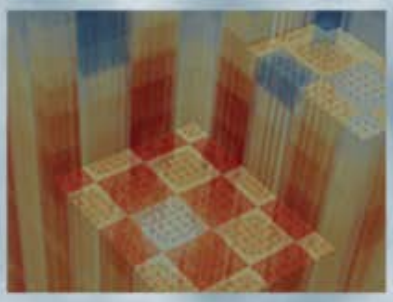
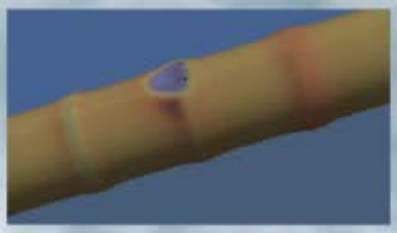
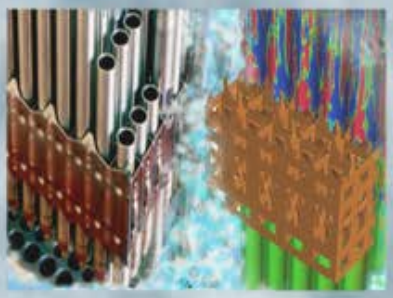
CASL-U-2015-0202-000

CASL Overview at International Atomic Energy Agency (IAEA) Meeting on Accident Tolerant Fuel (ATF) Concepts for LWRs







Douglas Kothe and Jess Gehin
Oak Ridge National Laboratory

October 16, 2014

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

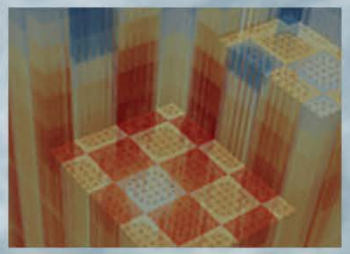
A DOE Energy Innovation Hub

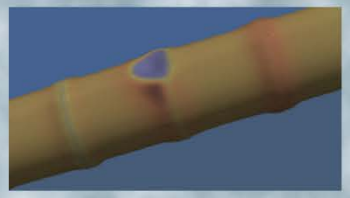
CASL: The Consortium for Advanced Simulation of Light Water Reactors

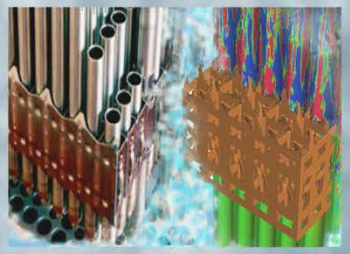
A DOE Energy Innovation Hub

Doug Kothe (ORNL)

CASL Director



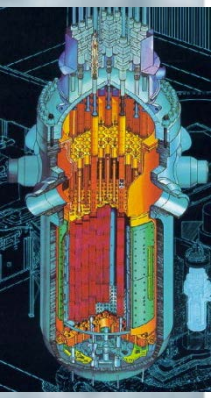


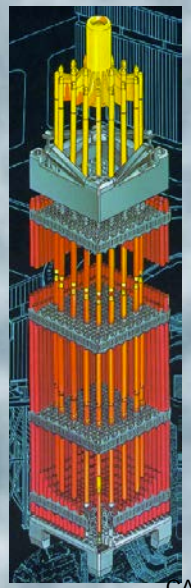


U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

CASL-U-2015-0202-000

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

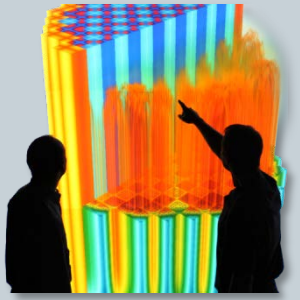
Nuclear Energy Industry Dependencies and Capabilities in Modeling and Simulation (M&S)

- 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.

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

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

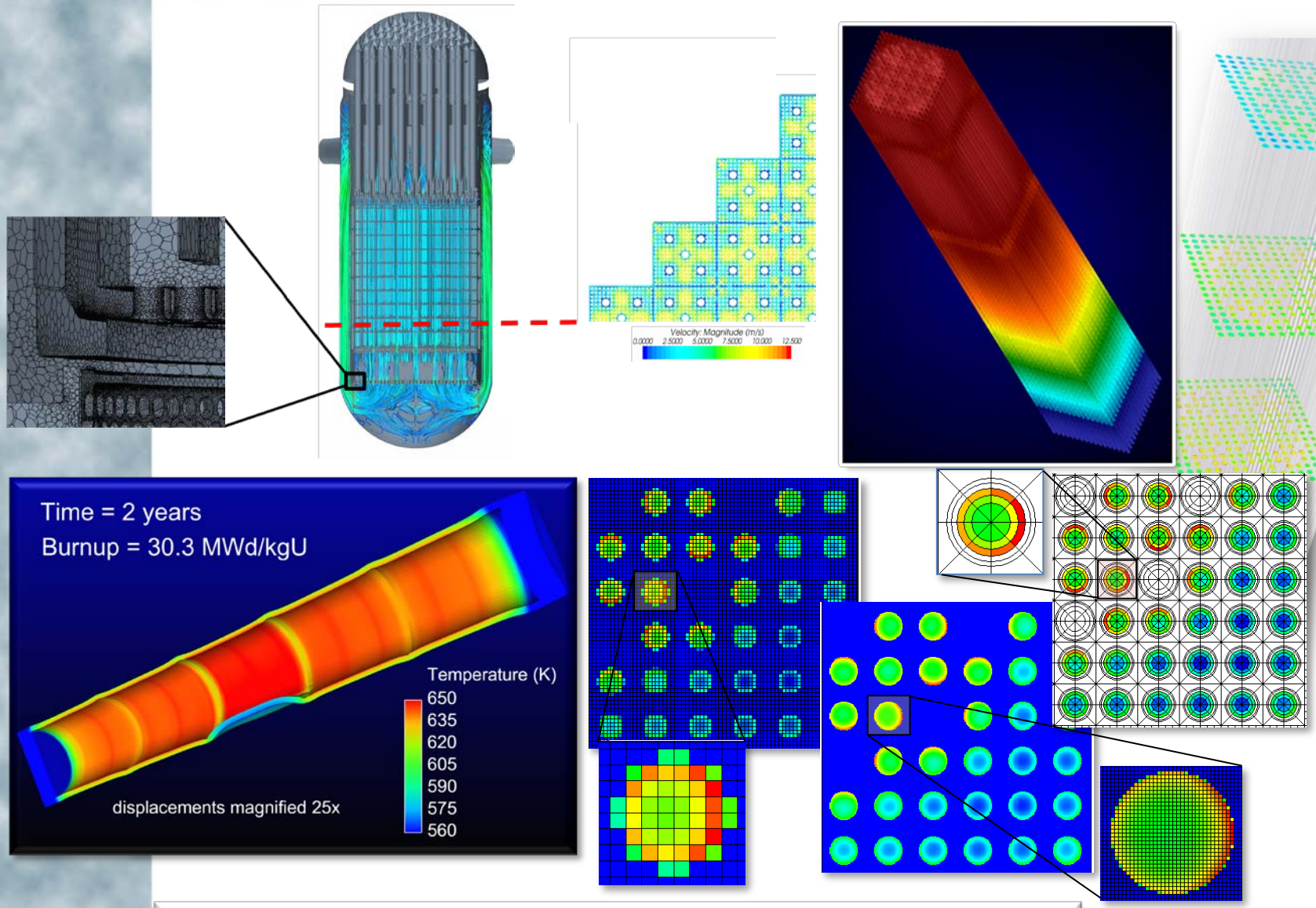
University of Texas at Austin

University of Texas at Dallas

University of Tennessee – Knoxville

Pacific Northwest National Laboratory

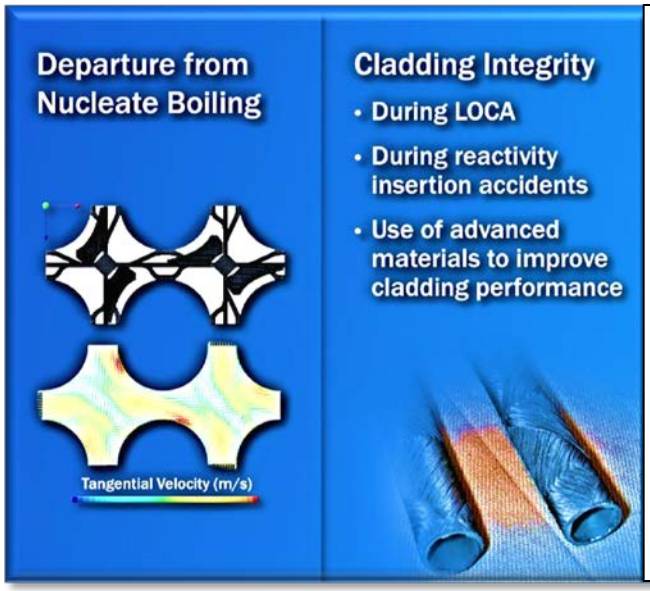
CASL Tackles the Multi-Scale Challenge of Predictively Simulating a Reactor Core



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

CASL Challenge Problems

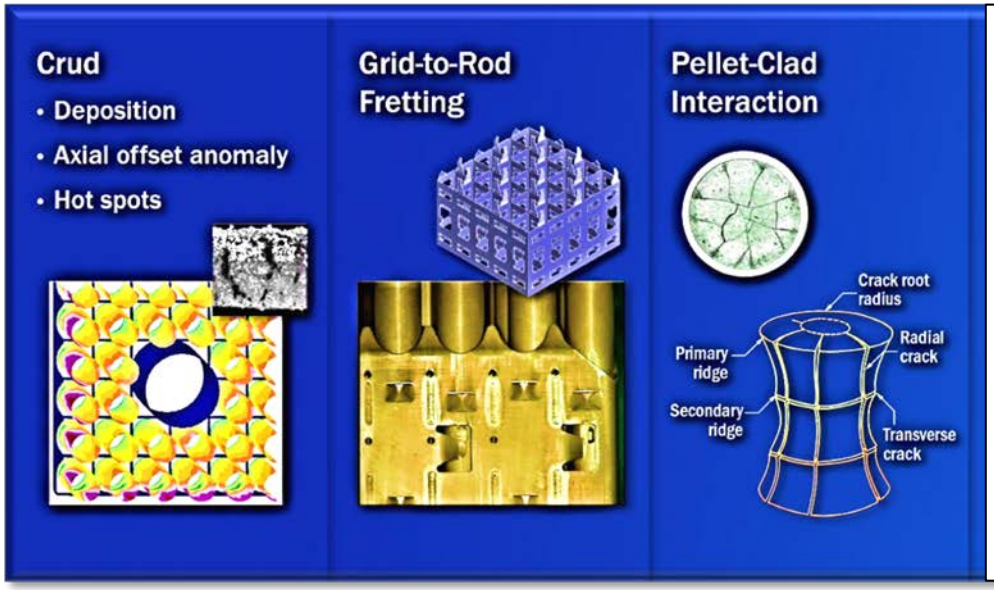
Key safety-relevant reactor phenomena that limit performance



Safety Related Challenge Problems

CASL Challenge Problems

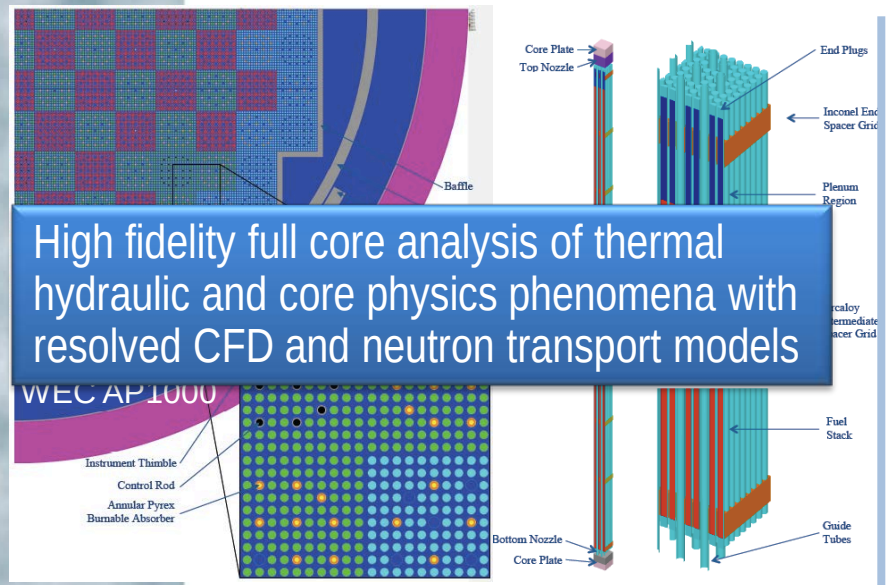
- Are relevant industry problems whose solutions remain elusive
- Are amenable to insight afforded by advanced M&S
- Help to direct RD&D activities on CASL M&S technology
- Help to establish clear performance metrics



Operational Challenge Problems

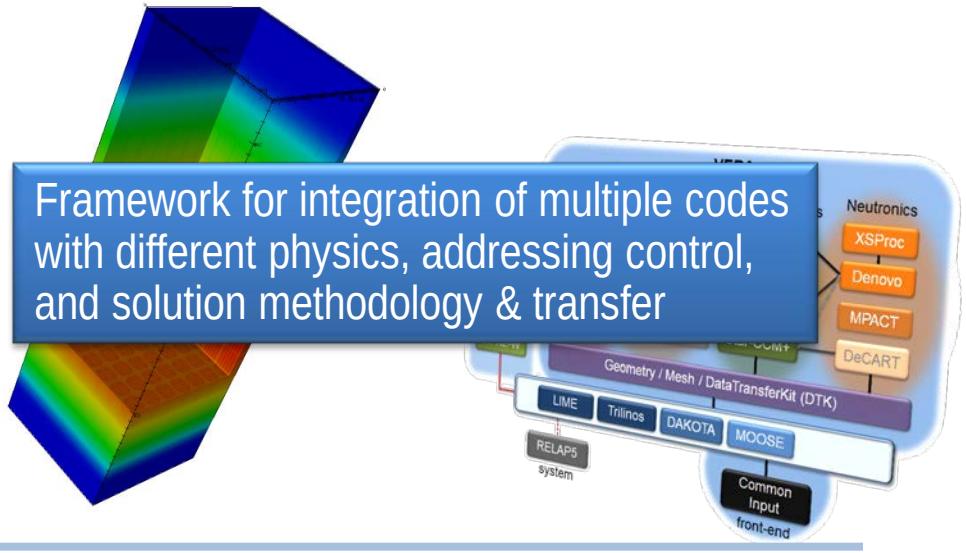
CASL Innovations

Advanced Modeling Applications



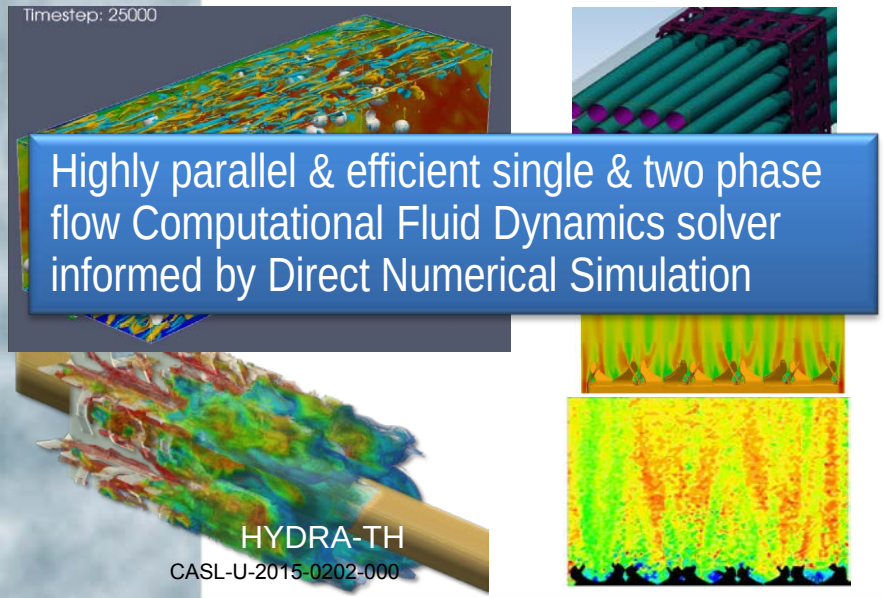
High fidelity full core analysis of thermal hydraulic and core physics phenomena with resolved CFD and neutron transport models

Physics Integration



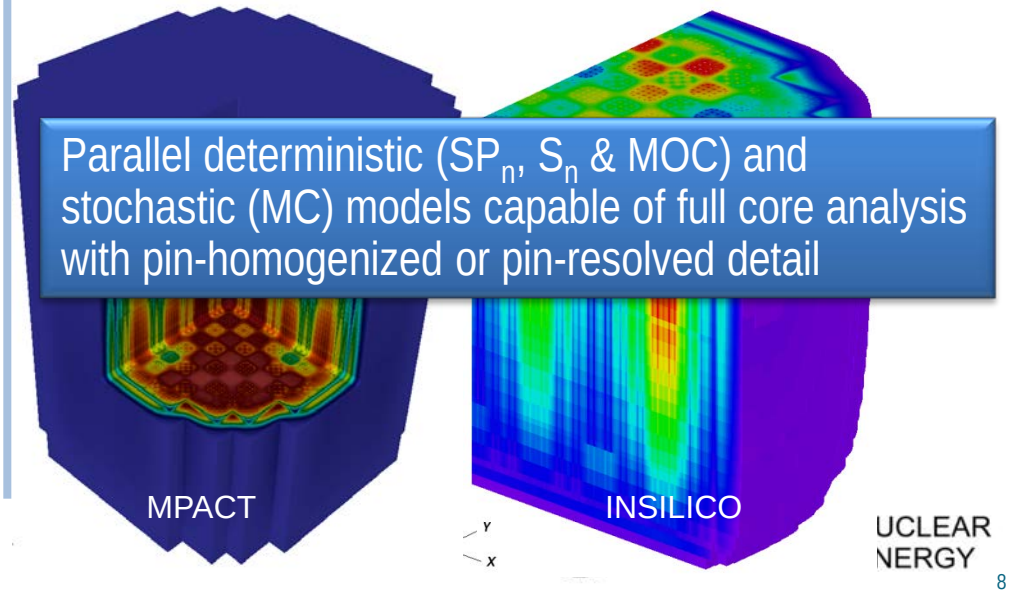
Framework for integration of multiple codes with different physics, addressing control, and solution methodology & transfer

Thermal Hydraulic Methods



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

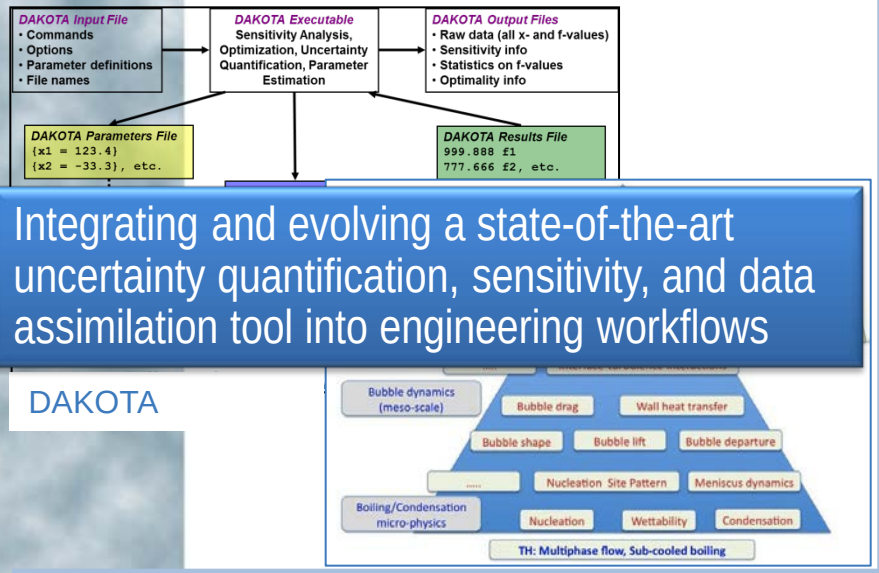
Radiation Transport Methods



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



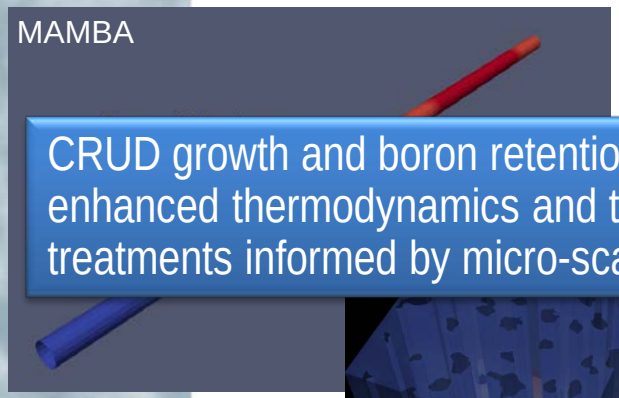
Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows

DAKOTA

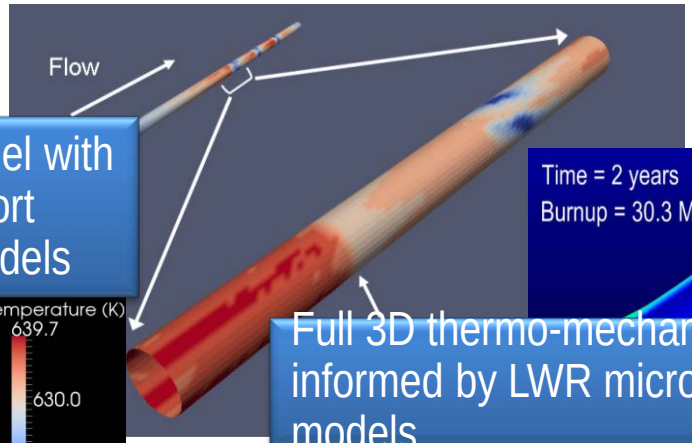
VOCC

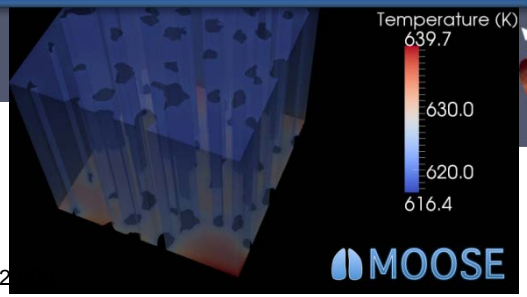
Bringing together local ("physical") and geographically distributed ("virtual") contributors in a meaningful and productive way

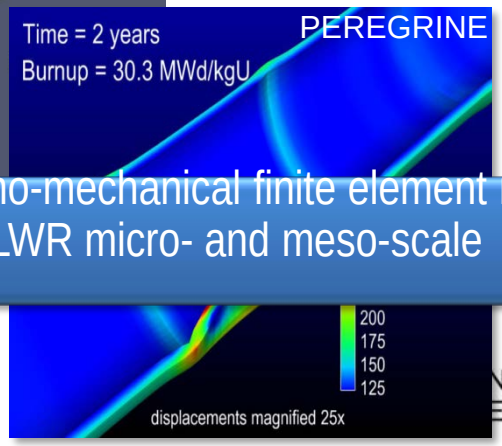
Fuel Materials and Chemistry



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



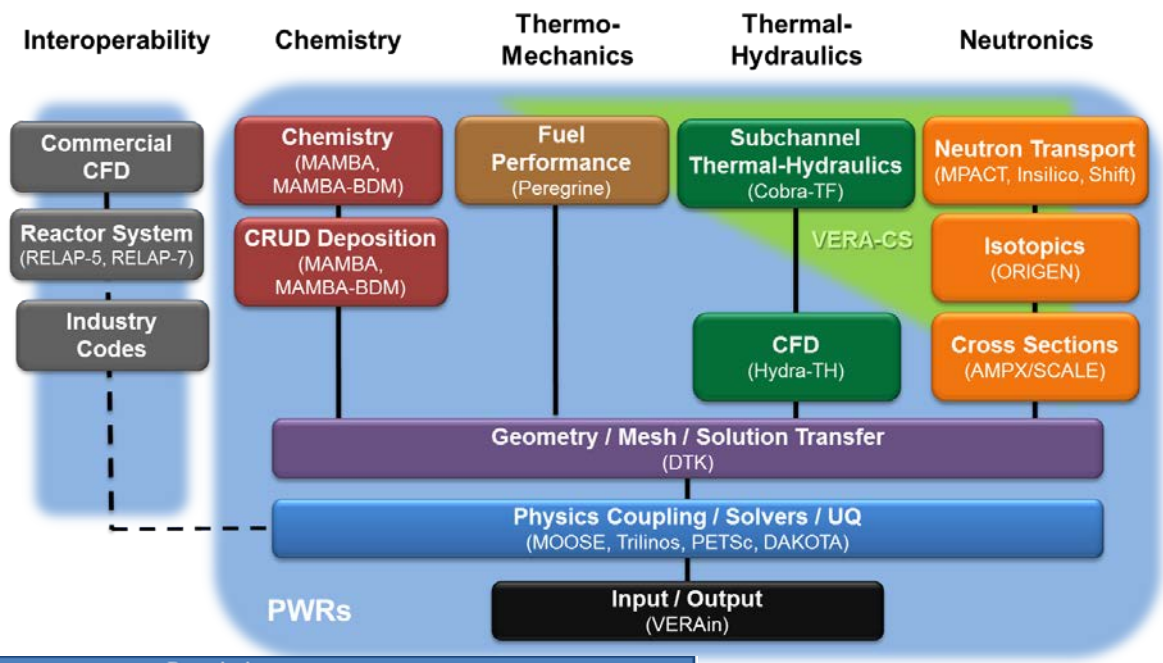




Full 3D thermo-mechanical finite element model informed by LWR micro- and meso-scale models

CASL's Virtual Environment for Reactor Applications (VERA)

VERA capabilities expected at Phase 1 conclusion (Apr 2015)

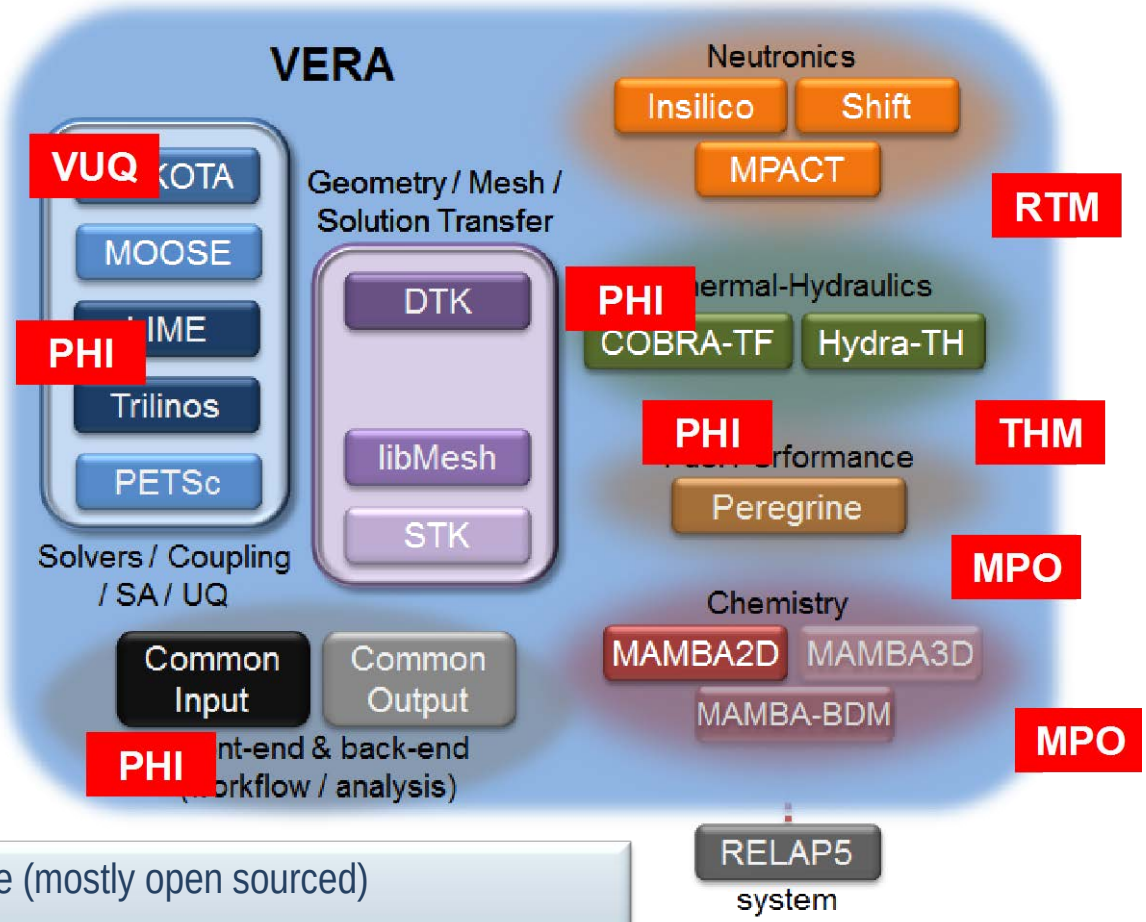


Item	Description
S/W Development Tools and Computational Infrastructure	Standardized set of compilers and configuration tools Git revision control system and S/W repository management Build & test infrastructure (TriBITS, CMake, CTest, CDash) 17 geographically dispersed code repositories, 205 TriBITS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

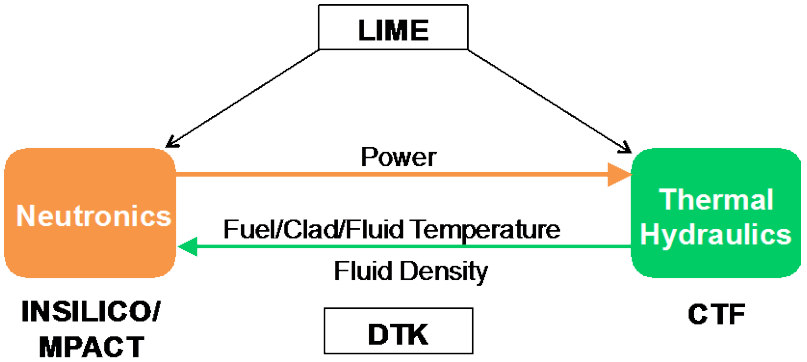
Integrates physics components from focus areas

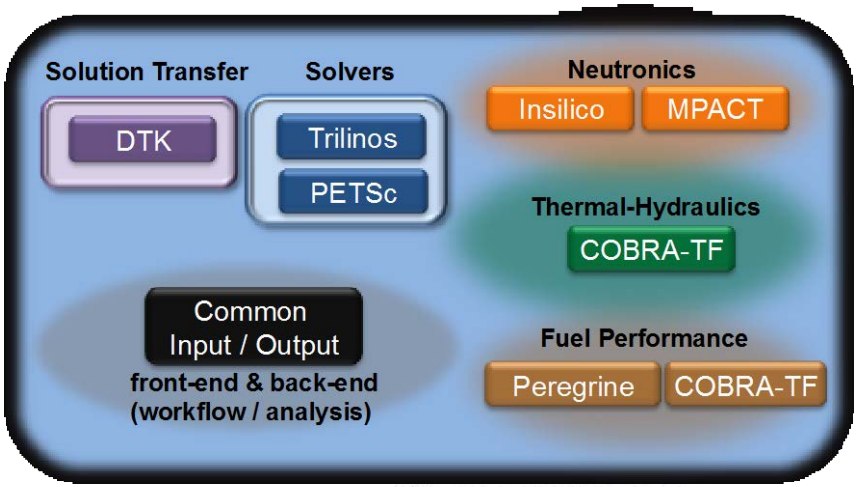


- Mature infrastructure (mostly open sourced)
- Automated testing and growing test base
- Many new coupling developments and implementations
- Rapidly-evolving Core Simulator (VERA-CS)
- 2014 RSICC release (later this CY) will have major functionality upgrades relative to 2013 release

VERA 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





VERA-CS

Painfully easy to measure progress with our 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

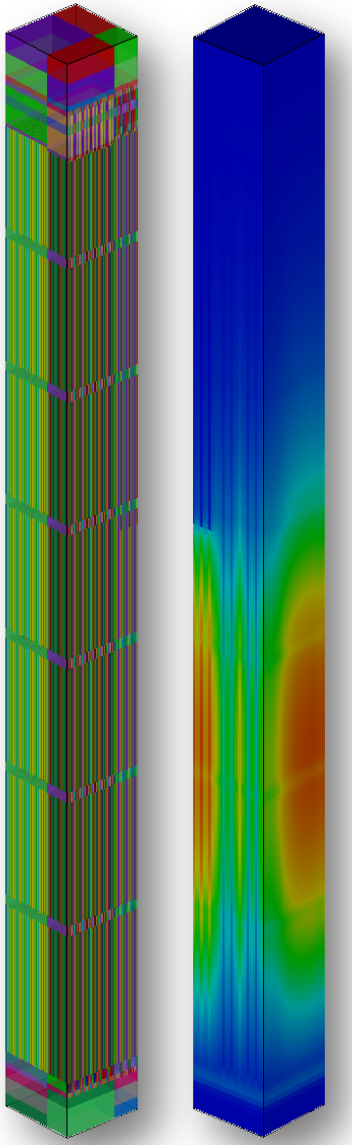
demonstrable progress

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

CASL Core Simulator

Relative to 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

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

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 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			

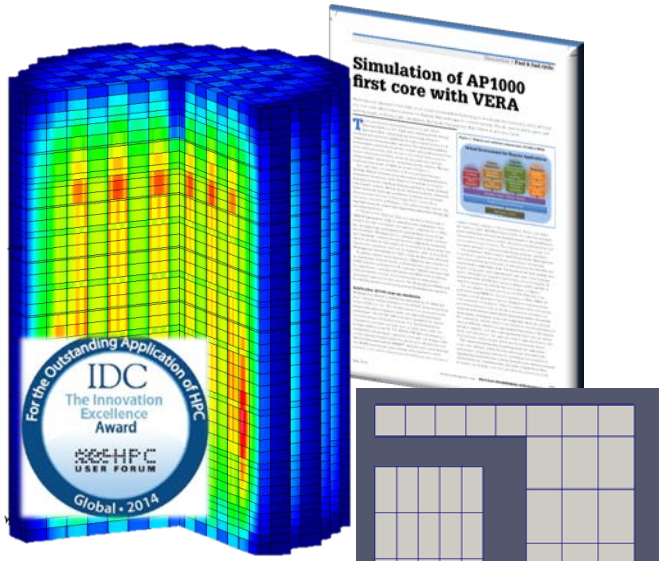
CASL Core Industry Partners Represent 3 Pillars of Nuclear Industry

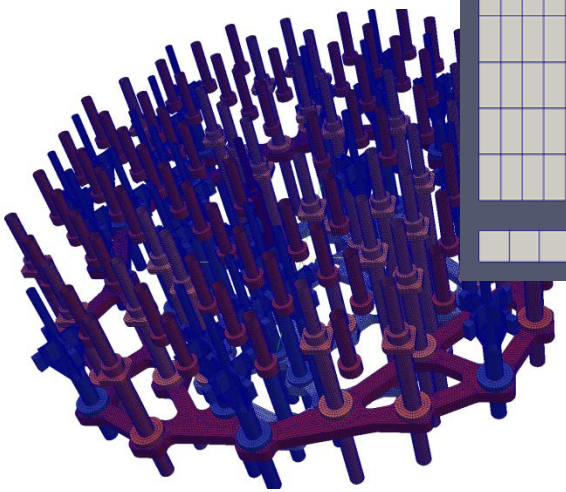
- EPRI: *R&D arm* of industry as driven by near-term utility (owner/operator) needs
  - Power uprates, license extensions, new fuel designs
- TVA: *owner/operator* of 6 nuclear reactors – also brings operational reactor data for validation
  - Address power-limiting operating scenarios
- Westinghouse: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

Technology Deployment

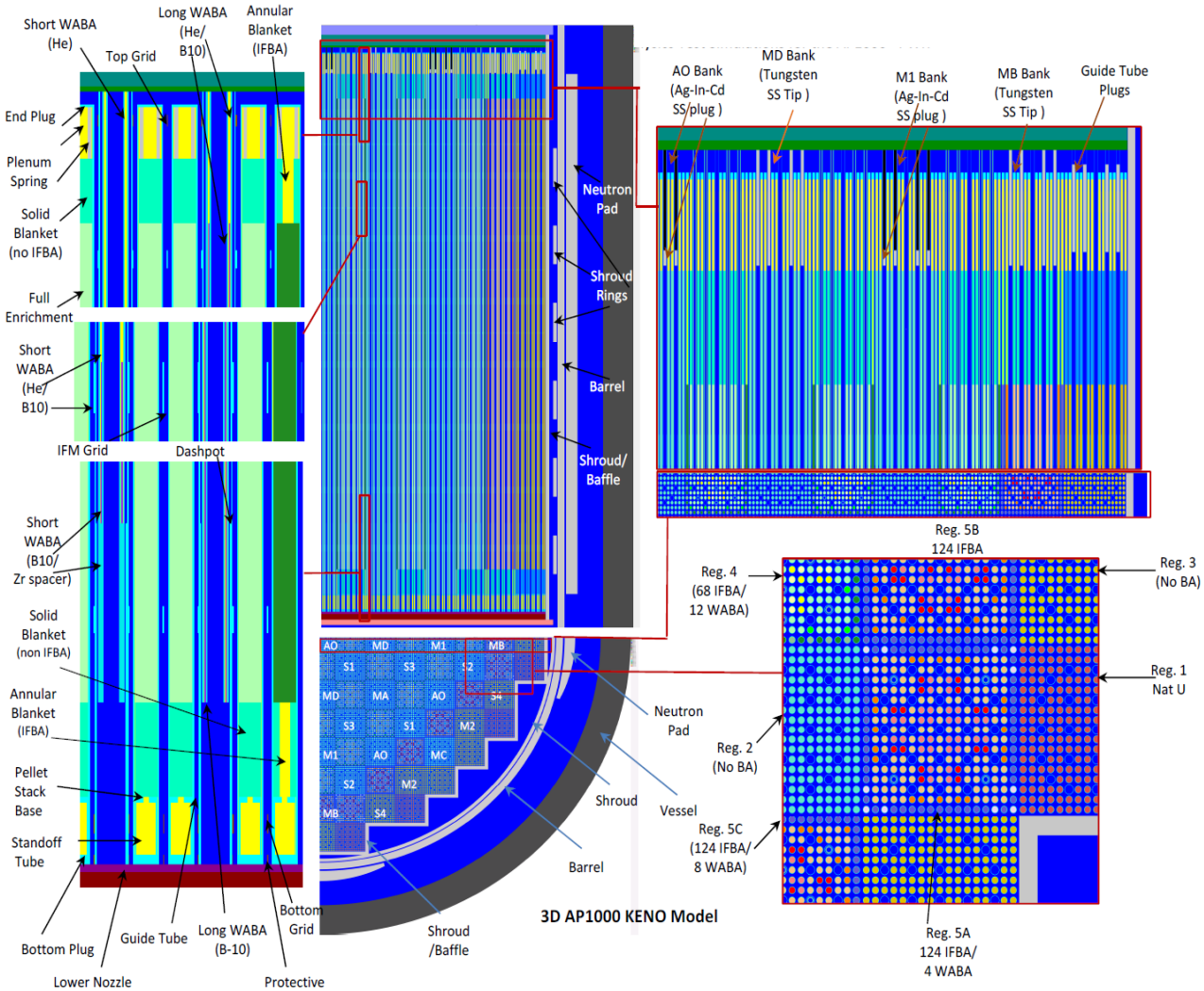
We have now deployed 3 Test Stands

- 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





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.

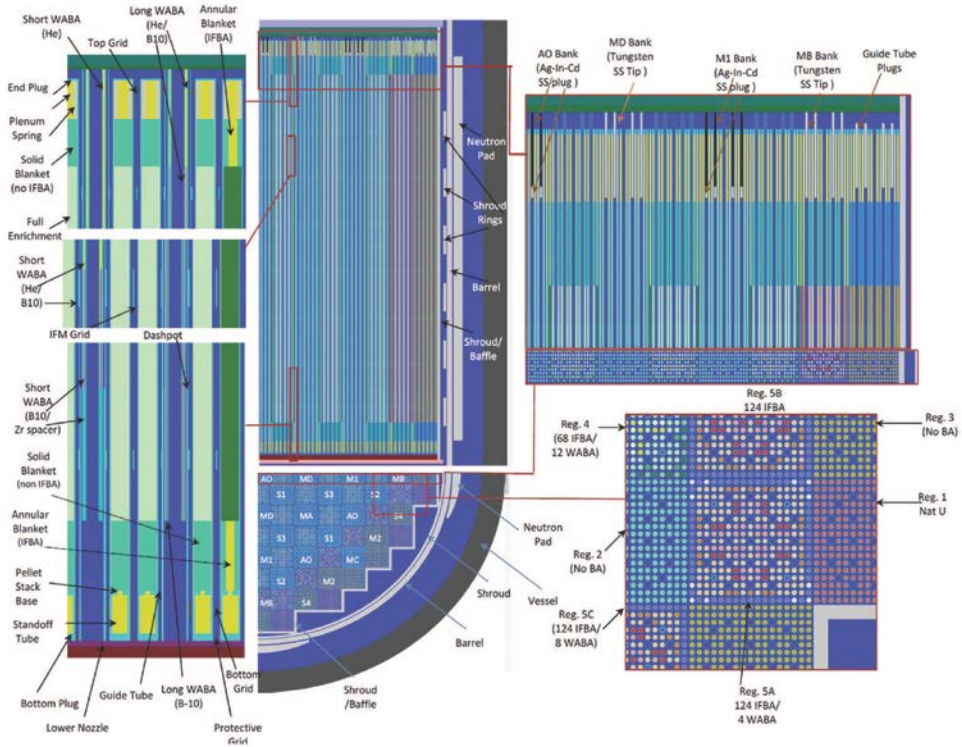
The advanced first core is a major economic advantage since it reduces the number of transition cycles before equilibrium but it also poses challenges to the simulation.

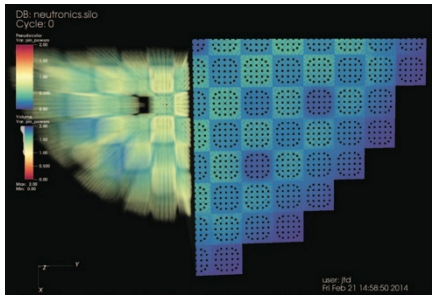
VERA high-fidelity physics provided an ideal match for simulating this challenging core and gain confidence in the start-up predictions

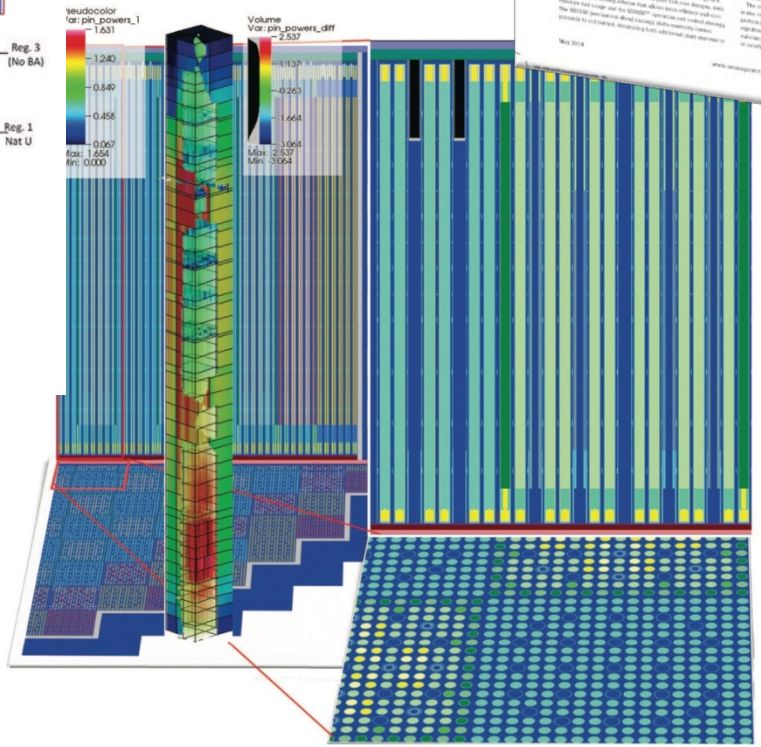
CASL Test Stand at Westinghouse

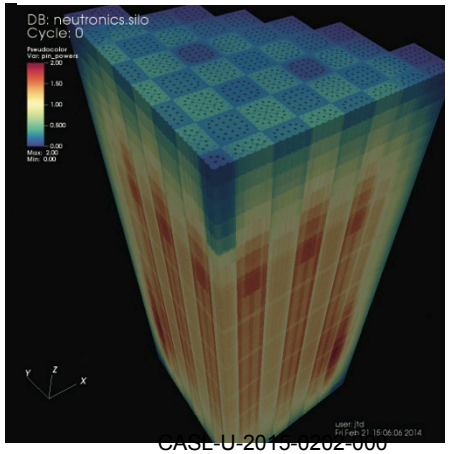
Highlighted in Nuclear Engineering International Magazine

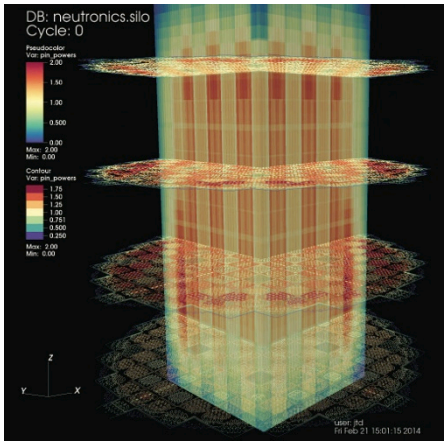
Recipient of IDC HPC Innovation Excellence Award

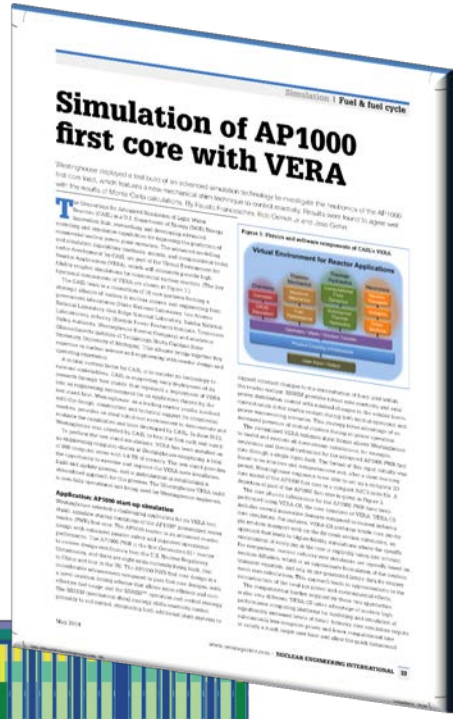












Simulation | Fuel & fuel cycle

Simulation of AP1000 first core with VERA

Westinghouse employed a test build of an advanced simulation technology to investigate the neutronics of the AP1000 first core design, which features a more heterogeneous core than previous designs. Results were found to agree well with long results of Monte Carlo calculations. By Paulo Ansuategui, Rick Gerlach Jr and Jesse Gehre

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

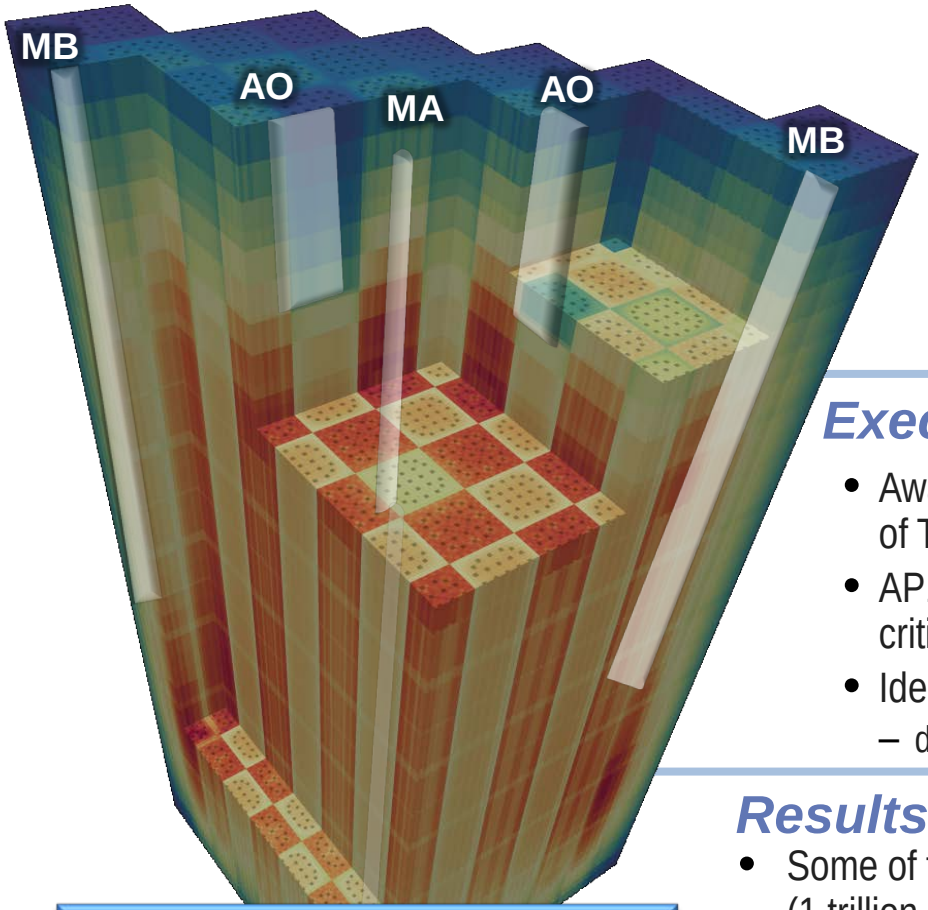
Virtual Environment for Reactor Applications

Application: AP1000 start-up simulation

May 2014

NUCLEAR ENGINEERING INTERNATIONAL 19

Shift: VERA Continuous-Energy Monte Carlo
AP1000 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

CASL Test Stand at Westinghouse

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

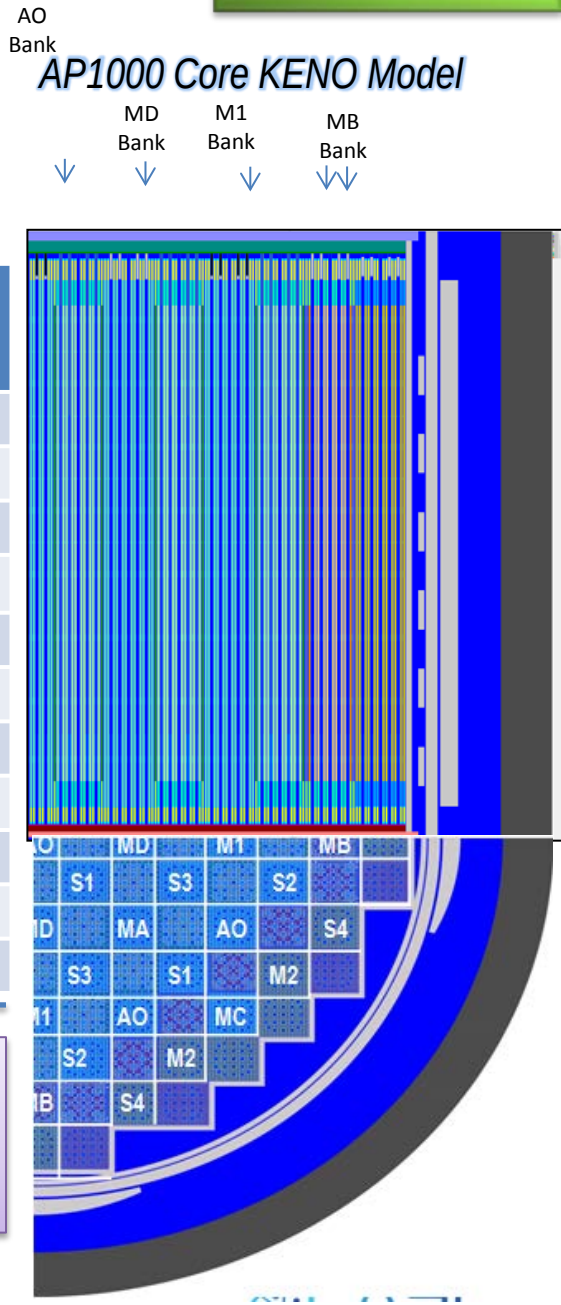
Start-up Boron and Reactivity Coefficients

	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

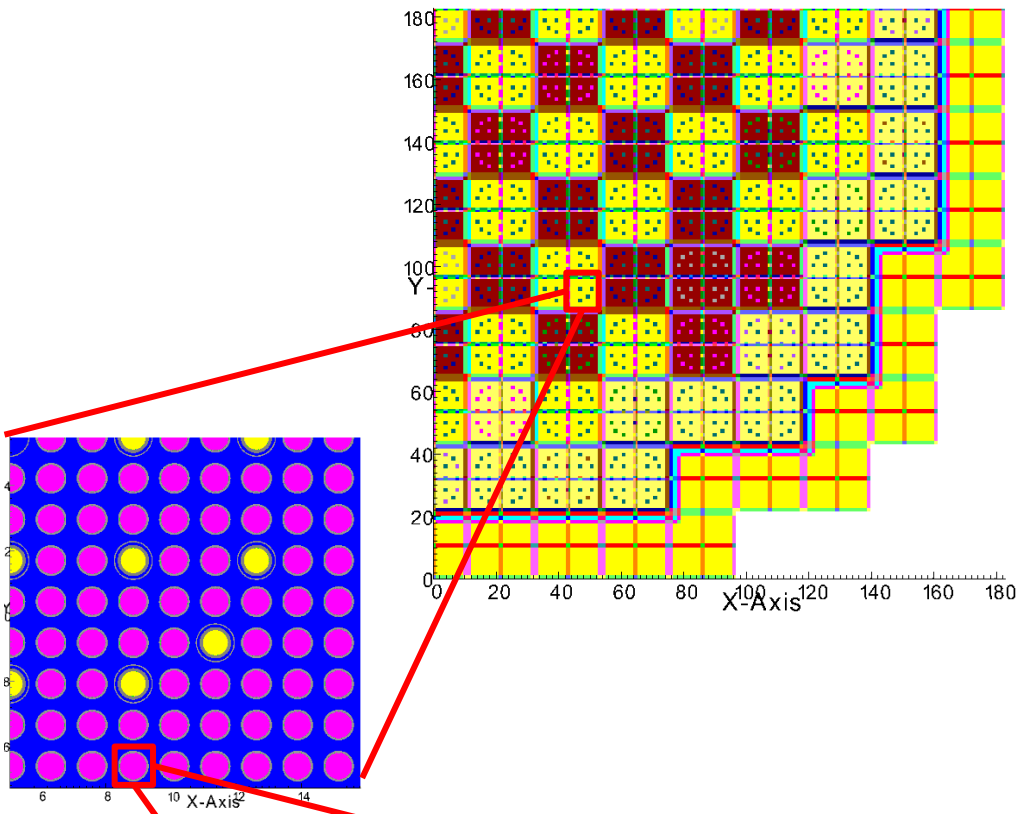
AP1000 Core KENO Model

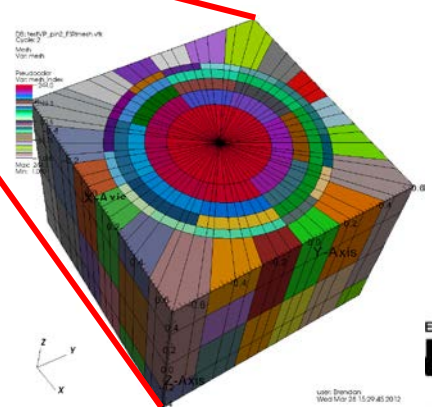


CASL technology deployed at the industry proves beneficial for challenging simulation scenarios

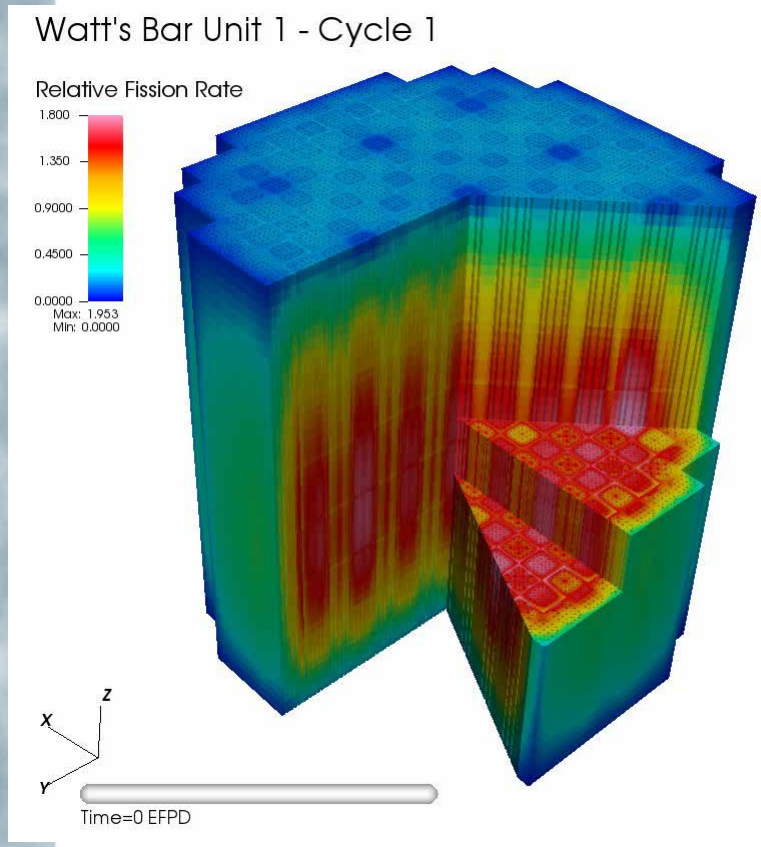
Whole-Core Pin Resolved Transport
(implemented in MPACT)

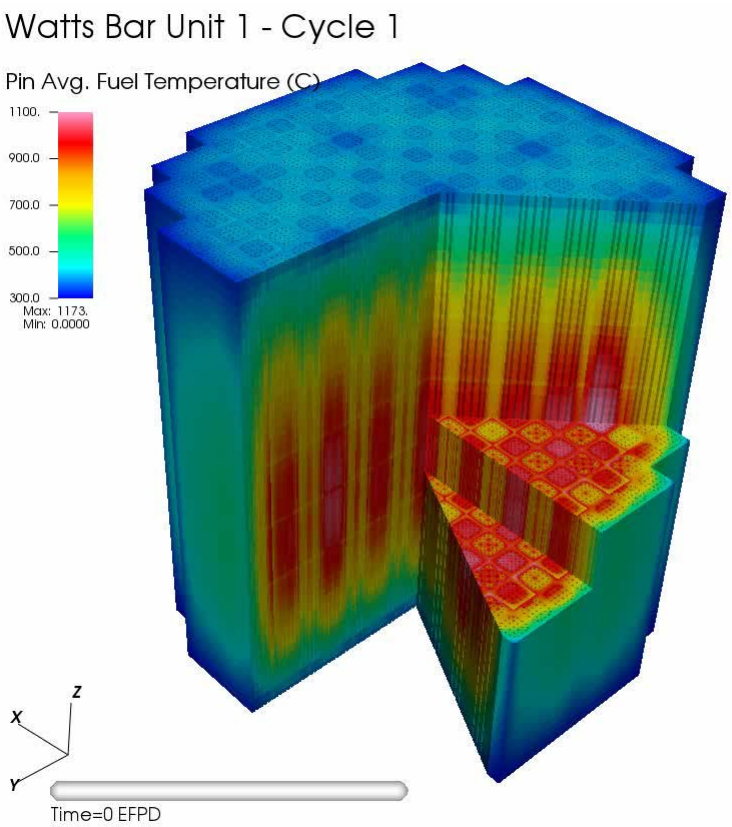
- Explicit Geometry Representation
- No pre-homogenization or cross section tabulation
- Deterministic 3-D Transport
  - 2-D/1-D Method
- Works on Desktops for small problems and scales to leadership class computers for realistic whole core problems
- Processes easy-to-use VERA Input
- Coupled to T/H
  - COBRA-TF (subchannel)
- Isotopic depletion with ORIGEN



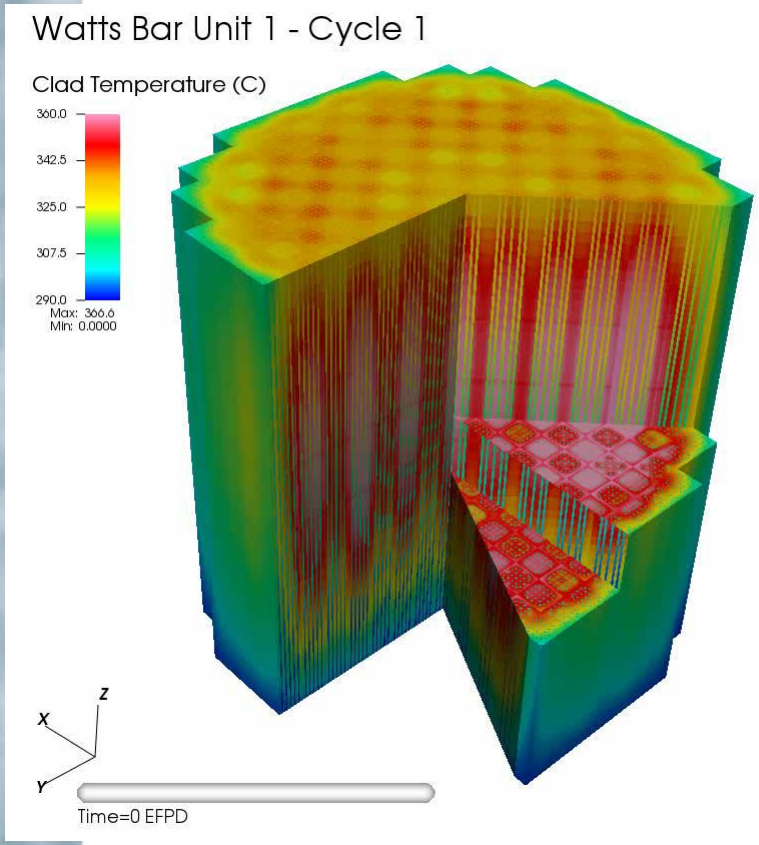


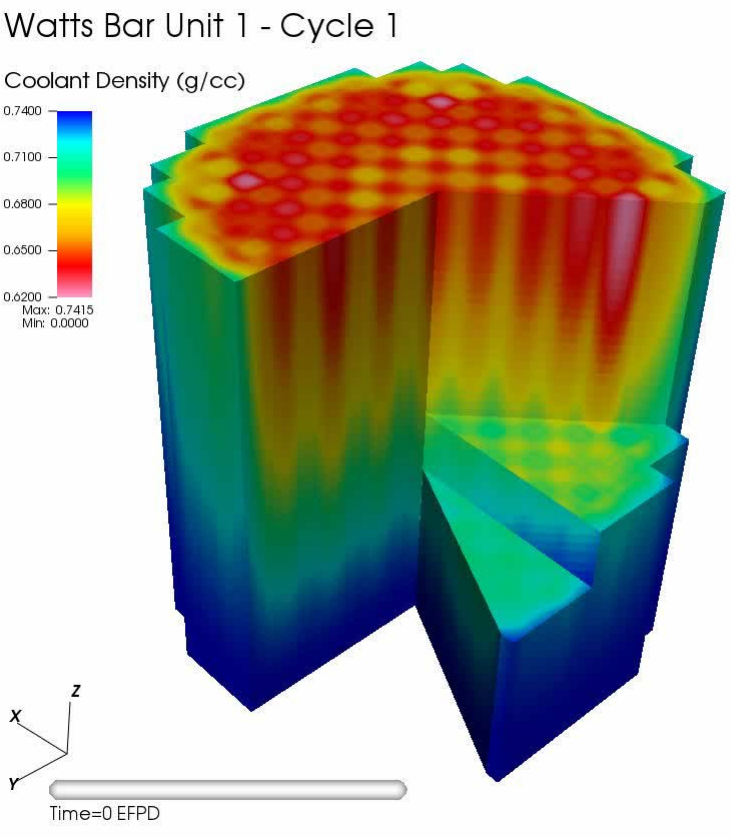
Power and Fuel Temperature



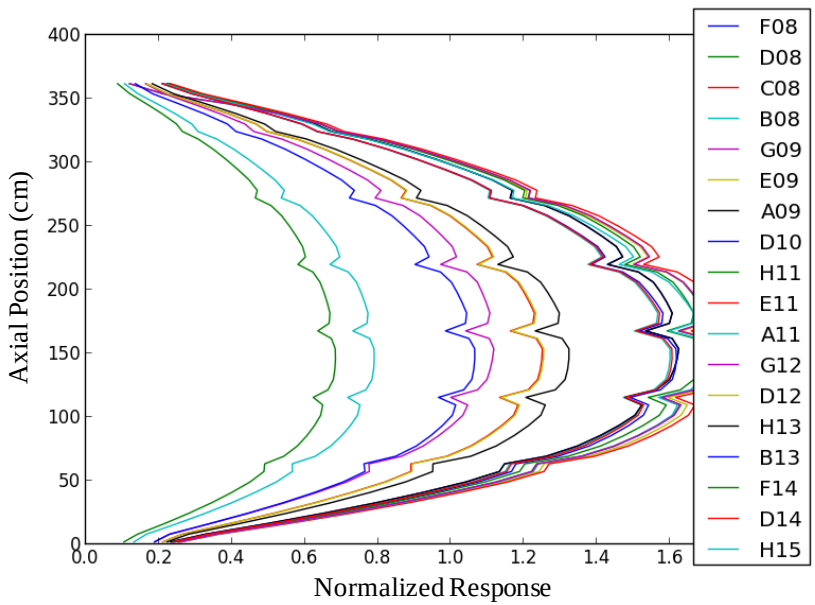


Clad and Moderator T/H





Detector Responses



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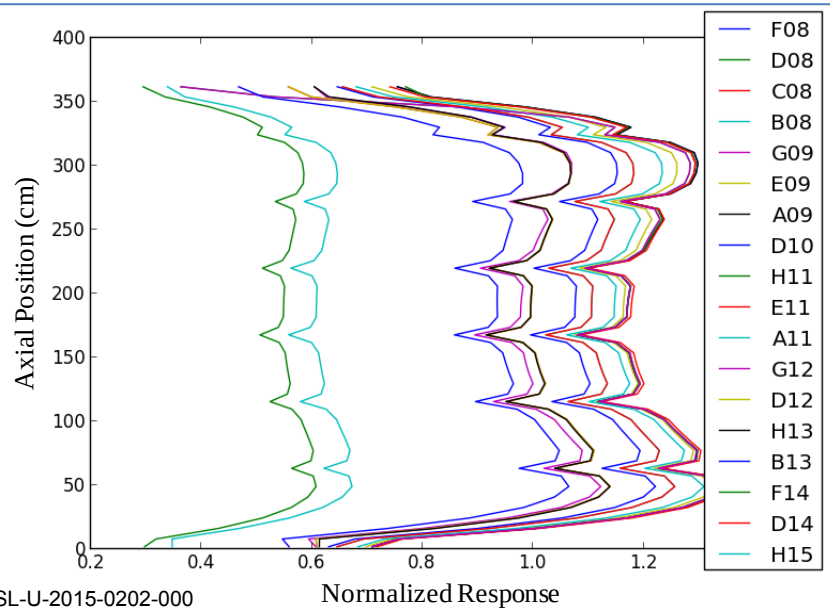
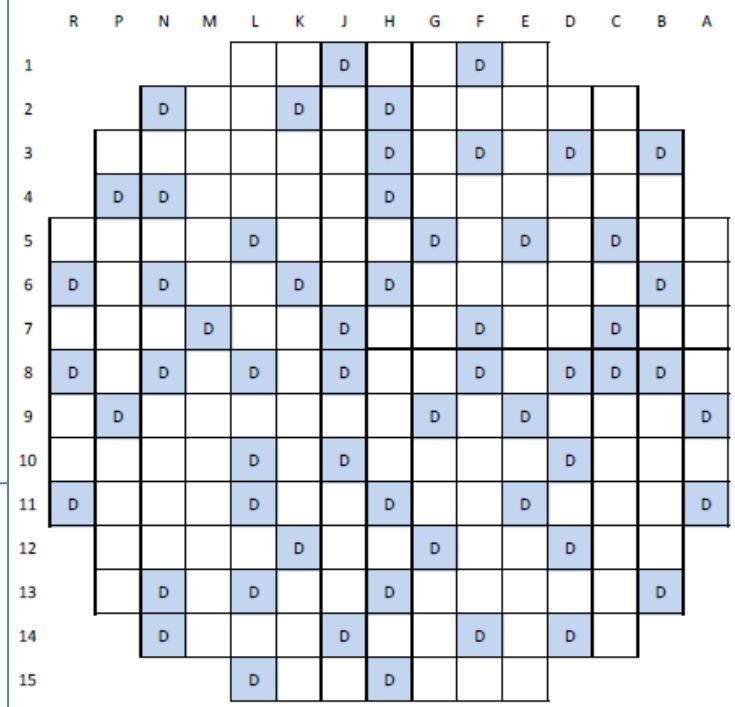


EOC

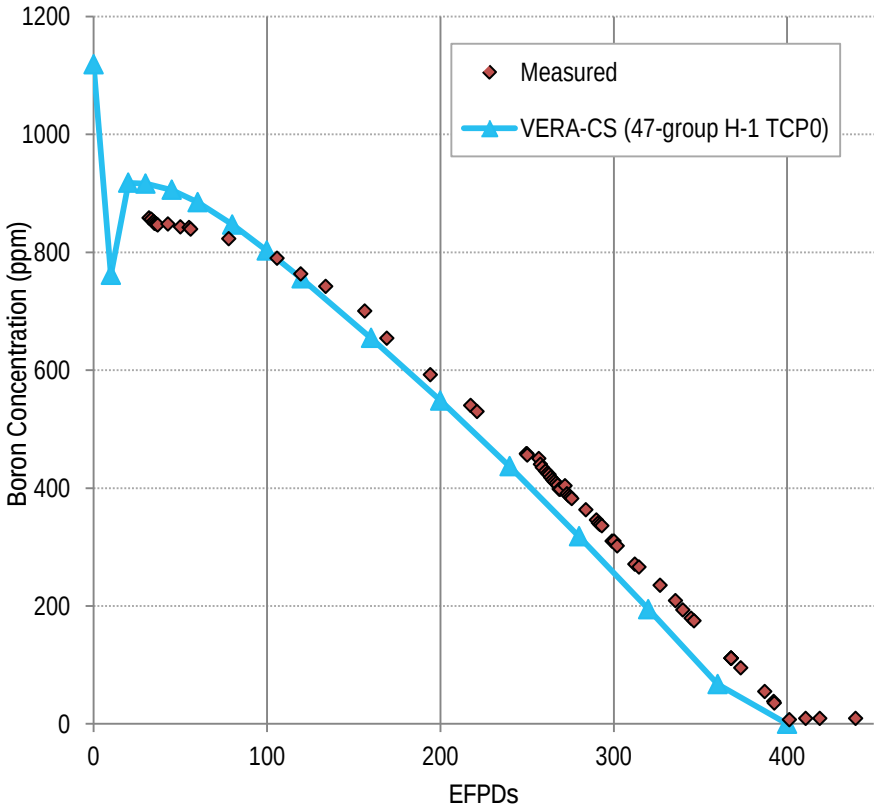
Detector Map



Operational Reactor Depletion Analysis Capability

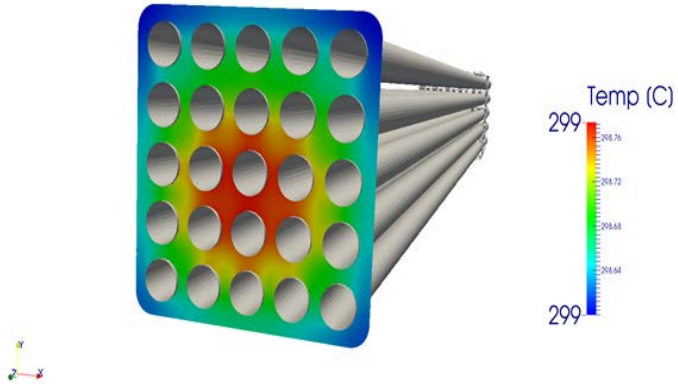
Simulation of Watts Bar Unit 1 Cycle 1

- MPACT coupled to Cobra-TF
- MPACT's internal depletion
- 47 energy group library
- Transport Corrected P0 with neutron leakage conservation
- Constant HFP depletion
  - Approximated operating history due to computational burden
- Quarter symmetry
- Run on Eos and Titan 4076 cores

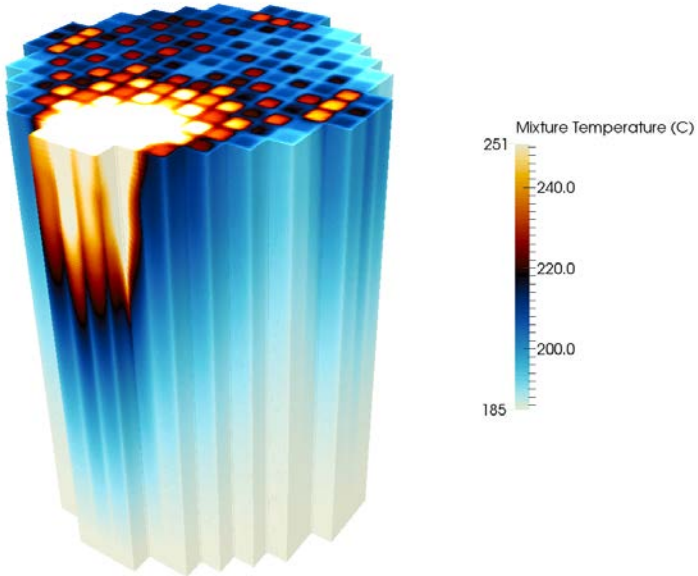


Multi-Scale Thermal Hydraulic Model Applications to the DNB Challenge Problem

- Multi-Scale thermal-hydraulic (T/H) codes applied to modeling and simulations of coolant conditions within subchannels and in reactor cores:
  - High-fidelity Hydra-TH CFD code
  - Subchannel code COBRA-TF (CTF)
  - DAKOTA for uncertainty and sensitivity analyses
- Results demonstrate VERA T/H capabilities for addressing Departure from Nucleate Boiling (DNB) Challenge Problem:
  - Hydra-TH for turbulent mixing prediction in subchannels of rod bundles
  - COBRA-TF for whole reactor core DNB margin predictions under steady-state and transient conditions
  - DAKOTA/CTF calibration process for turbulent mixing based on test data



Hydra-TH Prediction of Coolant Temperature Distribution in Subchannels



CTF Prediction of Reactor Core Coolant Temperature Distribution during PWR Steamline Break Accident

Progress in Validation of the COBRA-TF (CTF) Subchannel Capability for Nuclear Reactor Thermal Hydraulics Phenomena

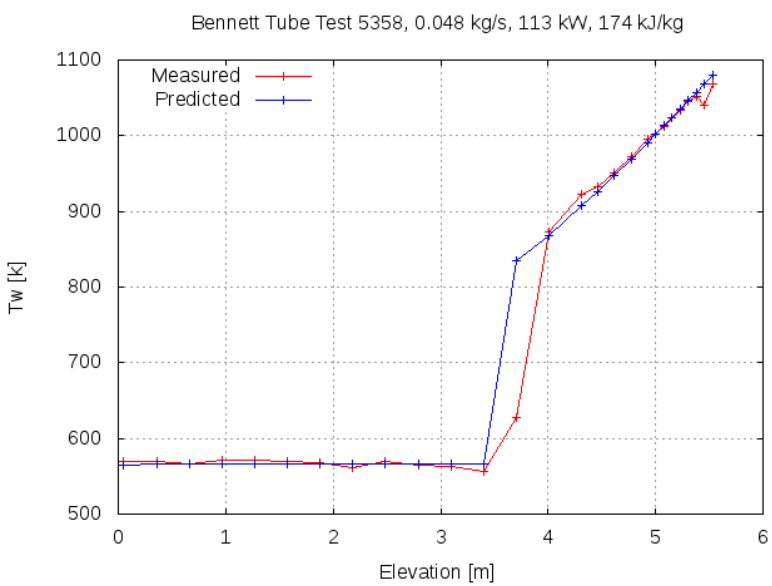
Science Highlight

Background

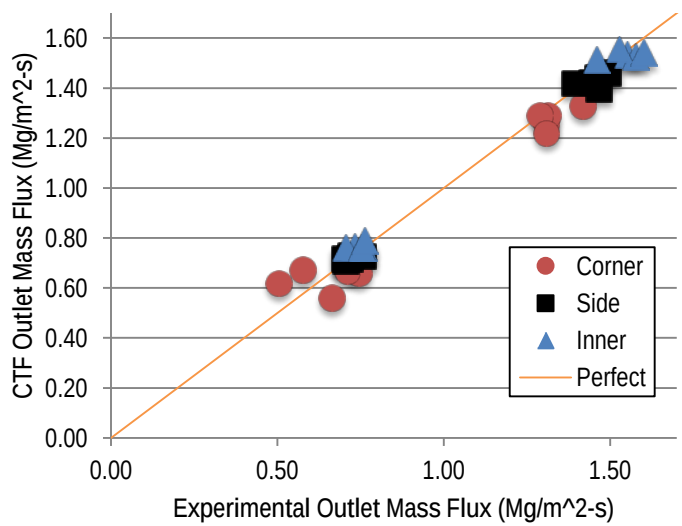
- CTF is a reactor thermal-hydraulics code being developed in the CASL program
- CTF documentation suite includes theory and user manuals, but lacked validation document

Details

- A broad range of experiments were modeled with CTF to build a validation test suite
- Experiment physics included vertical rod-bundle geometries with operating conditions ranging from natural circulation to boiling and accident conditions
- Document summarizing test matrix and code comparisons has been created and included in CTF repository

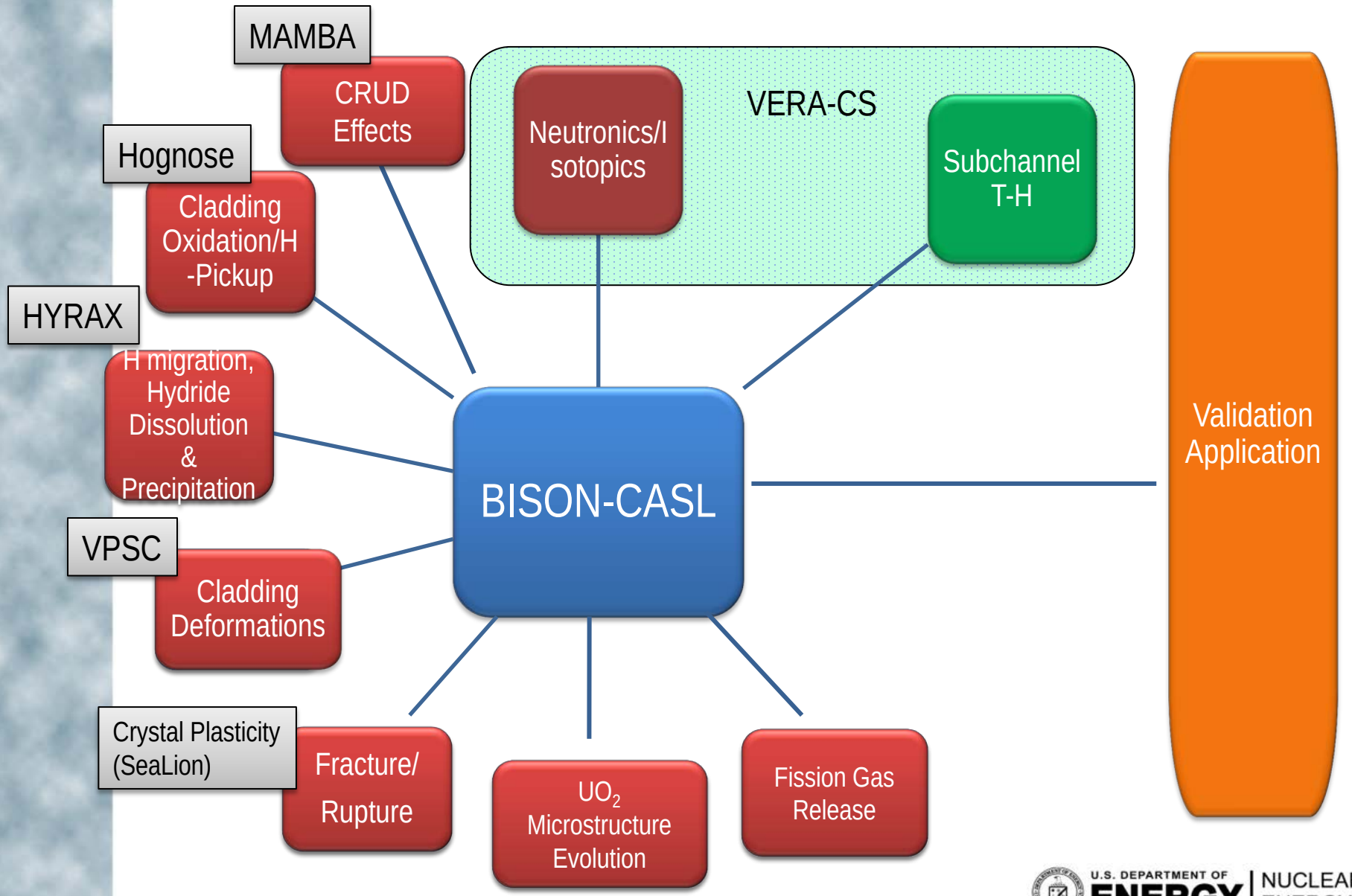


CTF prediction of wall dryout



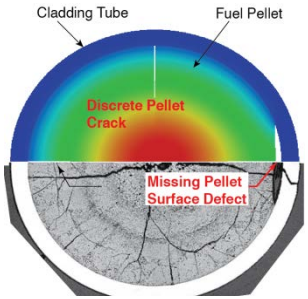
CTF channel flow distribution prediction

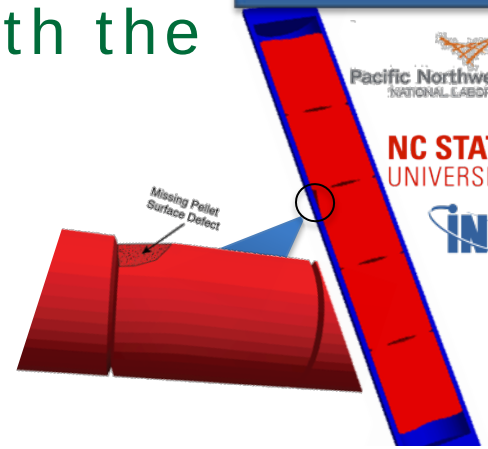
BISON-CASL Fuel Performance Modeling in Support of RIA and LOCA



High Fidelity 3D Simulation of a Nuclear Fuel Pellet-Cladding Interaction with the BISON-CASL Modeling Capability

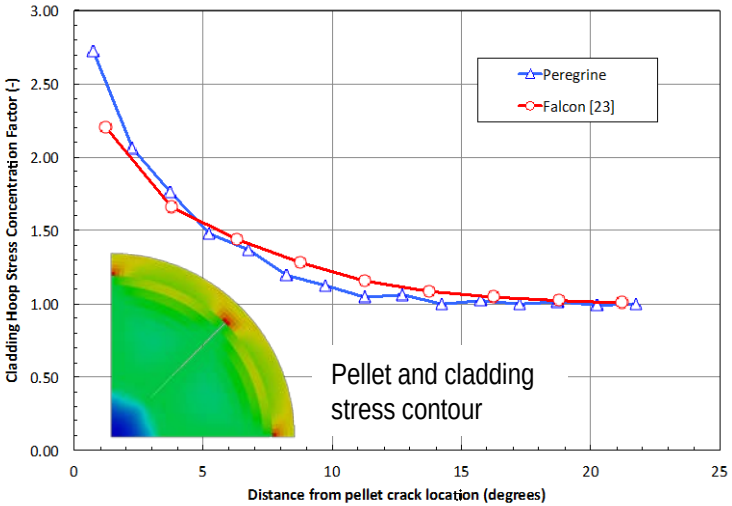
Science Highlight

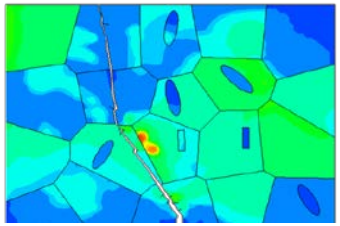




Key Achievements

- 2-D PCMI modeling is consistent with current state of the art in fuel behavior modeling for PCI

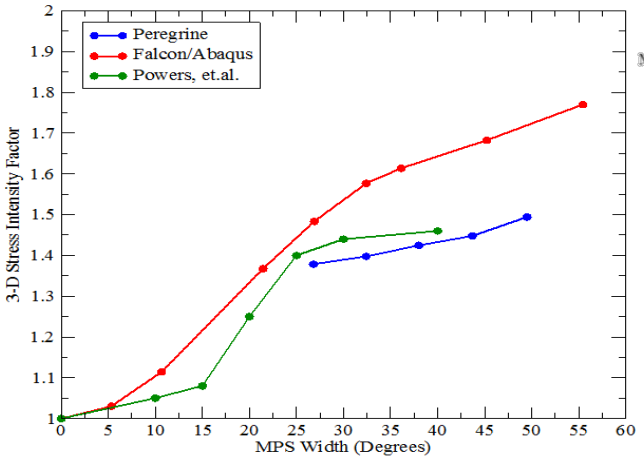


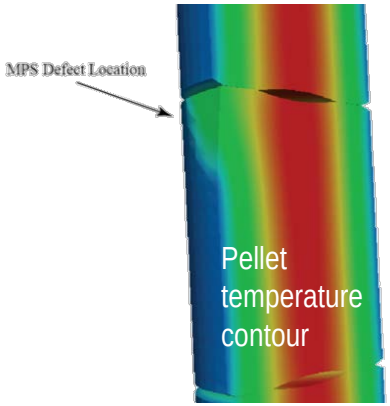


Dislocation density contour

- Able to characterize crack growth evolution unique to Zr-alloys using dislocation-density crystal plasticity model coupled with microstructural features

- Impact of MPS defect size on stress concentration factors are similar to industry assessments (with Falcon/ABAQUS/ANSYS)



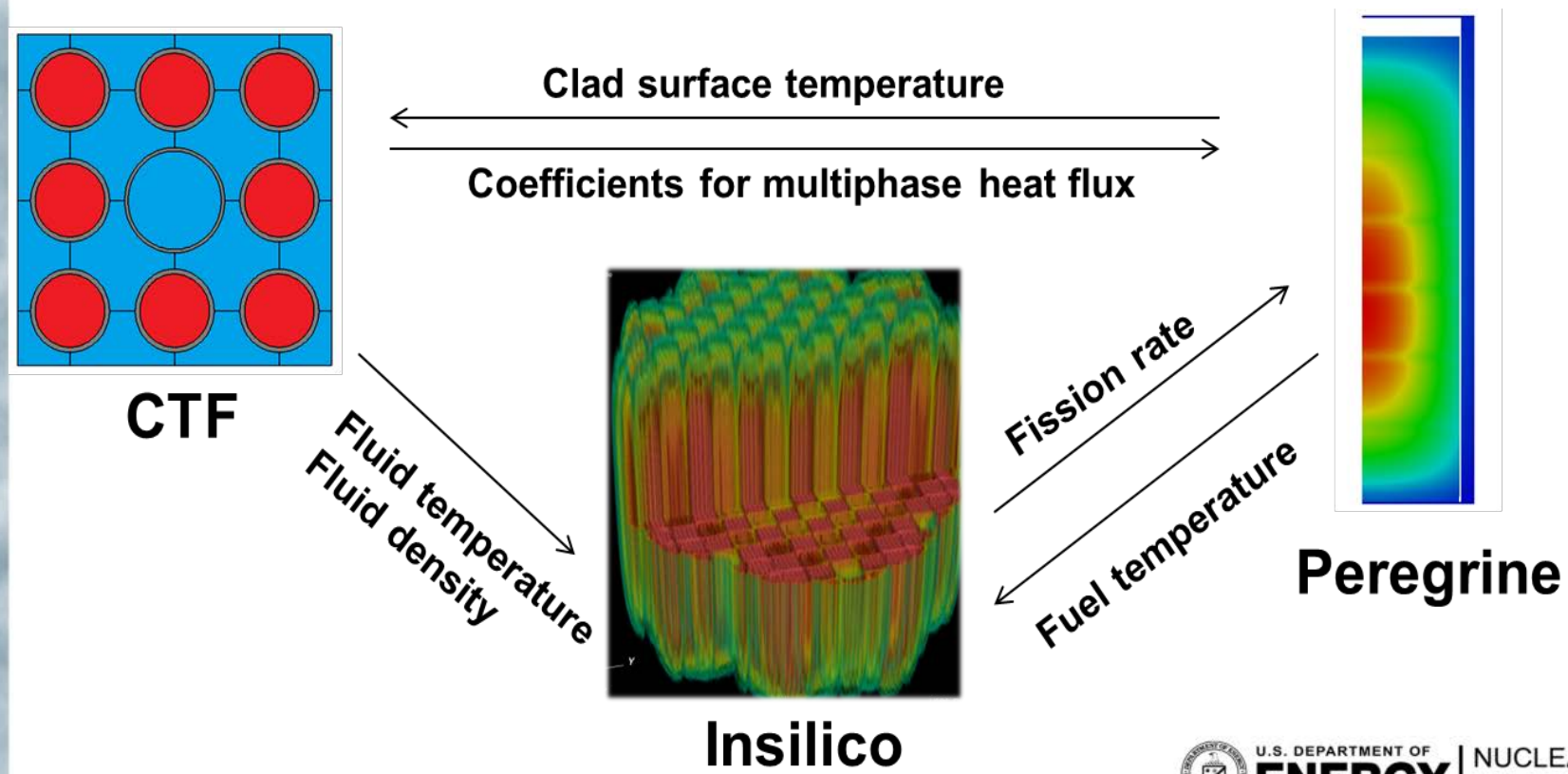


Path Forward

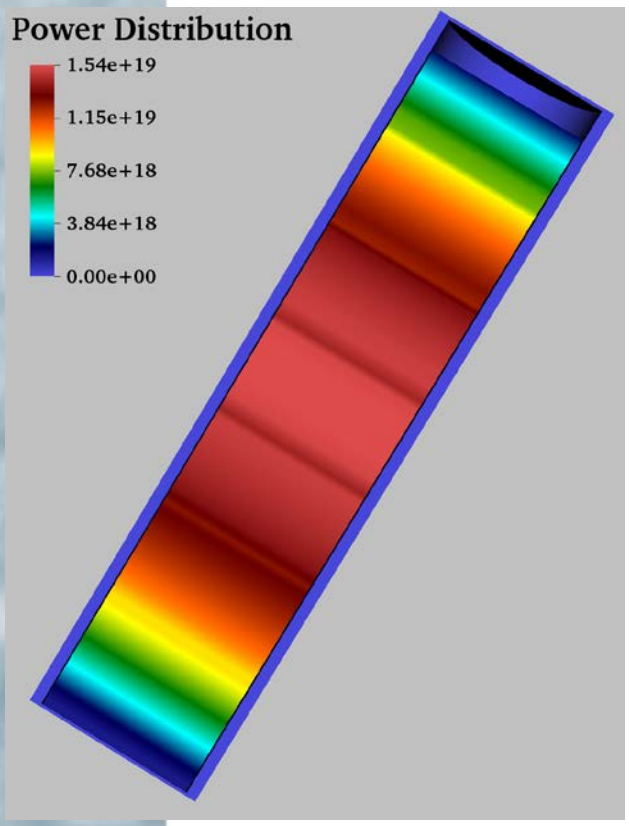
- Implement robust 3-D mechanical contact algorithm
- Develop smeared crack and relocation models based on fracture and deformation behavior of ceramic UO_2 pellets
- Interface with a fission product chemistry and reaction model for initiation and propagation of cladding cracks by SCC

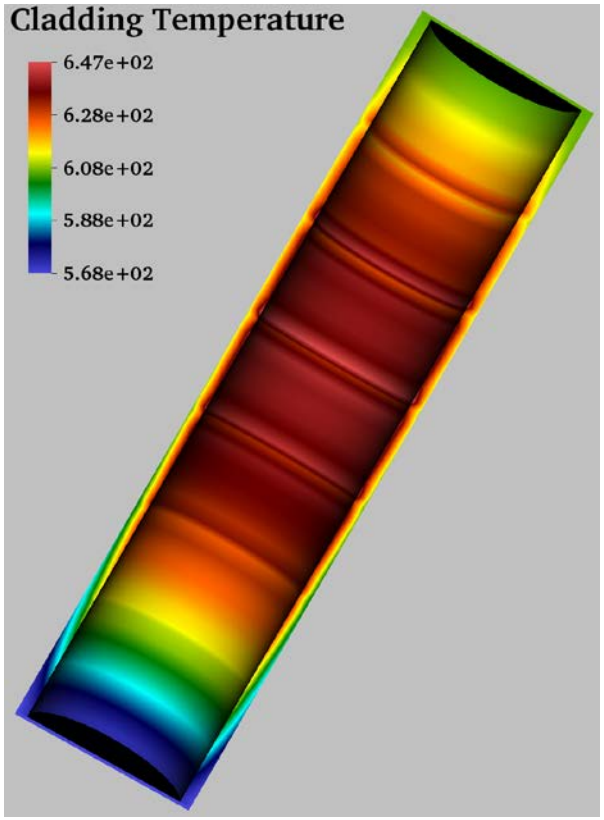
VERA Coupled Capability: PCI Challenge Problem

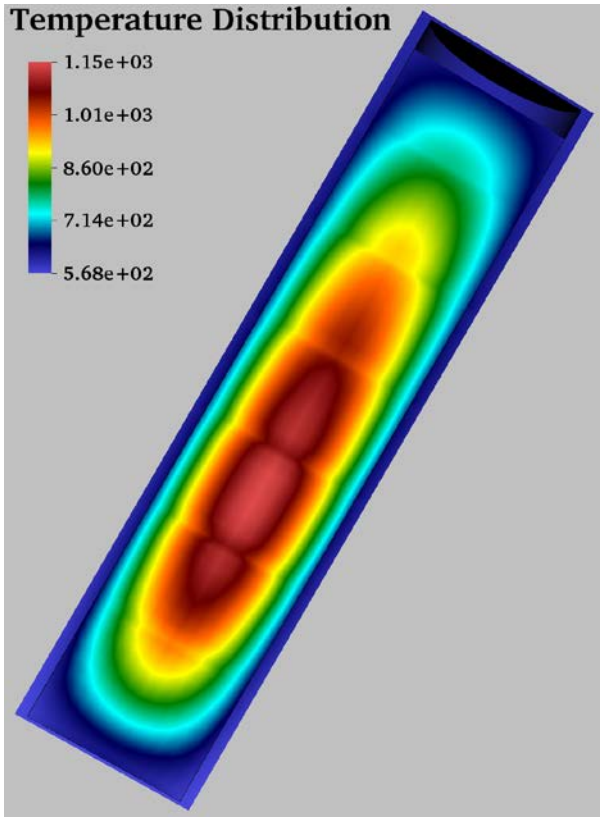
- Tiamat-based coupling of CTF-Insilico-Peregrine
- All applications are run in their own MPI process space
- Data Transfers are handled through DTK with MPI sub-communicators
- Extends core simulator functionality with improved fuel performance capability
  - CTF has simplified model that has been replaced here with 2D Peregrine fuel rod model



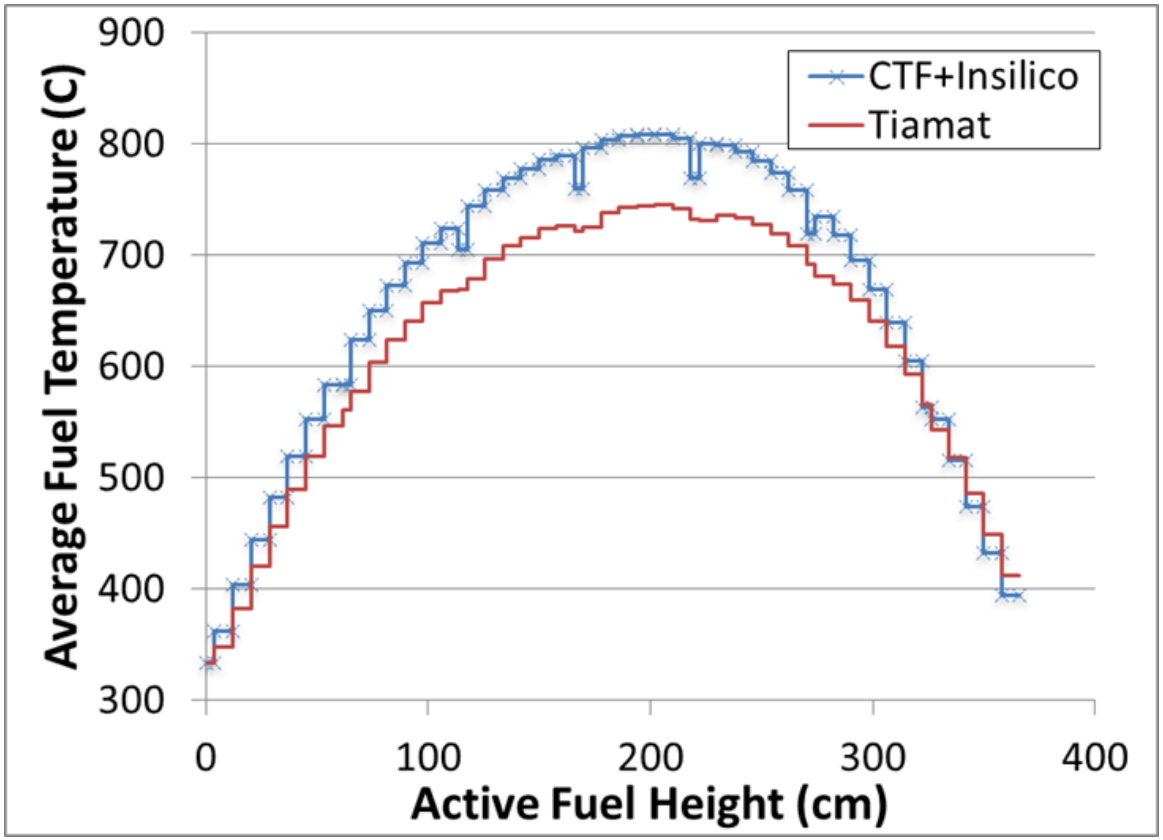
CASL Core Physics Progression Problem 6
(Single Assembly Watts Barr)







Comparison: Average Axial Fuel Temperature

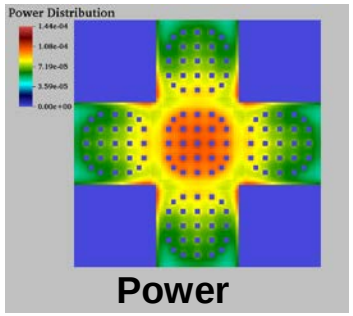


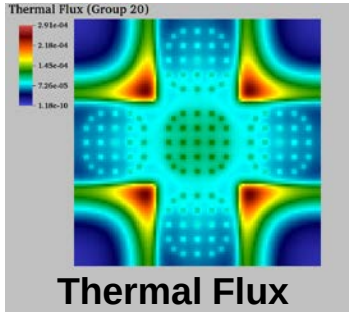
- Average values for each axial edit bound region (plotted as piecewise constants)
- Temperature is higher in CTF+Insilico
- Likely due to:
  - Gap heat transfer coefficient value that was arbitrarily chosen in CTF for VERA.
  - Number of radial rings in CTF+Insilico simulation
  - Offline study puts temperatures within error for realistic gap htc and radial ring values

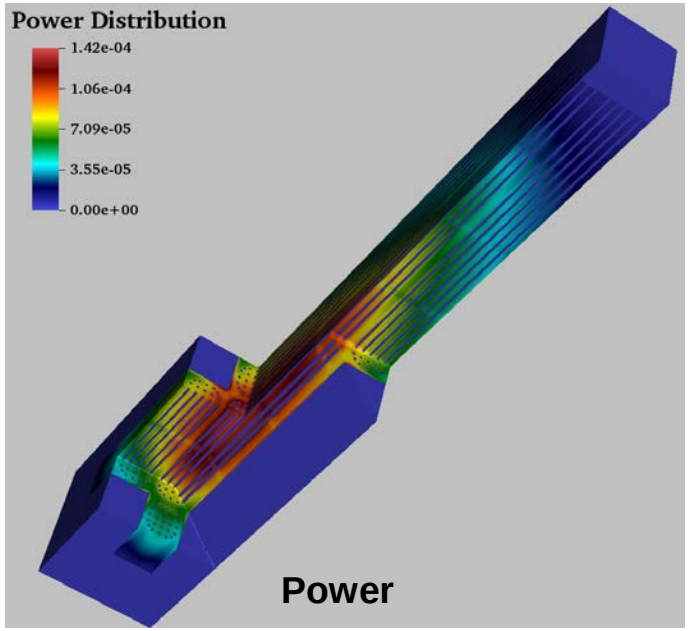
A Preliminary Capability for Novel Investigation of Pellet Clad Interaction

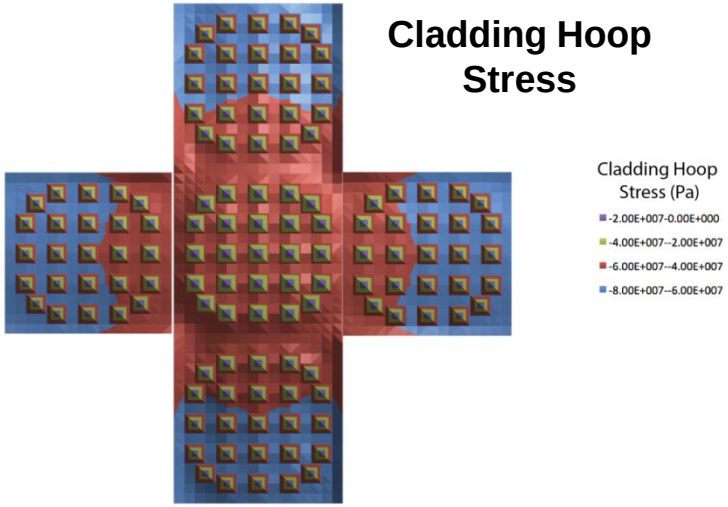
Tiamat is a multiphysics coupled code for assessing pellet clad interaction failures.

- Couples COBRA-TH for thermal hydraulics, Insilico for neutronics and Peregrine for fuels performance.
- Strong coupling of transient physics
- Targets large-scale parallel architectures
- Initially focused on ramp to hot-full power









Outcome:

- Tiamat can be used to identify regions in the reactor where PCI is likely to occur due to high hoop stress in the cladding.
- Demonstrated on 5-Assembly Cross for Watts-Barr Cycle 1

CFD Overall Review: Year 1-4

- Three fundamental Steps aimed at "capability" and "delivery"

Code Evaluation: methods, capabilities, performance, extensibility

Candidate Codes: CFDLib, CartaBlanca, Drekar, Fuego, TRUCHAS, NPHASE, TransAT, STAR-CD, STAR-CCM+, …

V&V Pedigree: Necessary to have a V&V culture embedded in development
- Documentation base
- Testing infrastructure
- Existing regression & verification tests

Integration in VERA: Source code accessible for extension/integration

1

Phase-1: single phase capabilities supporting CP's

Hydra-TH:
- Meshing assessment for CFD -> Hexpress/Hybrid
- Validation studies for GTRF, VUQ turbulence model effects
- Extended LES and RANS models for GTRF, DNB mixing studies
- Rich suite of LES statistics output delegates
- Conjugate heat transfer, porous drag
- User, theory, V&V documentation
- VERA integration with automated nightly pushes

2

Phase-2: advanced multiphase framework

Hydra-TH:
- Code infrastructure to handle multiple phases, parsing, output, restarts
- Implementation for arbitrary number of phases, i.e., multifield
- Demonstration of parallel scaling to 36,000 cores
- Transient flow
- Framework for momentum closures: lift, drag, turbulent dispersion, etc.
- User, theory manuals

3

Single Phase Validation of Computational Fluid Dynamics for Fuel Applications

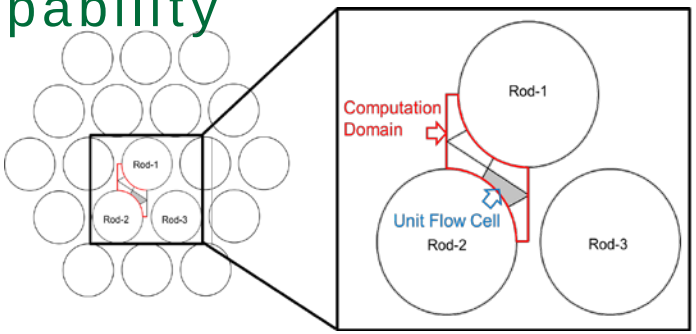
With the CASL-developed Hydra-TH capability

Purpose

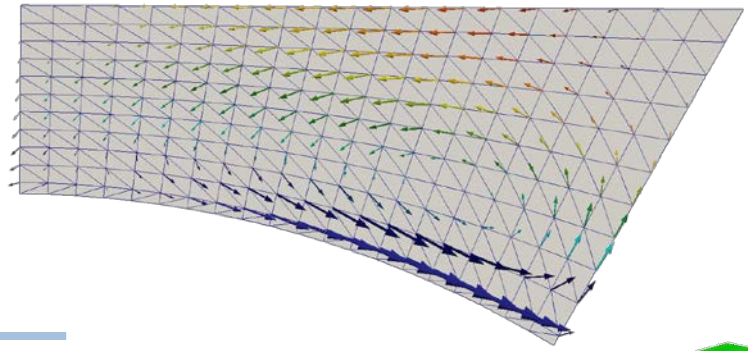
- Demonstrate and assess Hydra-TH capabilities for fuel related single phase applications.
- Implement advance turbulence approaches to deliver a robust capability in support of CRUD and GTRF CPs.

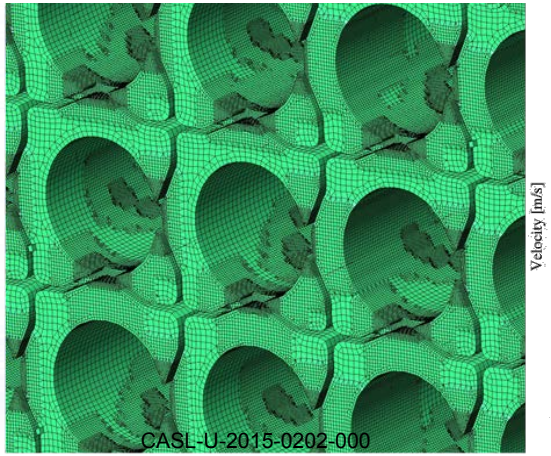
Execution

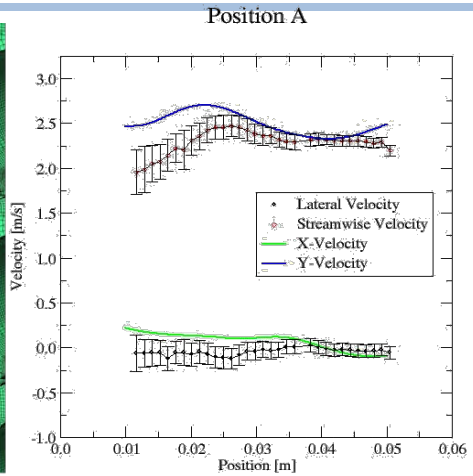
- Advancement and assessment of Hydra-TH solution algorithms.
- Extension of turbulence modeling framework for RANS/URANS simulations.
- Implementation and assessment of an advanced non-linear turbulence model for fuel related applications.
- Assessment of Hydra-TH capabilities for application to GTRF predictions.
- Testing and best practice development for fuel related applications of Hydra-TH.



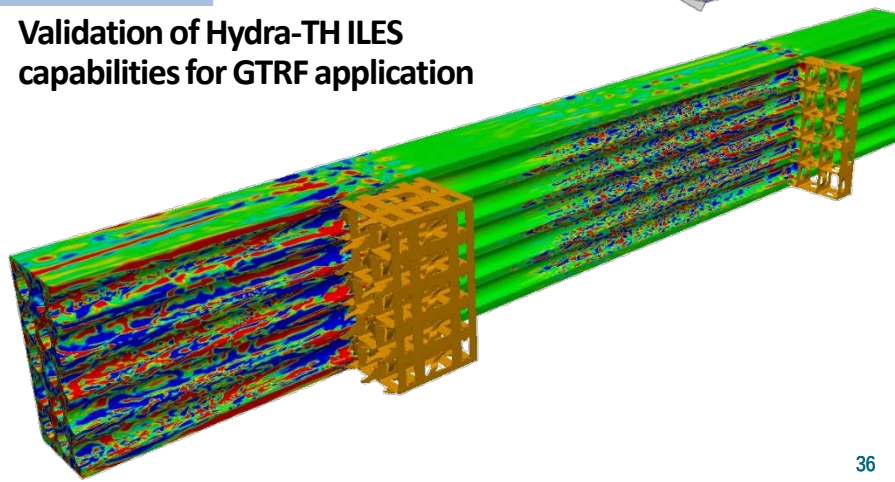
Turbulence Driven Secondary Flows predicted by new Quadratic NLEVM





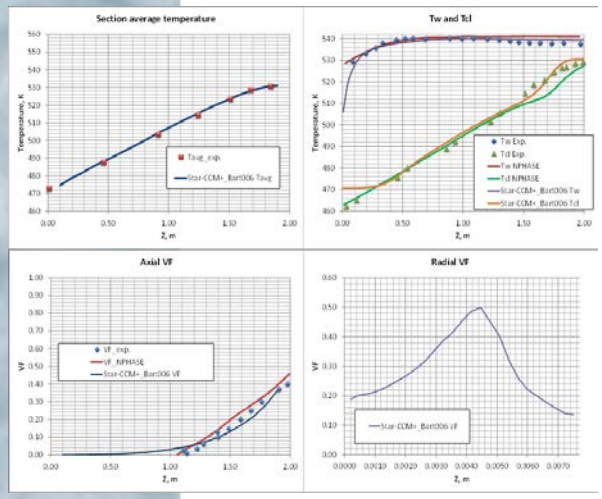


Validation of Hydra-TH ILES capabilities for GTRF application



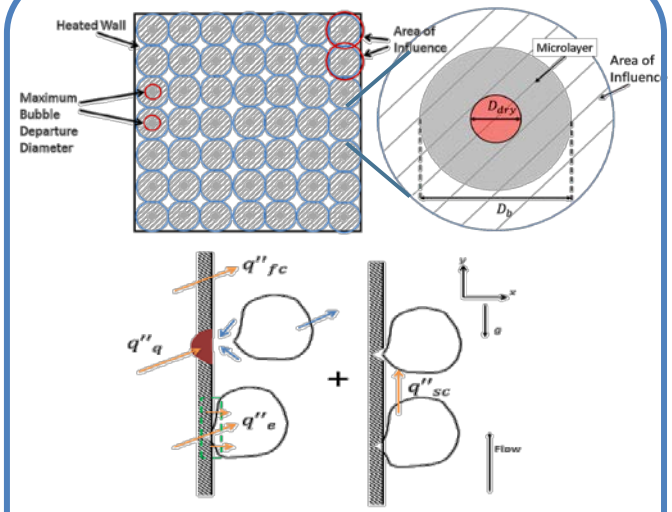
2014 Focus:
GEN-II Boiling → towards DNB

Robust Baseline Closure



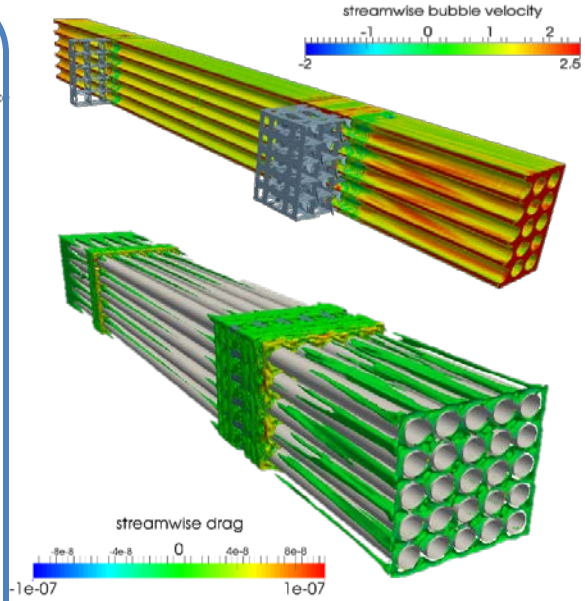
- First Generation Closure in Hydra-TH should leverage existing experience
- Implementation of baseline closure in STAR-CCM+ allows direct comparison to CD-adapco baseline closure results (platform independent)
- Sensitivity of model parameters should confirm PoR-3 studies

Innovative GEN-II Closure



- Second Generation Closure should incorporate new physical understanding
- Increased synergy with experimental "micro" measurements
- Extended applicability (lower/ higher vapor generation)
- Include modeling toward limiting behavior (CHF)

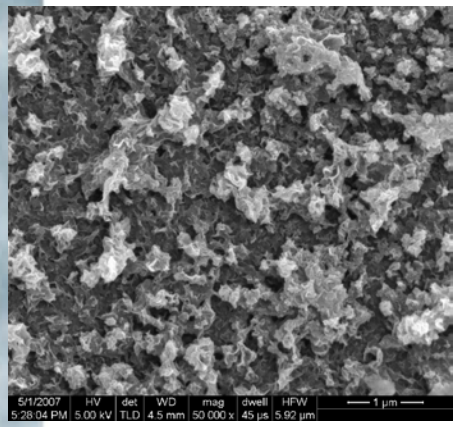
New M-CFD Platform

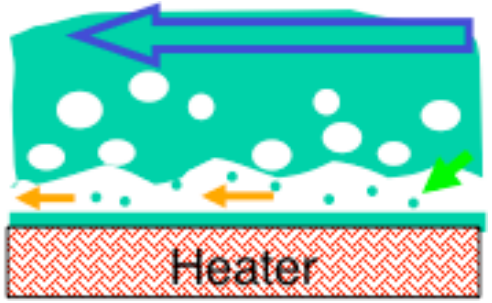


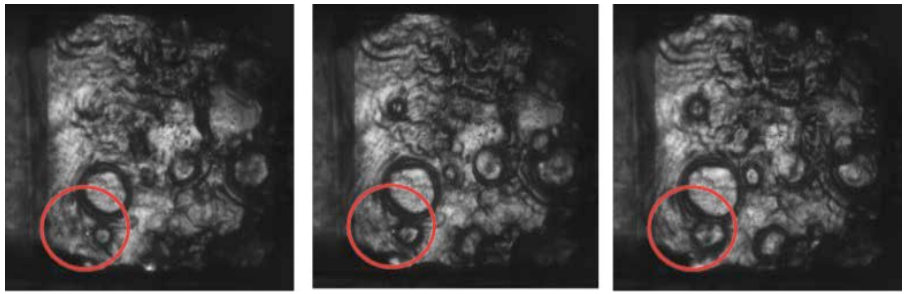
- Hydra-TH baseline multiphase capabilities first shakedown
- Hydra-TH Multiphase implementation targets enhanced applicability towards transient simulations (including fast transients)

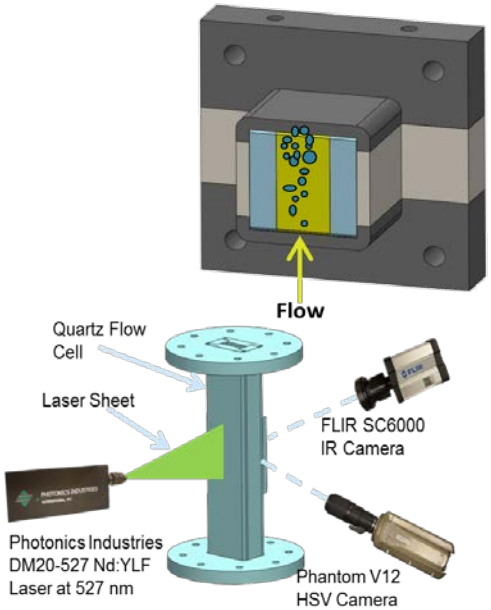
New Physical Understanding: Subgrid Surface Representation

- Extension to DNB requires physical representation of heater surface
- Includes bubbles interaction



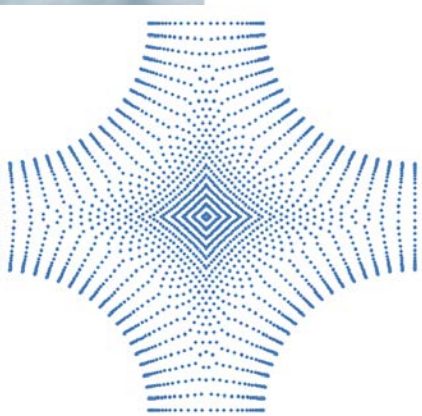


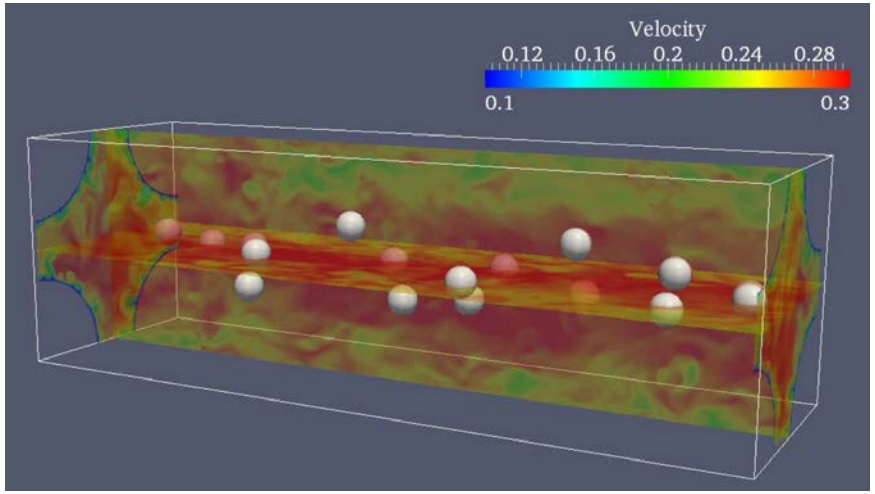


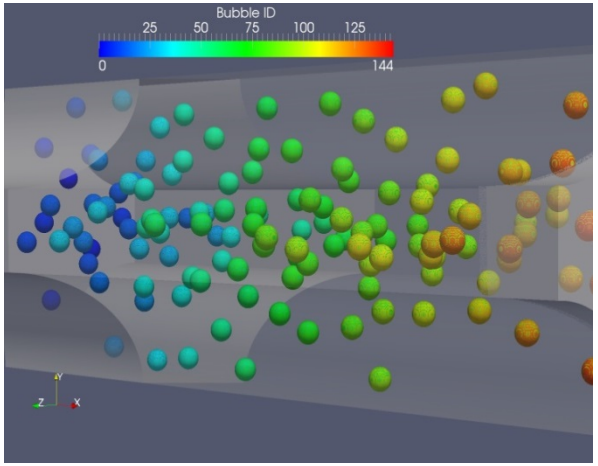


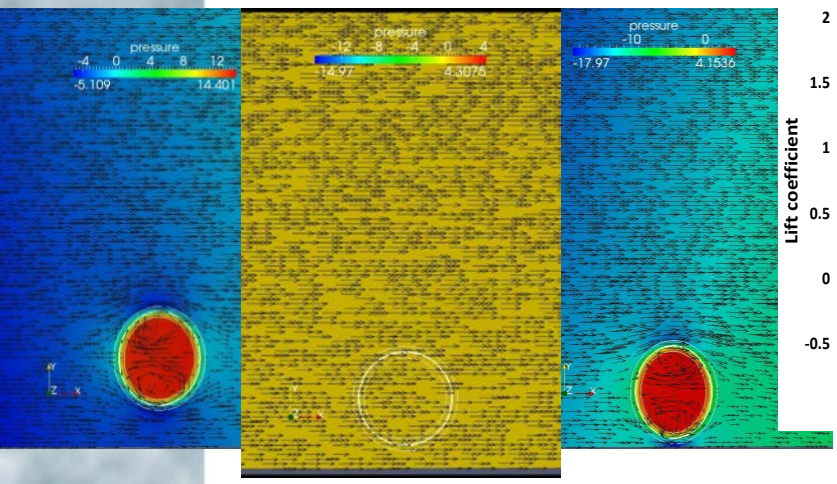
- Platform must include the modeling capabilities
- Experiments/DNS are used for continuing improvement of physical understanding
- Understand/agreement on boiling microhydrodynamics

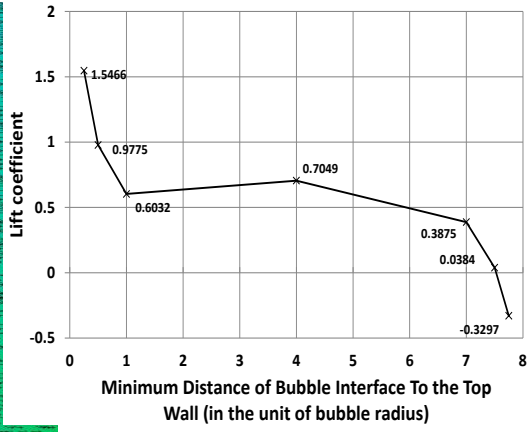
Microscale Modeling

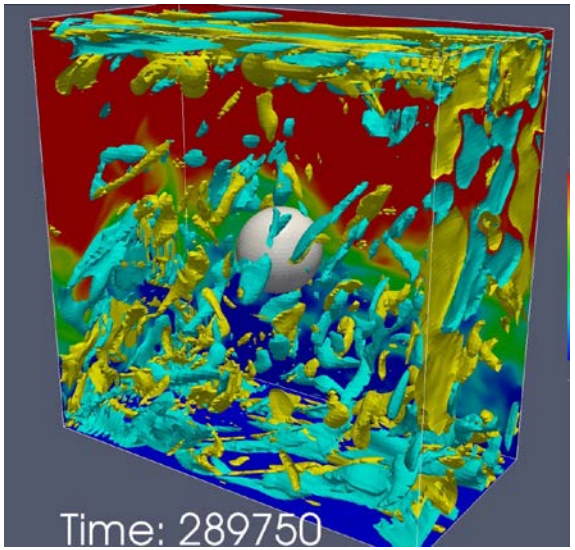










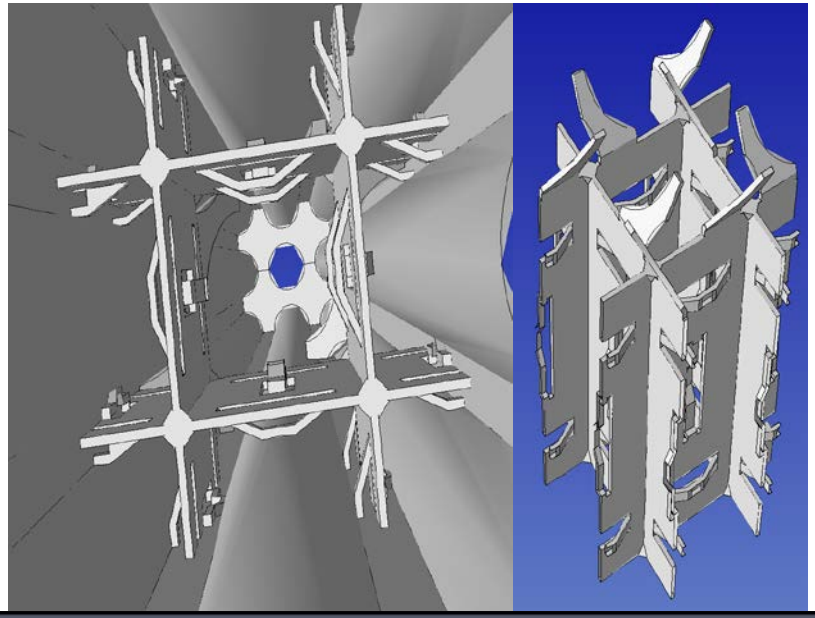


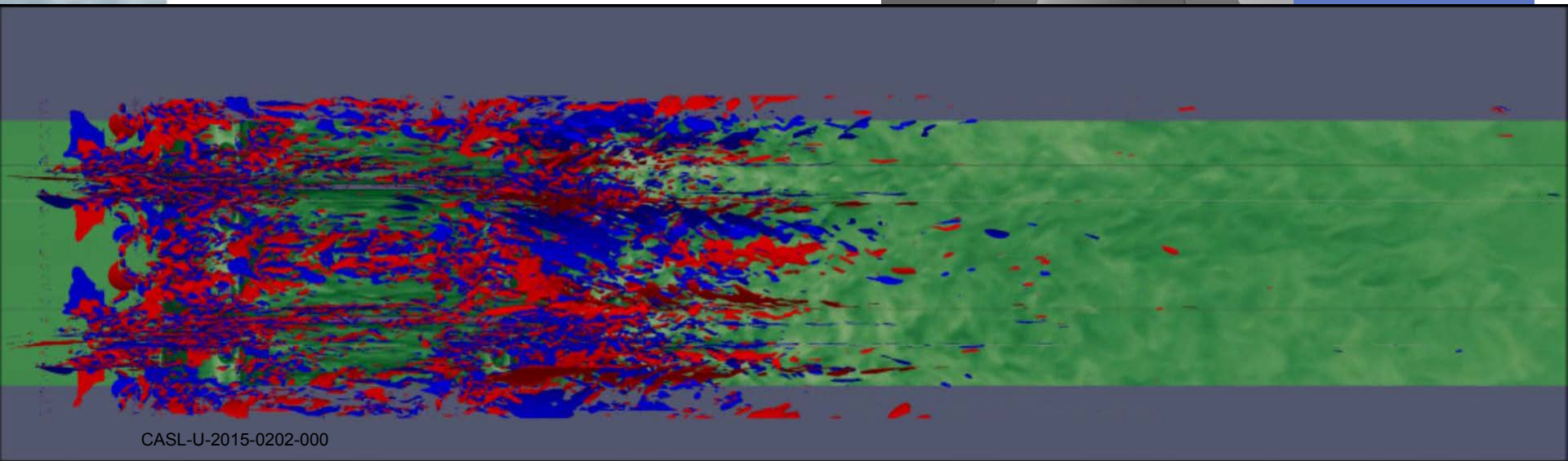
2x2 Subchannel Modeling

Realistic reactor spacer grids and mixing vanes used for turbulent flow simulations.

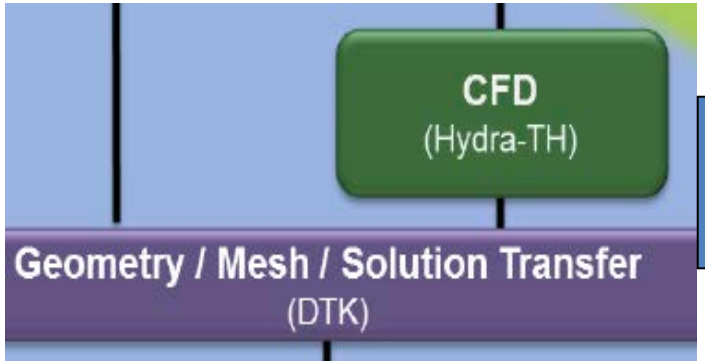
190M mesh on 18,000 cores on Titan:

Simmetrix meshing: includes boundary layers on spacer grids / mixing vanes. Larger meshes (up to 10B) will be used for bubbly flow simulations

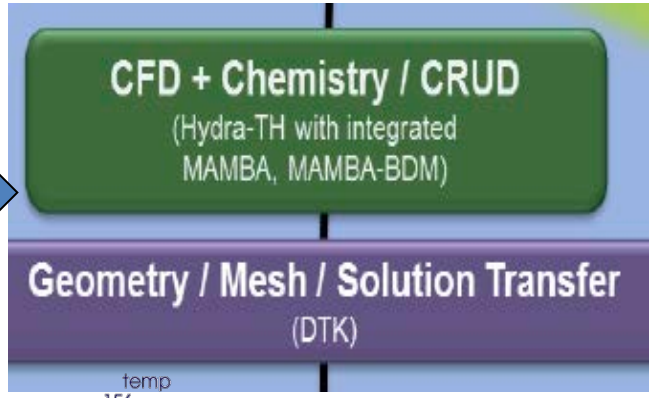


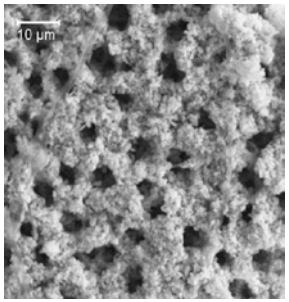


Innovation Highlight: Integration of Surface Chemistry Capability as sub-grid model in Hydra-TH

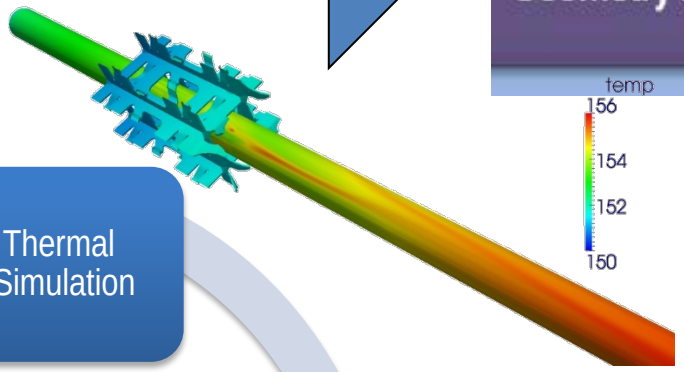


Evolution of Hydra-TH in VERA From End of Phase 1 to Phase 2





- Local CRUD Chemistry
- Boiling, chimney formation
- CRUD deposition
- Thermal resistance



Hydra-TH Thermal Hydraulics Simulation

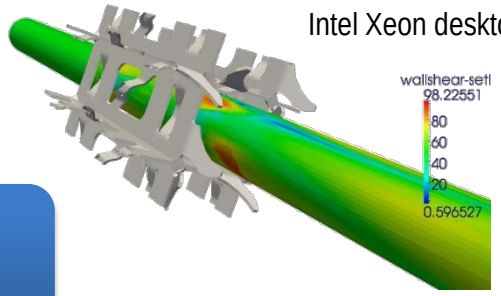
- CRUD Induced Power Shift
- CRUD Induced Localized Corrosion
- Difficult to Predict
- Drive to Zero Fuel Failure

MAMBA Sub-Grid Scale Model

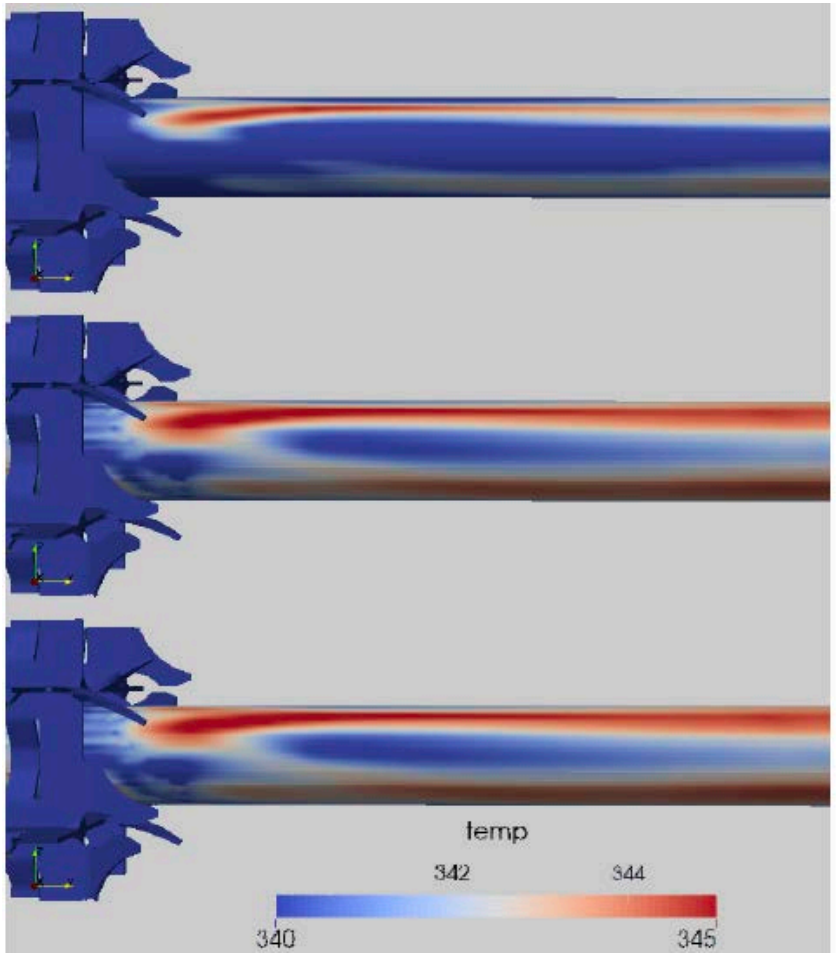
Wall-Shear, Temperature, Heat Flux

Fully-Implicit Projection

- RNG k-ε model
- Re ~ 4.0×10^5
- $q_w = 10^6$ W/m^2
- 2.4M elements, ~18M DoF
- ~ 4.75 hours on 16-core Intel Xeon desktop



CRUD leads to Higher Clad Temperatures



No Surface Chemistry

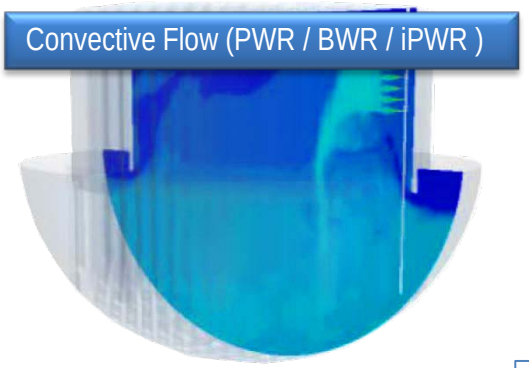
With Surface Chemistry

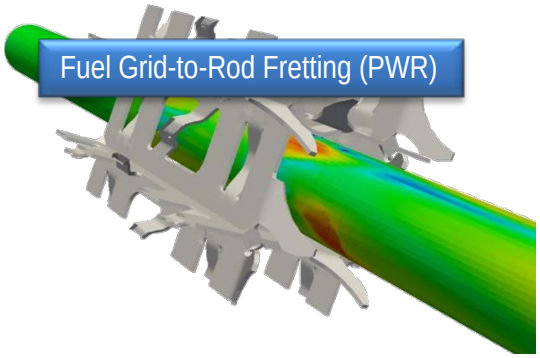
CASL Status
and looking forward

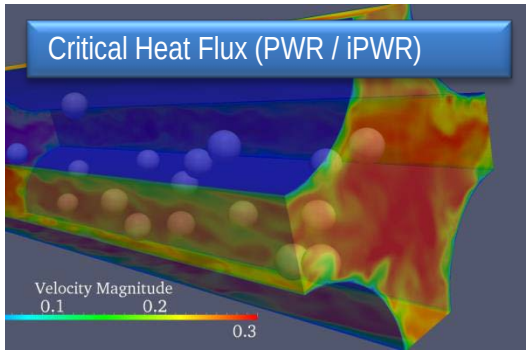
- ✓ Year 1: Build the foundation
- ✓ Year 2: Advance the science basis of the M&S technology components
  - Guided by challenge problem requirements baselined against industry capabilities
- ✓ Year 3: Assess, refine, integrate, and beta test the M&S technology components within the multi-physics Virtual 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

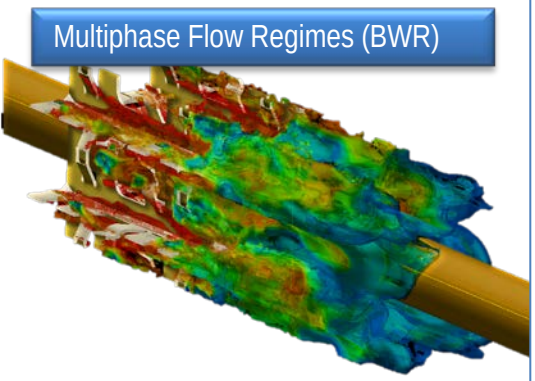
Document Type	Quantity (May 2014)
Journal Articles, refereed	68
Conference Papers	341
Technical Reports	37
Milestone Reports	520
Presentations	52
Workshop/Seminars	95
Reference Documents	7
Record/NR Publications	53
Management Documents	154
Awards	4
Thesis, Poster, Manual, Patent, Images	10
Total	**1,321**

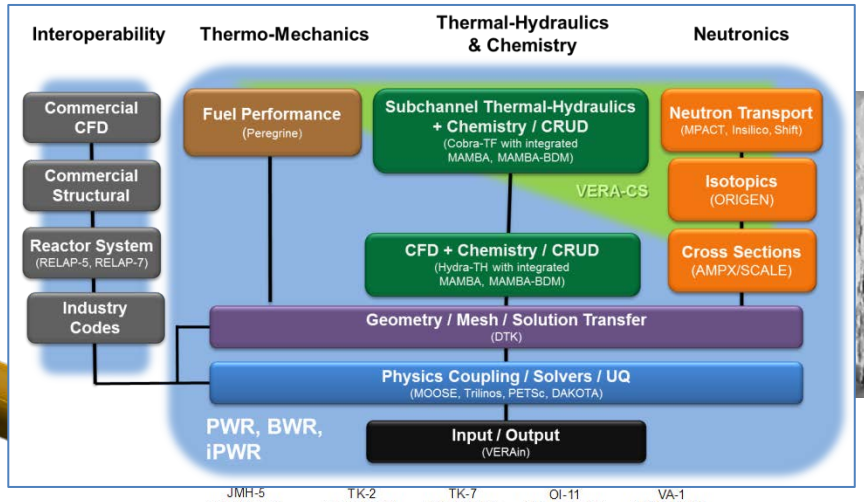
CASL Proposed Phase 2 Scope: 2015 – 2019

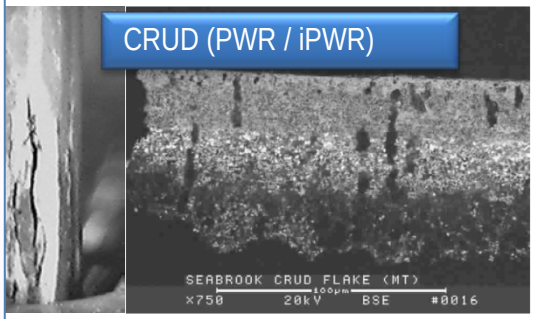


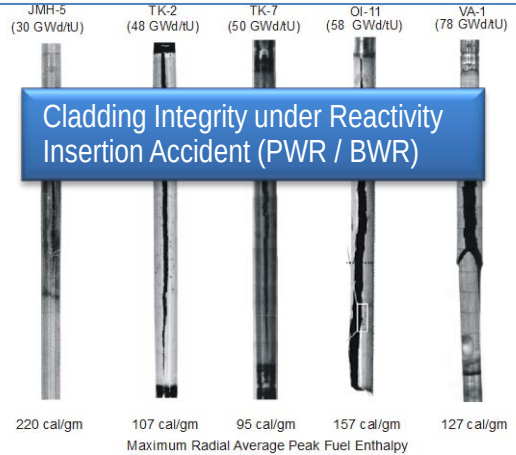


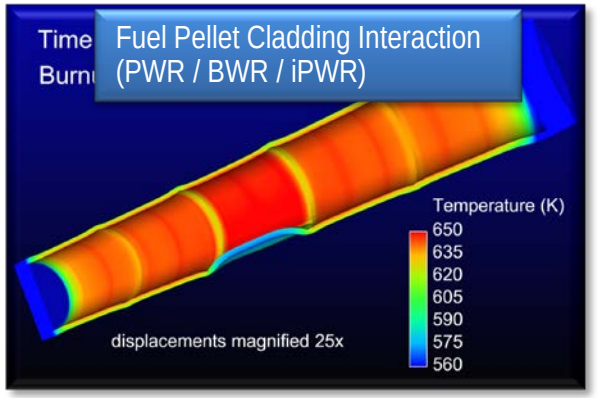












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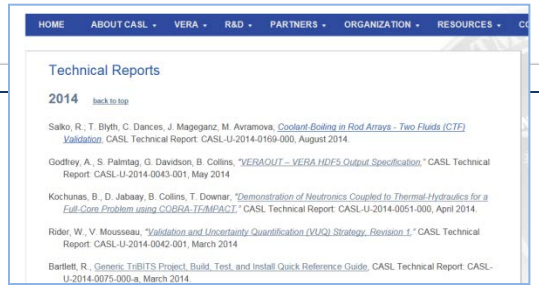
Rák, Z., C. J. O'Brien, and D. W. Brenner, "First-Principles Investigation of Boron Defects in Defects in Nickel Ferrite Spinel," Journal of Nuclear Materials, Volume 452, Issues 1-3, Pages 446–452, September 2014.

Palmtag, S., K. Clarno, G. Davidson, R. Salko, T. Evans, J. Turner, K. Belcourt, R. Hooper, R. Schmidt, "Coupled Neutronics and Thermal-Hydraulic Solutions of a Full-Core PWR Using VERA-CS," *Proceedings of PHYSOR 2014*, September 28 – October 3, 2014.

Jessee, M. A., W. Wieselquist, T. Evans, S. Hamilton, J. Jarrell, K. Kim, J. Lefebvre, R. Lefebvre, U. Mertyurek, A. Thompson, M. Williams "Polaris: A New Two-Dimensional Lattice Physics Analysis Capability for the Scale Code System," *Proceedings of PHYSOR 2014*, September 28 – October 3, 2014.

O'Brien, C. J., Rák, Zs., Bucholz, E.J., and Brenner, D. W., "First Principles Calculations Predict stable 50nm Nickel Ferrite Particles in PWR Coolant," *Journal of Nuclear Materials*, Volume 454, Issues 1–3, November 2014, Pages



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Technical Reports

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Salko, R.; T. Blyth, C. Dances, J. Mageganz, M. Avramova, *Coolant-Boiling in Rod Arrays - Two Fluids (CTF) Validation*, CASL Technical Report: CASL-U-2014-0169-000, August 2014.

Godfrey, A., S. Palmtag, G. Davidson, B. Collins, "*VERAOUT – VERA HDF5 Output Specification*," CASL Technical Report: CASL-U-2014-0043-001, May 2014.

Kochunas, B., D. Jabaay, B. Collins, T. Downar, "*Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using COBRA-TF/MPACT*," CASL Technical Report: CASL-U-2014-0051-000, April 2014.

Rider, W., V. Mousseau, "*Validation and Uncertainty Quantification (VUQ) Strategy, Revision 1*," CASL Technical Report: CASL-U-2014-0042-001, March 2014.

Bartlett, R., Generic TriBITS Project, Build, Test, and Install Quick Reference Guide, CASL Technical Report: CASL-U-2014-0075-000-a, March 2014.

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Franceschini, F. ; M. Kromar, D. Čalić, A. Godfrey, B. Collins, T. Evans, J. Gehin, ORNL, "Simulation of the NPP KRSKO Startup Core with CASL Core Simulator VERA-CS," *Proceedings of the International Conference Nuclear Energy for New Europe (NENE)*, Portorož, Slovenia, September 8..11, 2014.

Short, M., C. Stanek, D. Gaston, S. Yipp, "A Perspective on Coupled Multiscale Simulation and Validation in Nuclear Materials," *MRS Bulletin*, Volume 39, Issue 01, pp. 71-77, January 2014.

Kulesza, J., F. Franceschini, T. Evans, J. Gehin, "Overview of the Consortium for the Advanced Simulation of Light Water Reactors (CASL)," *Proceedings of the International Symposium on Reactor Dosimetry (ISRD-15)*, April 17, 2014, Aix en Provence, France, Paper A133, 2014.

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