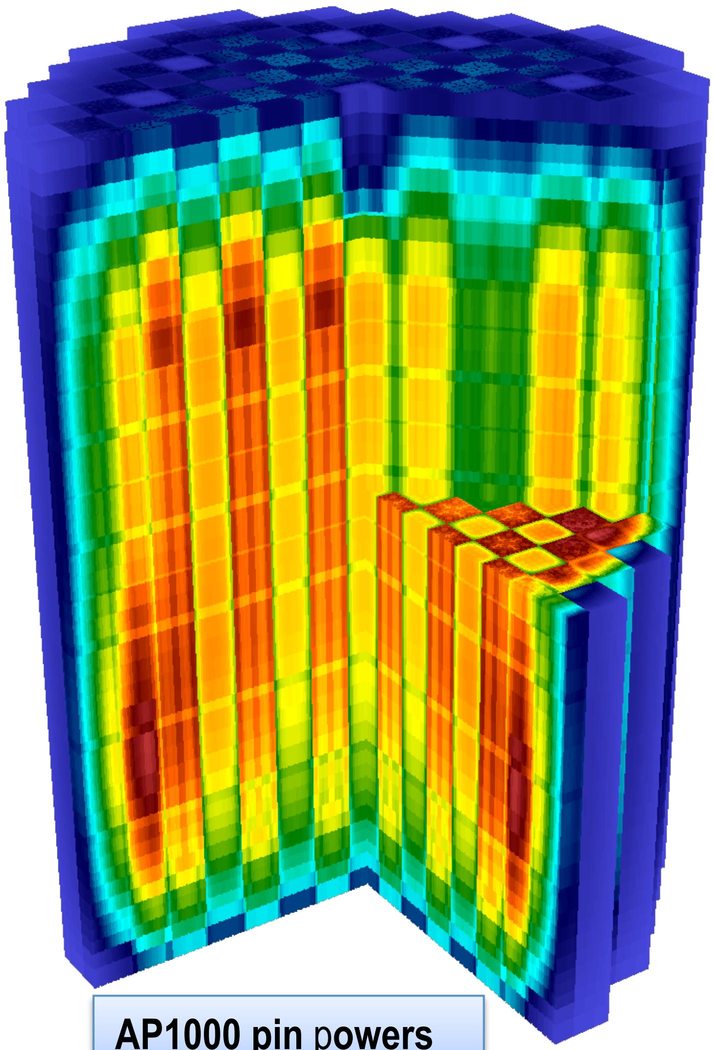
- Compare fidelity and performance of Shift against Keno, SP_N, and S_N (Denovo)
- Generate high-fidelity neutronics solution for code comparison of solutions for predicting reactor startup and physics testing

Execution

- Proposal submitted to OLCF as part of Titan Early Science program
- Awarded 60 million core-hours on Titan (worth >$2M)
- 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 use 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

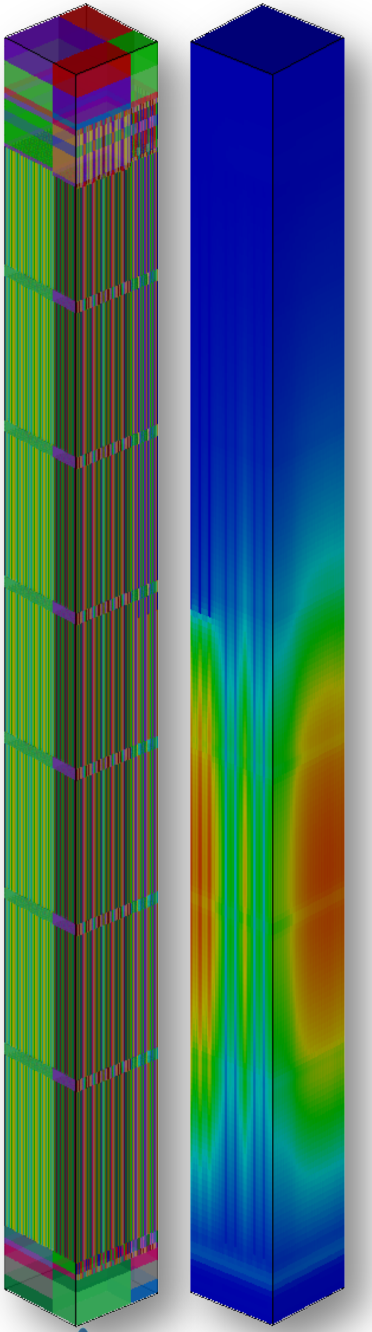


AP1000 pin powers

CASL

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

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

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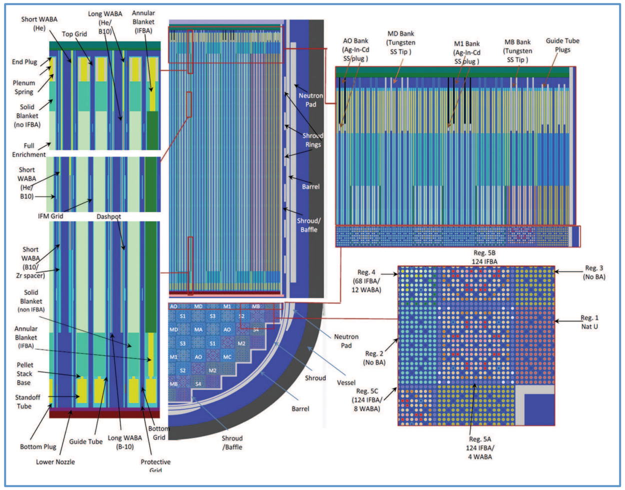
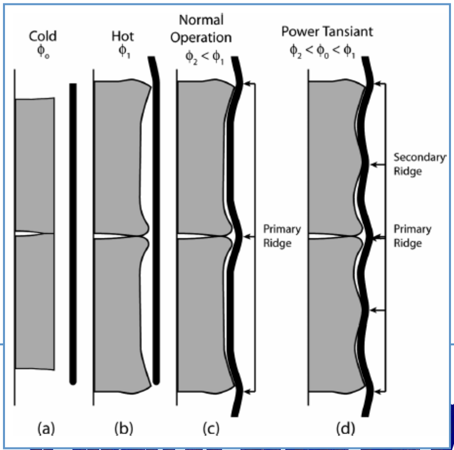
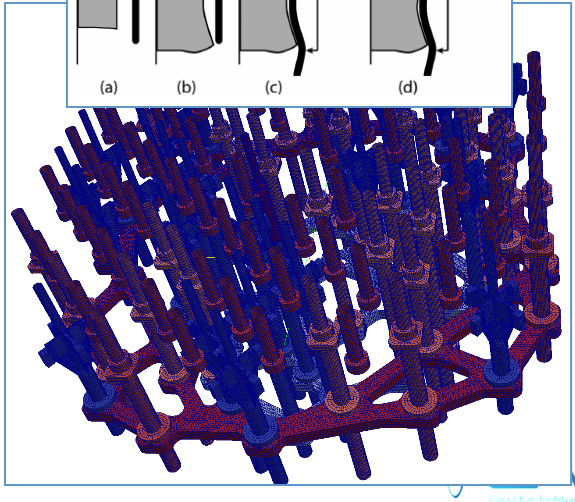
CASL Technology Deployment

Test Stands to Beta Releases to Broad Releases

- CASL is committed to ensuring its products are deployed to the broader nuclear industry
- 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): Use VERA core simulator to analyze AP1000 first core startup
  - EPRI (Nov 2013): new EPRI computing capabilities will be utilized to test VERA fuel performance (Peregrine) applications
  - TVA (Mar 2014): test VERA CFD capability (Hydra-TH) on lower plenum flow anomaly observed in operational reactors







First CASL Test Stand Highlighted in Nuclear Engineering International Magazine

CASL

- **Highlights Simulation of AP1000® First Core by Westinghouse (May 2014)**
- Strong demonstration of deployment of CASL tools and use by Westinghouse
- NEI Magazine has broad international circulation

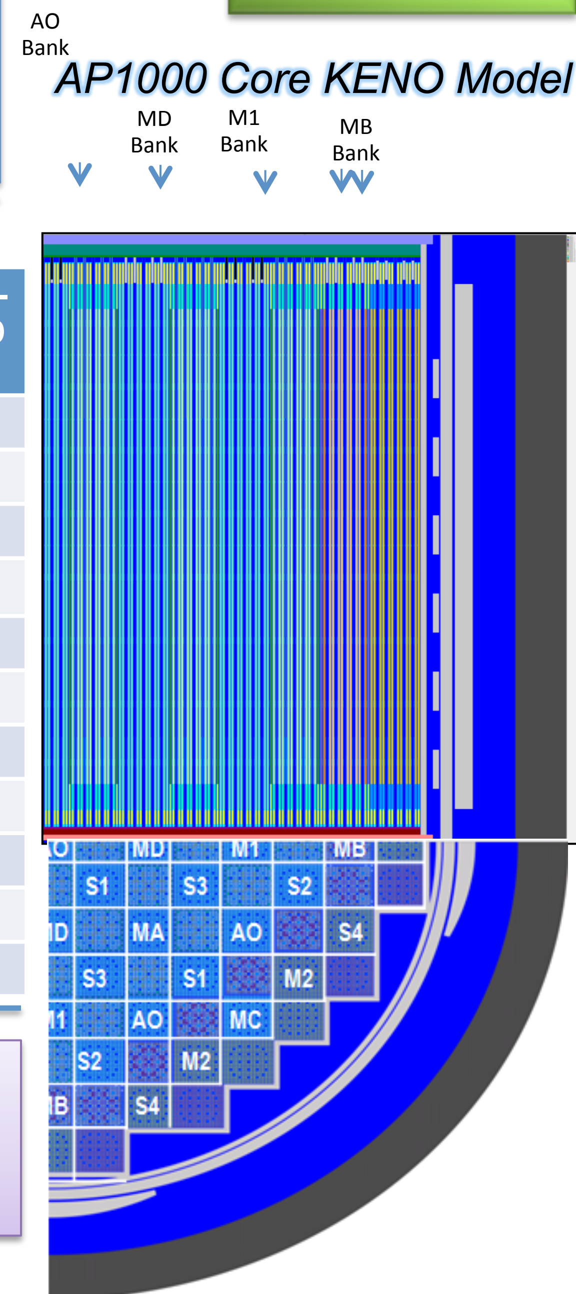
Start-up Boron and Reactivity Coefficients

	KENO	VERA
Critical Boron (ppm)	1314	1311
Isothermal Temperature Coefficient (pcm/F)	-2.7	-3.2
Doppler Temperature Coefficient	-1.6	-1.7
Moderator Temp. Coeff.	-1.1	-1.5

Control Rod Worth

	KENO	VERA-KENO (pcm)	VERA-KENO (%)
MA	258	-1	-0.5
MB	217	-5	-2.1
MC	188	-2	-1.1
MD	234	0	0.0
M1	651	-4	-0.6
M2	887	3	0.4
AO	1635	-4	-0.3
S1	1079	0	0.0
S2	1096	-9	-0.8
S3	1124	0	0.0
S4	580	-3	-0.4

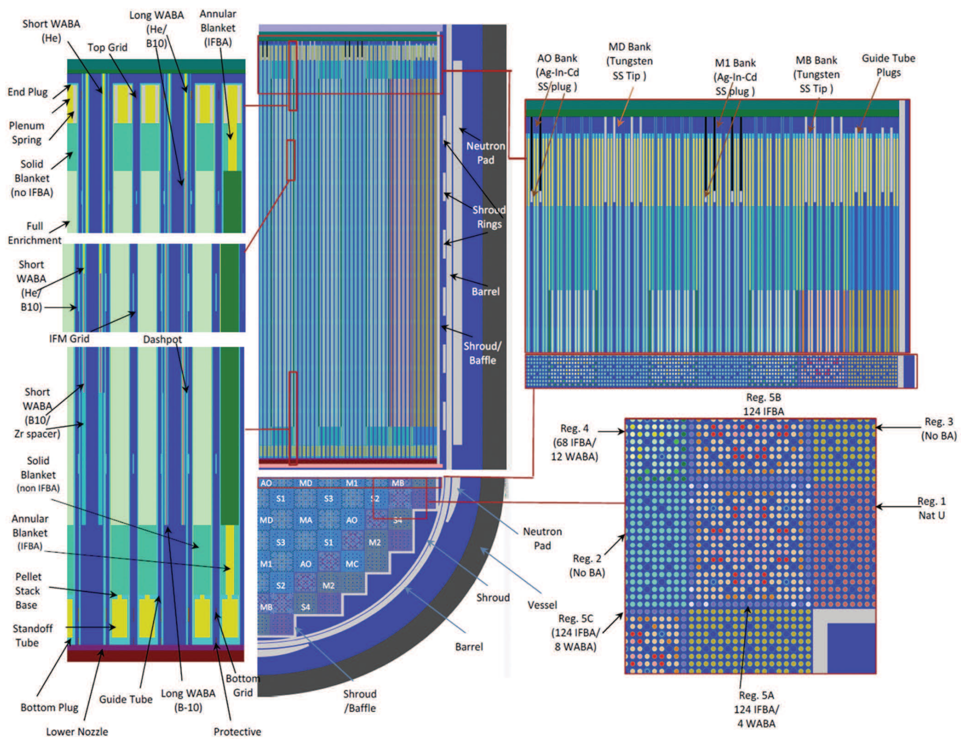
AP1000 Core KENO Model

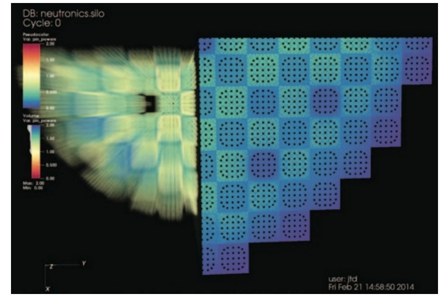


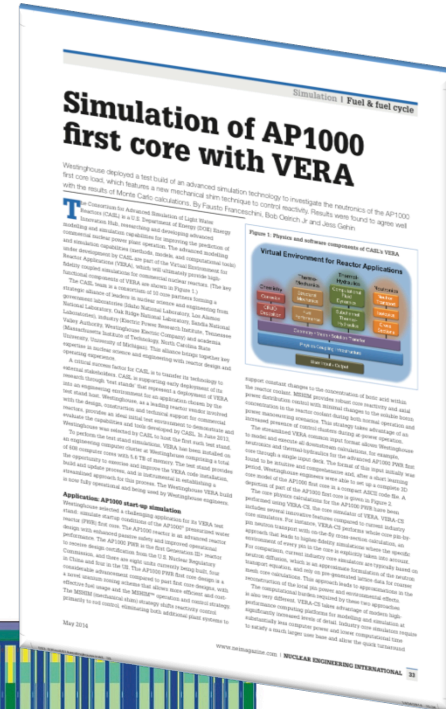
CASL technology deployed at the industry proves beneficial for challenging simulation scenarios

CASL Test Stand at Westinghouse

Highlighted in Nuclear Engineering International Magazine
Recipient of IDC HPC Innovation Excellence Award







Simulation | Fuel & fuel cycle

Simulation of AP1000 first core with VERA

Westinghouse deployed a test build of an advanced simulation technology to investigate the neutronics of the AP1000 first core load, which features a new mechanical shim technique to control reactivity. Results were found to agree well with the results of Monte Carlo calculations. By Fausto Franceschini, Bob Oelrich Jr and Jess Gehin

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is a U.S. Department of Energy (DOE) Energy Innovation Hub, researching and developing advanced modelling and simulation capabilities for improving the prediction of commercial nuclear power plant operation. The advanced modelling and simulation capabilities (methods, models, and computational tools) under development by CASL are part of the Virtual Environment for Reactor Applications (VERA), which will ultimately provide high-fidelity coupled simulations for commercial nuclear reactors. (The key functional components of VERA are shown in Figure 1.)

Figure 1: Physics and software components of CASL's VERA

Virtual Environment for Reactor Applications

Application: AP1000 start-up simulation

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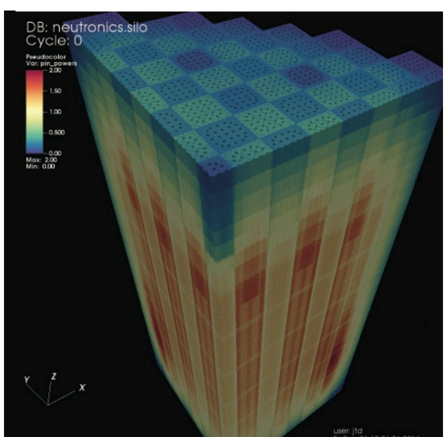
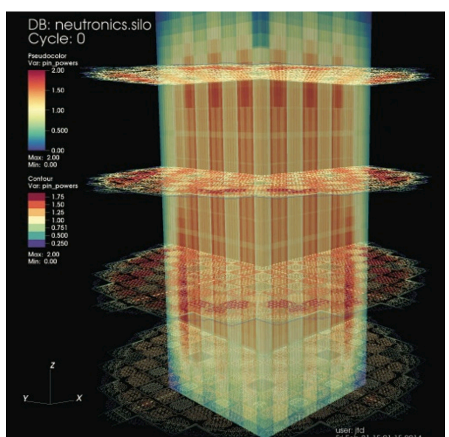
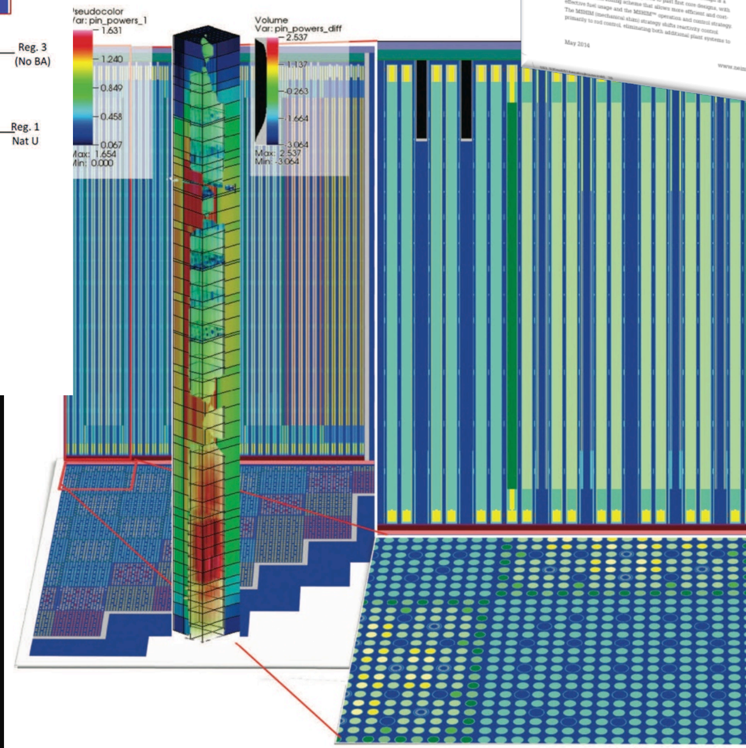
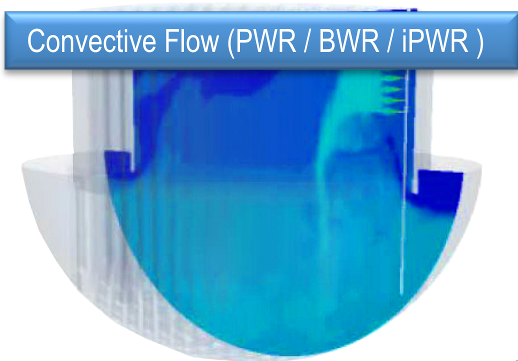
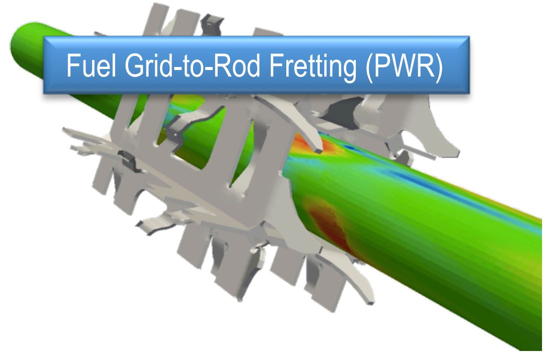


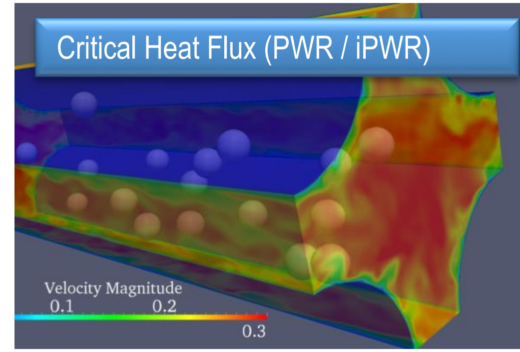


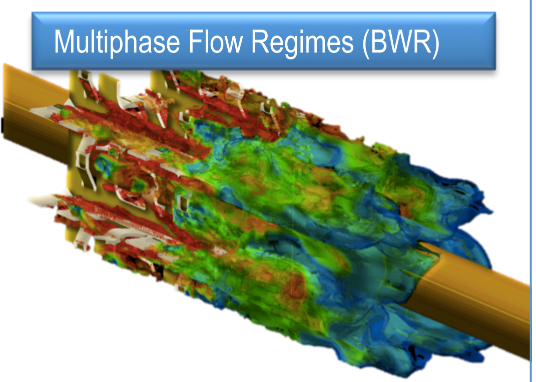


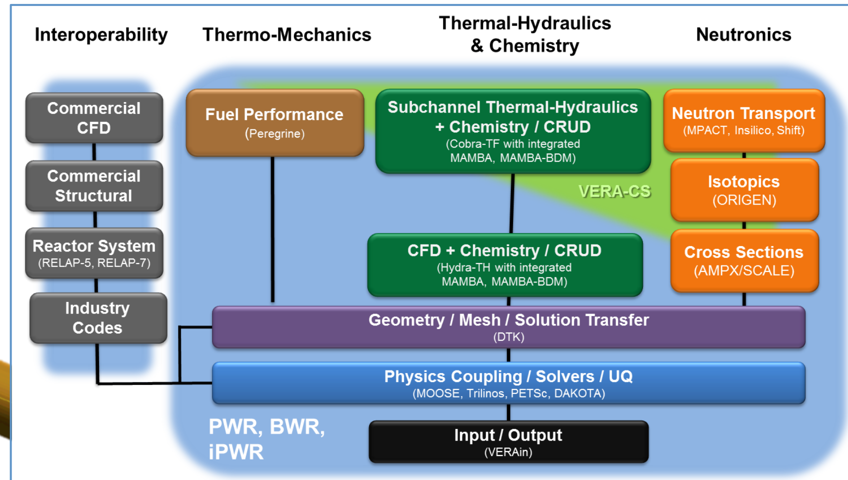
CASL Proposed Phase 2 Scope: 2015 – 2019

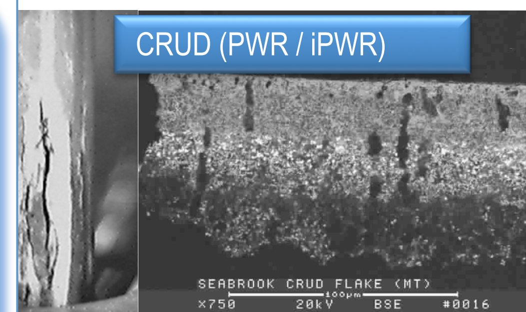


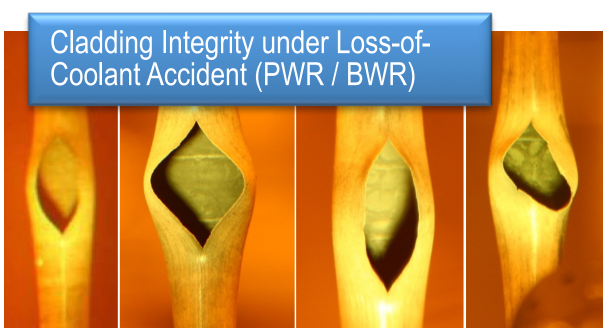


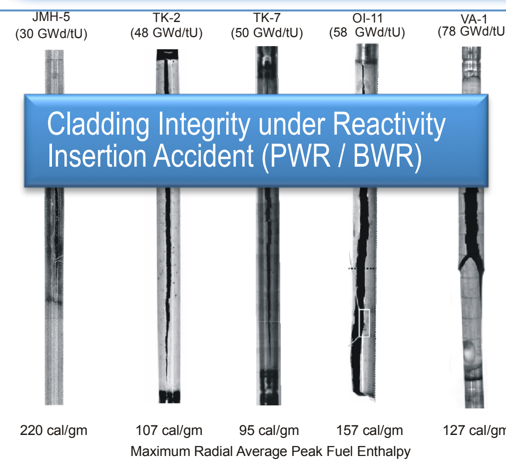


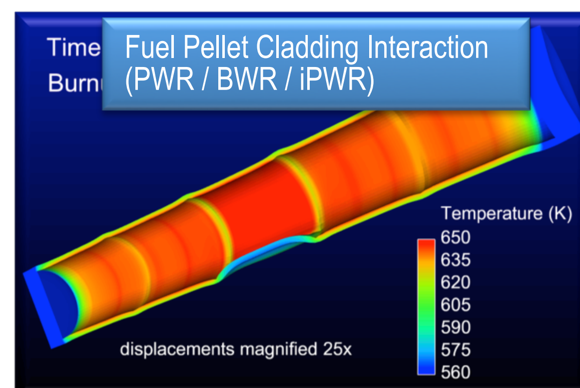




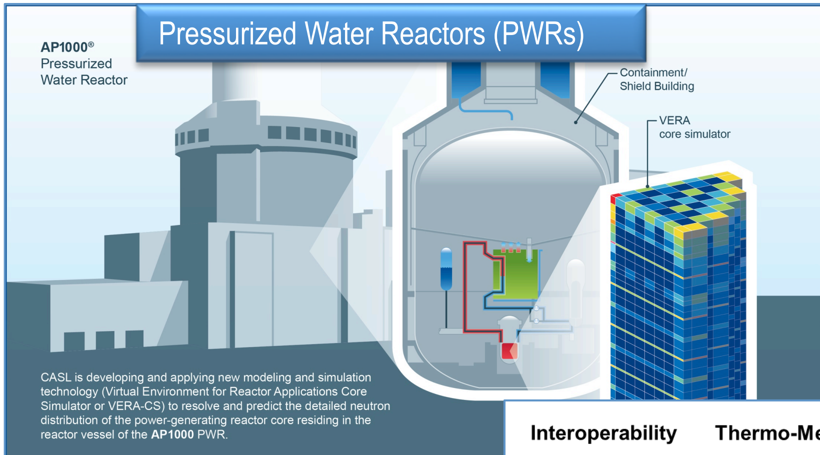


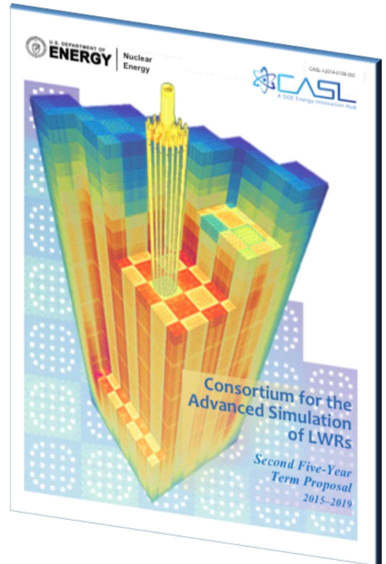


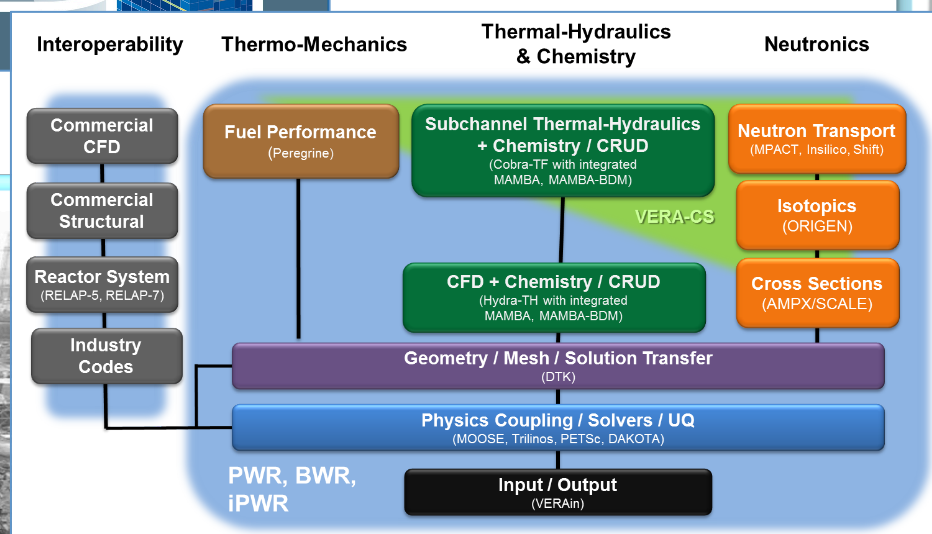




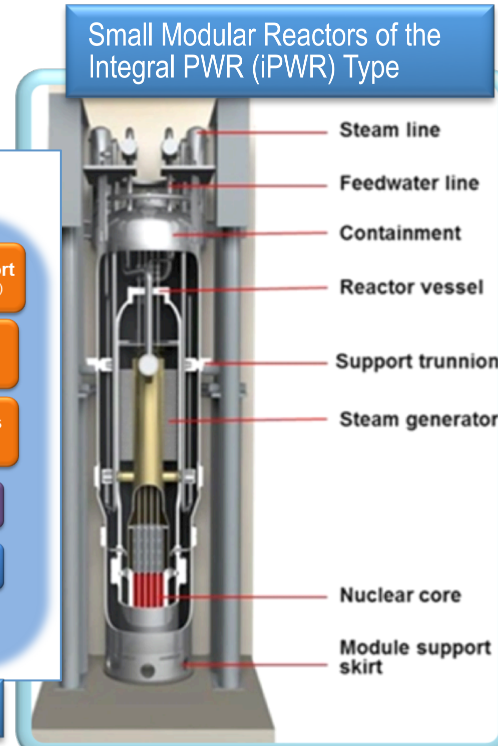
CASL Phase 2 Scope
Proposed for 2015 – 2019







CASL's Virtual Environment for Reactor Applications (VERA)



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 er
  - ◆ Perform initial verification and validation (V&V), sensitivity analys uncertainty quantification (UQ) analyses
- ✓ Year 4: Harden for robustness & efficiency and deploy coupled multi-physics Virtual Reactor technology for br assessment and continuous improvement
  - ◆ Prepare for possible 5-year renewal that leverages development
- ✓ Year 5: Continue maturation of the multi-physics Virtua technology thru increased breadth and depth of testing 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?

www.casl.gov or *info@casl.gov*