Consortium for Advanced Simulation of LWRs

CASL Industry Council Meeting
September 9-10, 2014 – Oak Ridge, TN
Minutes

The ninth meeting of the Industry Council (IC) for the Consortium for Advanced Simulation of Light Water Reactors (CASL) was held on September 9-10, 2014 at Oak Ridge National Laboratory in Oak Ridge, TN. A joint meeting of the Science Council and the Industry Council was held the first day and chaired by Paul Turinsky (CASL Chief Scientist) and Dennis Hussey (IC Chairman). The Industry Council meeting on the second day was chaired by Dennis Hussey.

The meeting attendees and their affiliations are listed at the end of these minutes. Attendance was by invitation only. Industry Council representatives from 22 member organizations were invited. Eleven members of the Industry Council attended representing eight organizations. Members of the CASL project team participated in the meeting including the program director, chief scientist, the quality manager, the project manager, focus area leads, and technical staff. The DOE-NE Director of Advanced Modeling and Simulation also participated by teleconference on the first day.

The meeting followed the agenda included at the end of these minutes.

Doug Kothe began the Joint Science and Industry Council meeting with a welcome and extended his appreciation to the Industry Council and Science Council members for their active participation in CASL.

Doug Kothe, CASL Director, and Paul Turinsky, Chief Scientist, provided an overview of the CASL project technical accomplishments over the last year (as noted in the Plans of Record 8 and 9). In 2013, 11 DOE-reportable milestones were completed, covering various challenge problems and focus areas. One milestone (VERA demonstration to couple neutronics and thermal hydraulics for a full core) was delayed by three months and completed in December 2013. In FY14, there are 13 DOE-reportable milestones, most are on track with some risks.

The enhanced capabilities of the CASL tools were described. Challenge problems were focused on improving physics and integrating the modules within VERA. CRUD challenge problems have advanced to include coupled CTF and Star-CCM+ with MAMBA for CIPS/CILC (5x5 Seabrook Cycle 5 Array). PCI has extended to 3D development for full rods and local geometries. GTRF progress includes an engineering wear model and there are experimental fretting wear tests. DNB had CTF rod bundle mixing and DNB test simulations. Hydra-TH rod bundle studies were performed on an industry computer. RTM supported integrated cross-section generation/transport solver capabilities with Insilico, and MPACT with additions of depletion and thermal hydraulic feedback.

Scott Palmtag, deputy lead for CASL Physics Integration (PHI) Focus Area (FA), presented an overview of the current VERA capabilities. The components and hierarchy of VERA components were highlighted. Key additions were the inclusion of SHIFT, Insilico and MPACT were coupled with CTF, and Insilico-CTF-Peregrine were also coupled. Integration is enabled using TriBITS, and support requests are tracked using the CASL Support, Improvement and Corrective Action Tracking System (CSICAT). Additional descriptions of the coupling methods were presented. The Data Transfer Kit (DTK) and PIKE were improved, and offered on github and in Trilinos (SNL – trilinos.org). Tiamat was developed to support

three-way coupling (CTF-Insilico-Peregrine). Progression problems were highlighted from FY11 to FY14, modeling Watts Bar Unit 1 Cycle 1 with depletion is expected to be demonstrated by September 30, 2014, refueling will demonstrated by November 11, 2014. Problem 7 2D and 3D Fast and thermal flux results were shown, as well as the multi-assembly test problem based on Watts Bar Unit 1 Cycle 1.

Bill Martin, lead for the CASL Radiation Transport Methods (RTM) FA, provided a detailed review of the progress of the RTM neutronics codes including MPACT, Insilico, and Shift. Highlighted were the pin-resolved transport that modeled the fuel pellet, clad, and surrounding moderator regions. Radial, azimuthal and axial resolution of the pin is obtained. The predicted boron rundown for Watts Bar Cycle 1 was compared with the measured plant data and the agreement is good. Shift is a continuous-energy Monte Carlo code that is under development for benchmark calculations. Initial Shift validation results against critical experiments were presented. A review of the quarter-core zero power physics tests for the AP-1000 was presented, highlights were how the results obtained from 230,000 cores, or 60 million core-hours, agreed well with KENO-IV. Insilico results were validated with Watts Bar startup data. Milestones were reviewed, and the Level 1 milestone of implementing an operational reactor depletion analysis with TH feedback is on schedule. The Level 2 milestone, advanced pin-resolved depletion with MPACT, was completed on time. Initial validation results of MPACT depletion capability with Takahama 3 assay data were discussed. Results for additional milestones are in the presentation.

Dennis Hussey, Industry Council Chair and lead for Technology Deployment and Outreach (TDO), provided a description of the planned TDO focus area during the working lunch. TDO is to be the liaison between the CASL hub and the industry, and has four objectives: developing the post-CASL entity, user community outreach, managing release and support, and managing test stands. The post CASL entity is intended to be the primary VERA distribution and user support vehicle after Phase 2 of CASL. Early milestones will be determining the market for VERA and CASL tools, and building a revenue model and business case based on the market review and expected resource requirements. Outreach will be accomplished via training and coordinating the VERA Working Group (WG), as well as actively engaging other utility groups (Owner's Groups, INPO, EPRI) and regulatory bodies (NRC). Demonstrations and workshops will offer users the opportunity to work with VERA, including a planned workshop to be held at the Advances in Nuclear Fuel Management conference in Hilton Head, March 29-April 1, 2015. The VERA WG was discussed. The WG is expected to serve as an administrative body for VERA users to receive product information and updates and to facilitate user communication. Initially, WG fees are expected to be minimal, but it is expected the WG will be self-sustaining and managed by the post-CASL entity. Annual VERA update releases are planned. User support tracking (CSICAT) is available to coordinate user support requests. VERA users can use support@casl.gov for issue reporting. Test stands will remain active in TDO, with the goal of one test stand per year.

Igor Bolotnov presented the highlights of recent accomplishments in the Thermal Hydraulics (THM) focus area. Highlights of the THM focus area includes computational fluid dynamics solutions, closure (boiling) modeling for CFD systems, single phase/multiphase V&V, and direct coupling of MAMBA/Hydra. Highlights of Hydra-TH include porous drag capabilities, native conjugate heat transfer between the fuel and coolant. Experimental work applying synthetic crud nanoparticles was used to help understand the mechanistic representation of bubble liftoff and evaporative heat flux. Phase 2 will focus on CFD closure for onset of DNB, and extend work to the BWR applications.

Jeff Secker, CRUD Challenge Problem Integrator, Brian Wirth, deputy lead for the Materials Performance and Optimization (MPO) FA, and Paul Turinsky presented an overview of the following challenge problems:

- CRUD (CIPS/CILC)—Progress was made in both CIPS and CILC areas. CILC model validation was performed by assessing assembly failures of Seabrook Cycle 5. Thermal hydraulics was assessed using STAR-CCM+. Both axial and azimuthal T-H effects affected the crud deposition patterns, and the variations were consistent with plant observations. A comparison of azimuthally averaged axial liftoff showed similar trends for two of the affected rods. Current efforts are including MAMBA as a module in HYDRA, continue validation, improve thermodynamic correlations, complete validation and uncertainty quantification efforts, and develop CIPS modeling cases.
- Departure from Nucleate Boiling—Work in Critical Heat Flux/Departure from Nucleate Boiling using COBRA-TF subchannel code was completed in rod bundle mixing and DNB test simulations. Reactor core modeling for loss of flow, steamline break, and RIA accident scenarios has been recently completed. Hydra-TH work in single phase mixing has had limited work completed, there have been clad surface temperature predictions for mixing grids using the Westinghouse HPC platform.
- Pellet Clad Interaction—Brian Wirth presented the PCI challenge problem status update on behalf of Robert Montgomery. Peregrine has been developed for 2D and 3D modeling for full length and local effects geometry. Lower length scale material modeling of cladding involved visco-plastic self-consistent models (VPSC) for thermal and irradiation creep and growth, as well as corrosion and hydriding behavior. Peregrine has been successfully integrated into VERA-CS. The 3D modeling capabilities for the PCI challenge problem were demonstrated as a L1 milestone, and the EPRI test stand showed favorable comparisons to the EPRI Falcon model.
- Grid to Rod Fretting—Brian Wirth presented the update for Grid to Rod Fretting. The CASL approach to GTRF was modified in 2013 to focus on developing a wear model and focus less on developing a first principles model using thermal hydraulics. An engineering wear model has been developed that focuses on the oxide-oxide interaction, friction coefficient, normal forces during time t, and the frequency and amplitude of the oscillation. The model was compared to bench-scale experimental results taken at ORNL. Preoxidation was shown to reduce wear depth and the wear coefficient significantly.
- LOCA and RIA Challenge Problems—Paul Turinsky presented the LOCA and RIA challenge problem strategies. Results to date show the fuel rod conditions have been modeled using Peregrine, whole core models were developed using COBRA-TF, and initial steady-state modeling of the SPERT reactor was discussed. Refer to the presentation for validation activities.

Rose Montgomery and Paul Turinsky discussed the Phase 2 Workscope. Phase 2 will continue Challenge Problems to target the simulation capability for the R&D efforts. The criteria are to enhance the maturity level of the current codes to facilitate industry usage, broaden the applicability to simulate a wider class of LWRs, and deepen the capabilities developed in Phase 1. There were many relevant challenge problems suggested including BWR and SMR reactors, fuel assembly distortion, and accident tolerant fuel. Mini charters were created for each of these potential new challenge problems. A survey of CASL partners and industry was created to help select the Phase 2 challenge problems. The surveys were collected and ranked according to criteria including programmatic feasibility, industry impact, innovation, and institutional interest. The surveys were ranked according to Industry Council and CASL

criteria, the risks and rewards were considered, and the topics were down-selected. The Phase 2 challenge problems were built from that survey and presented in the Phase 2 proposal. Refer to the proposal and supporting presentations for details.

Alex Larzelere discussed the CASL DOE Annual Review and Renewal Proposal Reviews.

The meeting was adjourned for the day.

The next morning the Industry Council and Science Council held separate meetings. Dennis Hussey opened the Industry Council meeting with an overview of the Industry Council scope, members, website, and action items. The Industry Council website contains links to resources including minutes and presentations (http://www.casl.gov/IndustryCouncil.shtml). 3DS/Simulia has joined the Industry Council and attended the meeting. Dennis reviewed the meeting agenda. Dennis noted CASL documents that are planned to be provided. The meeting dates and location have not been finalized for the upcoming Spring 2014 Industry Council meeting. The presentation is included as Attachment 7.

Steve Hess (TDO Test Stand Manager) presented an overview of Test Stands. Test Stands, a mechanism for beta testing VERA outside of the in-house development process, are a key component of the deployment process.

- Westinghouse: Completed January 31, 2014, focus on neutronics of the AP-1000®
- EPRI: Completed August 1, 2014, focus on fuel performance (pellet-cladding interaction).
- TVA: Test Stand established March 31, 2014, topic is Watts Bar 1 lower plenum flow anomaly

Dennis Hussey presented slides prepared by Brenden Mervin about the EPRI Test Stand Experiences. Highlights of the test stand showed that Peregrine was able to predict fuel performance trends that were comparable to Falcon, and comparison of clad temperature and cladding stress were shown. It was noted the contact algorithm for actual power histories where contact occurs and relaxes was a challenge point, and several iterations between developers and Test Stand users were needed to resolve the issues. Visualizations showing the contact pressure and clad temperature over the cycle length were presented. Recommendations for Test Stand implementation, in particular supporting frequent and productive communication between the developers and the Test Stand users were offered.

Kelly Kenner, University of Tennessee, Knoxville, presented the results of core cycle design and economic studies of a typical small modular reactor completed for TVA. The configuration of the iPWR SMR modeled is different from a commercial PWR reactor (no soluble boron, control rod reactivity management, fuel height of 2.41 meters). Standalone VERA Neutronics capabilities were used, including the MOC subcomponent (MPACT), the SPn subcomponent (Insilico), and the Monte Carlo subcomponent (Shift). The core cycle design was created using 2D MPACT simulations (3D simulations with depletions were not yet available). 3D full core simulations with depletion followed as the capabilities became available in VERA. The results showed the planned 1400 EFPD cycle was not possible using the simulation assumptions (note there were no control rods modeled and inclusion of the control rods should yield a longer cycle time). The simplified public design used to model the SMR provided a good demonstration of VERA capabilities and flexibility in modeling alternative geometry.

Dennis Hussey opened up a Phase 2 Industry Council planning session with a few slides that as the VERA development continues in Phase 2, Industry Council feedback will be important. An open discussion began with Dennis Hussey asking about modeling strategies by utilities (i.e. many NRC licensed calculations are deterministic, are there probabilistic strategies that could be used), and whether VERA codes could be valuable without licensing.

Discussion was active and some key points were:

- Meshing strategies remain a challenge. There is a need for developing a strategy to build meshes as efficiently as possible.
- Licensing codes with the NRC takes a lot of time. For a plant to update their licenses with new models, there would need to be life extension for most domestic plants to greater than 60 years to justify the cost.
- Many plants are moving towards probabilistic risk assessments.
- Some applications do not require NRC-approved models (fuel reliability risk assessments are an example); therefore, there is potential value in the CASL codes. Another high value application that doesn't require approved methods is product development and optimization (for example, grid design).
- CASL code value is generated through industry use cases. An understanding of the fidelity difference, or difference in margin confidence, between existing codes and the CASL tools needs to be quantified for these use cases.
- The industry should be surveyed to find detailed use case needs.
- An ideal framework would be to set up 'model' plants to streamline the input requirements. For example, have one test case for each NSSS design.

Doug Kothe presented his thoughts on Phase 2 proposal scope. He noted the phase 1 accomplishments were significant: there were 1,300 publications and related records throughout the first four years of CASL, including 450 journal articles, conference proceedings, and technical reports, the CASL team has had a significant impact on the nuclear energy communities (test stands, EPRI advisory committees, Owner's Groups, NRC) as well as the DOE. Phase 2 will have a revised organization chart with the addition of Technology Deployment and Outreach, the combination of Validation and Uncertainty Quantification (VUQ) and the Advanced Modeling Applications (AMA) into VMA, and a change in the name of the MPO Focus Area to the Fuels Materials and Chemistry (FMC) Focus Area. More contributing partners will be added; for example, AREVA and GNF will be added as partners. Milestones were reviewed. It is recommended to review the CASL Phase 2 proposal for details.

Chris Lewis from AREVA provided a fuel vendors input on the benefits of CASL codes. Three areas were potential areas for use: 1) Product Development, 2) Evaluation of Operational Issues, and 3) Licensing Applications. Product development would be valuable for down selecting assembly designs before expensive testing were implemented. In addition, conditions that cannot be tested could be evaluated. Reasonable lengths of computation time are allowed (a month for a thermal hydraulic CHF calculation would be acceptable) if the predictions were accurate from a relative, or preferably absolute, perspective. Proprietary models would need to be incorporated. Operational issues generally would require more rapid analysis turnaround, the accuracy needs to sufficient to predict relative change. For licensing applications, the models may be usable to provide additional licensing margin. However, the models must be benchmarked against measured data and there must be adequate uncertainty analysis. NRC approval is also required. The conclusions were that there are several areas where VERA can

provide value to the industry and vendors, in particular product development and operational issues. Challenge problems, benchmarking and validation are key requirements for this to be achievable.

During the Open Discussion, each IC member was invited to provide their views of the meeting. A summary of the feedback is given below.

Alan Copestake—Rolls Royce

- Impressed with CASL overall, TDO is needed early.
- Phase 2 challenge problems seem right, but ambitious.
    - The simulations need to have results that can be validated understanding there are software and platform limitations.
    - Natural circulation is a high need problem, be sure to include decay heat removal, structural heating (control rod heating).
- Thermal hydraulics progress is good. CFD is going well. BWR and accident condition modeling are needed.
- Strongly recommend benchmarking calculations against available data.
- Agrees with the comment that gaining speed given loss of fidelity can be advantageous, but be certain to quantify the loss of fidelity.
- Fuel performance is doing well.
- Reducing the scope of the GTRF challenge problem was the proper choice, there no need to bring in the structural mechanics code when other tools are available.

Scott Thomas—Duke Energy

- Technical nature of the presentations, including SC with the IC was helpful, keeping the joint meeting once a year is a good idea.
- Challenge problem update was high value, and would recommend more time from the meeting devoted to these topics.
- Continue to focus on the test stands.
- TDO, the concept and structure are well done. However, there is uncertainty, for example, Year 1 or Year 2 decisions for the post CASL entity may be rushed, it may be better to wait to see what the value will be and what the proper structure. One post CASL entity may be overburdened.
- Interested in the comparing the predictions and highlighting the benefits compared to current production codes, for example, Westinghouse didn't show ANC results for AP1000.
- Catawba data may be shared for comparing to VERA.
- MPACT presentation was well done. Jump start capability for mid-cycle outages will be needed.

Walter Schwarz—Ansys

- Impressed with record of performance.
- Phase 2 is well developed.
- Looking forward to testing finished products. Verification and validation of each code will be necessary.
- Interoperability is a key goal, other tools will allow advantages to users.
- Understanding that software evolves, ensure that there is life after CASL by focusing future users of the product.

Atul Karve—GNF

- Clarification of Phase 2 activities was appreciated, especially with BWR two-phase work.
- There are other challenge problems of significance (especially in BWRs), for example, shutdown margin.
- For manufacturing, instrumentation, and modeling, quantifying modeling uncertainty is high value.
- Rollout of VERA-EDU should be communicated and implemented, there is a need to train the future generation of nuclear fuel engineers. Having a common framework as an education tool is very important.
- There is a need to resolve the export control, technology transfer, and intellectual property issues.

Action Items

The following Action Items were identified as a result of this meeting:

Action	Owner	Date
Develop a strategy for meshing (pre-planning a meshing implementation guidelines). Highlight CFD and perhaps fuel performance. (compilation of best practice guidelines)	TDO	Next IC meeting
Summary on Hydra progress/challenges, in particular with regards to BWR	Yixing, THM leadership	Next webcast
Develop a table of use cases, needed VERA functionality, resource requirements, value added and timescale (map to specific benchmarks). Include as an outreach activity	Dennis Hussey	Update at webcast, document by next in person meeting
Define plans for working group	Rose Montgomery	Next webcast
Develop a statement of Chairperson commitments, including planned compensation.	Dennis Hussey	One month
Select an Industry Council Chairperson	IC Director	Before next webcast
Document distribution (tech notes, documents)	Dennis Hussey	Monthly

Prepared: September 19, 2014
Distributed to Senior Leadership Team for Review: September 19, 2014
Finalized: September 27, 2013

By Dennis Hussey, Industry Council Chair

CASL Science / Industry Council Meeting

Agenda

September 9-10, 2014

Location: Oak Ridge National Laboratory

Tuesday, September 9

Joint Industry and Science Council Meeting (SNS-Building 8600, Room C156)

8:00	Check In (Building 5200, Visitor's Center)	
8:30	CASL technical accomplishments past 12 months (PoR8 and PoR9)	Doug Kothe Paul Turinsky
9:45	*Break*	
10:00	VERA: Description, Status, Plans	Scott Palmtag
11:00	Spotlight on Radiation Transport Focus Area	Bill Martin
12:00	Working Lunch – Description of new Technology Deployment & Outreach organization	Dennis Hussey
1:00	Spotlight on Thermal Hydraulic Focus Area	Igor Bolotnov
2:00	Challenge Problems – Progress Made	Jeff Secker Brian Wirth Paul Turinsky
3:30	*Break*	
3:45	Work Scope for Phase 2	Rose Montgomery Paul Turinsky
5:00	Status of DOE annual & renewal proposal reviews (ReadyTalk Connections – see below)	Alex Larzelere
5:15	Adjourn	

Wednesday, September 10

Industry Council Meeting (SNS-Building 8600, Room C156)

8:30	Welcome and Introductions	Dennis Hussey
9:00	Test Stands – EPRI Test Stand Presentation (ReadyTalk Connections – see above) – SMR modeling highlights – Future Test Stands	Steve Hess Brenden Mervin Kelly Kenner Steve Hess
10:15	Break	
10:30	Phase 2 Industry Council Planning	Dennis Hussey
11:15	VERA Working Group	Rose Montgomery
11:45	Working Lunch – Thoughts on Phase 2 (2015-2020) Scope	Doug Kothe
12:45	Fuel Vendor Perspective on CASL	Chris Lewis, AREVA
1:15	Open comments for IC meeting	Dennis Hussey
1:30	Break	

Science Council Meeting (SNS-Building 8600, Room C152)

8:00	Update on FY15 S&T Plans and Beyond (Phase 2)	Doug Kothe/Paul Turinsky
8:45	Charge to Science Council regarding S&T Annual Review	Bill Oberkampf (Chair)
9:00	Response to Science Council Recommendations for RTM	Tom Evans
9:20	Response to Science Council Recommendations for THM	Doug Kothe Paul Turinsky
9:40	Response to Science Council Recommendations for MPO	Brian Wirth
10:00	Break	
10:20	Response to Science Council Recommendations for VUQ	Brian Adams
10:40	Response to Science Council Recommendations for PHI	Jess Gehin
11:00	Response to Science Council Recommendations for AMA	Steve Hess
11:20	Breakout Meetings with Focus Area Leads	Science Council and FA Leads
12:00	Science Council Working Meeting on S&T Annual Review Preparation, *working lunch*	Science Council
1:30	Break – Walk to Room C156	
Joint Industry Council/Science Council Meeting (SNS-Building 8600, Room C156)		
1:45	*Science Council Joins Industry Council* Industry Council Round Robin **(opportunity for individual IC members to comment)**	All Industry Council Members
2:45	Industry Council Action Items	Dennis Hussey
3:00	Science Council Out Briefing of Major Findings	Bill Oberkampf (Chair)
4:00	Adjourn	
4:10	Pictorial Communicating VERA Structure (Optional)	John Turner Jess Gehin

Industry Council Attendees

1. Chris Lewis, AREVA, Christopher.Lewis@areva.com
2. Scott Thomas, Duke Energy, Scott.Thomas@duke-energy.com
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4. Atul Karve, Global Nuclear Fuels (Alt), Atul.Karve@ge.com
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6. Brian Aviles, KAPL, brian.aviles@unnpp.gov
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8. Alan Copestake, Rolls Royce, Alan.Copestake@rolls-royce.com
9. Ian Stevenson , Simulia, Ian.STEVENSON@3ds.com
10. Simon Huffeteau, Simulia, simon.huffeteau@3ds.com
11. Bob Oelrich, Westinghouse, oelricrl@westinghouse.com

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2. Richard Lahey, RPI-retired, laheyr@rpi.edu
3. Elmer Lewis, NWU-retired, e-lewis@northwestern.edu, participation via teleconference
4. William Oberkampf, ,SNL-retired, wloconsulting@gmail.com
5. Kord Smith, MIT, kord@mit.edu, participation via teleconference
6. Finis Southworth, Areva, finis.southworth@areva.com
7. James Tulenko, UFL, tulenko@ufl.edu
8. William Weber, UTK/ORNL, wjweber@utk.edu, Sept 9 only
9. Mary Wheeler, UT-Austin, mfw@ices.utexas.edu, unavailable

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20. Bill Martin, UMI, wrm@umich.edu

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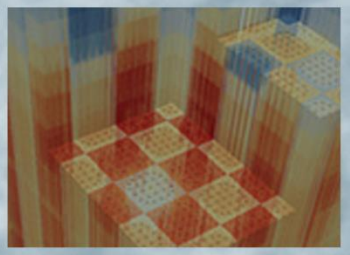
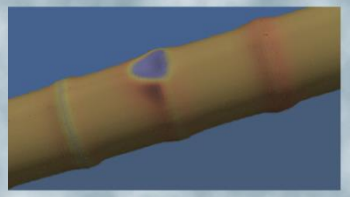
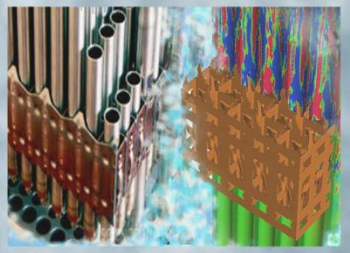
CASL Technical Accomplishments Past 12 Months (PoR8 and PoR9)

Doug Kothe
Director

Paul Turinsky
Chief Scientist







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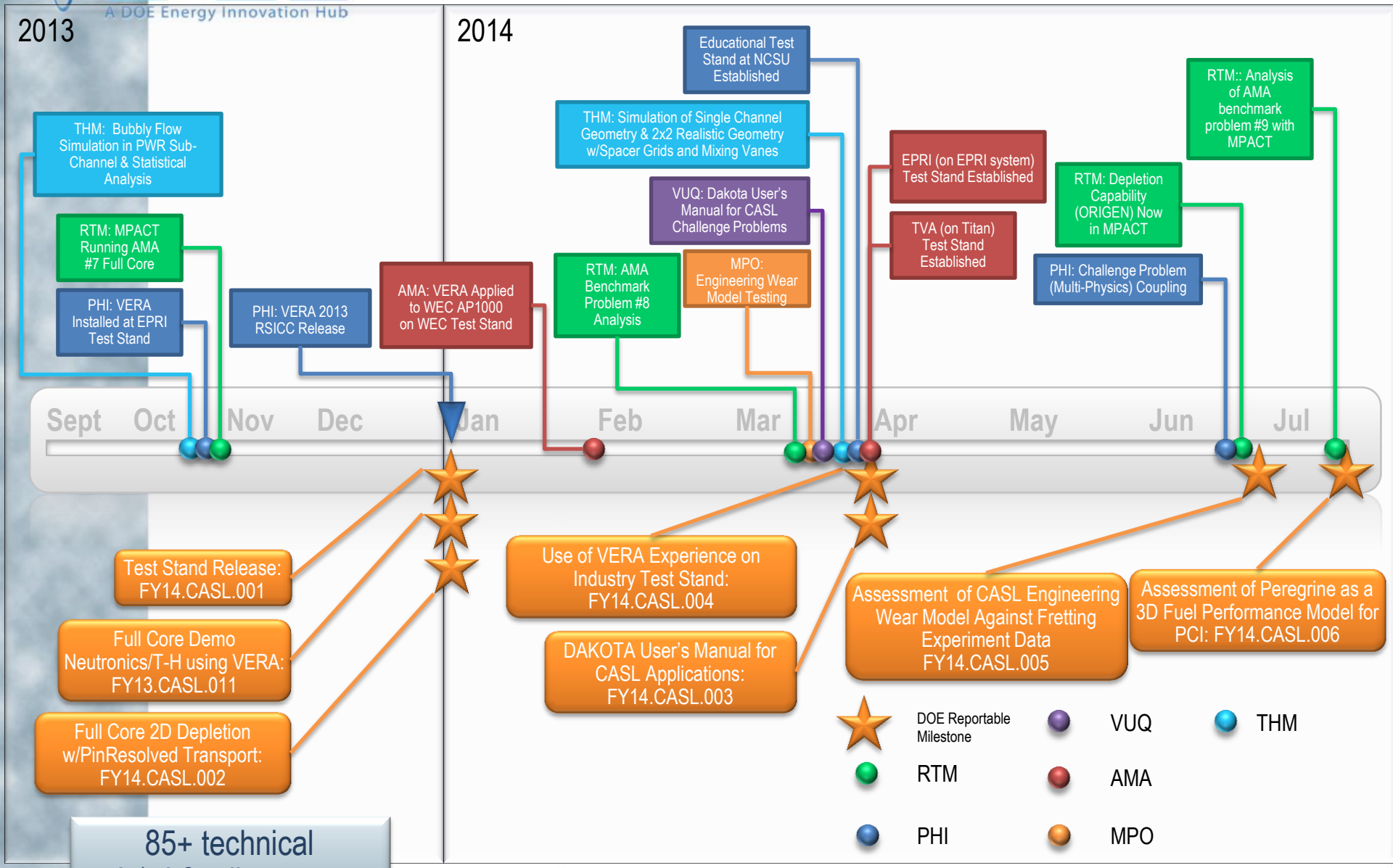
S&T Program: Presentation Outline

- Milestone Performance
- M&S Current Practice versus CASL Practice
- FY14 Challenge Problems Accomplishments (to date)
- FY14 Highlighted Accomplishments (to date)
- Organization changes to be implemented in FY15

Subsequent presentations
will provide more details

Selected Accomplishments



85+ technical L1–L3 milestones

FY13 CASL Milestones

Formally reportable to DOE

Reportable #	Milestone ID	Milestone Description	Finish Date
FY13.CASL.001	L3:RTM.PRT.P6.01	Demonstration of advanced pin-resolved method of characteristics (MOC) capabilities for neutron transport	Dec 2012
FY13.CASL.002	L2:AMA.P6.01	DNB Relevant Experimental Data Collection and Modeling with CASL Tools	Mar 2013
FY13.CASL.003	**L1:CASL.P7.01**	Operational Reactor Model Demonstration with the VERA Core Simulator	Jun 2013
FY13.CASL.004	**L1:CASL.P7.02**	Peregrine: Validation and Benchmark Evaluation of Integrated Fuel Performance of Halden Test Reactor Data and Falcon	Jun 2013
FY13.CASL.005	L2:VRI.P7.02	Initial demonstration of Peregrine integration into the VERA Core Simulator	Jul 2013
FY13.CASL.006	L3:SLT.PP.P7.01	Issue an updated CASL Program Plan	Jul 2014
FY13.CASL.007	L2:THM.P7.01	Demonstration & assessment of an advanced modeling capabilities for multiphase flow with subcooled boiling	Aug 2013
FY13.CASL.008	L2:VUQ.P7.02	Uncertainty quantification and data assimilation (UQ/DA) study on a VERA component for CRUD analysis	Aug 2013
FY13.CASL.009	**L1:CASL.P7.05**	Multiphysics modeling of CRUD deposition on PWR fuel	Sep 2013
FY13.CASL.010	**L1:CASL.P7.04**	VERA Release thru RSICC	Sep 2013
FY13.CASL.011	L2:AMA.P7.02	Demonstration of neutronics coupled to thermal-hydraulics for a full-core scenario using VERA.	~~Sep 2013~~ Dec 2013

- 11 milestones with a broad coverage of CPs and FA capability development
- As noted at the 2013 review, "Other outstanding milestones on track but not without risk (e.g., full core coupling)"; this milestone (VERA-CS BPP #7 with Insilico + CTF) was delivered 1Q late but represented an *important* demonstration capability
- All other milestones were delivered on time, meeting >90% DOE completion metric

VERA Analysis of Watts Bar 1 Hot Full Power

Milestone L2:AMA.P7.02 delivered Dec 2013

Purpose

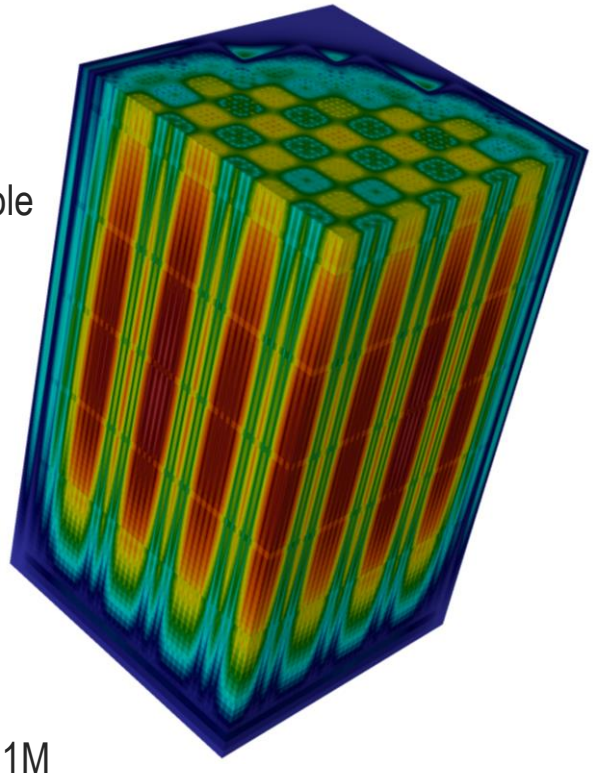
- First large-scale coupled multi-physics model of operating PWR reactor using Components of CASL's Virtual Environment for Reactor Applications (VERA)
- Features resolved are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1: geometry for fuel, burnable absorbers, spacer grids,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

Execution

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

Next Steps

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



Thermal Flux Profile in Reactor Core

Remarkable resolution of physics and geometry

FY14 CASL Milestones

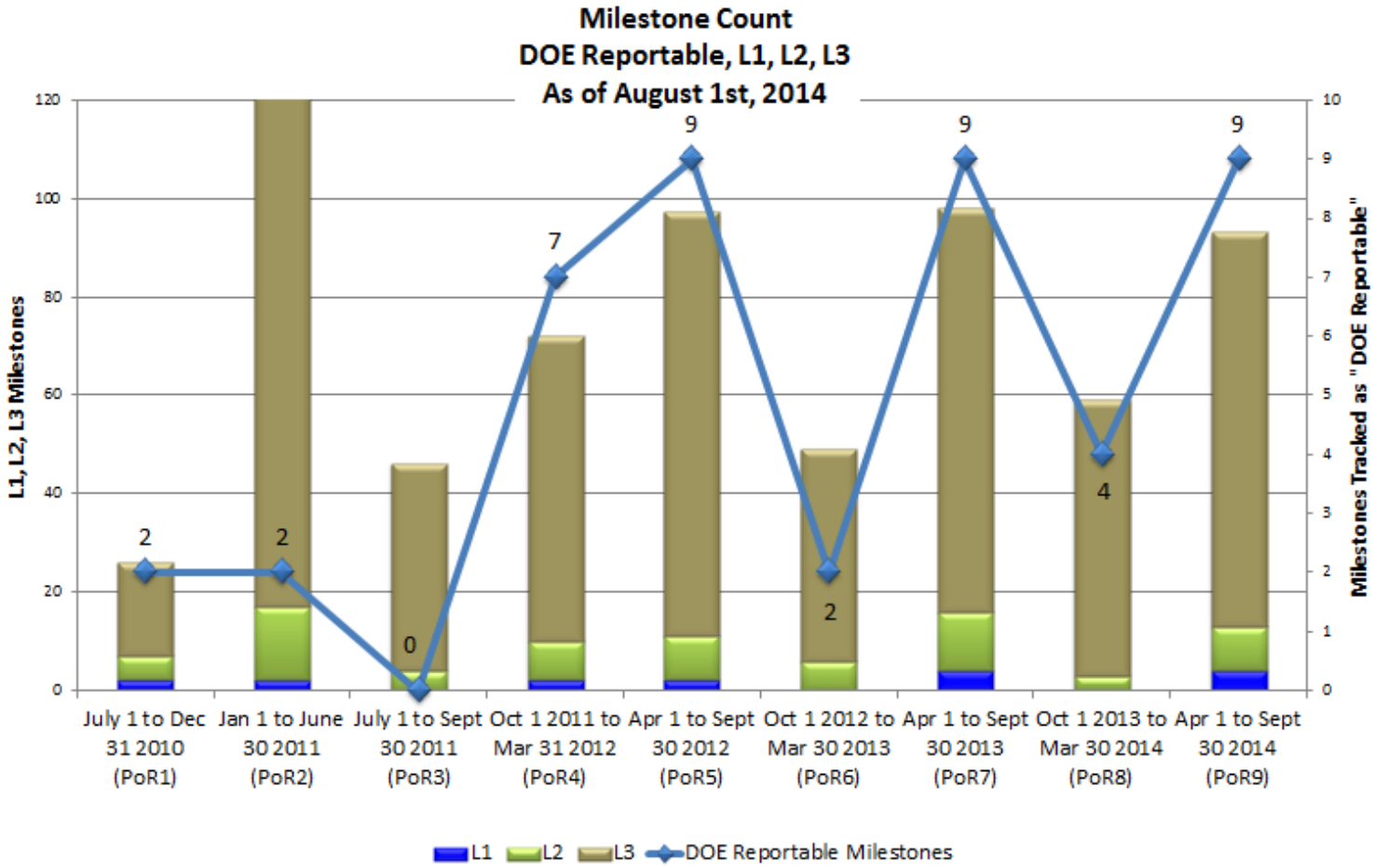
Formally reportable to DOE

Reportable #	Milestone ID	Milestone Description	Finish Date
FY13.CASL.011	L2:AMA.P7.02	Demonstration of neutronics coupled to thermal-hydraulics for a full-core scenario using VERA.	~~Sep 2013~~ Dec 2013
FY14.CASL.001	L2:PHI.P8.01	VERA Deployment for EPRI Test Stand on PCI	Dec 2013
FY14.CASL.002	L2:RTM.P8.01	PWR Full Core 2D Depletion Capability with Pin Resolved Transport	Dec 2013
FY14.CASL.003	L3:VUQ.V&V.P8.01	User Guidelines and Best Practices for CASL UQ Analysis using DAKOTA	Mar 2014
FY14.CASL.004	L2:AMA.P9.01	Experience with use of VERA in Industry Test Stands	Mar 2014
FY14.CASL.005	L2.MPO.P9.01	Assessment of CASL Engineering Wear Model Against Experimental Fretting Measurements	Jun 2014
FY14.CASL.006	**L1:CASL.P9.01**	**Assess Peregrine as a 3D Fuel Performance Model for the PCI Challenge Problem**	Jul 2014
FY14.CASL.007	**L1:CASL.P9.02**	**Application of Multi-Scale Thermal Hydraulic Models to DNB Analysis**	Aug 2014
FY14.CASL.008	**L1:CASL.P9.03**	**Demonstrate integrated VERA-CS for the PCI Challenge Problem**	Aug 2014
FY14.CASL.009	L2:VUQ.P9.01	Demonstration of Integrated DA/UQ for VERA-CS on a Core Physics Progression Problem	Aug 2014
FY14.CASL.010	L2:THM.P9.01	Single Phase Validation of Hydra-TH for Fuel Applications	Aug 2014
FY14.CASL.011	**L1:CASL.P9.04**	**Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback**	Sep 2014
FY14.CASL.012	L2:MPO.P9.02	Demonstration of Coupled CFD and Crud/Corrosion Chemistry for a Fuel Sub-region	Sep 2014
FY14.CASL.013	L2:MPO.P9.03	Demonstration of Atomistically-informed Multiscale Zr Alloy Deformation Models in Peregrine for Normal Operation and Accident Scenarios	Sep 2014

- 13 milestones with a broad coverage of CPs and FA capability development
- FY13 milestone delivered 1Q late (VERA-CS BPP #7 with Insilico + CTF)
- All remaining milestones on track with some risks in play due to innovative nature of scope (e.g., crud/corrosion chemistry coupling to T-H)

CASL Milestone Statistics

Milestones delivered since CASL start (Jul 2010)



Milestone count: 13 L1s, 62 L2s, 474 L3s

1887 milestone documents in the CASL records management system

Phase 1 Milestone Progress

Milestone delivery has led to *many* technical reports

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

Milestone reports by Focus Area

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

Milestone reports outside of Focus Areas

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

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

Phase 1 Milestone Progress

Risks encountered and mitigated or being managed

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

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

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

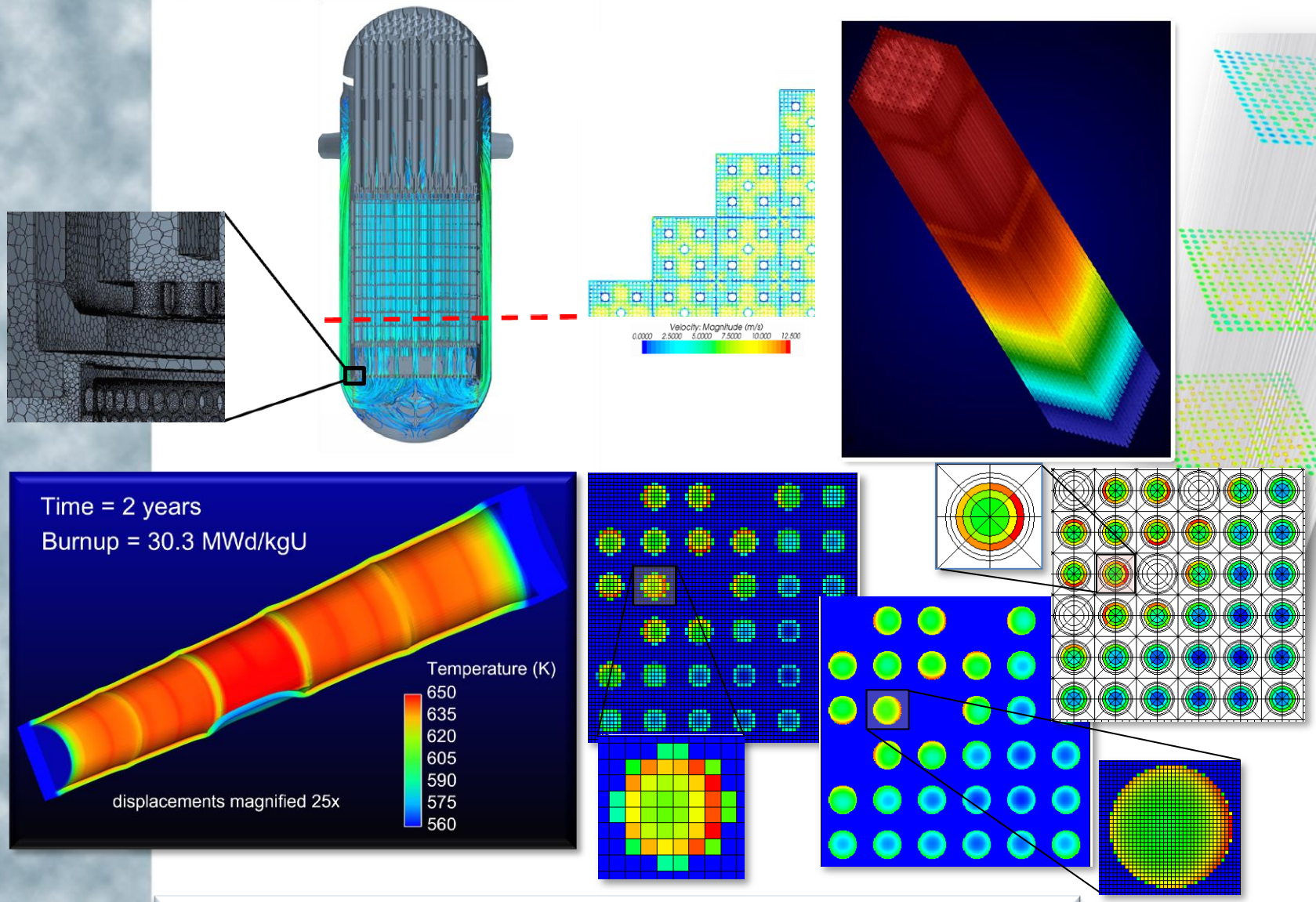
Phase 1 Milestone Progress

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.

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

What enhanced capabilities over current practices will CASL provide?

Predictive capabilities

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

Phase-space resolution

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

VUQ practices

- Verification & validation
- Data assimilation
- Uncertainty quantification

Computational resource utilization

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

What enhanced capabilities over current practices will CASL provide?

Fluids (HYDRA-TH)

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

Radiation Transport (MPACT & INSILICO)

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

High level differences of current versus CASL capabilities

Fuel Performance (PEREGRINE)

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

Crud Chemistry (MAMBA & MAMBA-BDM)

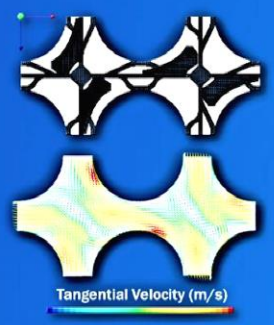
- Current Practice: 2D with limited chemical species & experimentally derived models' parameters
- CASL Practice: 1D, 2D and 3D with expanded chemical species, experimentally & micro modeling derived models' parameters, and new cladding corrosion model

Multiphysics (VERA)

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

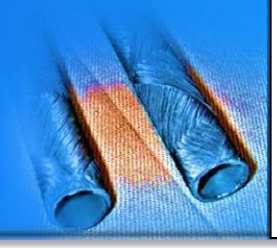
CASL Challenge Problems

Departure from Nucleate Boiling



Cladding Integrity

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



Safety Related Challenge Problems

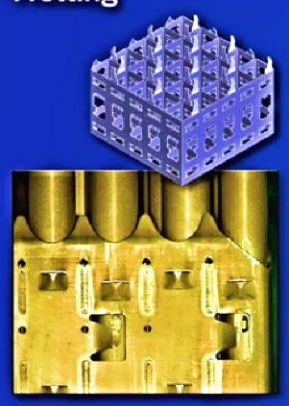
CASL is committed to delivering simulation capabilities for

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

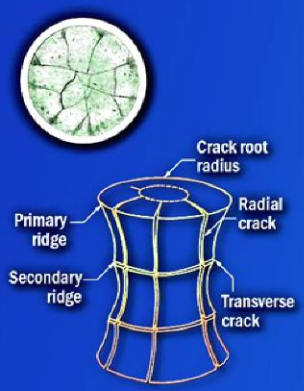
Crud

- Deposition
- Axial offset anomaly
- Hot spots

Grid-to-Rod Fretting



Pellet-Clad Interaction



Operational Challenge Problems

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

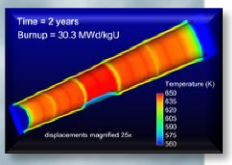
- Predict Minimum GTRF Margin in Core using **PEREGRINE2D** – grid to rod gap, **STAR/HYDRA-TH** excitation force

Brian Wirth

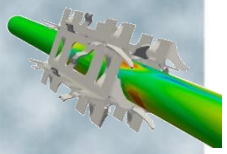
For each Challenge Problem apply DAKOTA using coupled tools for UQ

Challenge Problem Updates

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



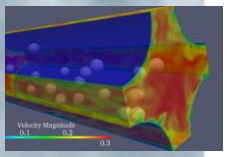
- PCI
  - ✓ Peregrine 2D/3D development for modeling full-rod and local geometries
  - ✓ Lower-length scale material modeling of cladding (VPSC)
  - ✓ Peregrine integration into VERA-CS for multi-rod/multi-assembly simulations
  - ✓ EPRI Test Stand PCI testing and benchmarking of Peregrine



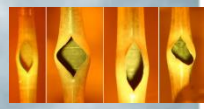
- GTRF
  - ✓ Engineering wear model development and experimental fretting wear tests
  - ✓ Parametric study of influences of key GTRF phenomena

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

Challenge Problem Updates



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



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

Good overall progress since last year

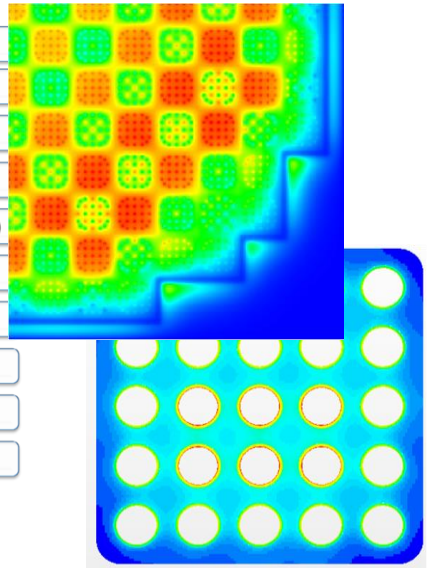
VERA Usage for Challenge Problems

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

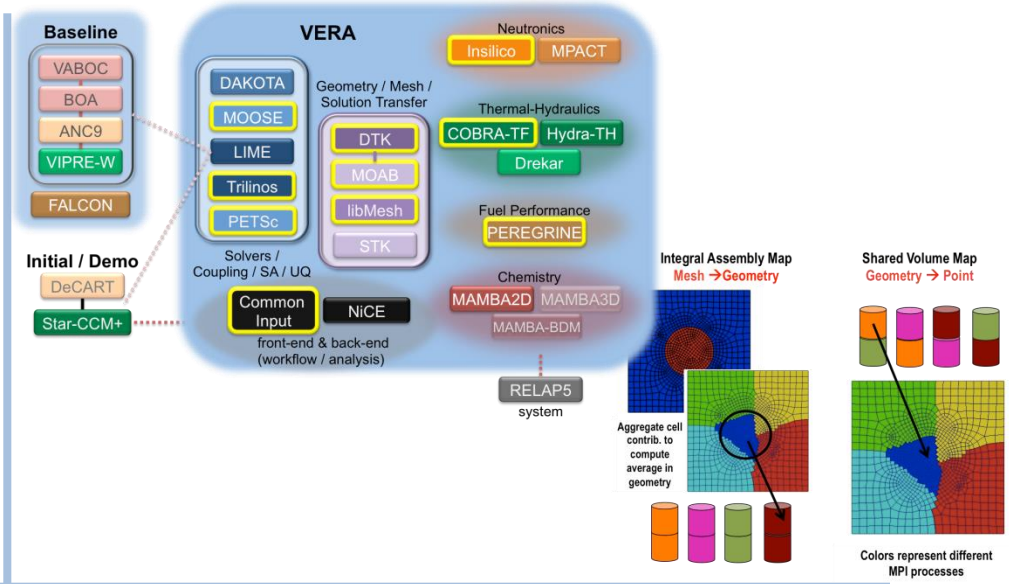
Technical Execution This Past Year

Advanced Modeling Applications

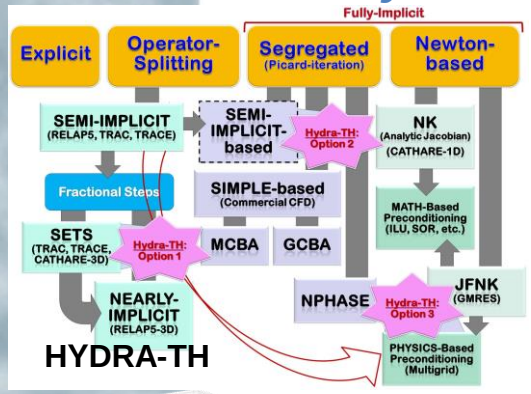
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- **#5 Physical Reactor Zero Power Physics Tests (ZPPT)**
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical Reactor Refueling

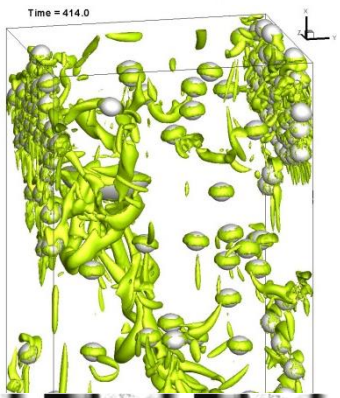


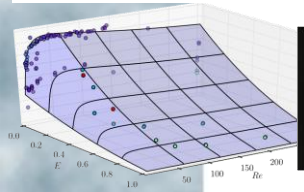
Virtual Reactor Integration

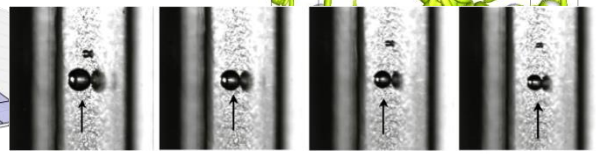


Thermal Hydraulic Methods

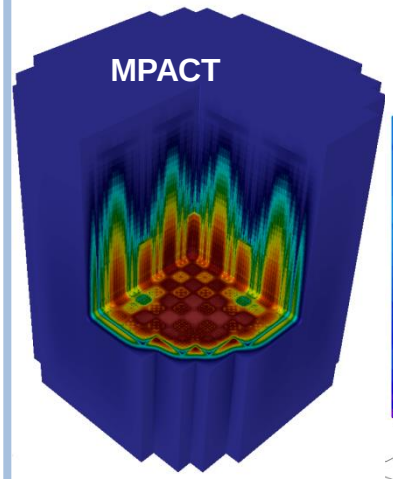


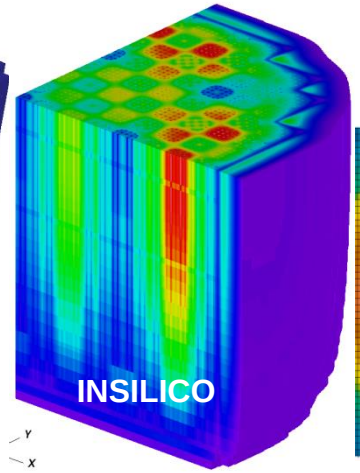


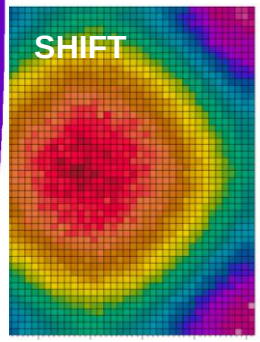




Radiation Transport Methods







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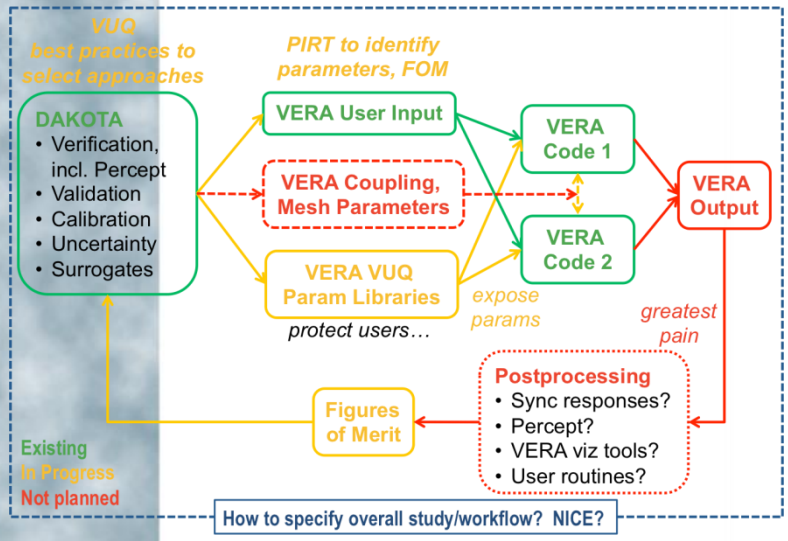
Technical Execution This Past Year

Validation & Uncertainty Quantification



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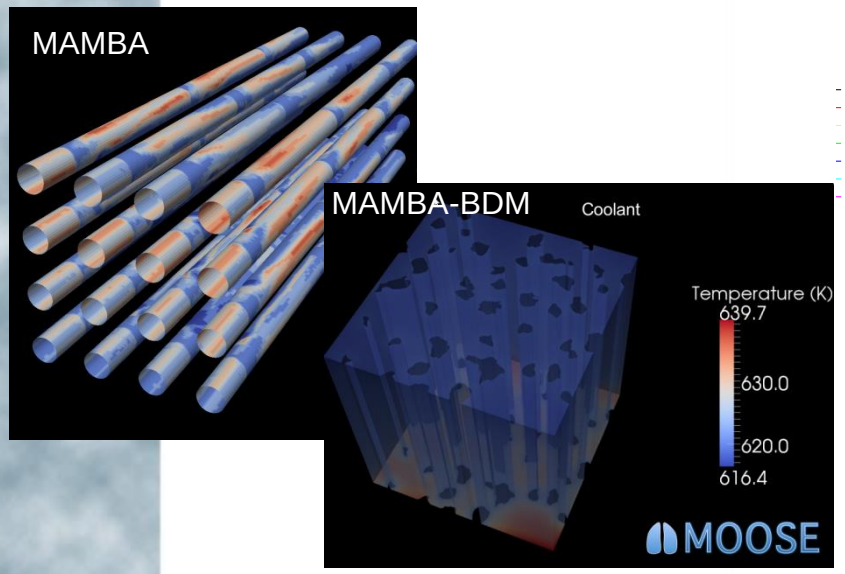
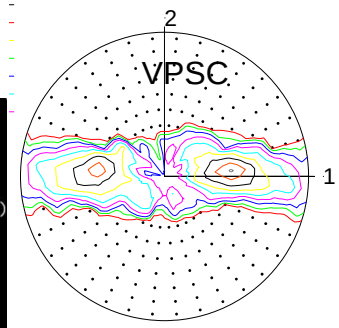
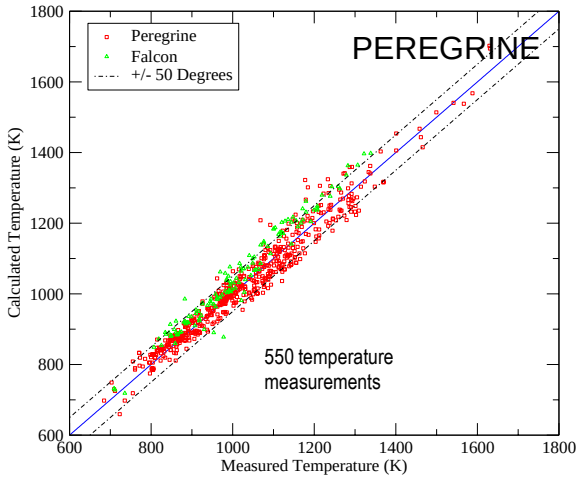
Materials Performance and Optimization





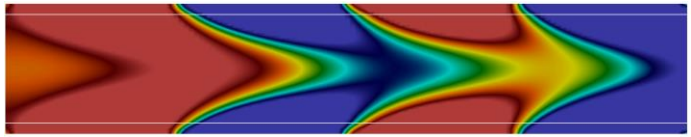


S&T Program: FY14 Highlighted Accomplishments (to date)

- Thermal-Hydraulic Methods (THM)

❖ Hydra-TH Capabilities Enhancements

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



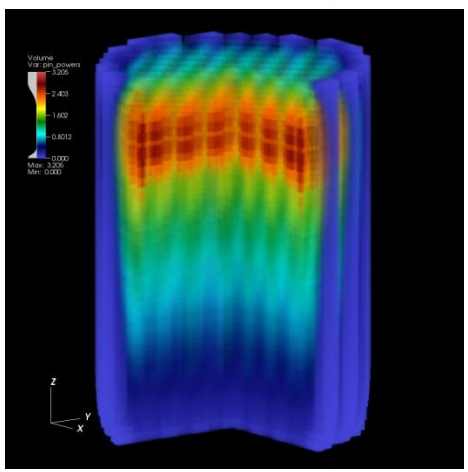
❖ Closure Relationships Development

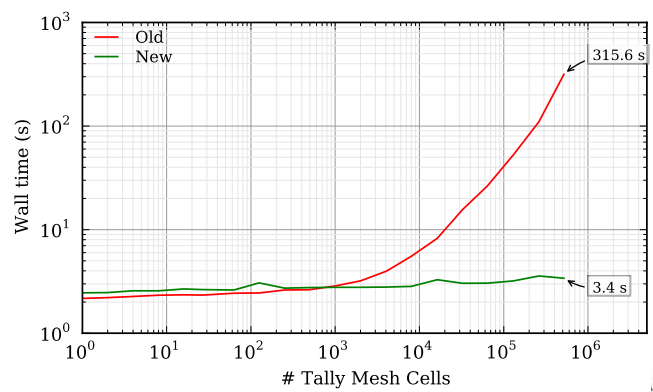
- Experimental work: Subcooled flow boiling database, gas-liquid two-phase flow experiments, effects of CRUD on boiling
- Interface tracking / DNS: Lift force on a single bubble, phase change
- Large scale ITM / data analysis: Transient motion of large number of bubbles, simulations and analysis of two-phase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

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

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

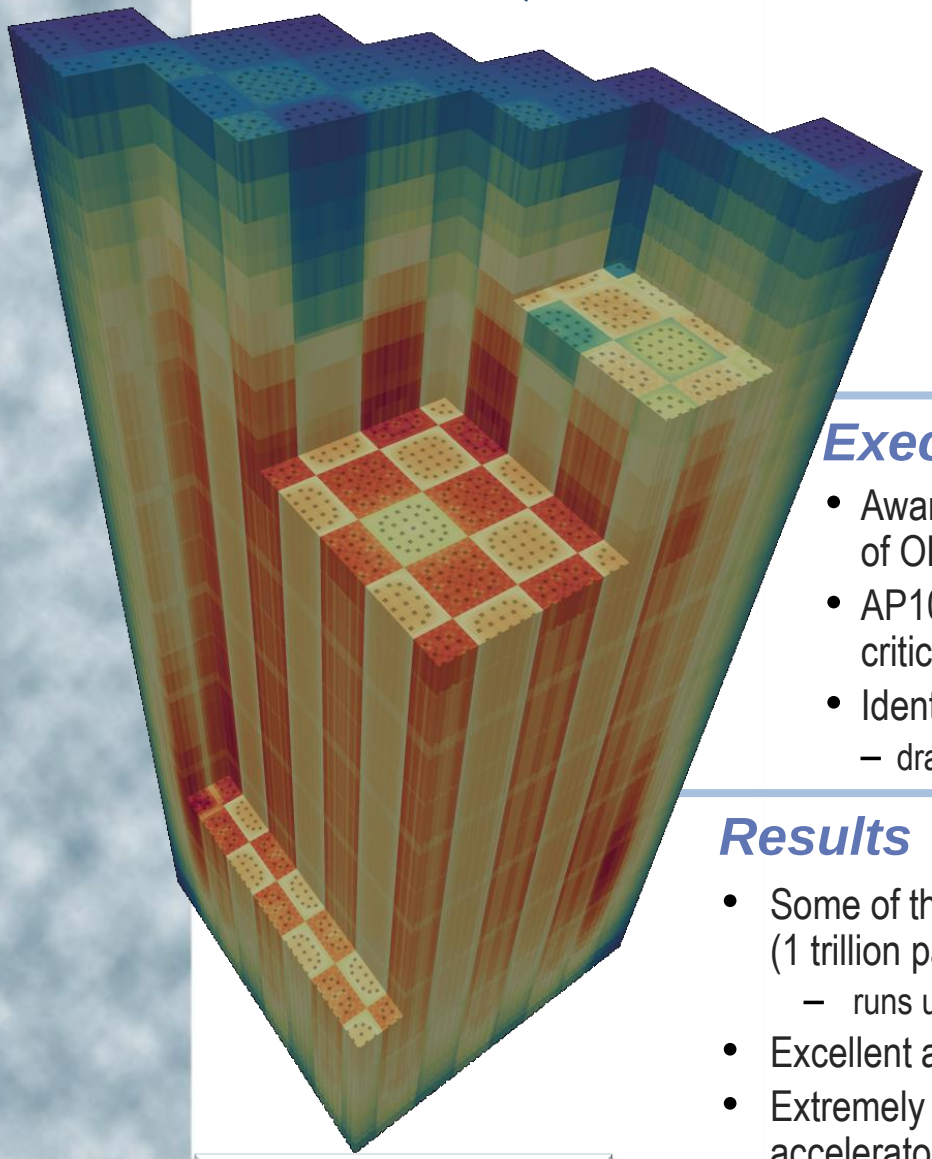
Bringing together Insilico (ORNL) & MPACT (UM) teams has proven effective





Evaluation of Shift: VERA Continuous-Energy Monte Carlo Capability

Quarter-Core Zero Power Physics Test



AP1000 pin powers

Goals

- Compare fidelity and 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

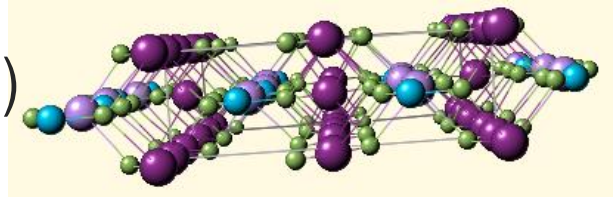
Execution

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

Results

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

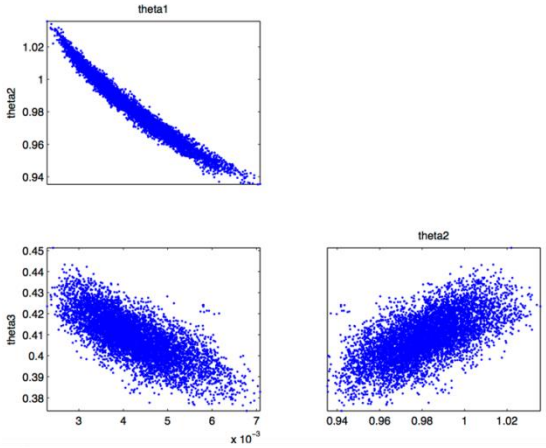
S&T Program: FY14 Highlighted Accomplishments (to date)



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

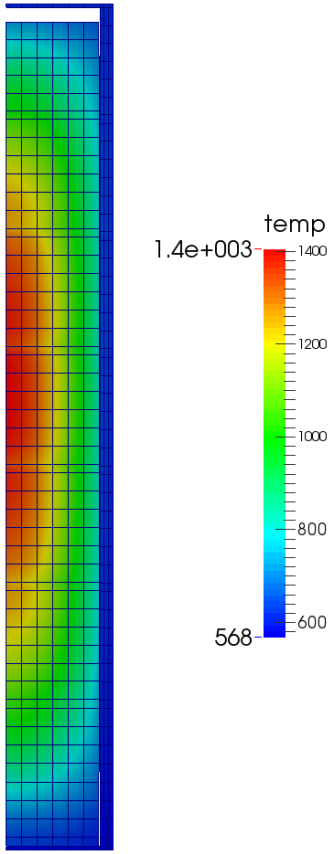
S&T Program: FY14 Highlighted Accomplishments (to date)

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



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

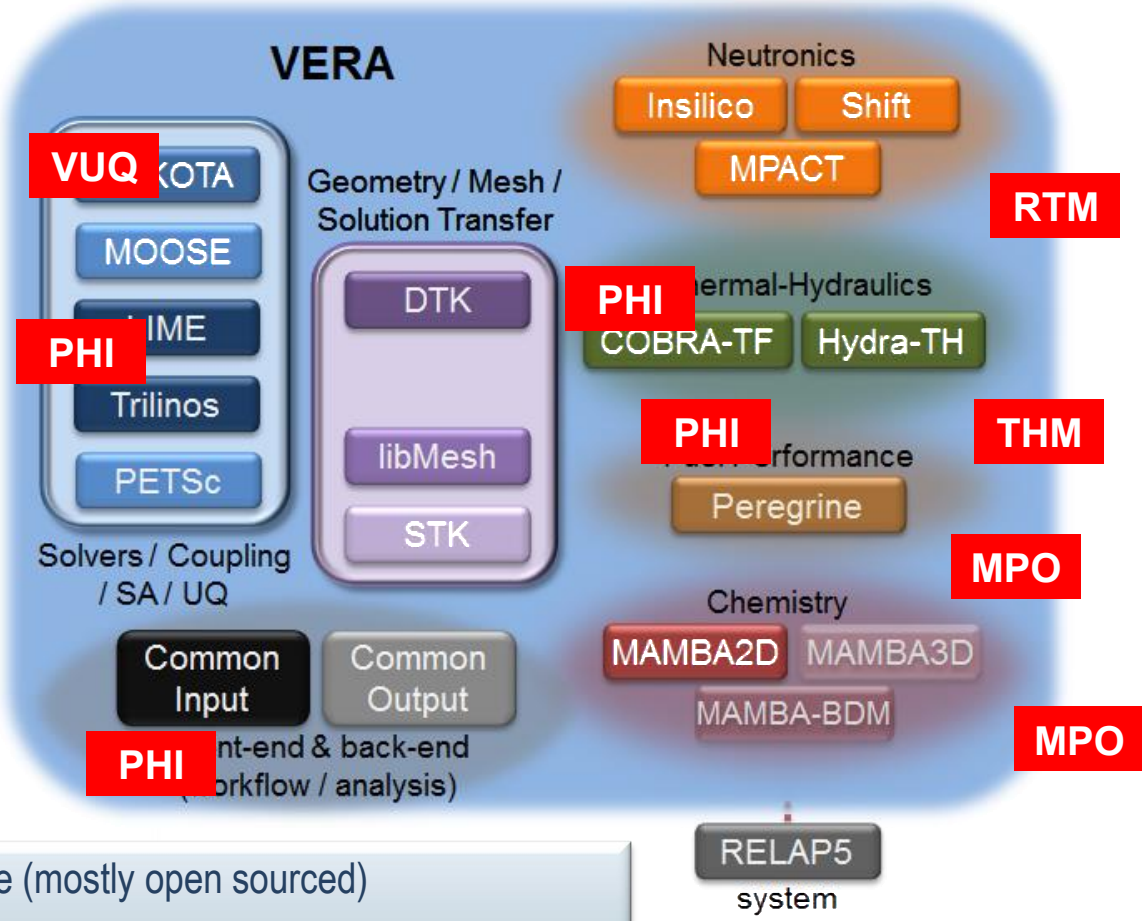
- Physics Integration (PHI)
  - Advancement of VERA-CS to Progression Problem 9 using MPACT-CTF (addition of depletion (Origen API), transient fission products, incore detector response).
  - Coupling of VERA-CS to Peregrine using improved coupling infrastructure using Tiamat (then PIKE) and DTK conserving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



VERA Status

Integrates physics components from focus areas

Congrats to lead COBRA-TF developer Bob Salko for receiving the 2014 CASL Knight award for outstanding technical accomplishments



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

VERA-CS

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

FY11

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

FY12

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

FY13

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

FY14

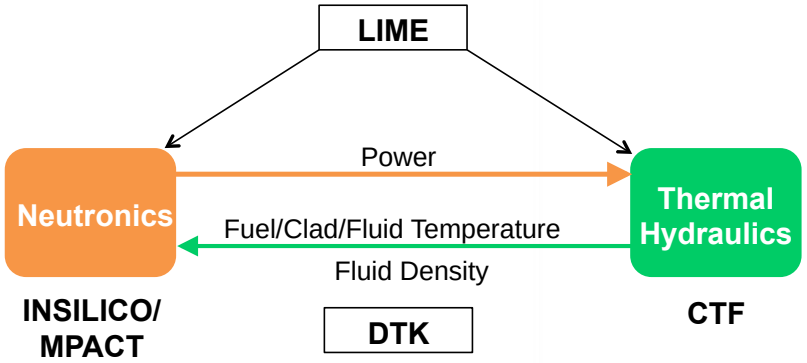
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical Reactor Refueling

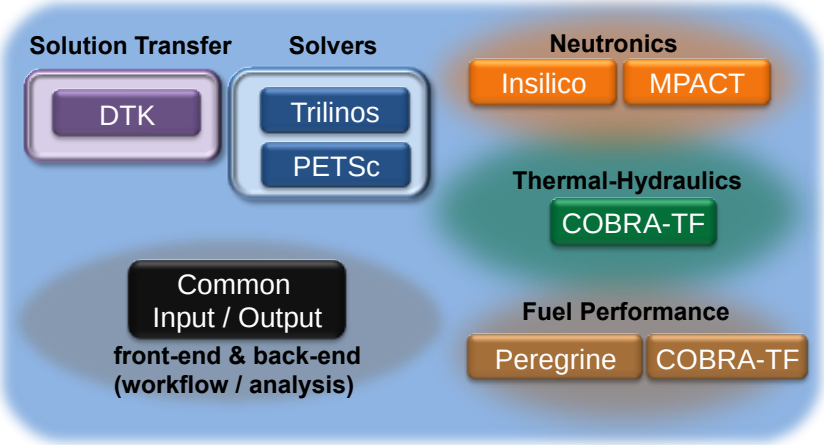
demonstrable progress

DOE reportable L1 milestone (*Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback*) on track for completion by Sep 30 2014

VERA Coupled Capability
The Core Simulator (VERA-CS)

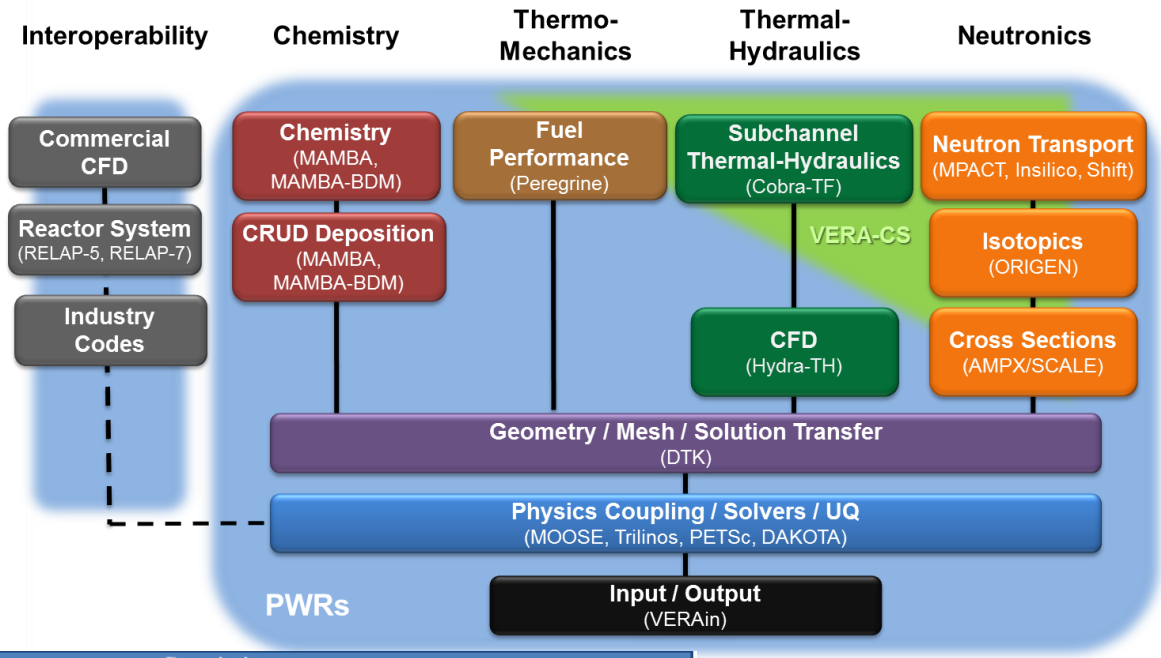
- VERA-CS is a subset of VERA components that are used to model the steady-state operation of the reactor and depletion
- Contains neutronics, thermal-hydraulics and fuel rod temperature components
- Key Achievements/Applications:
  - Insilico/CTF full-core hot-full power capability
  - MPACT/CTF full-core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





Near-Term Expectations for VERA

VERA capabilities expected at Phase 1 conclusion (Apr 2015)



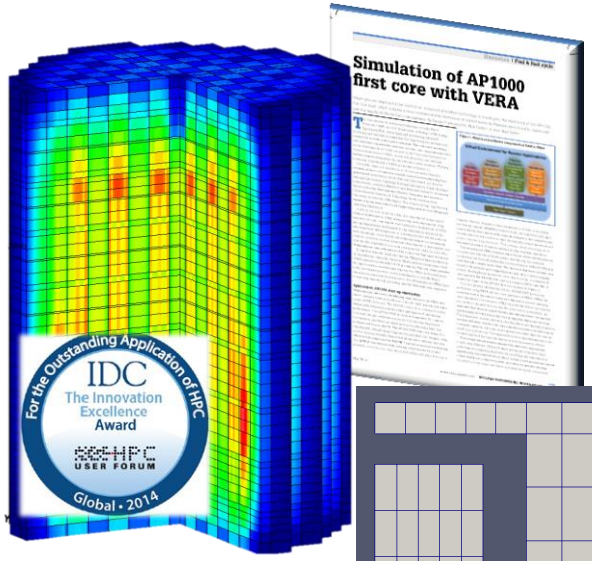
Item	Description
S/W Development Tools and Computational Infrastructure	Standardized set of compilers and configuration tools Git revision control system and S/W repository management Build & test infrastructure (TriBITS, CMake, CTest, CDash) 17 geographically dispersed code repositories, 205 TriBITS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

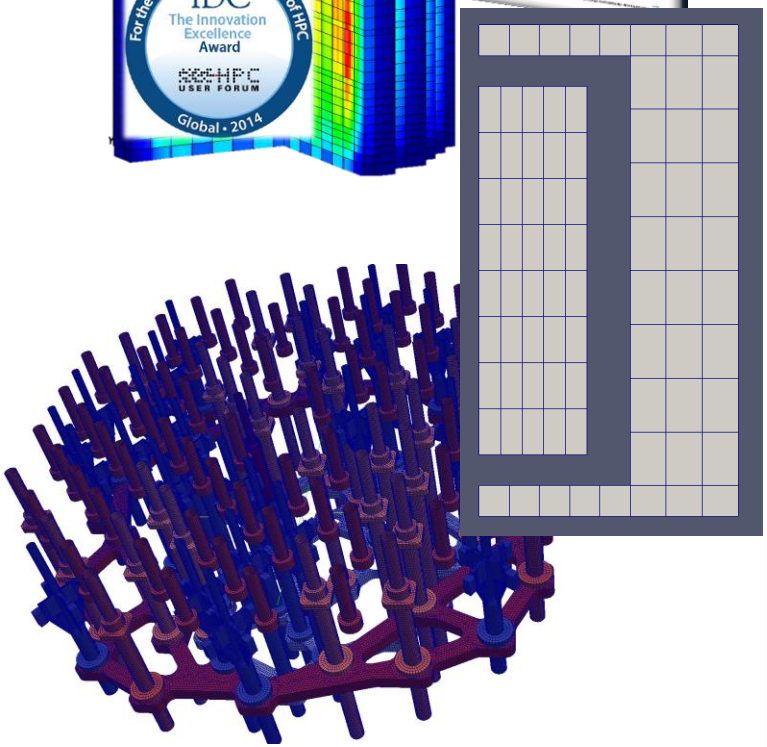
VERA current technology portfolio

Technology Deployment

We have now deployed 3 Test Stands

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





Validation Accomplishments

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

CPIs & FAs will give more details during their presentations

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

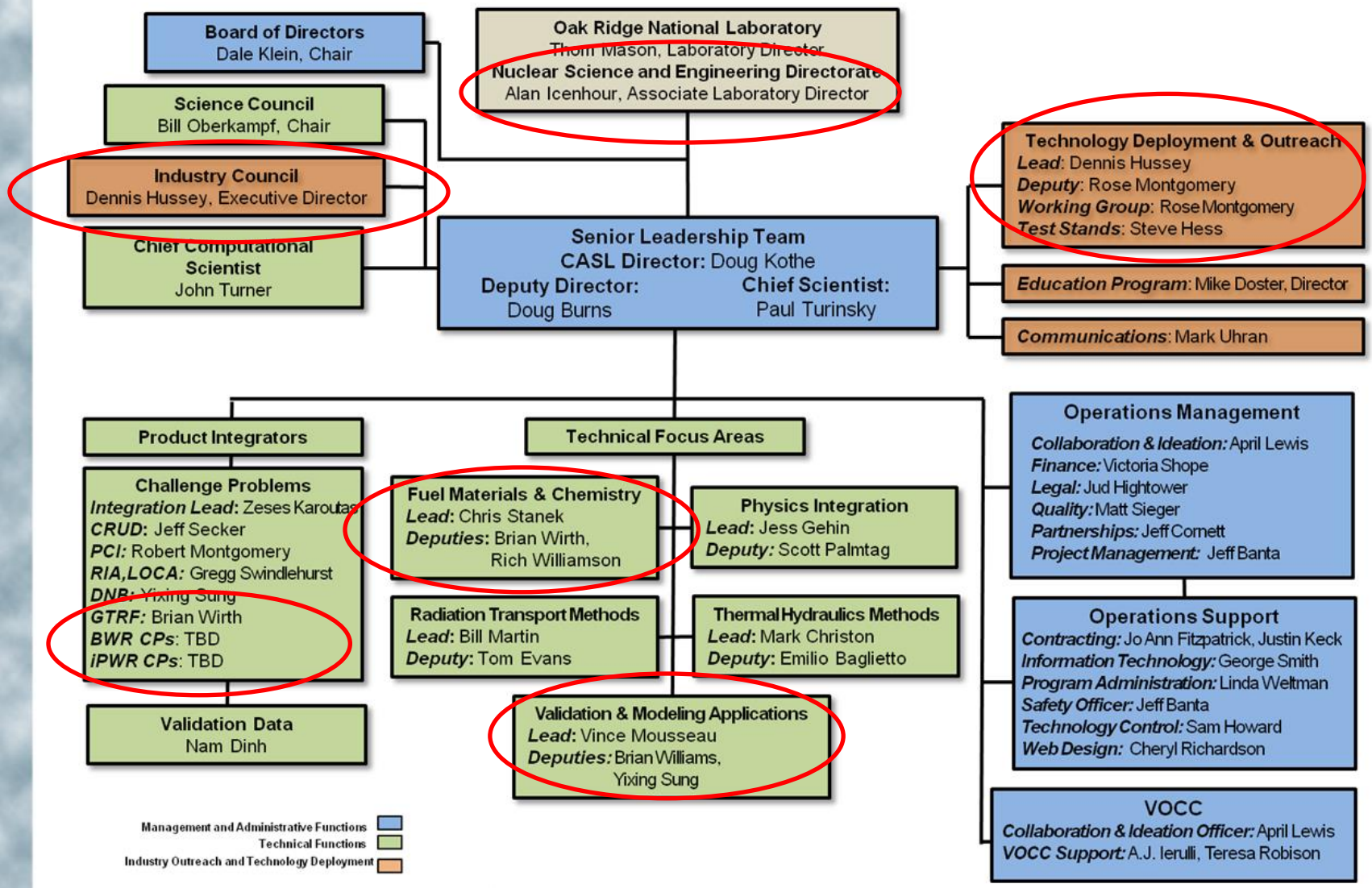
Physics Integration
Lead Jess Gehin
Deputy Scott Palmtag

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

Congrats to Finance Officer Victoria Shope for receiving 2014 CASL Jester award

We are Planning to Evolve our Structure Moving into FY15

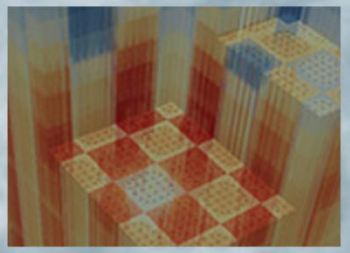


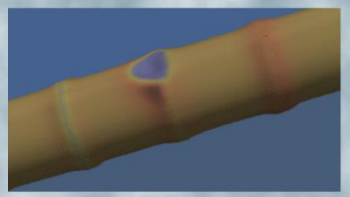
A DOE Energy Innovation Hub

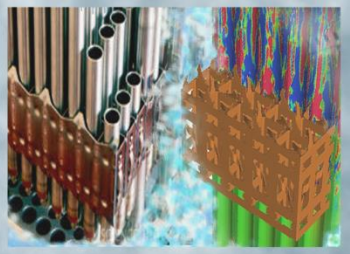
VERA: Description, Status, Plans

Jess Gehin, PHI FA Lead

Scott Palmtag, PHI FA Deputy Lead





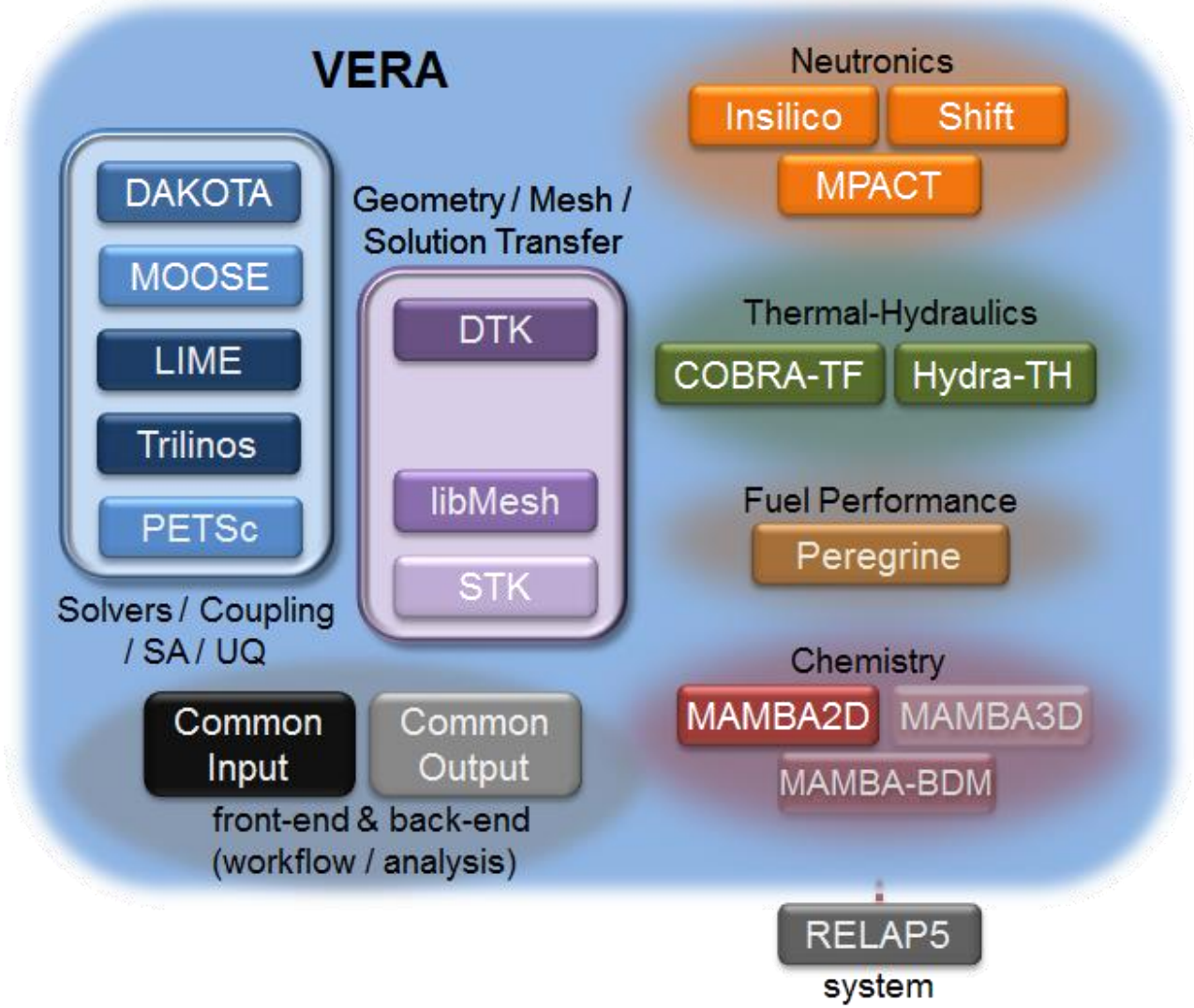


U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

VERA Status Summary

- The VERA development, testing and release infrastructure is in place and mature
- Key advancements are being made in coupling including coupling infrastructure and coupling methods research
- Physics components developed by all FAs are being improved and integrated in to VERA
- In FY14 an increased emphasis is being placed on coupling codes to support challenge problem applications
- The VERA release process is maturing and supporting several releases to Test Stands and through RSICC

VERA Components



Evolving Components to meet Requirements

VERA Components by Release in Phase 1

Date	VERA Snapshot	Infrastructure Components Added**	Physics Components Incorporated**	Component Coupling Implemented**	CP Supported	Notes
12/2010	0.5	Trilinos LIME	ANC9[I] VIPRE-W[I] DeCART[p] Star-CCM+[c]	DeCART+Star-CCM+[c]	PWR CIPS (initial) PWR PCI (initial) PWR GTRF (initial) All	Investigative work with industry / commercial / proposed tools. Basic infrastructure established.
03/2011	1.0	DAKOTA	Insilico	ANC9+VIPRE-W[I] DAKOTA+VIPRE-W[I]	PWR CIPS (initial) PWR PCI (initial) PWR GTRF (initial) All	Investigative work continued. Basic UQ capability added. S_N capability added.
03/2012	2.0	Common Input	Drekar[p] BOA[I] Mamba RELAP5	ANC9+VIPRE-W+BOA[I] DAKOTA+VIPRE-W+BOA[I]	PWR CIPS PWR PCI (initial) PWR GTRF (initial) PWR RIA (initial) All	Investigative work continued. Common input added. Initial CRUD capability added.
06/2012	2.1	DTK STK MOAB	VABOC[I] COBRA-TF Hydra-TH	N/A	PWR CILC PWR DNB PWR LOCA All	Advanced infrastructure components integrated. CFD code integrated.
01/2013	2.3	N/A	MPACT	CTF+Insilico DAKOTA+CTF	All (VERA-CS)	MOC capability added. Subchannel T/H coupling achieved.
07/2013	3.1	PETSc libMesh MOOSE	Peregrine Shift	TIAMAT: CTF+Insilico+Peregrine (Figure A-7)	PWR PCI All (VERA-CS)	Three-code coupling completed. Initial thermo-mechanics capability added. FEM and underlying solver integrated.
03/2014	4.0	N/A	N/A	CTF+MPACT	All (VERA-CS)	MOC coupling with subchannel T/H implemented.

*Many components were investigated for capability and coupling development and are currently inactive in VERA, including industry codes (I), commercial codes (c), and proposed tools (p). Figure 2 provides the active codes at the end of Phase 1, with interoperability maintained for commercial and industry tools as possible.

**Note that the components and coupling listed are cumulative.

Key Capability Developments Since August 2013

- VERA is being optimized to a stable set of components to support challenge problem analysis
- Key Additions
  - SHIFT Monte Carlo code has matured and been added as a VERA capability
  - Insilico coupling with CTF development completed
  - MPACT has matured significantly and been coupled with CTF
  - Insilico-CTF-Peregrine coupling matured to support PCI
  - Many improvements to individual components
- Deprecated capabilities
  - "Baseline" ANC-VIPRE-BOA has been updated and deployed to Westinghouse for future development and use
  - Star-CCM+/DeCART demonstrated of neutronics+CFD
  - Drekar CFD code
- Additional adjustments are anticipated in the future, but most effort will be in improving individual components and their coupling

A Mature VERA Infrastructure Has Been Established

- The VERA infrastructure coordinates a diverse set of software components
  - Multiple distributed development groups
  - 18 repositories hosted on casl-dev with different access lists
  - 96 software packages, 14+ third party libraries (TPLs)
- Tribal Build, Test, and Integrate System (TriBITS) enables integration of distributed repositories
  - Emphasis in FY14 on documentation of TriBITS
  - Open source and has been adopted by non-CASL development teams
- Releases taken off of “master” branches
  - Supports snapshots, Test Stands, and RISCC releases
- CASL Support, Improvement and Corrective Action Tracking System (CSICAT)

Automated Testing and Growing Test Base

- CASL utilizes a continuous integration (CI) build/test environment (TriBITS)
- CTest/CDash - Use for testing and monitoring
- Continuous, nightly and weekly testing
- Test base is continually growing

Login All Dashboards Friday, March 22 2013 14:02:57 EDT

VERA

Dashboard Calendar Previous Current Project

March 2013 – 936 Tests

Project

Project	Configure			Build			Test			Last submission
	Error	Warning	Pass	Error	Warning	Pass	Not Run	Fail	Pass	
VERA	0	138	139	0	27	112	0	0	936	2013-03-22 13:59:08

Login All Dashboards Monday, August 04 2014 16:30:44 EDT

VERA

Dashboard Calendar Previous Current Project

August 2014 – 2063 Tests

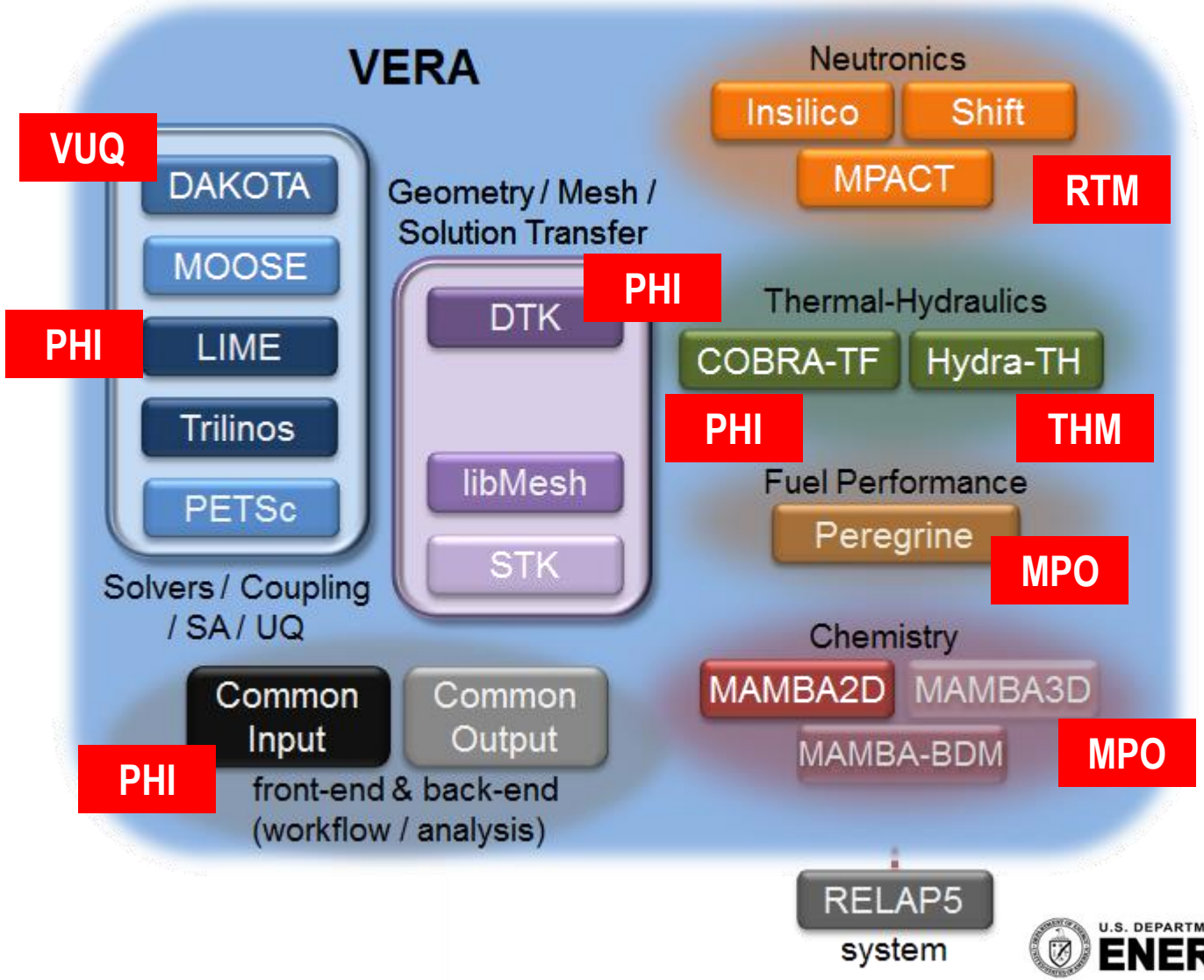
Project

Project	Configure			Build			Test			Last submission
	Error	Warning	Pass	Error	Warning	Pass	Not Run	Fail	Pass	
VERA	0	39	39	0	24	15	0	6	2063	2014-08-04 10:17:57

Coupling Developments

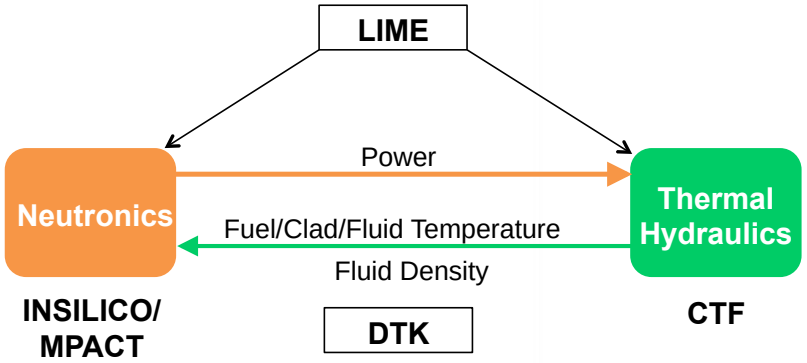
- A coupling infrastructure has been developed to support coupled code capabilities
- Data Transfer Kit (DTK)
  - Provides for grid data transfer between components provides mapping for use parallel computing environments
  - Key 2014 developments include performance improvements, support for mesh-free methods
  - CASL open source product available on github and integrated into MOOSE
- Physics Integration KErnels (PIKE)
  - Evolution of LIME to provide a improved multiphysics driver capability
  - Developed based on CASL experience with LIME in coupling components and need for additional features (POR3 milestone on needs: “LIME 2.0 Design Report”).
  - CASL product to be released in as open source in Trilinos (SNL – trillinos.org)
- Tiamat
  - Generalized driver for multiple couplings – applied to CTF-Insilico-Peregrine coupling
  - Contains light-weight tools to assist in setting up applications with unique communicators
- Coupling Methods Research
  - Current capability based on Picard iteration
  - Research on Jacobi-Free Newton Krylov and Anderson Acceleration Methods

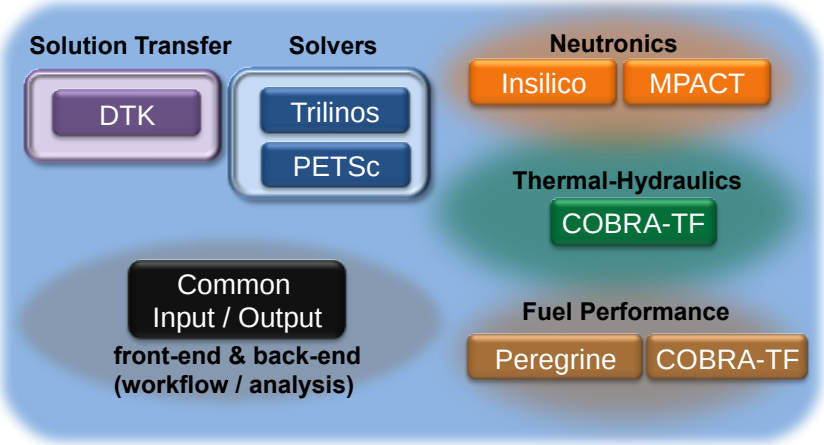
VERA Integrates Physics Components Developed by All Focus Areas



VERA Coupled Capability: Core Simulator

- The VERA Core Simulator provides the sub-set 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/UT





Progression Problems Progress

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 ✓
- #4 HZP 3x3 Assembly CRD Worth ✓

FY13

- **#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** September 30, 2014
- #10 Physical Reactor Refueling November 11, 2014

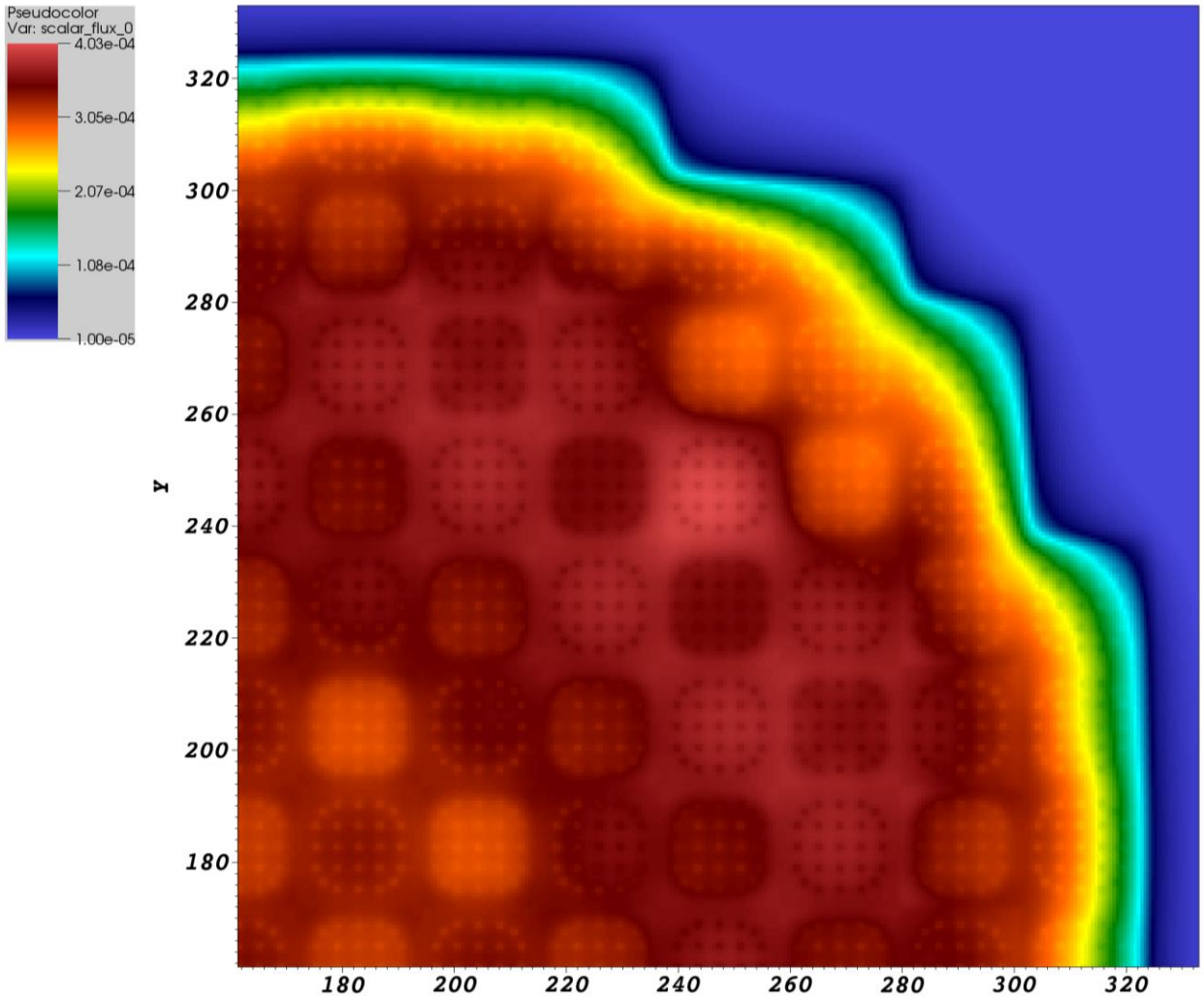
*** Bold text signifies ability to compare to measured plant data**

Problem 7 – Operational Reactor at HFP

- Hot Full Power (HFP)
- Full-core model from Problem 5
- Coupled physics from Problem 6
- Operating "real" reactor with all the geometry detail
- No reference results available due to feedback
  Future Problems will include flux maps and depletion
- Problem 7 solved with both Insilico/CTF (L2.AMA.P7.02) and MPACT/CTF (L3:RTM.PRT.P7.05)

- SCALE cross-section processing for DENOVO in VERA
- DENOVO pin cell capability with SCALE in VERA
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #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
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical Reactor Refueling

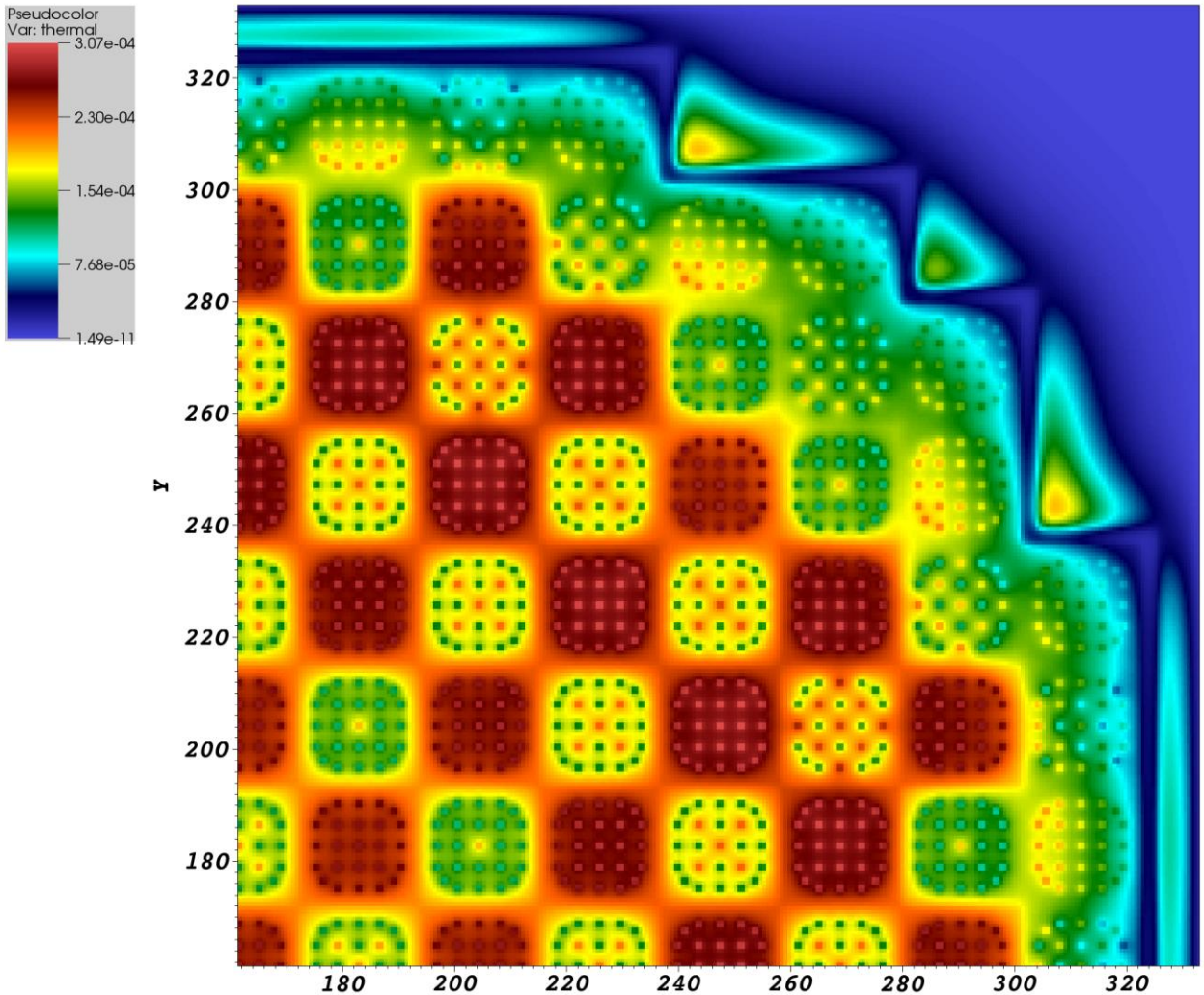
Problem 7 - Fast Flux Results



Fast Flux
at mid-plane

Highest energy
neutrons,
Longer mean-free-
paths

Problem 7- Thermal Flux Results



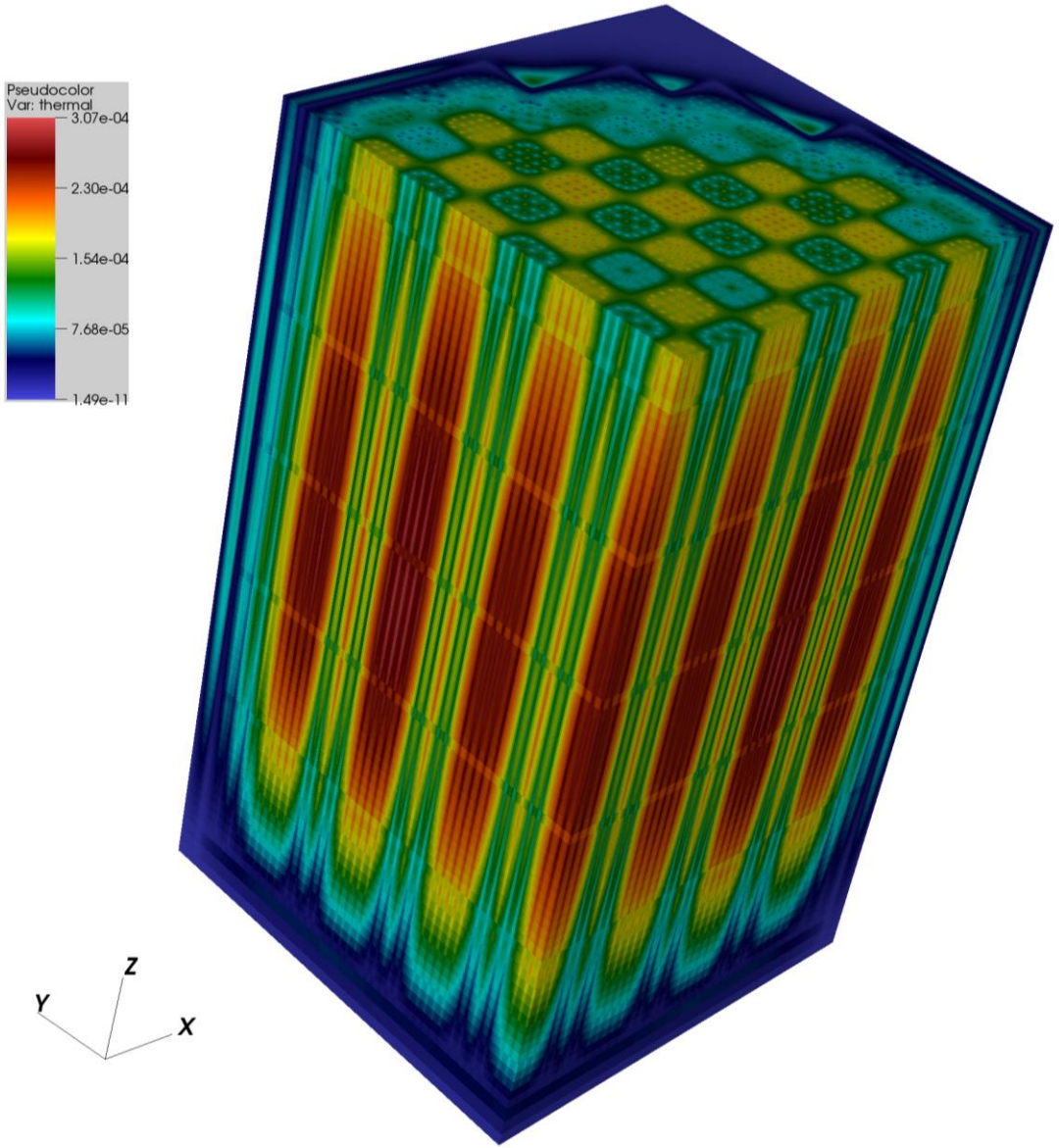
Thermal Flux at midplane
(0.625 eV cutoff)

Low energy neutrons,
Short mean-free-paths

Peaks formed in reflector from downscatter source

Low flux in baffle

Problem 7 – 3D Thermal Flux Results

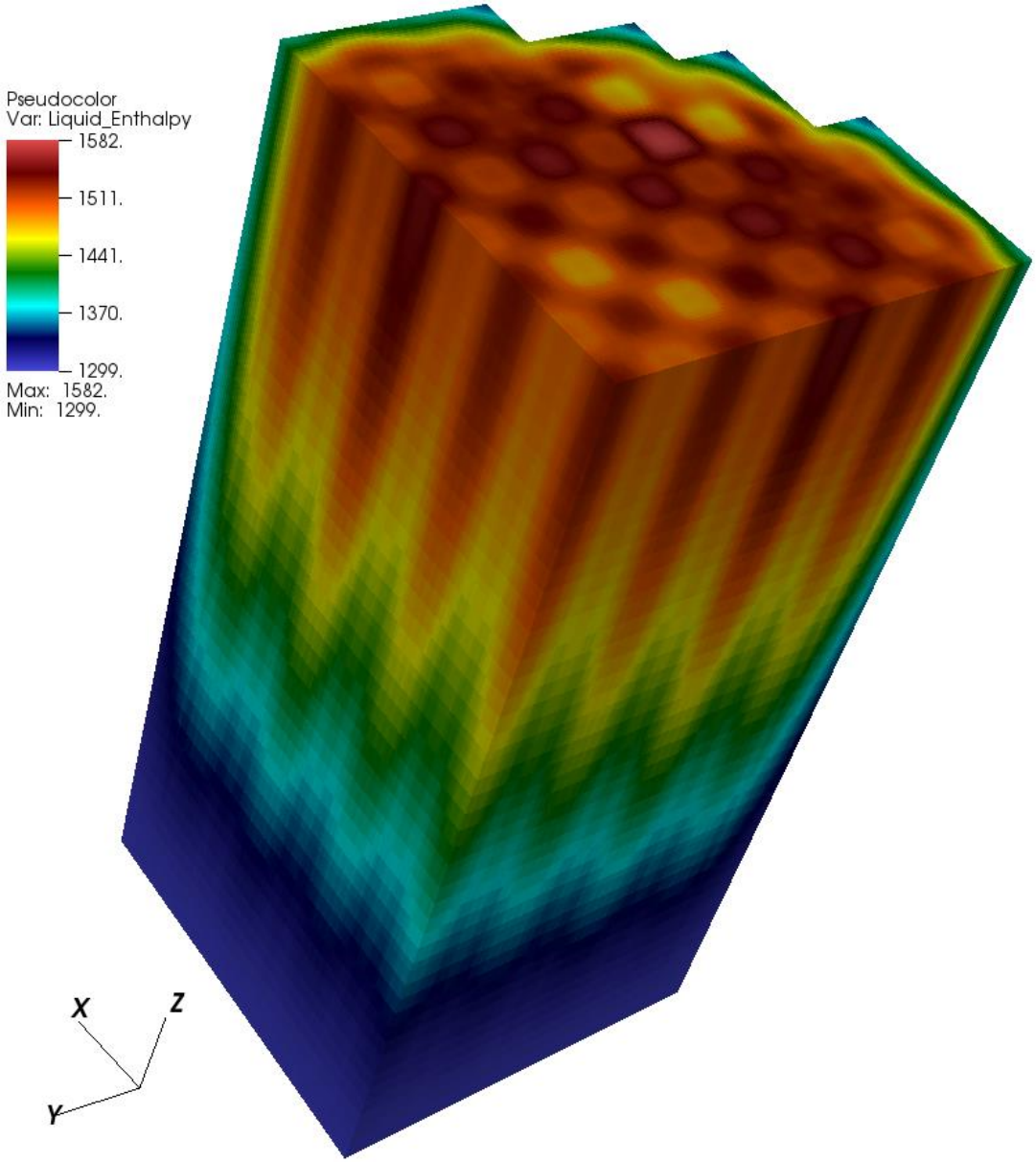


Thermal Flux
(0.625 eV cutoff)

Flux depressed in assemblies with Pyrex absorbers

Can observe geometry features such as baffle, nozzles, and spacer grids

Problem 7 - 3D Coolant Enthalpy



VTK output file created by CTF

Enthalpy increases with core height

Note the lower enthalpy in assemblies with Pyrex absorbers

Problem 7 – Significant Performance Improvements

- Milestone L2.AMA.P7.02 (Dec 2013)
  - Insilico/CTF – 56/8 energy groups
  - 18,769 cores, 17.5 hours wall time
- Milestone L3:RTM.PRT.P7.05 (Apr 2014)
  - MPACT/CTF – 56 energy groups
  - P2 Scattering
  - 2,784 cores, 12.25 hours wall time
- Current (Aug 2014)
  - MPACT/CTF – 56 energy groups
  - Transport Corrected P0 Scattering
  - 2,784 cores, 3.75 hours wall time

328,457 CPU-hr

↓

34,104 CPU-hr

↓

10,440 CPU-hr

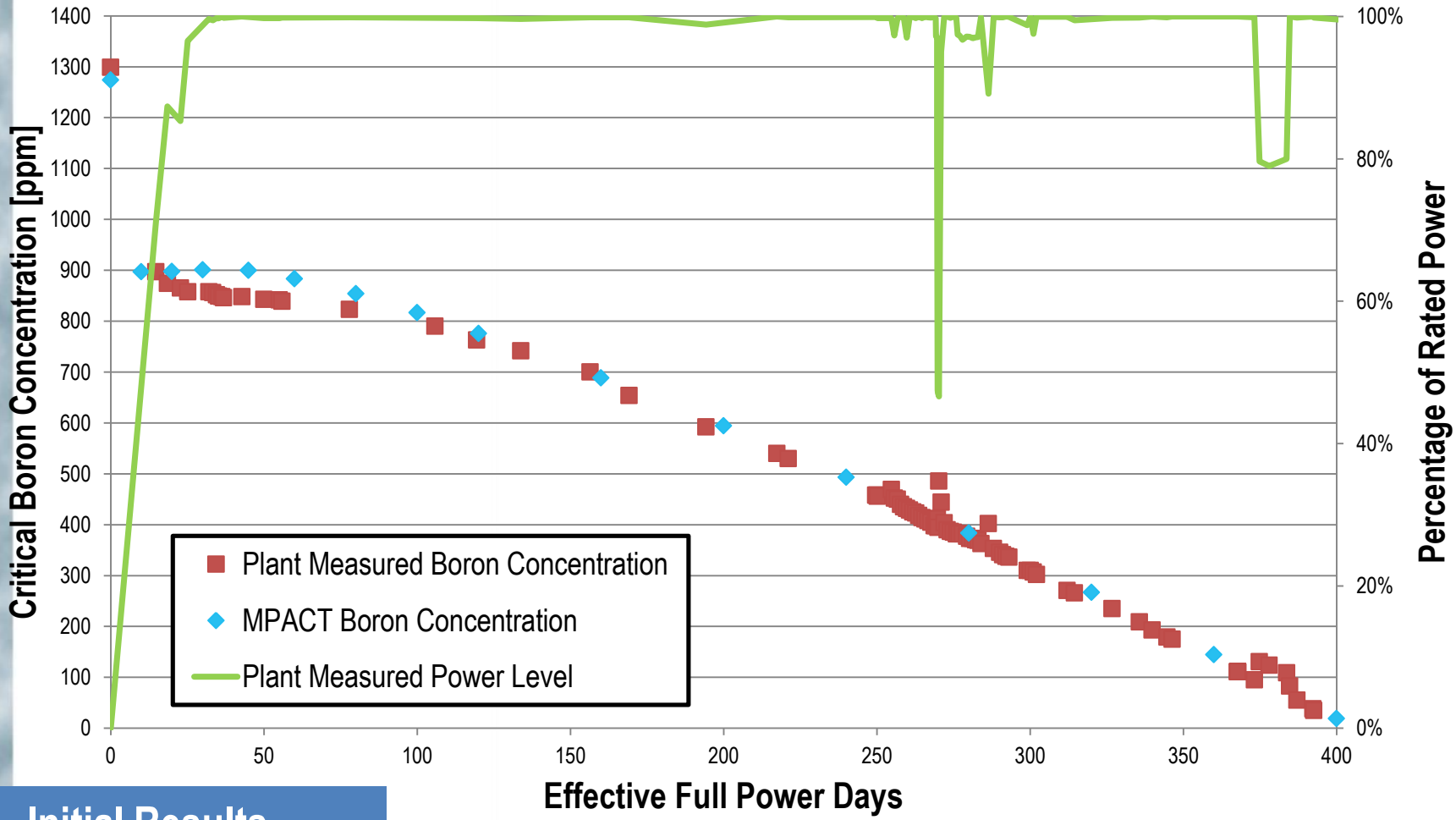
↓

More Improvements in Progress

Problem 9
Watts Bar Cycle 1 Depletion

- Simulation of WBNP1 Cycle 1 was performed with MPACT at 100% power for 400 Effective Full Power Days (EFPD)
  - Escalation to full power was neglected (131 days or 36 EFPD)
  - Neglected other down-powers and outages
  - Neglected coast down at end of life
- P0 scattering was used for increased speed.
  - BOC tests showed critical boron concentration was not very sensitive to isotropic scattering approximation.
  - Enhanced cross-section library will allow for stable transport correction or memory improvements will allow for P1 or P2 scattering.
- Run on EOS on 2096 cores for 21 hr 18 min
  - Critical boron search
  - Simplified TH feedback (assembly axial energy balance without cross-flow + 1D fuel temperature – no CTF)

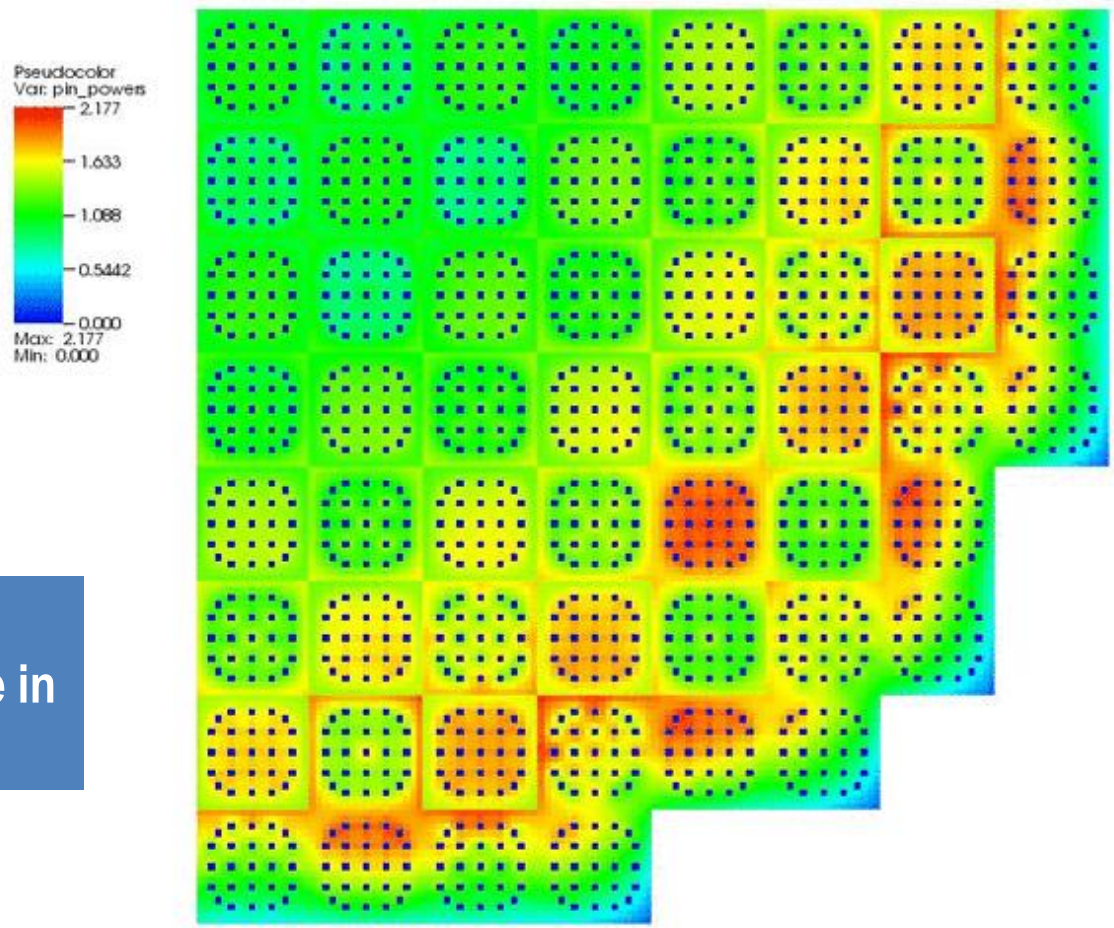
WBNP1 Cycle 1 Boron



Initial Results – Problem 9 Milestone in Progress

WBNP1 Cycle 1 Power

2D Power Distribution vs. Exposure



Initial Results – Problem 9 Milestone in Progress

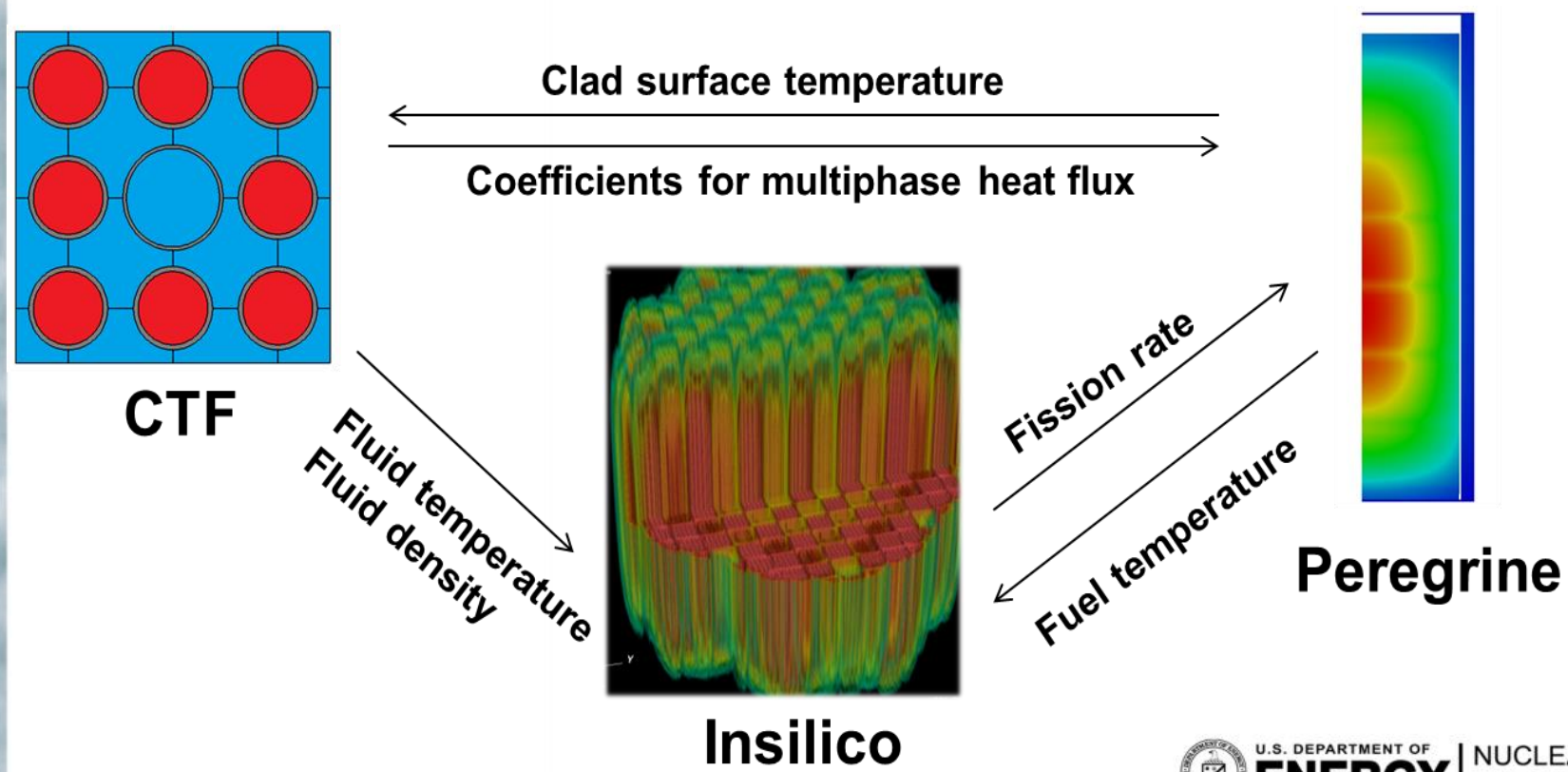
Exposure 0 GWd/MT

VERA Coupled Capability: PCI Challenge Problem

- Extend Core Simulator Capability with Fuel Performance Model
  - Replace CTF fuel rod model with MOOSE-based Peregrine fuel performance capability (keep CTF T/H solver)
- 2D R-Z Peregrine model for every rod
- Milestones completed this year:
  - L3: PHI.CMD.P8.02 (2/28/2014) “MOOSE development”
  - L2: PHI.P9.01 (6/30/2014) “Single Assembly”
  - L1: CASL.P9.03 (8/31/2014) “Multi Assembly”
- Tiamat used to perform three-way coupling (CTF-Insilico-Peregrine)
  - Successfully integrated Peregrine with VERA environment
  - Successfully coupled Peregrine with CTF and Insilico
  - Developed new multiphysics driver (PIKE)
  - Developed data transfers for this specific application using DTK

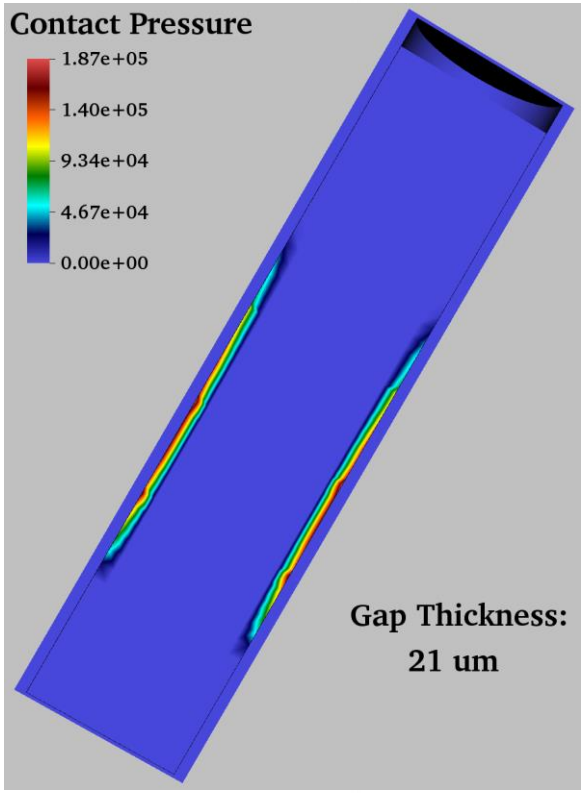
VERA Coupled Capability: PCI Challenge Problem

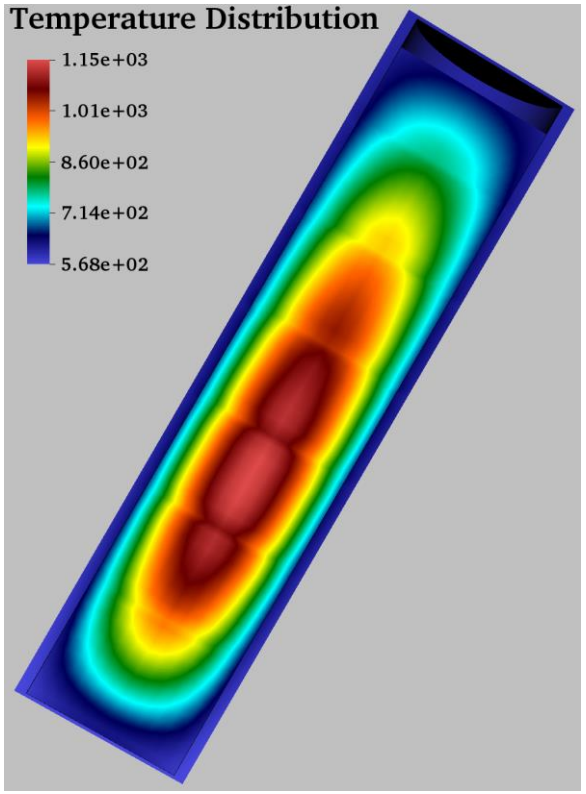
- Tiamat-based coupling of CTF-Insilico-Peregrine
- All applications are run in their own MPI process space
- Data Transfers are handled through DTK with MPI sub-communicators
- Extends core simulator functionality with improved fuel performance capability
  - CTF has simplified model that has been replaced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



Demonstration of PCI on Single Rod Problems

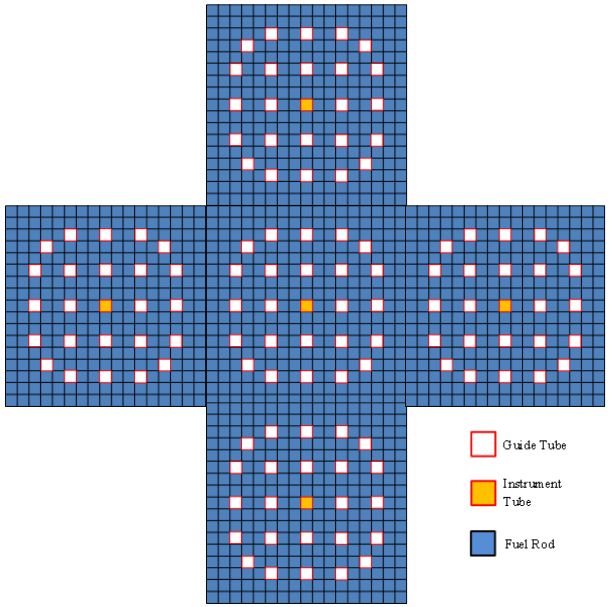
- Problems run with differing gap thickness to demonstrate fuel performance pellet-clad contact model.
- Example result for 21 micron gap





Applied to Multi-Assembly Test Problem

- Based on Watts Barr Unit 1 Cycle 1
- Extended Assembly to Multi-Assembly
  - Layout of 5 assemblies
  - 1320 fuel rods modeled



- DOE Reportable milestone completed August 29th
- Next Step is ¼ core (~13,000 fuel rods)

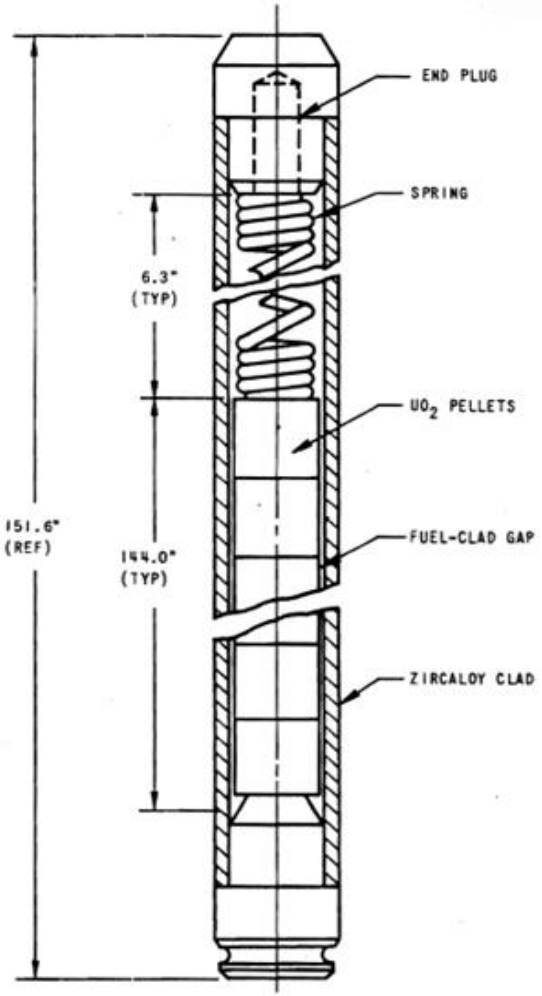
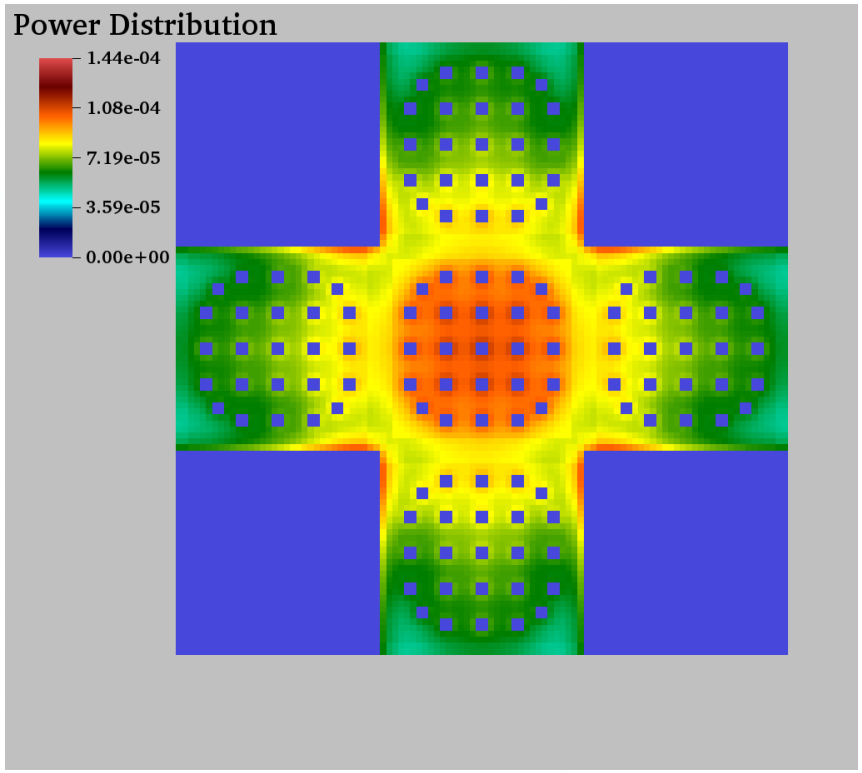
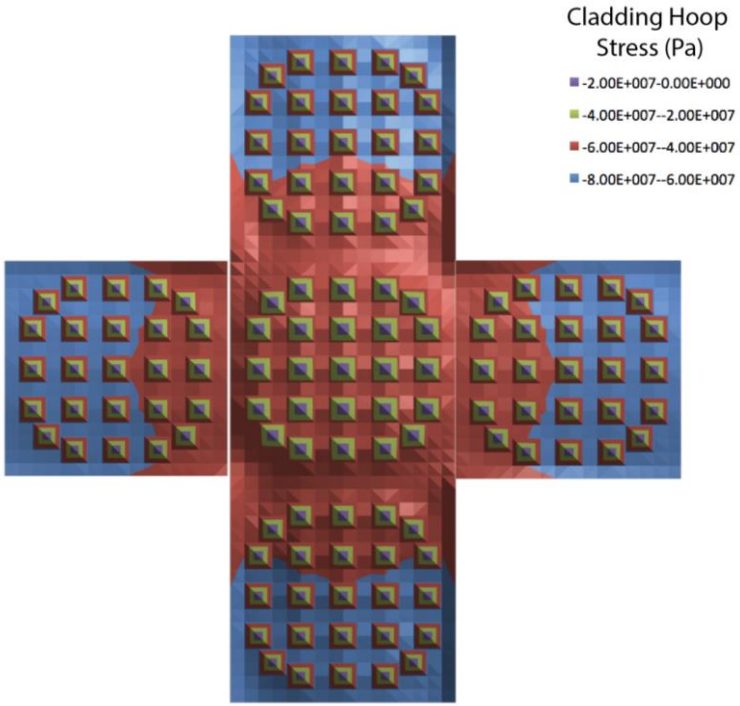


Figure from Watts Bar Unit 2 Final Safety Analysis Report (FSAR), Amendment 93, Section 4, ML091400651, April 30, 2009. Figure 4.2-3

Results – Power Distribution and Cladding Hoop Stress



Power Distribution

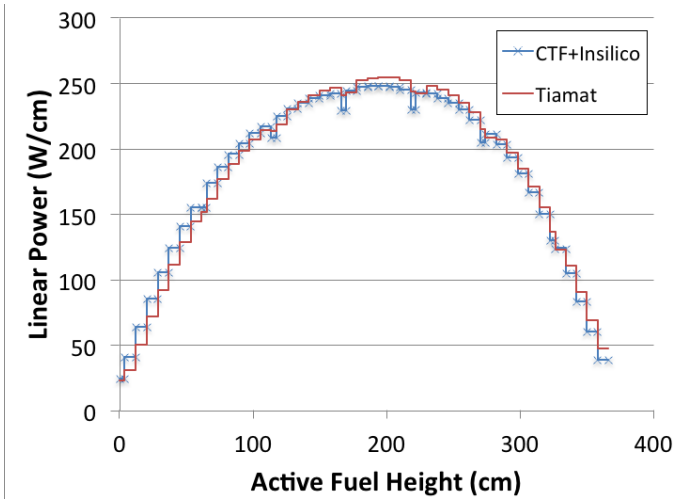


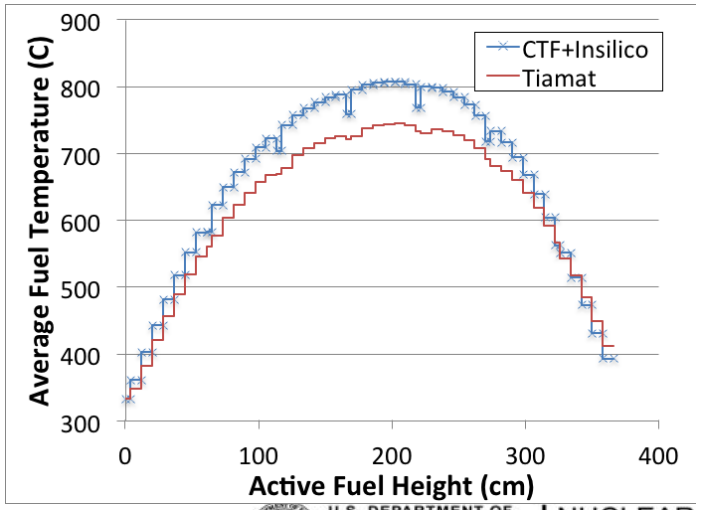
Cladding Hoop Stress

Comparison To CTF+Insilico
(Single Assemby Case)

- A comparison of CTF+Insilico with Tiamat provides a reasonable benchmark for timings and results.
- The CTF pin heat transfer model is very different from Peregrine
  - CTF used with a fixed gap-heat transfer coefficient and does not account for change to the gap thickness.
  - Differences in thermal conductivity models of the fuel and cladding
  - Future project planned to improve the models used in CTF through comparisons with Peregrine.

	keff	Avg. Fuel Temp (C)	Peak Power (W/cm)
Tiamat	1.189805	623	255
CTF+Insilico	1.188200	664	248

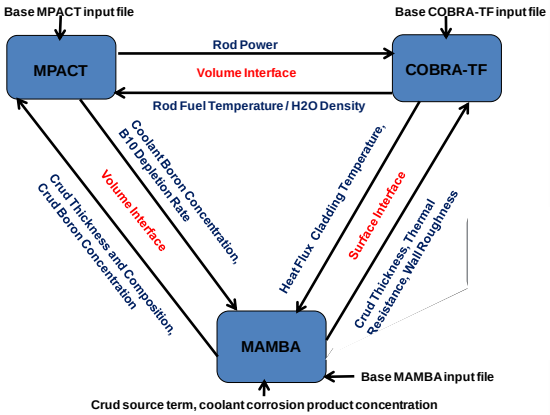


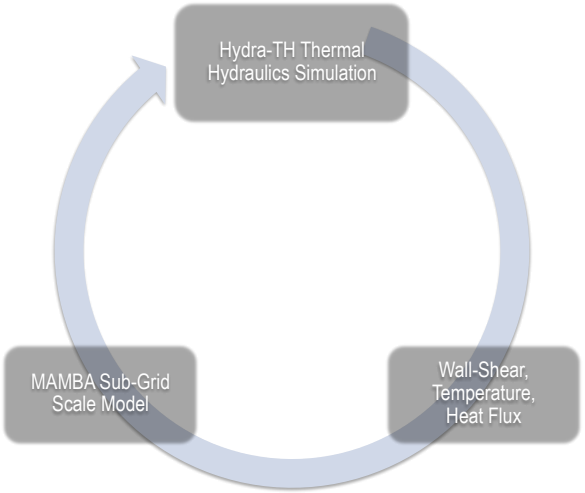


Timings (S)	Tiamat	CTF/Ins
Num Cores	326	36
Total time	2162	1544
Setup	53	-
HFP Est/HFP Ramp	1374	-
Solve	735	-
Num fixed-point Iterations	4 (+6)	8

VERA Coupled Capability
CRUD (CIPS/CILC) Challenge Problem

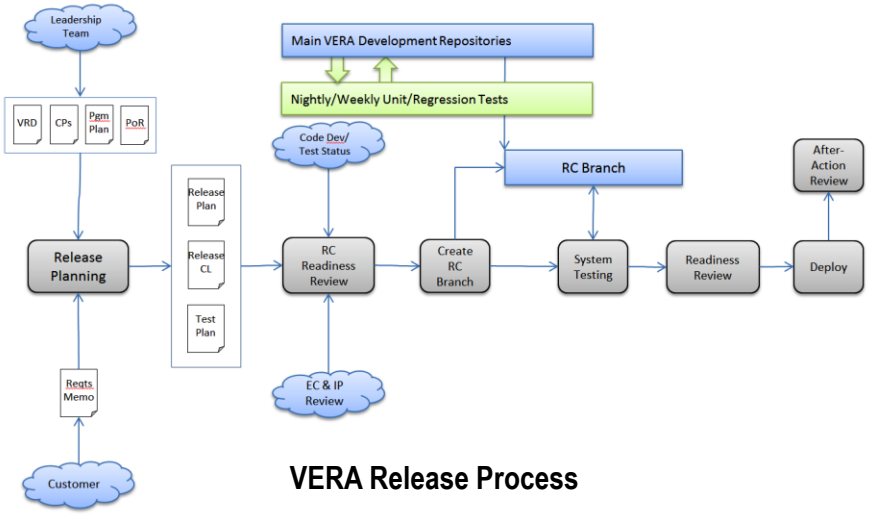
- CIPS requires modeling coupled neutronics-T/H-CRUD capability at full-core level to simulate impact on core power distribution
  - Approach is to integrate CRUD layer capability into CTF
  - Addition of simple CRUD model into CTF - L3:PHI.VCS.P9.01 (Sept 2014)
  - FY15 work will be to replace simple model with MAMBA and to add the CTF+MAMBA capability to the core simulator to couple with neutronics
- CILC requires modeling detailed spatial CRUD deposition on the fuel rod to simulate localized CRUD deposits
  - Approach is to develop integrated surface chemistry capability in Hydra-TH
  - Coupling of MAMBA and HYDRA-TH - L2:MPO.P9.02 (Sept 2014)





VERA Releases

- VERA has been released to Test Stands for deployment on non-CASL computers and to RSICC for further distribution
- Release process developed first with Westinghouse Test Stand and then improved through subsequent releases
- On track for full release including all VERA components in Nov. 2014



VERA Release Process

Release	Date of Release	Associated Milestone
2012 Limited Beta Release	September 2012	L2:VRI.P5.02
Westinghouse Test Stand	June 2013	L3:VRI.VERA.P7.02
2013 RSICC Release	December 2013	L1:CASL.P7.04; L3:PHI.REL.P8.02
EPRI Test Stand	December 2013	L2:PHI.P8.01
2014 RSICC Release	November 2014 (planned)	L2:PHI.P9.02
VERA-EDU	Q2 FY2015 (planned)	L3:EC.P8.06

VERA Accomplishments

- A mature infrastructure to support development has been established
  - Continuous integration and test system
  - Kanban-based agile development process
  - Repository syncing
  - An exercised release process
- CASL physics components have increased capabilities
- CASL physics components have been integrated into the VERA infrastructure
- Coupling of physics components is well underway for core simulator and challenge problem coupling
- VERA is being used to support applications in AMA and Test Stands and VUQ studies

VERA is Ready for Phase 2!

Questions?

A DOE Energy Innovation Hub

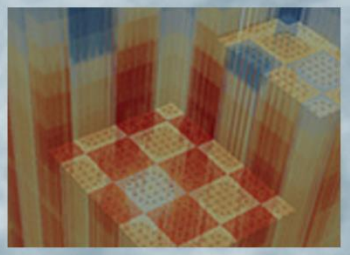
Radiation Transport Methods (RTM)

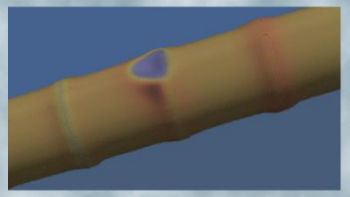
Joint Science Council & Industry Council Meeting

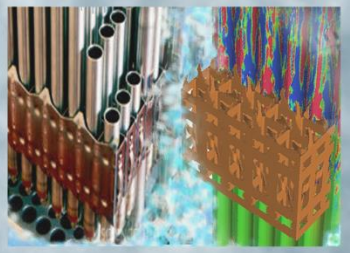
ORNL 9-9-14

Bill Martin, Lead

Tom Evans, Deputy Lead







U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Outline of talk

- RTM: overall summary
- Brief descriptions of key neutronics modules
- RTM: Year 4 Projects and Budget
- Status and progress of Year 4 milestones
- Response to 2013 DOE Review Comments
- Summary of June 2014 RTM Workshop
- An example of risk management, mitigation, and resolution
- Overall Phase 1 Progress
- Phase 2 Plans
- Background Slides

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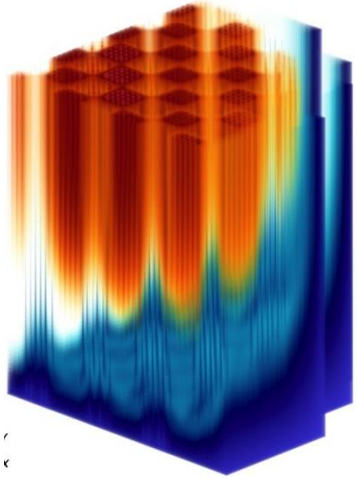
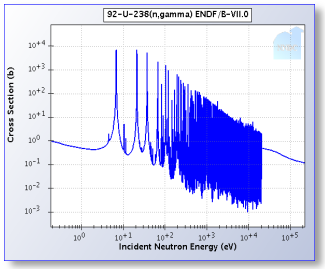
RTM Vision Statement

Objectives and Strategies

- Objective: Deliver next-generation, non-proprietary, scalable radiation transport simulation tools to VERA, incorporating the latest VUQ technologies
- Strategy: develop and deploy deterministic and Monte Carlo methodologies for 3D pin-resolved transport with coupled multiphysics capability





Requirements Drivers

- Challenge problems require pin-resolved (radial, azimuthal, and axial) 3D full-core transport with depletion and TH feedback
- Accommodate tight coupling to subchannel, CFD, structural analysis, and fuel performance models
- Integrated within VERA and VERA-CS and used with coupled physics modules or as standalone neutronics module

Outcomes and Impact

- Outcomes:
  - Development of validated deterministic and stochastic radiation transport modules for VERA to support reactor analysis with multiphysics coupling
  - Publication and dissemination of new methods that will enhance the state-of-the-art of reactor neutronics
- Impact:
  - Provides radiation transport capability to address all CASL Challenge Problems
  - Advance state of the art in computational radiation transport
  - Contribute to other DOE/NNSA needs/missions

RTM Team

- **University of Michigan**
  - Reactor physics
  - Transient and multiphysics coupling
  - Deterministic and Monte Carlo transport methods
  - Co-developers of MPACT
- **Oak Ridge National Laboratory**
  - Reactor physics
  - Deterministic and Monte Carlo transport methods
  - Linear/nonlinear solvers
  - Multigroup and CE physics
  - Co-developers of MPACT
  - Developers of Shift/Insilico
- **MIT**
  - Monte Carlo transport methods
  - Doppler-broadening of CE data
  - Reactor physics/SC
- **North Carolina State**
  - Linear/nonlinear solvers
  - Multiphysics coupling

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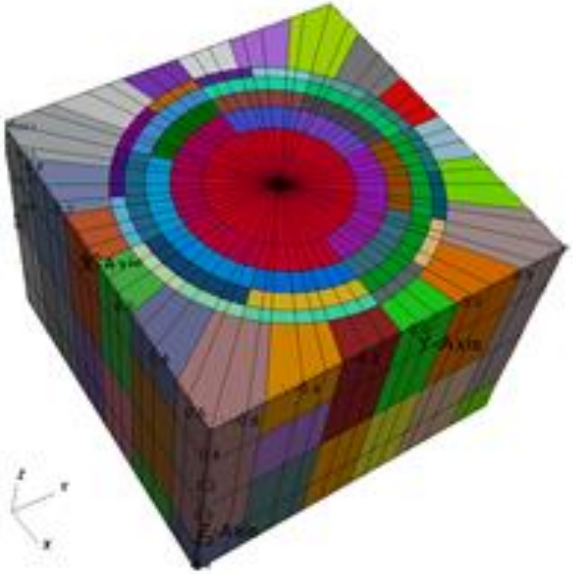
Pin-Resolved Neutronics - MPACT

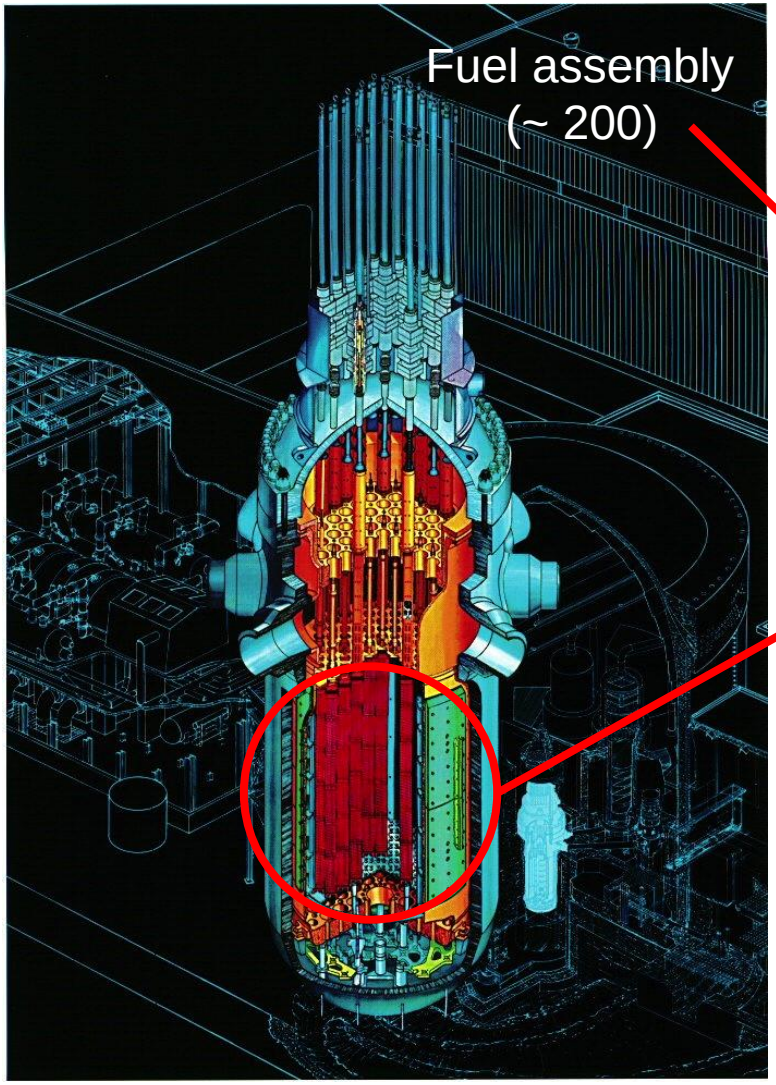
- Completed 2D/1D solver and resolved accuracy/convergence issues with refined axial mesh by developing and implementing a theory
- Completed initial coupling to COBRA-TF for single assembly and demonstrated full core TH feedback capability with internal TH
- Demonstrated capability to deplete 2D full core and carrying out 3D depletion
- Developed 3D MOC within MPACT
- Performed initial transient demonstration
- Integrated the ORIGEN API for depletion
- Will leverage Insilico success with advanced solvers to speed up MPACT
- Uses common VERA I/O (VERAIN, VERAOUT)



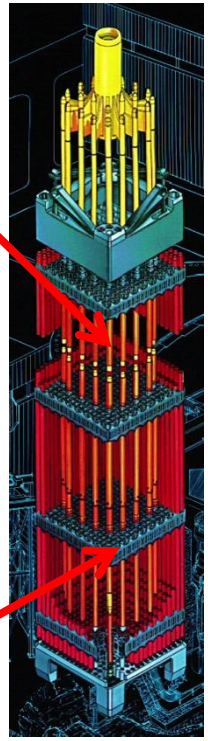
"Pin-resolved transport" illustrated for a pin cell. Radial, azimuthal, and axial resolution of a fuel pin and surrounding clad/moderator regions with MPACT.

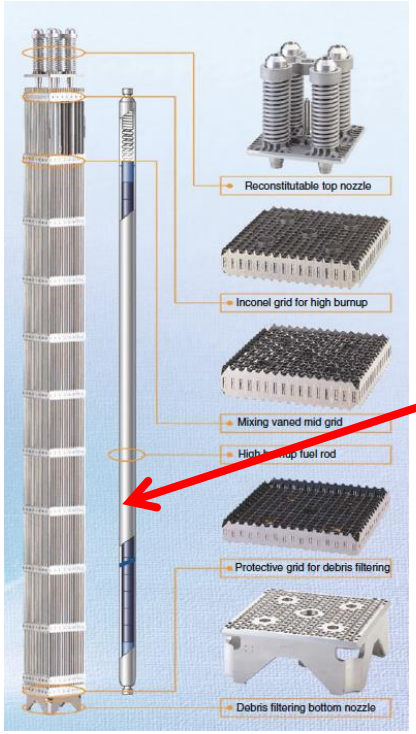
MPACT is providing accurate and reliable pin-resolved neutronics for engineering analysis

The nuclear reactor has over 40,000 fuel pins that need to be individually modeled with high resolution

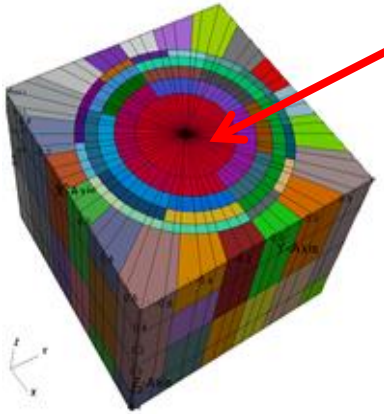


Nuclear reactor core (PWR)



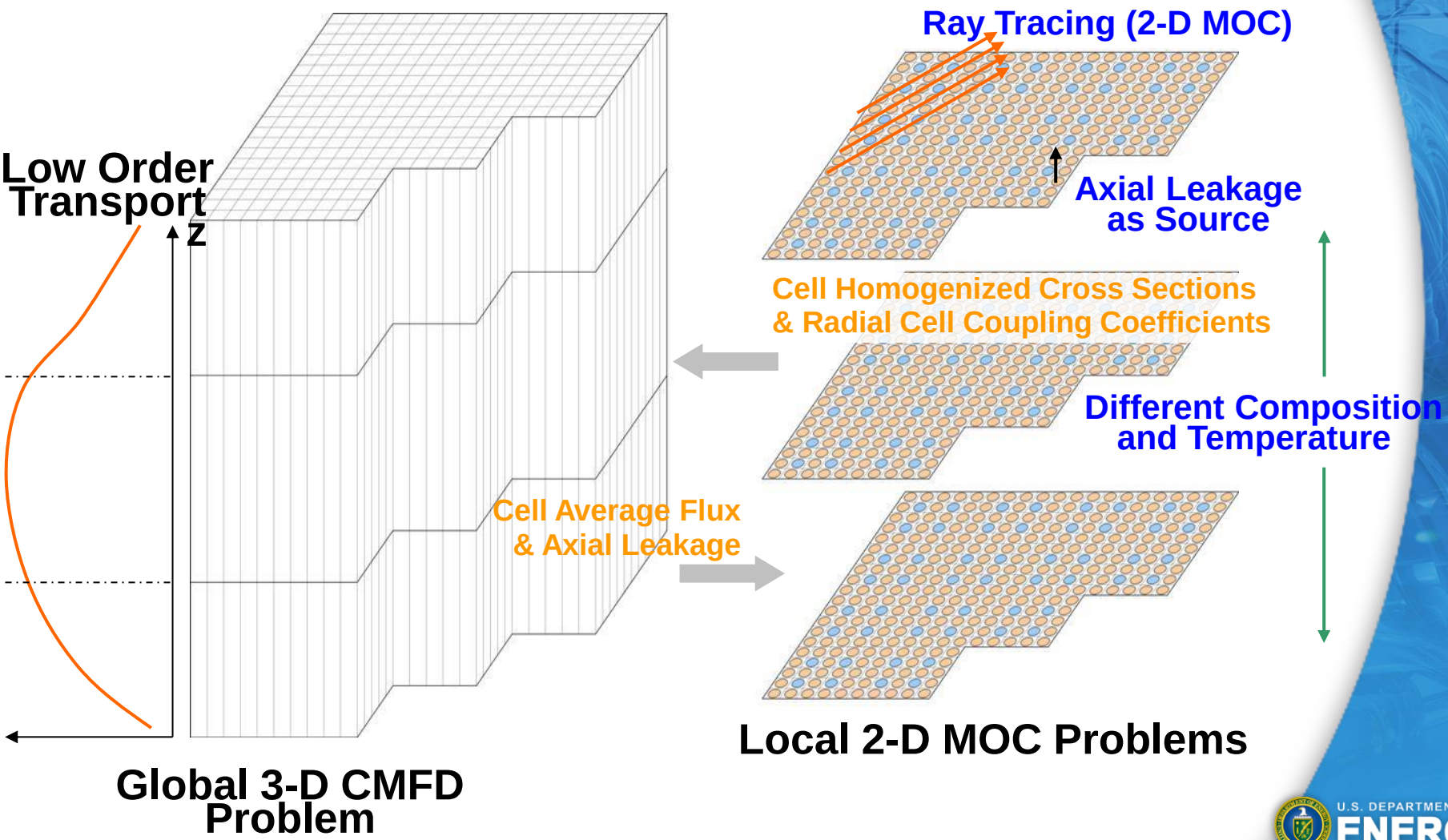


Fuel pin
(~ 40,000)



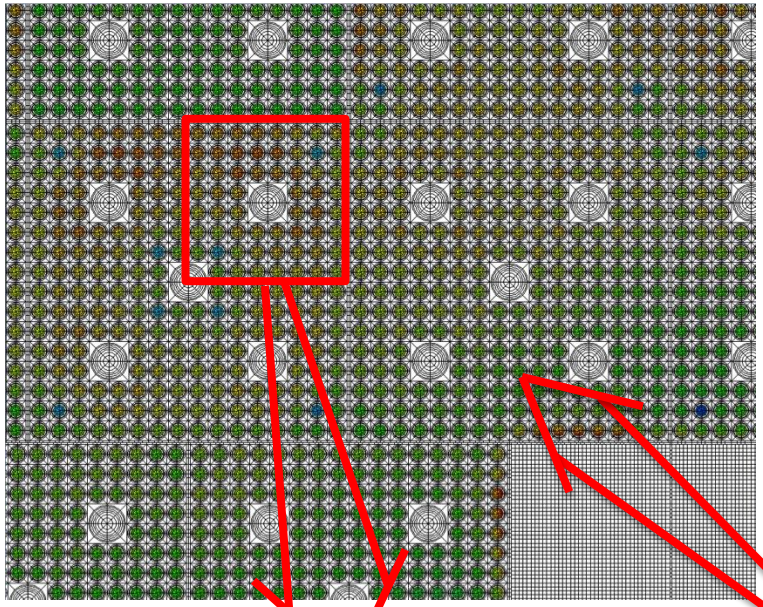
"Pin-resolved transport" illustrated for a pin cell. Radial, azimuthal, and axial resolution of a fuel pin cell with MPACT.

2D/1D Full Core Transport Methodology

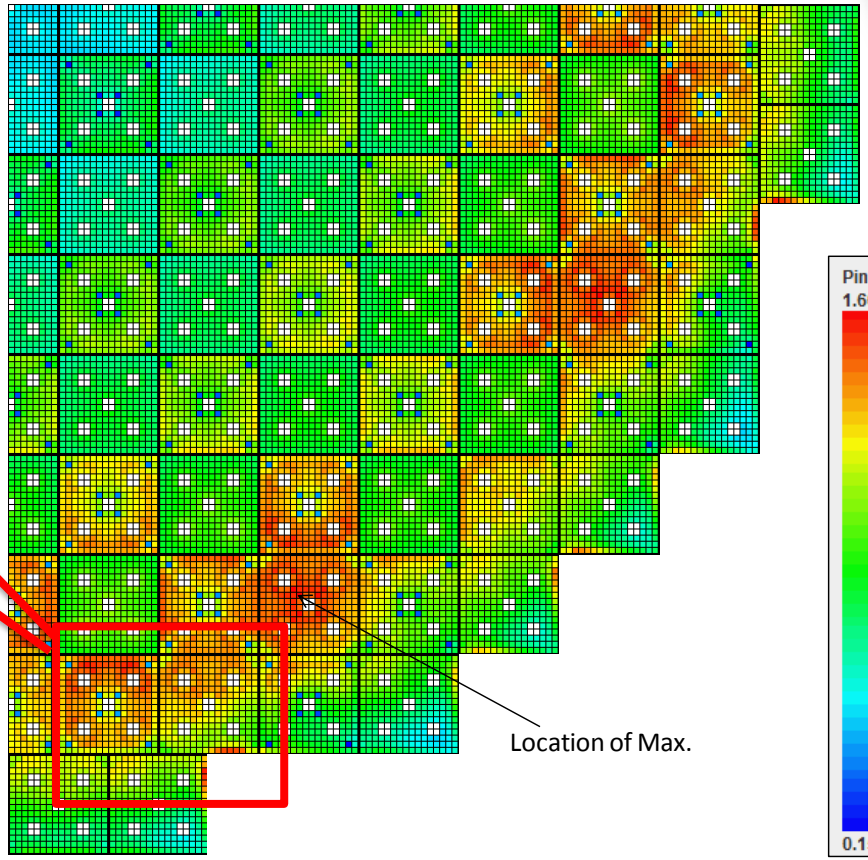


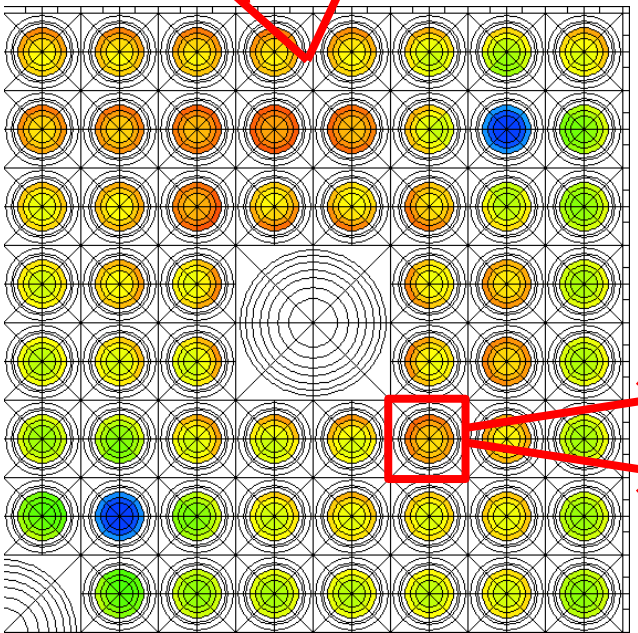
Coupled CFD/Pin-resolved transport (2D)

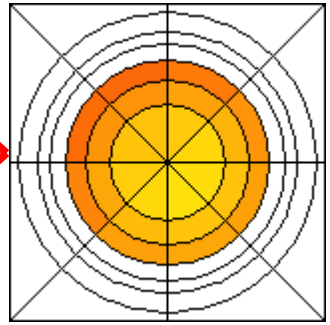
Progression from ¼ Core to Resolved Fuel Pin



¼ core







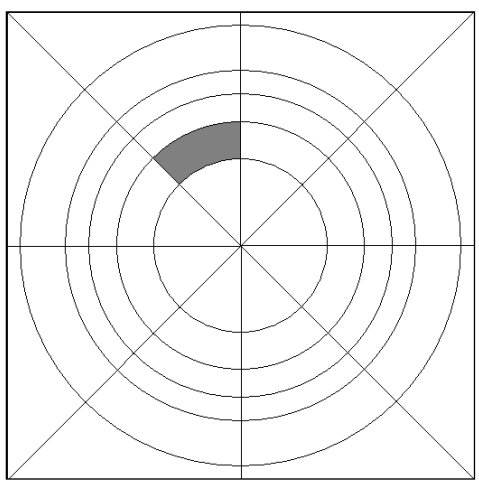
"Pin-resolved" with coarse radial mesh (20 rings may be needed)

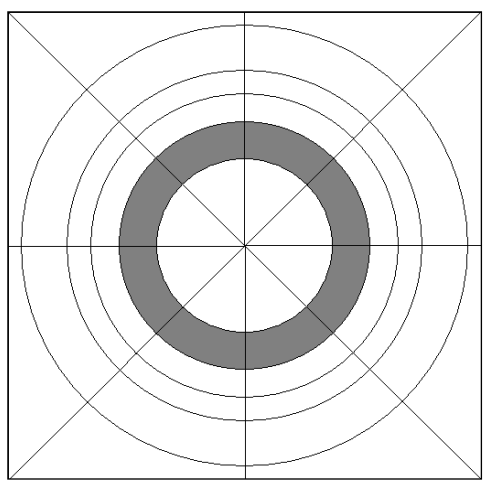
Depletion Methodology

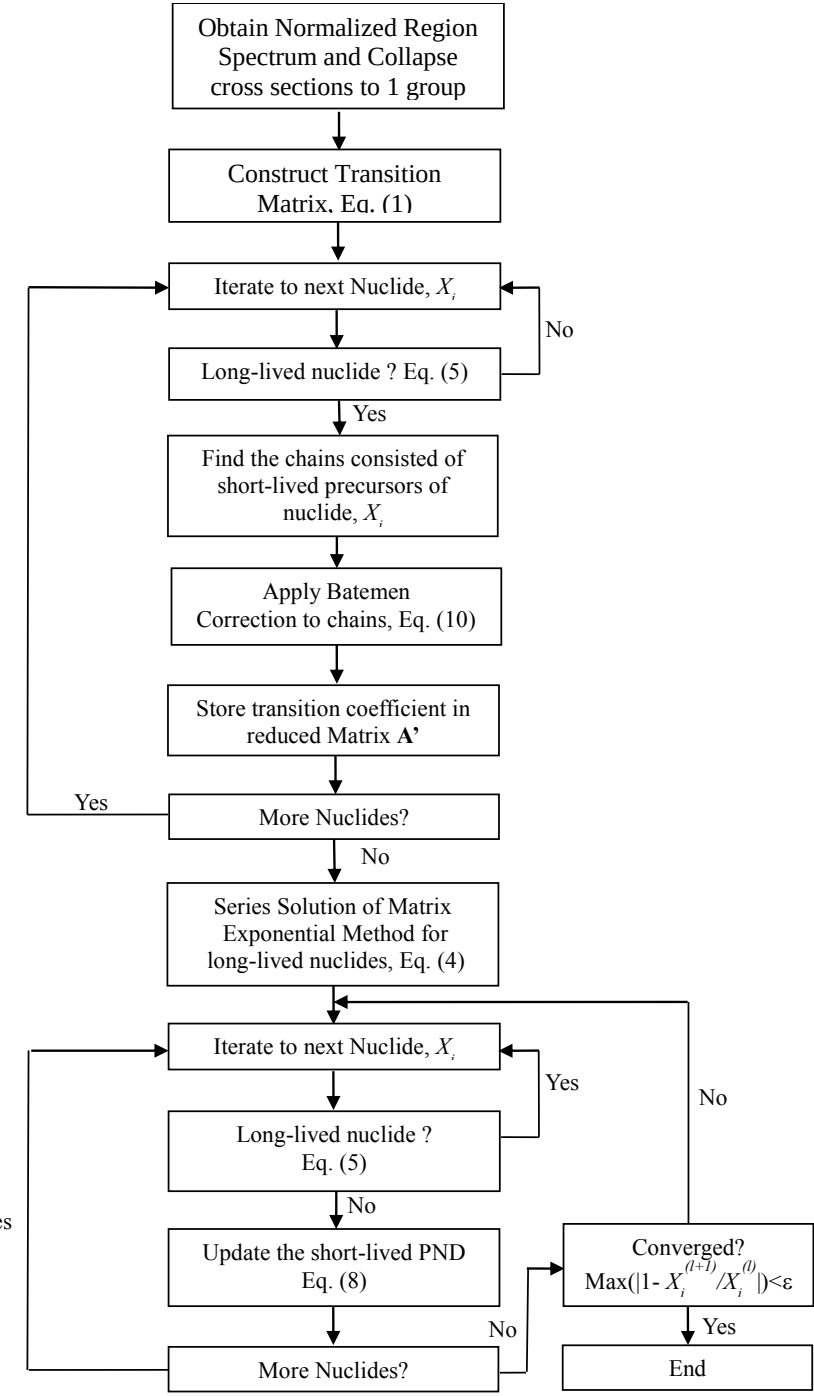
$$\frac{dX_i(t)}{dt} = \sum_{j=1}^{N} \ell_{ij}\lambda_j X_j + \bar{\varphi}\sum_{k=1}^{N} f_{ik}\sigma_k X_k - (\lambda_i + \sigma_i\bar{\varphi})X_i$$

$$\vec{X}(t) = \exp(\mathbf{A}t)\cdot\vec{X}(0)$$

- Exponential matrix is broken into two components; short lived and long lived
- Nuclides are tracked on a different mesh than transport





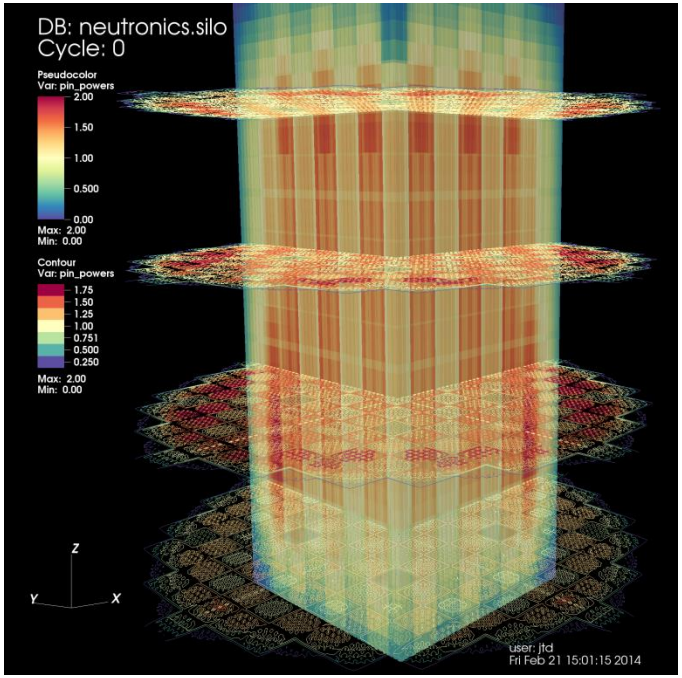


MPACT development effort planned and underway (UM and ORNL)

- Capability
  - Transient capability including multiphysics coupling
  - Allow BOC at arbitrary cycle with knowledge of isotopics
- Performance
  - Address memory usage
  - Optimize steady state iteration scheme
    - More efficient solvers (take advantage of Insilico success)
    - Runtime improvements in subgroup calculation
  - Optimize coupled TH iteration scheme
- Cross section development
  - ENDF/B7.1
  - Improved multigroup MPACT library
  - Incorporate extended ESSM (embedded self-shielding method) into MPACT
    - Accounts for radial variation of fuel cross sections and temperatures
    - Accounts for resonance interference

Monte Carlo Neutronics - Shift

- Integrated Shift into Insilico so that it automatically runs through VERA
  - Common I/O
- Integrated and optimized SCALE CE physics
- Implemented a *O(1)* tally system in arbitrary number of bins
- Integrated and testing depletion
- Fully operational in multiple parallel modes
  - Domain replication
  - Domain decomposition w/overlap
  - Multiple sets
  - Nearest-neighbor, scalable fission bank communication
- FW-CADIS and hybrid infrastructure in place
- **Benchmarking validation** against B&W 1484 and 1810 experiments and Watts Bar startup data



Shift simulation of WEC AP1000 core

Shift is available to provide benchmarking/validation for core-simulator neutronics

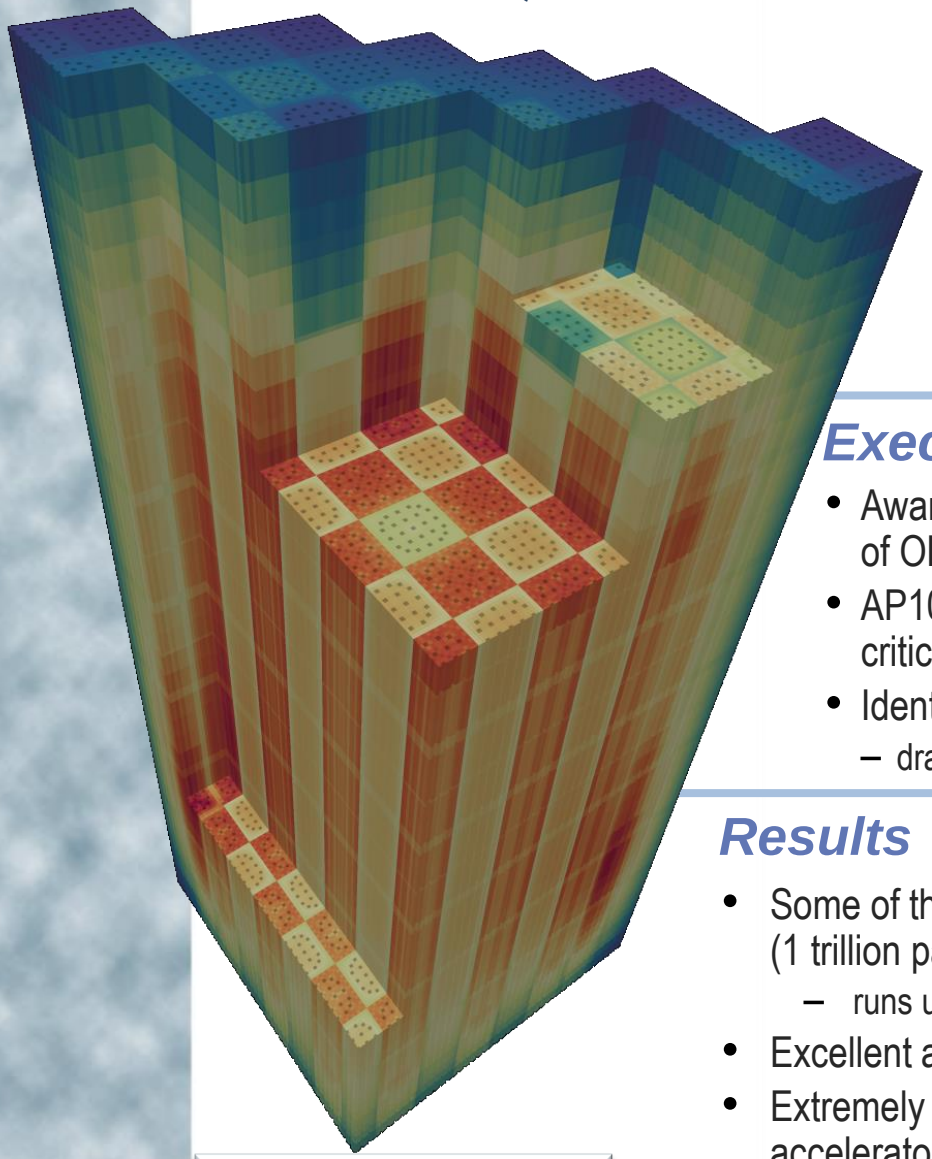
Shift Validation – B&W 1810 Lattice Critical Experiments

Core	Shift Gad Worth Error		OpenMC Gad Worth Error	
	(Boron ppm)	%	(Boron ppm)	%
III	-3.5	3.5	6.3	6.4
V	-5.3	4.1	4.8	3.7
Va	-6.1	4.2	4.5	3.0
Vb	-5.1	3.9	5.1	3.9
VII	-5.1	4.0	5.0	3.9
VIII	-4.7	2.8	6.1	3.6
XIV	3.6	1.5	-1.0	0.4
XVI	4.0	1.3	-0.6	0.2
XIX	4.9	3.3	-2.2	1.5
XX	4.6	1.7	-0.4	0.2

Validation of Shift using experimental data and comparison with OpenMC (MIT) – collaborative effort suggested by K. Smith during RTM 2013 Workshop

Evaluation of Shift: VERA Continuous-Energy Monte Carlo Capability

Quarter-Core Zero Power Physics Test



AP1000 pin powers

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 OLCF-3 Early Science program
- AP1000 model created and results generated for reactor criticality, rod worth, and reactivity coefficients
- Identical VERA Input models used for Shift, SP_N, and S_N
  - dramatically simpler than KENO-VI input model

Results

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

Shift and Early Science

- Preliminary testing demonstrates remarkable agreement between Shift and KENO-VI, except:
  - ~1% radial tilt for quarter core cases
  - Fission rate uncertainties too low
- OLCF granted CASL 60M core-hours for AP1000® ZPPT: (note max difference = 25 pcm)

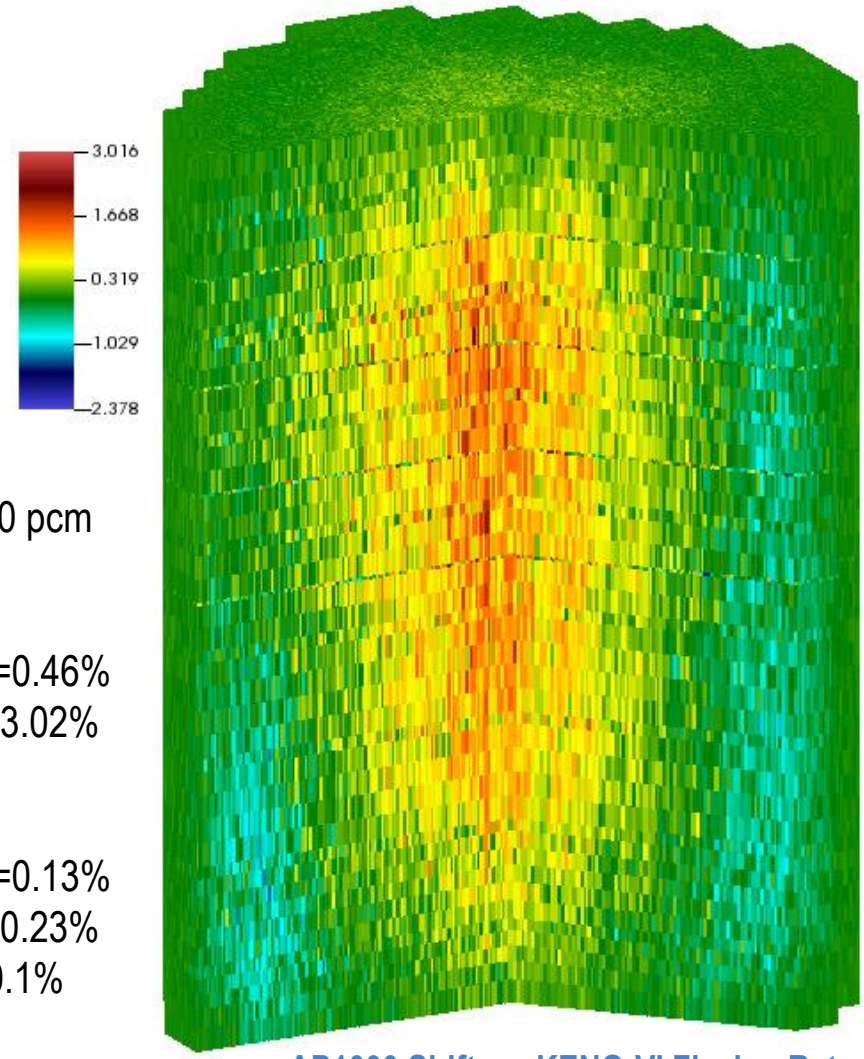
ID	KENO-VI	SHIFT	Diff (pcm)
ARO	1.000870	1.001030	**16**
DBW	1.003240	1.003450	**21**
MA	0.998258	0.998414	**16**
MB	0.998669	0.998909	**24**
MC	0.998956	0.999148	**19**
MD	0.998496	0.998643	**15**
M1	0.994350	0.994548	**20**
M2	0.992001	0.992185	**18**
AO	0.984609	0.984749	**14**
S1	0.990103	0.990200	**10**
S2	0.989935	0.990183	**25**
S3	0.989650	0.989739	**9**
S4	0.995055	0.995295	**24**
Average			**18**
St. Dev.			**5**

Δρ=50 pcm

Total:
RMS=0.46%
Max=3.02%

Axial:
RMS=0.13%
Max=0.23%
AO=0.1%

Radial:
RMS=0.38%
Max=1.15%



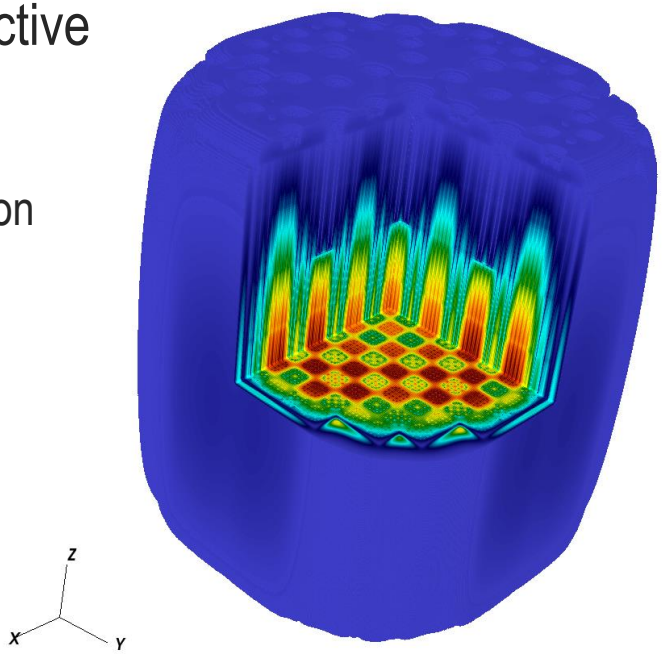
AP1000 Shift vs. KENO-VI Fission Rates

1 Trillion particles
240,000 cores
~ 3 hours
25M core-hours used

Avg σ ≈ 0.1%
Max σ ≈ 0.4%

Homogenized-Pin Neutronics – Insilico

- Alternative neutronics capability – no active development planned at this time
- Fully integrated advanced eigensolvers
  - Multigrid-preconditioned generalized Davidson
- Validated 1D pin-cell cross section generation models
- Full VERA integration
  - Automated meshing
  - Homogenization
  - I/O
- Multiple transport schemes
  - Discrete ordinates (SN)
  - Simplified Spherical Harmonics (SPN)
- Validated against Watts Bar startup data
- Excellent comparison with Shift on AP1000 (WEC)



Insilico-SPN simulation of HZP Watts Bar 1

Insilico provides a low-order, quick-running core-simulator capability

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- Status and progress of Year 4 milestones
- Response to 2013 DOE Review Comments
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- An example of risk management, mitigation, and resolution
- Overall Phase 1 Progress
- Phase 2 Plans
- Background Slides

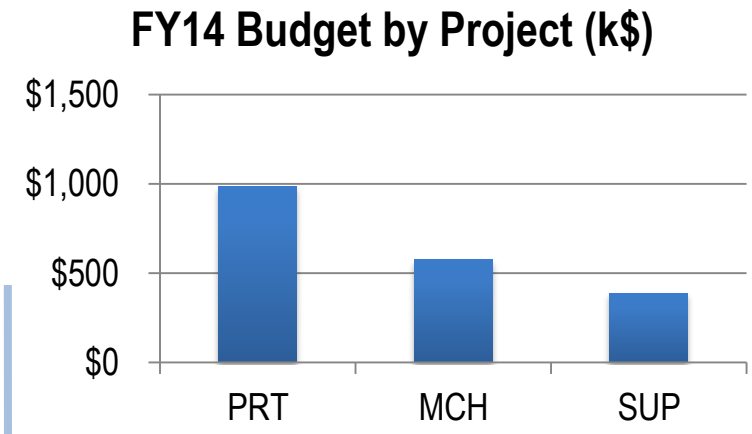
RTM Summary – Year 4

Oct 2013 – Oct 2014 (FY14)

Projects

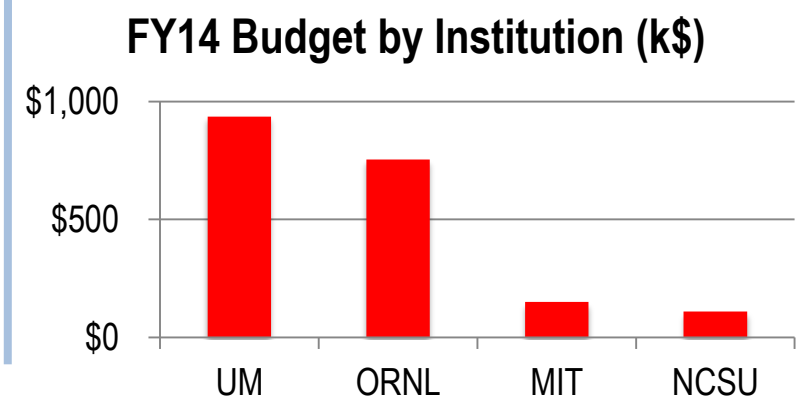
- **PRT** (Pin-resolved transport) - Develop 3D, full-core, pin-resolved deterministic transport capability (MPACT) with depletion (Origen) and TH feedback (CTF).
- **MCH** (Monte Carlo/Hybrid) - Develop efficient full-core hybrid Monte Carlo capability (Shift).
- **SUP** (Supporting Methodologies) - Generate multigroup (SCALE/ESSM) cross sections for MPACT and Insilico; develop transient capability for MPACT, continue V&V/UQ of MPACT, Insilico, and Shift.

RTM FY14 Budget - $1950k



Challenges

- Size and complexity of methods for 3D full-core pin-resolved transport with depletion and TH feedback.
- Sufficient human resources ($ and expertise) to develop new methods, fix old methods, maintain codes, write user manuals, and carry out V&V/UQ.
- Sufficient computing resources to allow development, debugging, and analysis of large 3D geometries.
- Improve code performance to allow use on industry-class clusters.



RTM projects – Year 4

- **Pin-resolved transport (PRT)**
  - MPACT development including coupling and depletion (UM + ORNL)
  - Insilico development (ORNL)
  - Improved 2D/1D axial model (UM)
  - 2D/3D method (UM + ORNL)
- **Monte Carlo / Hybrid (MCH)**
  - Shift development (ORNL)
  - Monte Carlo methods: OTF Doppler, data decomposition (ORNL + MIT + UM)
  - Hybrid methods: FW-CADIS, FMC, CMFD, and fission matrix (ORNL + MIT + UM)
- **Supporting Methodologies (SUP)**
  - Transient capability (UM)
  - Advanced coupling strategies (NCSU)
  - XS/Depletion (UM + ORNL)
  - ESSM (UM + ORNL)

RTM has done very well during Year 4 in meeting L1 / L2 / L3 milestones related to these projects …

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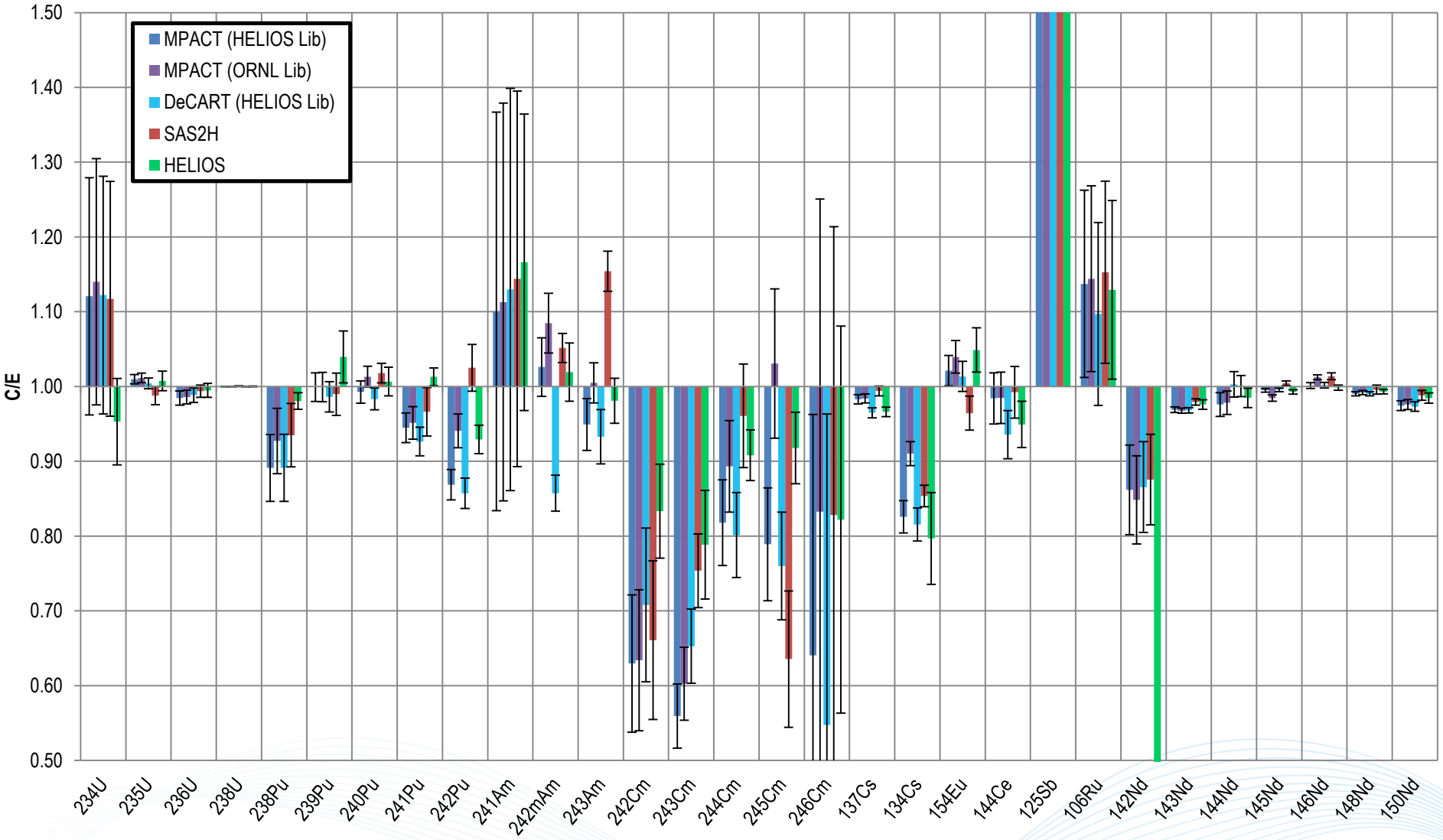
L1:CASL.P9.04 – Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback (# 917)

- DOE Reportable FY14.CASL.011 due 9/30/14
- Dependencies
  - 3D depletion with TH feedback (# 940)
  - Detector modeling, restart, and shuffling (# 944)
  - Restart (necessary due to machine constraints) - implemented in June (no ticket)
- Completion Criteria
  - The EOC1 power distribution and burnup distribution will be predicted for the specified cycle length and power history
  - Sufficient information will be provided to allow an assessment of the accuracy of the EOC1 power distribution when compared with **measured plant data**
- **Current status: on schedule to satisfy the milestone.**

L2.RTM.P8.01 – Demonstration of Advanced Pin-Resolved Depletion with MPACT (# 912) – Due 12/31/13

- Develop Code Features
  - Point Depletion based on ORIGEN Methodology (not ORIGEN code)
  - Predictor-Corrector Time Stepping Methodology
  - Addition of critical boron search for core follow calculation
- Verify Solution
  - Comparisons to computation benchmark does well for HELIOS library
  - Comparisons to **experimental benchmark** does well for both cross-section libraries
  - 2D core depletion agrees well compared to WEC methods
- **Completed on-time**
- **Selected results follow**

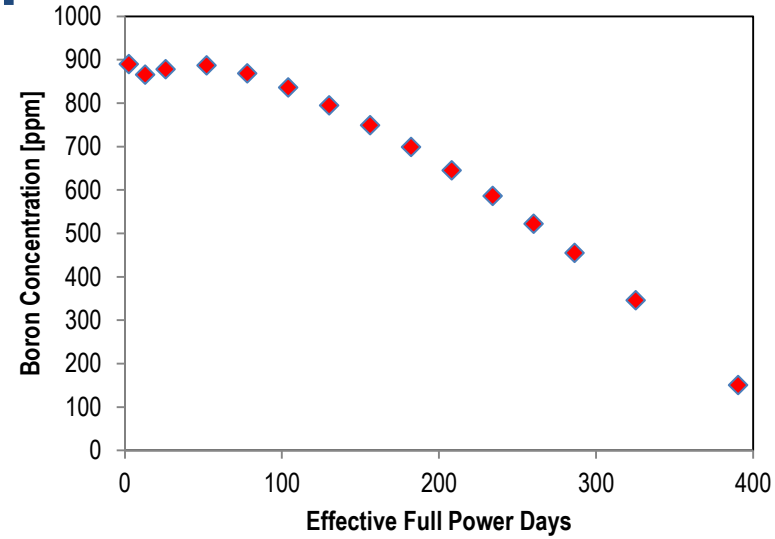
MPACT Validation - Takahama 3 Assay Data

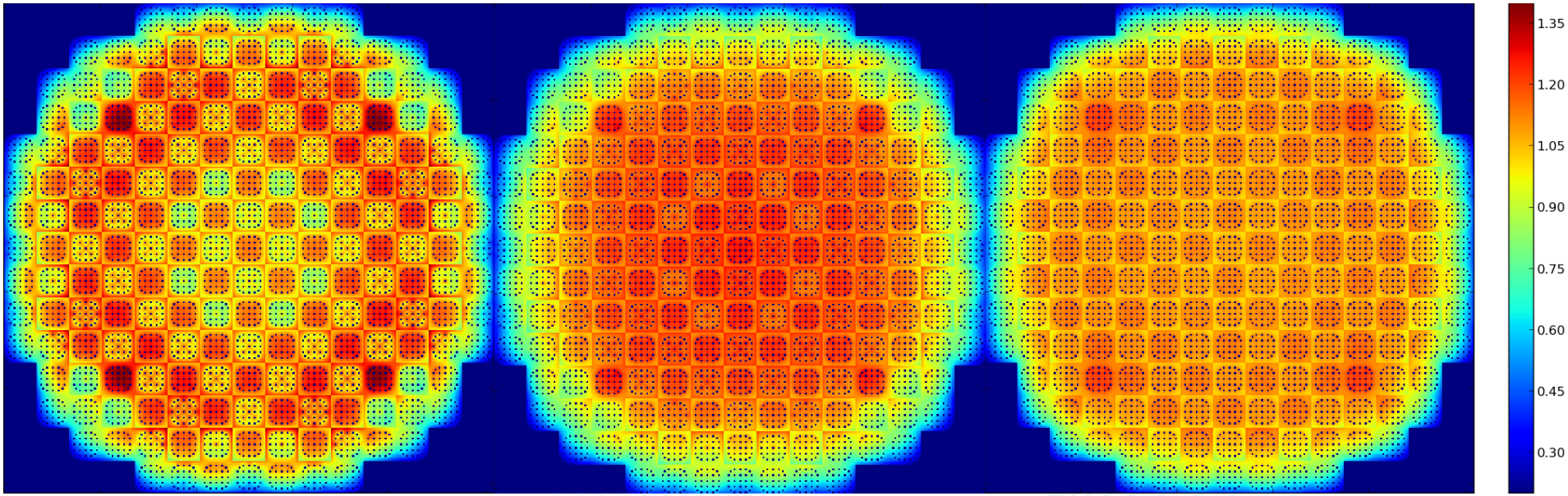


MPACT 2D depletion validated against experimental data

MPACT Validation - 2D Core Depletion

- 2D slice of Watts Bar Core was used at approximate core average temperature and density
- Boron search was used to make reactor critical
- Keff bias estimated for 2D core and used throughout cycle



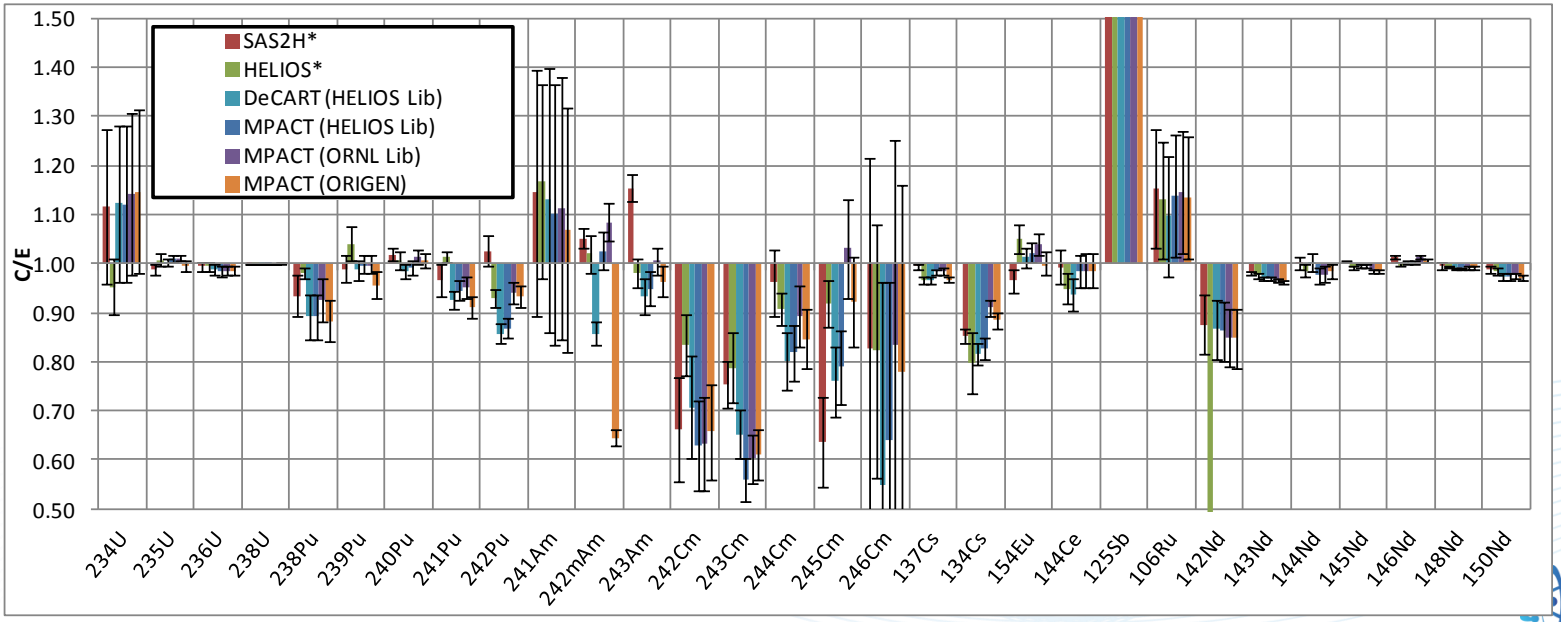


RTM.SUP.P9.03 - ORIGEN Integration in MPACT (# 941) – due 6/30/14

- In reactor applications, depletion of the fuel is a necessary capability.
  - ORIGEN has a long history of being applied to depletion problems and is extensively validated and is the industry-standard for depletion
  - MPACT has an existing depletion capability, but does not have a large validation base
- By integrating ORIGEN into MPACT we provide a better validated depletion capability
  - ORIGEN also has additional capability to compute decay heat and gamma sources
- Initial verification/validation compared to 2 benchmarks
  - Takahama-3 spent fuel isotopics
  - JAERI benchmark on Reactor Physics analysis of next generation LWR fuels
- Completed on-time
- Selected results follow

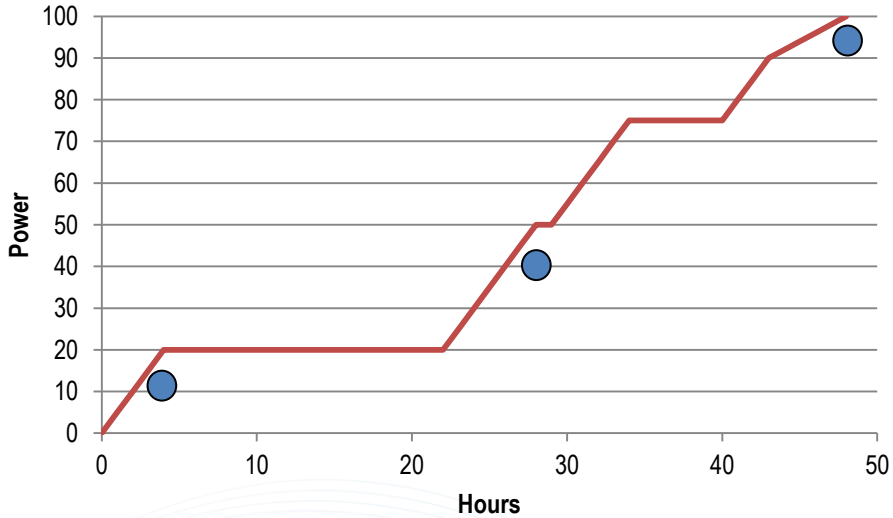
Selected Results for Initial Verification/Validation of MPACT+ORIGEN

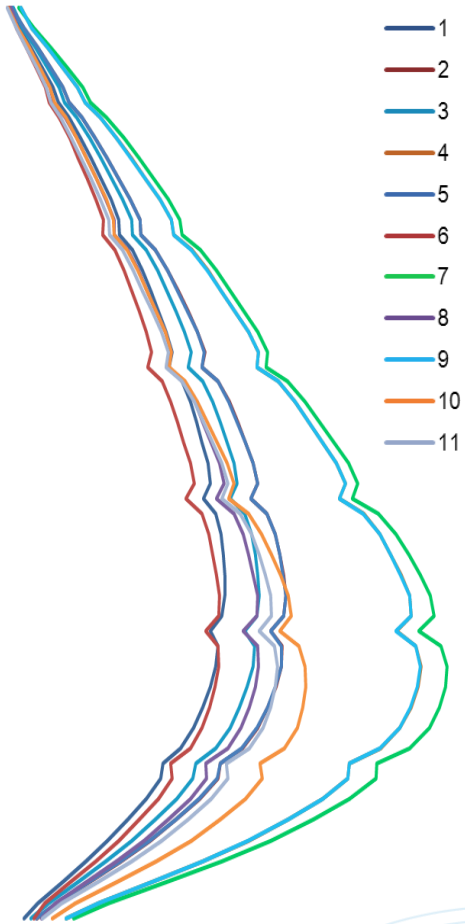
- Takahama-3 benchmark has PIE data and numerical results.
  - Fuel operated for 3 cycles in Takahama PWR reactor.
- ORIGEN results are consistent with other codes compared to experimentally measured values.
- Numerical and measured values are generally in good agreement.
- Poor agreement is seen for some fission products (Sb-125) and higher actinides (Cm) consistently by all codes.



RTM.PRT.P9.03 – Demonstration of Reactor Startup Flux Maps with MPACT (aka AMA #8) – due 4/30/14 (# 944)

- Simulate hour long time steps
  - Track important isotopes such as Xe during startup
  - Semi-predictor-corrector scheme
- Determine Incore Detector Response
- Move control rods between states



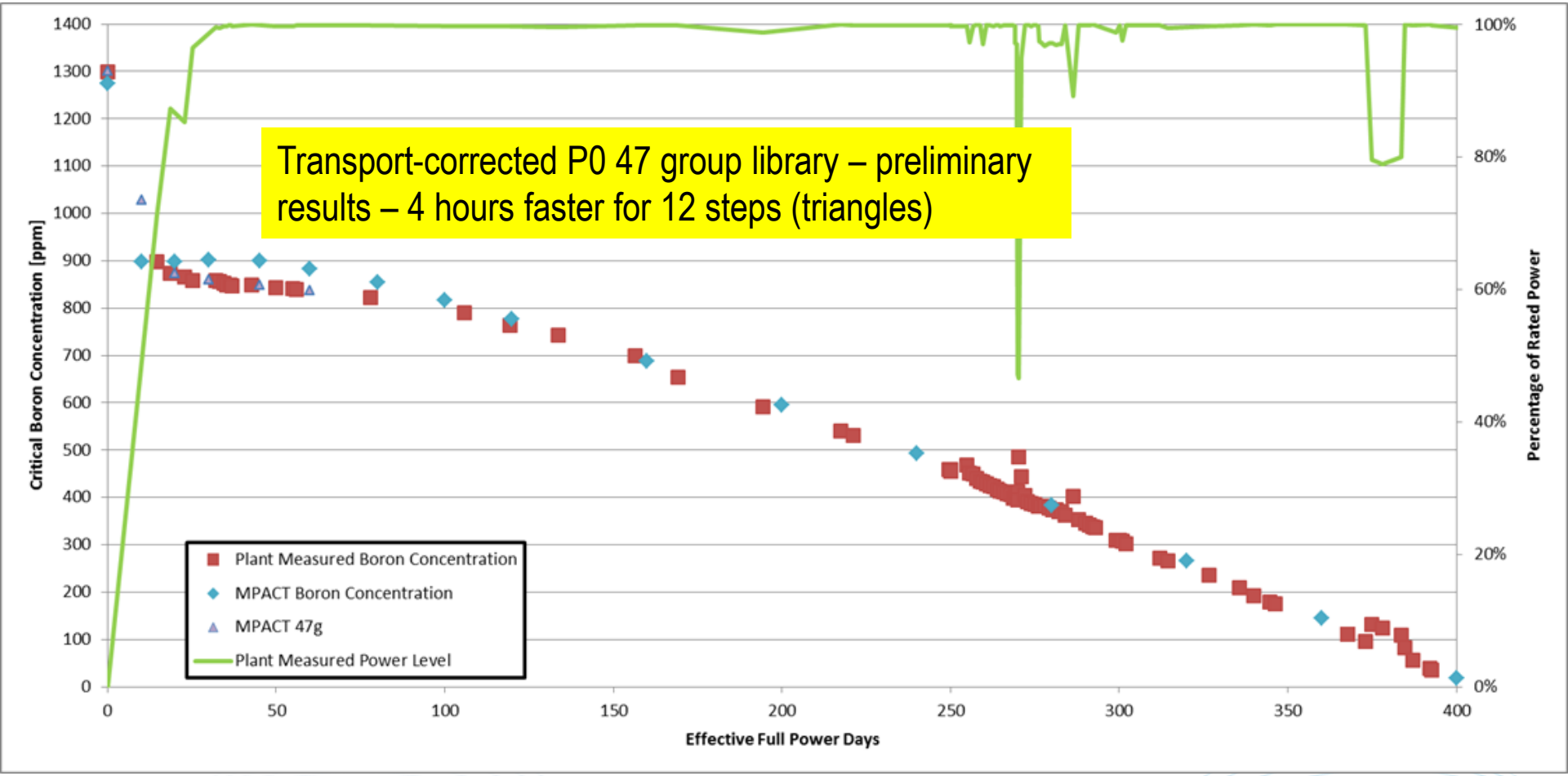


- Status – delayed due to complexity of modeling detectors and focus on completing AMA #9. Completion expected in August.

RTM.PRT.P9.01 – Analysis of AMA Benchmark Problem #9 with MPACT (# 940) – due 7/31/14

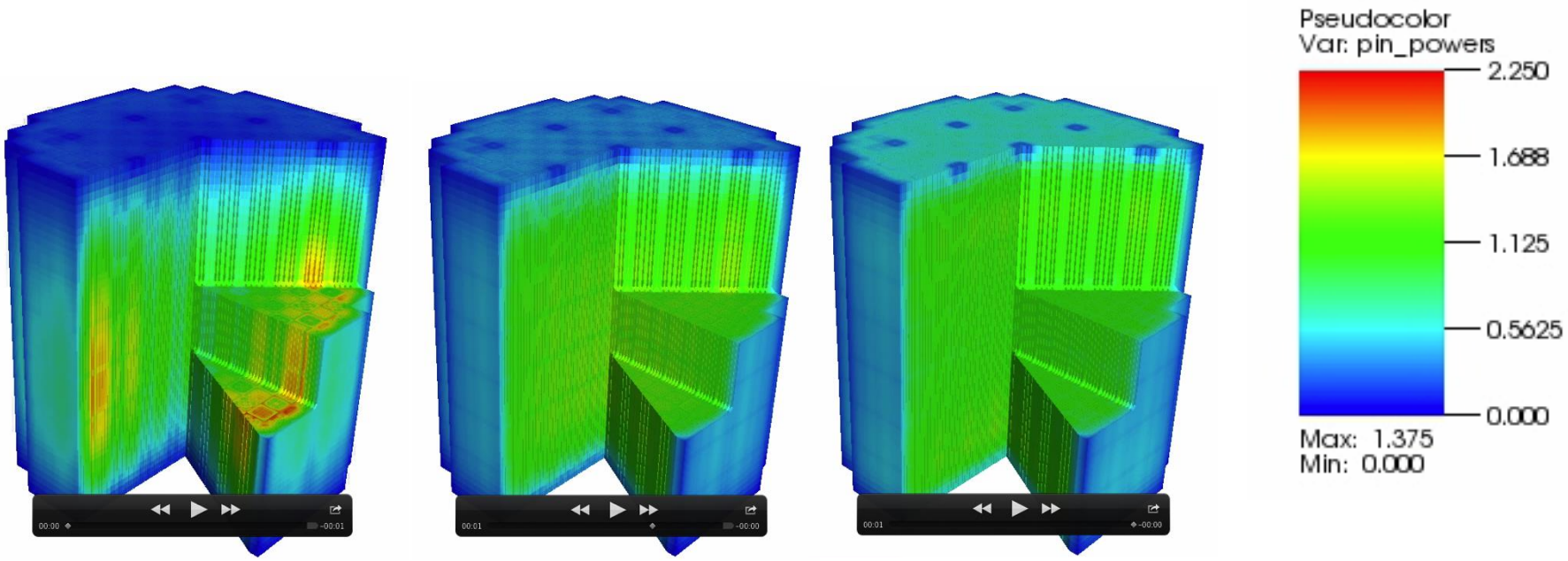
- Simulation of Watts Bar Cycle 1 was performed with MPACT at 100% power for 400 Effective Full Power Days (EFPD)
  - Escalation to full power was neglected
  - Neglected other down-powers and outages
  - Neglected coast down at end of life
- P0 scattering was used for increased speed.
  - BOC tests showed critical boron concentration was not very sensitive to isotropic scattering approximation.
  - Enhanced cross-section library will allow for stable transport correction or memory improvements will allow for P1 or P2 scattering.
- Run on EOS on 2096 cores for 21 hr 18 min
  - Critical boron search (results on next slide)
  - Internal TH feedback (assembly axial energy balance without cross-flow + 1D fuel temperature)
- **Status – essentially complete; report is being prepared**

Boron rundown thru 240 EFPD using new 47 group library from Kang Seog Kim



Shows the importance of cross sections

Predicted power distributions during Watts Bar Cycle 1



BOC1 **MOC1** **EOC1**

Plant Data

- Cycle length ~ 440 EFPD with a power coast down after 20% power reduction at 400 EFPD
- Plant measured boron concentration at 400 days = 11 ppm

Predictions

- Predicted boron concentration at 400 days = 18 ppm
- Have yet to model the 20% power reduction or power coast down.
- Improvements could be made to the startup power behavior and boron-10 depletion.
- Note: this is with internal T/H – still need to do CTF coupling

Performance on L3 milestones has been very good

#	Milestone ID	Due	Description	Status
938*	L3:RTM.SUP.P8.02	4/30/14	Development of transient capability for MPACT	Completed
939*	L3:RTM.SUP.P9.01	4/30/14	Extension of ESSM to treat multiple temp-dep fuel regions and resonance interference	Completed
944*#	L3:RTM.PRT.P9.03	4/30/14	Analysis of AMA Benchmark #8	Delayed
941*#	L3:RTM.SUP.P9.03	6/30/14	Development of API to allow MPACT depletion with Origen	Completed
940#	L3:RTM.PRT.P9.02	7/31/14	Analysis of AMA Benchmark #9	Completed
971	L3:RTM.PRT.P9.04	9/30/14	Analysis of AMA Benchmark #10	On schedule

*Milestone Report provided to Review Team

#Brief summary follows

Brief summaries of L3 milestone efforts (#) follow ….

Progress on MPACT milestones shows maturation of pin-resolved transport capability during Year 4

Completed milestones:

- **L2:RTM:P6.01** – Application of MPACT 2D/1D to AMA #5 (Watts Bar HZP with measured data): **11/13 (LATE)**
- **L2.RTM.P8.01** – Advanced Pin-Resolved Depletion with MPACT: **12/13**
- **L3:RTM.SUP.P9.01** – Extension of ESSM to treat multiple temp-dep fuel regions and resonance interference: **4/14**
- **L3:RTM.SUP.P8.02** – Development of transient capability for MPACT: **4/14**
- **L3:RTM.SUP.P9.03** – API to allow MPACT depletion with Origen: **6/14**
- **L3:RTM.PRT.P9.02** – Analysis of AMA Benchmark #9: **8/14**

Underway and on schedule:

- **L3:RTM.PRT.P9.04** – Analysis of AMA Benchmark #10: **11/14 (delayed due to L1)**
- **L1:CASL.P9.04** – Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback (full-core pin-resolved): **9/14**

Delayed but completion expected soon:

- **L3:RTM.PRT.P9.03** – Reactor startup flux maps (AMA #8)

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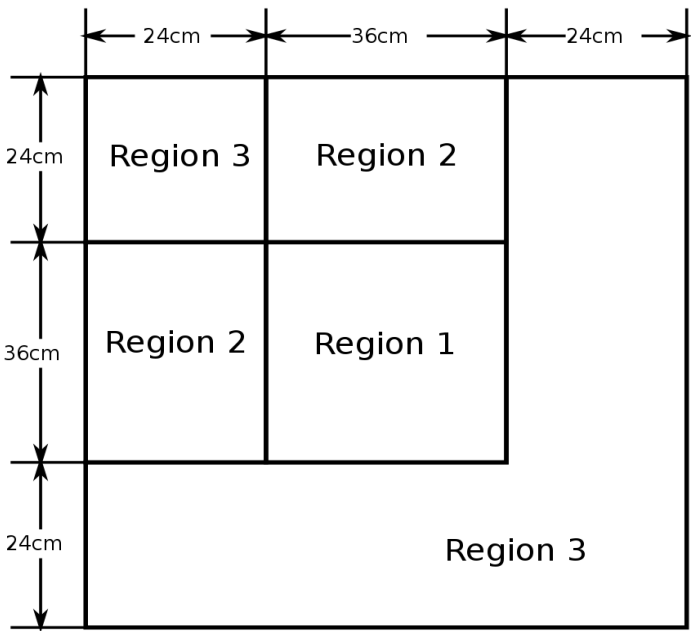
Resolution of RTM-related Findings from 2013 DOE Annual Review

- **Finding # 3**

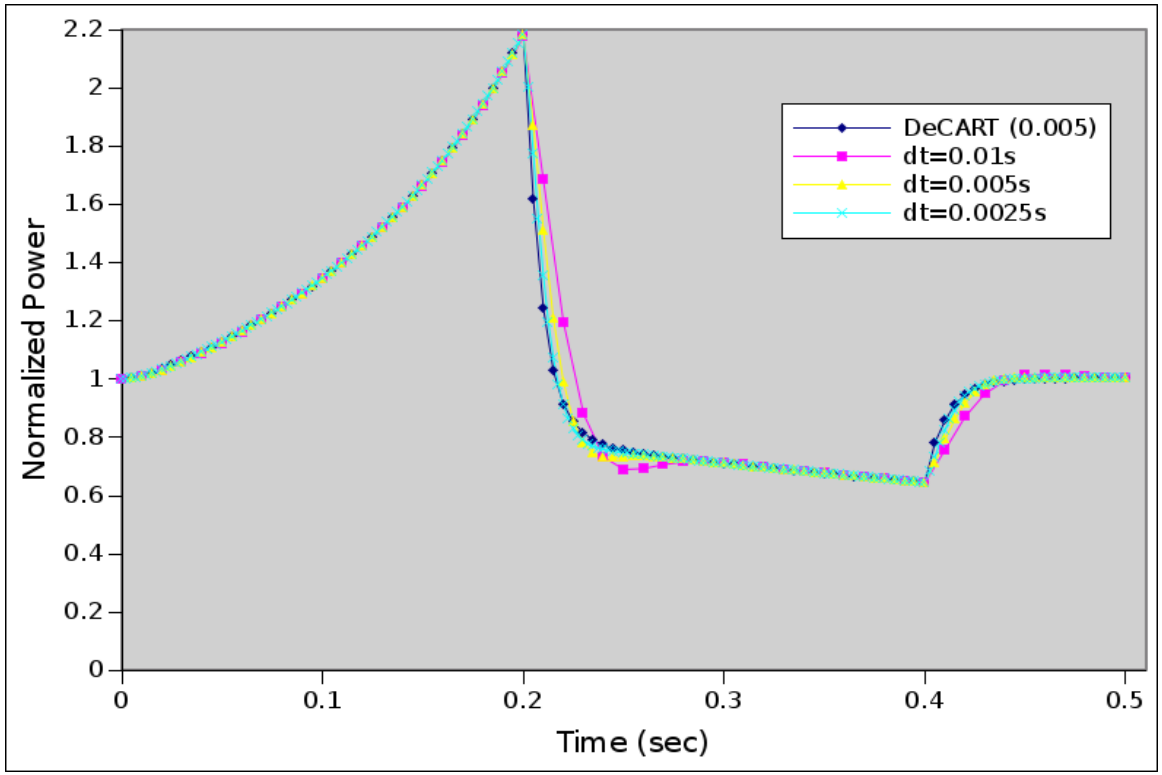
While the current focus in VERA is on creating simulations of the quasi-steady state of a reactor, it is not clear whether or not this approach will be sufficient to capture fast transient behaviors as seen in reactor accident conditions.

- **Resolution –** L3 and L4 milestones drive MPACT development
  - **L3:RTM.SUP.P8.02**: Development of transient methods in MPACT
    - The transient methodology in MPACT solves the transient fixed source problem on the MOC mesh rather than on the coarse finite difference mesh which was used in DeCART (and used successfully to analyze an RIA event for EPRI).
    - MPACT has been verified against the TWIGL benchmark, which is a computational benchmark with a specified cross section change.
    - Validation of the MPACT transient methodology is underway with the SPERT reactor power excursion test in 1958.
    - Selected TWIGL and SPERT results follow.
  - **L4:RTM.SUP.P9.03**: Assess capability of MPACT to perform a RIA (on schedule for 9/30 completion)

MPACT Transient Verification - TWIGL benchmark



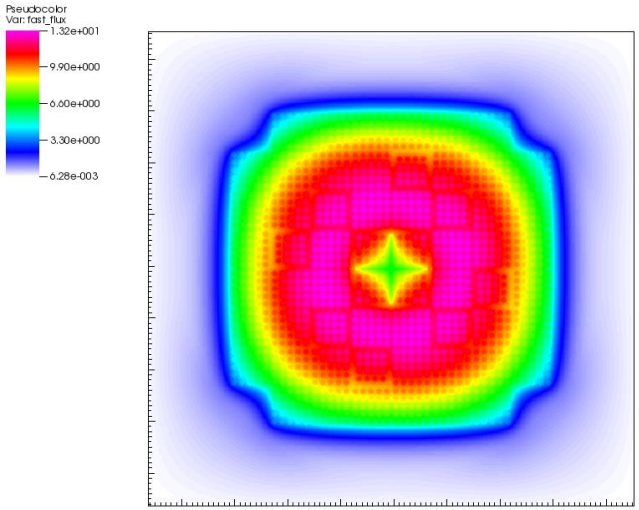
Time (sec)	Perturbation
0.0 -> 0.2	Ramp: 1 -> 4
0.2	Step: 5
0.2 -> 0.4	Ramp: 5 -> 6
0.4	Step: 1

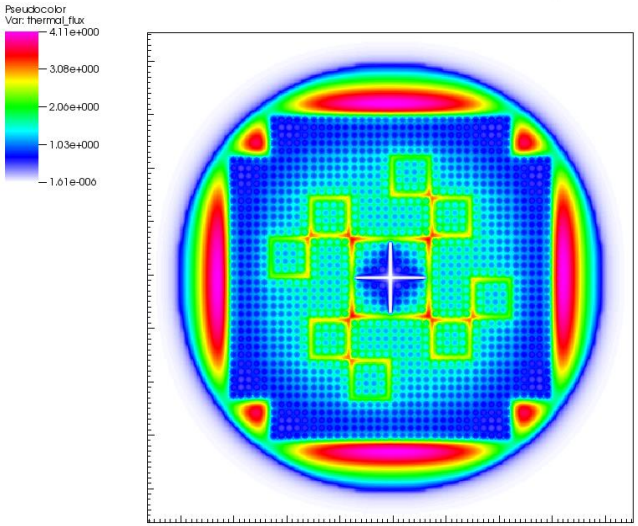


MPACT Discretization

- 0.03 cm ray spacing
- 4 azimuthal angles
- 2 polar angles

MPACT Validation - SPERT steady-state results





- **Discretization: MOC w/ 0.05 cm ray spacing,16 azimuthal angles, 4 polar angles, 20 axial planes with NEM kernel**
- **Xsecs: ORNL 56g library (P2 scattering)**
- **MPACT execution time: ~ 1 hour on 720 cores**

Comparison of Critical Condition w/ KENO-CE

Case	Temp (F)	Control rod Position (cm)	MPACT	KENO-CE
CZP	70	36.957	0.99411	0.99999 ±0.00082
HZP	550	71.755	0.99690	1.00242 ±0.00079

Comparison of Critical Rod Positions

Case	Temp (F)	Experiment	MPACT	S3K	PARCS
CZP	70	36.957	38.2	30.1	31.6
HZP	550	71.755	74.4	-	46.3

Preliminary results: transient results for SPERT Test 86

- Discretization: 16x less angular resolution than steady-state run; P0 scattering (vs P2)
- MPACT execution time: ~ 3 h for 100 time steps on 720 cores (~ 30 s /time step)
- Reasonable results given inaccurate initial conditions (keff ~ 1.04)

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RTM PI Workshop at ORNL June 14

- **Purpose**: annual meeting of the RTM PIs, research staff, and students to discuss status of RTM projects and Phase 2 plans – 4th RTM workshop
- **Attendance**
  - 37 total with 22 attendees at the ORNL meeting
  - 15 virtual attendees from MIT, UM, NC State, and WEC
  - CASL leadership (Doug Kothe and Paul Turinsky)
  - Science Council member (Kord Smith)
  - PHI Focus Area (Jess Gehin, Scott Palmtag, and others)
- **Agenda**
  - 17 technical talks
  - Phase 2 discussions
    - RTM capability development needs
    - BWR modeling and simulation challenges

RTM PI Workshop - Agenda

8:00	**Coffee and pastries**	
8:15	Bill Martin	Overview of RTM Focus Area
RTM Methods and Milestones		
8:30	Blake Kelley*	Improved 2D/1D
8:50	Ed Larsen*	Hybrid Monte Carlo
9:10	Yuxuan Liu*	Extended ESSM
9:30	Steve Hamilton	Advanced eigenvalue solvers
9:50	Ben Collins	2D/3D
10:10	**BREAK**	
10:30	Alex Toth	Advanced coupling methods
10:50	Tom Downar*	Transient capability
11:10	Tara Pandya	Shift analysis of B&W criticals
11:30	Ben Forget*	Data decomposition
11:50	Brendan Kochunas	MPACT milestones: AMA #7, Origen API, and status of AMA #10
12:20	**Lunch in cafeteria (no host)**	
1:00	Dmitriy Anistratov*	Advanced homogenization
1:20	Ben Collins	MPACT milestones: AMA #8 and status of AMA #9
1:50	Seth Johnson	Insilico/Shift development: selected milestones
RTM/PHI Coordination of Effort		
2:20	Scott Palmtag	VERA-CS Overview and PHI Responsibilities
2:40	Andrew Godfrey	VERA-CS Applications and Testing
3:00	**BREAK**	
3:20	Andrew Godfrey	Shift Early Science AP1000 Simulations
3:40	Kang Seog Kim	VERA-CS Development Plan for MPACT
RTM Plans for Phase 2		
4:00	Bill Martin	CASL L1 milestones + RTM L2 milestones
4:10	Tom Downar* , Brendan Kochunas, Ben Collins	This is a group discussion regarding the implications and challenges for RTM capability development given the Phase 2 milestones. It will be kicked off with a short presentation regarding where MPACT stands with regards to addressing BWR challenges noted by Kord Smith in his recent report to CASL following the PHI meeting.
5:30	**Adjourn (no host dinner TBD)**	

*** Via Vidyo**

RTM PI Workshop - Photos

RTM PI Workshop – Key Outcomes

- Interesting and important progress being made on a number of research and development projects
- RTM is on track to complete remaining Phase 1 milestones including 9/30/14 DOE reportable (full core depletion with TH feedback)
- Joint development effort between institutions (UM and ORNL) and between Focus Areas (RTM and PHI) for MPACT development is working very well
- Several MPACT modifications have been identified that should allow speedups by 3-5x
- Important to limit scope of BWR analysis effort in Phase 2
- Kord Smith submitted many candid and insightful comments regarding RTM projects that we are taking into consideration

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L2:RTM:P6.01 – Application of MPACT 2D/1D to AMA #5 (Watts Bar HZP with measured data) – due 3/27/13

An example of Risk + Mitigation + Cooperative Resolution

- MPACT had a core flux/power tilt that gave poor results for Watts Bar HZP compared with CE KENO predictions.
- ~ 5 experienced reactor analysts (Tom Downar's team) at UM were unable to find the problem. It happened in 2D as well as 3D. A number of possible causes were eliminated such as ENDF library difference, reflector cross sections, transport-corrected P0, etc.
- **Risk**: significant risk as full-core pin resolved capability is needed for essentially all the Challenge Problems as well as to meet an important AMA milestone that depended on the RTM L2.
- **Mitigation**: Since MPACT was pushing the state of the art in pin-resolved transport, this type of risk was anticipated and ORNL developed SPN in 3 months building upon the Sn Denovo framework to complete a related AMA milestone. The results were impressive, comparing very well with measured data. This resulted in an alternative VERA capability – Insilico SPN.
- **Cooperative resolution**: ORNL collaboration helped to identify and resolve the MPACT problems. The MPACT L2 was completed in November 2013, approximately 7 months late.

MPACT has proven to be an accurate and reliable core analysis tool. The next slide shows the MPACT results.

MPACT results ended up in good agreement with data

Criticality (pcm)

	KENO-VI†	Shift‡	MPACT
Initial	-67	-33	-144
ARO	-25	11	-98
D	-149	-113	-234
C	-153	-127	-255
B	-121	-85	-228
A	-177	-153	-275
SD	-160	-129	-267
SC	-159	-130	-262
SB	-125	-88	-222
SA	-155	-123	-267
Average	**-129**	**-97**	**-225**

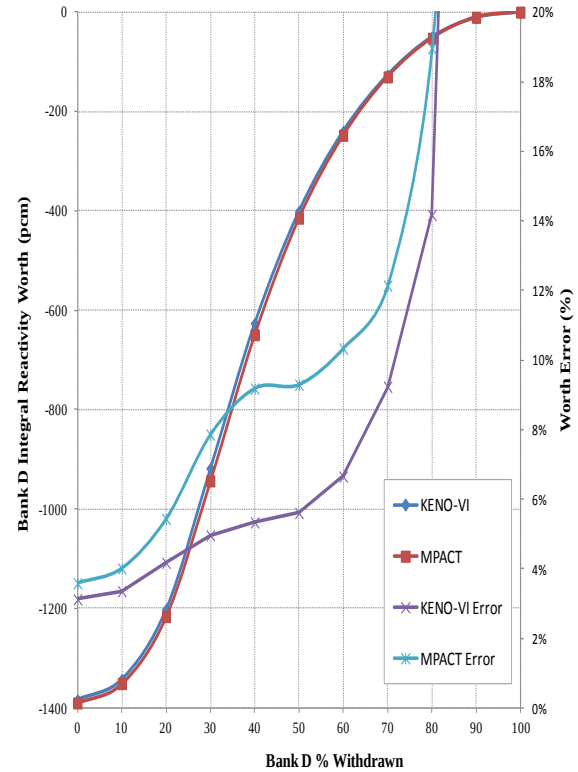
†KENO σ <= 1 pcm
‡Shift σ <= 6 pcm

Bank Worth Differences

Bank	Measured (pcm)	KENO-VI	Shift	MPACT
D	1342	3.3 ± 0.1%	3.4 ± 0.6%	3.6%
C	951	3.5 ± 0.1%	3.9 ± 0.9%	4.2%
B	879	-0.5 ± 0.2%	-0.8 ± 0.9%	1.2%
A	843	6.4 ± 0.2%	6.9 ± 1.0%	5.7%
SD	480	4.0 ± 0.4%	3.6 ± 1.7%	3.8%
SC	480	3.9 ± 0.4%	3.9 ± 1.7%	2.9%
SB	1056	1.0 ± 0.2%	1.1 ± 0.8%	1.4%
SA	435	2.6 ± 0.4%	1.3 ± 1.9%	3.9%
Total	**6467**	**2.9 ± 0.1%**	**2.9 ± 0.4%**	**3.3%**

*Meshes moved to match control rod tip

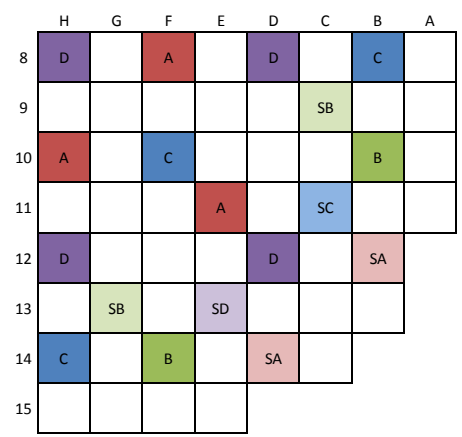
Bank D Integral Worth



Reactivity Coefficients

	Measured	KENO-VI	Shift	MPACT
Differential Boron Worth (pcm/ppm)	-10.77	0.56 ± 0.02	0.55 ± 0.07	**0.61**
Isothermal Temperature Coefficient (pcm/F)	-2.17	-1.01 ± 0.04	--	**-1.55**

*Doppler upscatter in KENO-VI worth an additional -66 pcm



Outline of talk

- RTM: overall summary
- Brief descriptions of key neutronics modules
- RTM: Year 4 Projects and Budget
- Status and progress of Year 4 milestones
- Response to 2013 DOE Review Comments
- Summary of June 2014 RTM Workshop
- An example of risk management, mitigation, and resolution
- **Overall Phase 1 Progress**
- Phase 2 Plans
- Background Slides

Phase 1 Progress – Overall

- The development of MPACT, Insilico, and Shift has been evolutionary with recent capability and achievements discussed in the Year 4 overheads, which in turn were built upon effort performed in Years 1 - 3.
- The following slides present a high level summary of RTM effort in Years 1 - 4.

RTM Progression in Years 1-4

- **Early Phase**
  - Lots of candidate codes
  - Lack of clear implementation strategy for incorporation of neutronics
  - Unclear roles between partners (working independently)
- **Middle Phase**
  - New strategy based on core-simulator begins to take shape
    - Multiple directions considered (2D/1D, SN, SPN)
    - Roles of partners still unclear
  - Attempts to use high-order SN fail
- **Current Phase**
  - Good partner collaboration on primary RTM CASL products
    - MPACT: shared ownership and collaboration between UM and ORNL
    - Shift: technologies developed in OpenMC at MIT have been integrated into Shift (ORNL)
  - Stable homogenized-pin core-simulator neutronics (Insilico-SPN)
    - Completed project (not under active development)
  - Pin-resolved deterministic neutronics (MPACT)
    - Primary vehicle for industry-class, core-simulator neutronics
  - Pin-resolved stochastic neutronics (Shift)
    - Primary vehicle for leadership-class neutronics

Collaboration between RTM partners is the big success in the current phase of CASL

RTM has met or exceeded the original Phase 1 milestones

RTM L2 Milestones (Table 2-12 in Original Proposal)

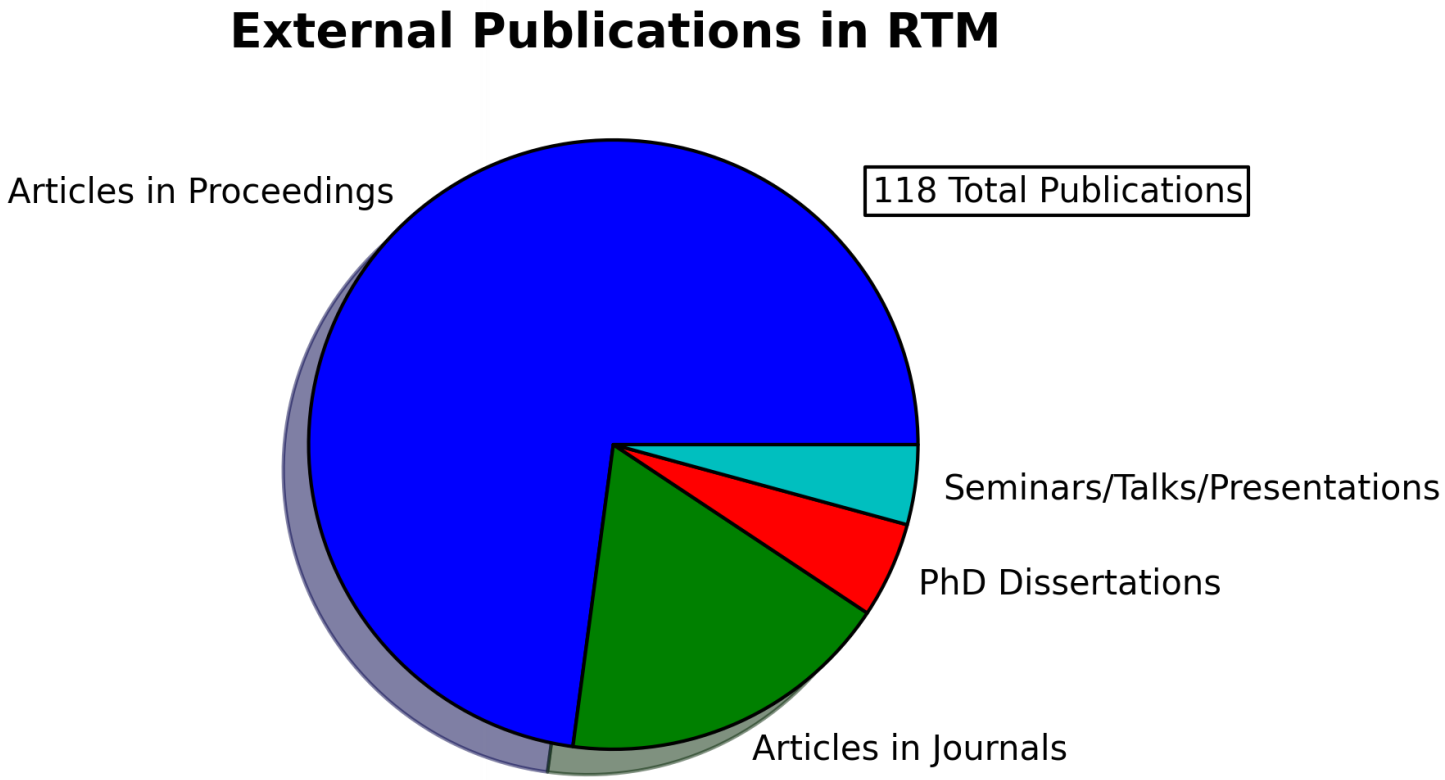
Challenge: Description	Yr	Outcome
Full-core 3D homogeneous cell deterministic transport capability with T-H coupling	2	Completed in Year 1 (pin-resolved: DeCART + Star-CD)
Full-core 3D pin-resolved deterministic transport capability	3	Completed in Year 3
Full-core 3D pin-resolved deterministic transport capability with T-H coupling	4	Completed in Year 4 (MPACT + CTF)
Full-core 3D domain-decomposition hybrid Monte Carlo transport capability	5	On schedule for early Year 5

Note: RTM was originally part of MNM, which split early in Phase 1 into the RTM and THM focus areas. The THM-related MNM L2 milestones are not shown here.

RTM has also delivered on the original RTM-related MNM L3 milestones

Year	L3 Milestones/Deliverables - Transport
1	1. Full-core pin-homogenized deterministic transport capability (✔) 2. Full-core 3D (2D/1D) coupled transport capability (✔) 3. Initiate evaluation of FW-CADIS and other candidate hybrid methods (✔) 4. Initiate domain-decomposition Monte Carlo code development (✔)
2	1. Improved 2D/1D coupled capability (✔) 2. Initiate unstructured mesh capability for 3D deterministic transport (✔) 3. Complete prototype domain-decomposition Monte Carlo code (✔) 4. Problem-dependent spectrum calculations and improved energy condensation schemes (✔)
3	1. Full-core 3D pin-resolved deterministic transport capability (✔) 2. Transient deterministic capability (✔) 3. Complete prototypic hybrid transport capability (✔) 4. Improved tally capabilities for Monte Carlo (✔)
4	1. Prototypic full-core 3D domain-decomposition hybrid Monte Carlo transport capability (✔) 2. Full-core 3D pin-resolved deterministic transport capability with T-H coupling (✔)
5	1. Improved full-core pin-resolved deterministic and hybrid Monte Carlo transport capabilities (✔) 2. Initiate advanced methods for Monte Carlo, deterministic transport and multiphysics codes for transformational changes in Years 6–10 (✔)

RTM Publications



Proceedings include refereed contributions only.

Discovery and Innovation

Innovation Target	CASL Innovation and Discoveries
✓ Hybrid Monte Carlo and deterministic transport methods with improved source convergence ✓ Optimized, portable, and extensible algorithms and software implementations for advanced architectures	• Theory exists for 3D converged/stable coupling of 2D planar MOC sweeps to 1D axial solvers. • ESSM yields accurate, inline calculation of core-level multigroup cross sections. • Multi-level energy partitioning yields scalable [O(100K) cores] discrete ordinates simulations on eigenvalue problems, and GPU-enabled sweep kernels can deliver further speedup (3-5x). • Angular collocation methods (S_N and MOC) exhibit much better convergence properties for k-eigenvalue problems with QR quadrature sets. • New cross-section extrapolation method for JFNK-coupled T/H + neutronics dramatically reduces compute requirements. • 1D on-the-fly cross section processing for pin-by-pin homogenized cross sections proves highly accurate on a wide class of problems when coupled to a low-order (SP_N) 3D solver. • Full core reactor core MC calculations on DOE HPC platforms can efficiently resolve pin-level detail resulting from several parallel algorithmic developments including tally servers; multiple-set/overlapping domain decomposition, and a scalable fission-bank rebalance algorithm. • Two new approaches for on-the-fly Doppler broadening have been developed to enable TH-coupled Monte Carlo reactor analysis including a multipole expansion method and a library-based approach.

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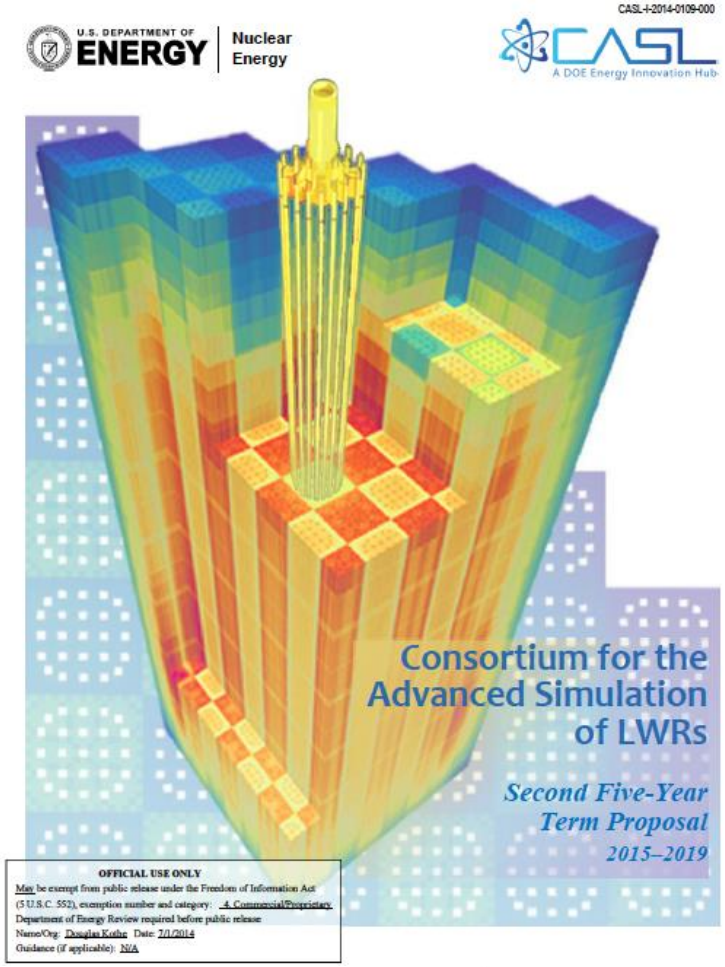
Phase 2 Plans



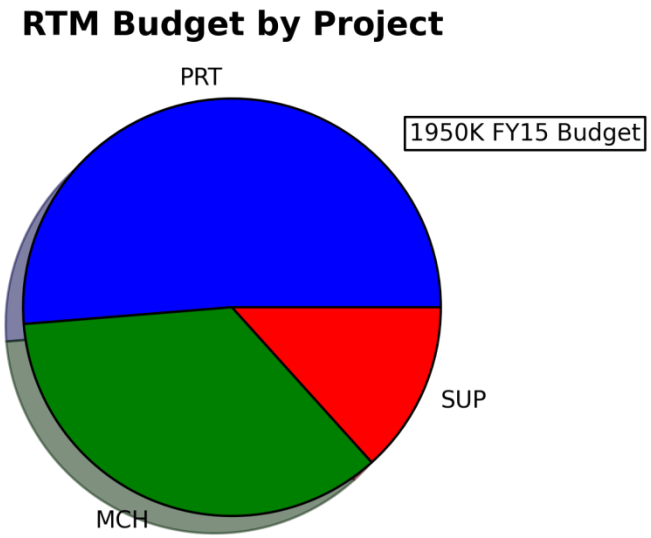
RTM Emphasis

- Broaden by extending methodology to BWRs and iPWRs
- Deepen by developing transient capability to model an RIA
- Optimize by improving computational performance.
- Emphasize V&V/UQ
- Develop high fidelity Monte Carlo benchmark tool for full core reactor simulation including TH feedback

RTM Phase 2

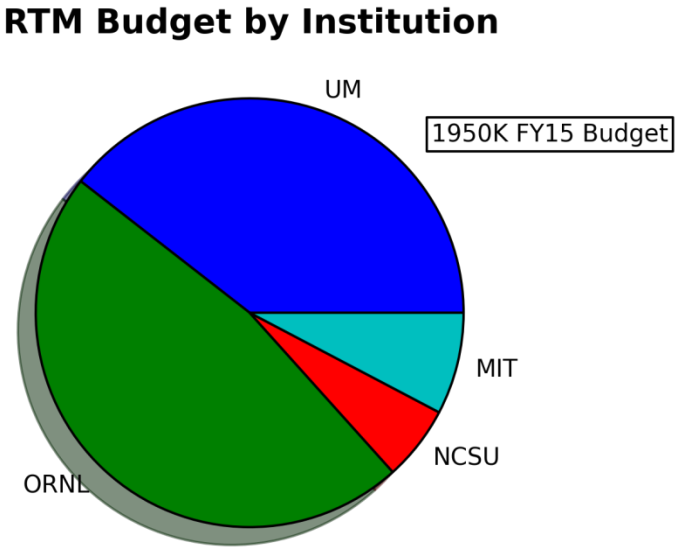
Goals

- Complete core-simulator in order to perform engineering analysis on industry-class platforms
- Extend neutronics methodologies to iPWRs and BWRs
- Develop Monte Carlo for fully-coupled reactor analysis



Capabilities at Conclusion

- Pin-resolved transport (MPACT)
  - Execute CASL progression problems on industry-class hardware
- Pin-resolved transport (Shift)
  - Fully-coupled Monte Carlo-TH for benchmarking and validation on leadership-class hardware



Phase 1 has set the stage for Phase 2

- MPACT has evolved into an accurate and reliable full core deterministic transport capability
  - Transient capability has yet to be proven but is expected soon.
  - Multiphysics capability is being demonstrated. Earlier successful efforts to couple DeCART with CFD (Star CCM+) and crud deposition/loss (Mamba) are encouraging for success with MPACT.
- With modest CASL funding, Shift has proven to be a powerful tool for high fidelity simulation of full core reactor configurations
  - WEC analysis of AP1000 with excellent comparison to CE Keno.
  - Common input allows convenient comparison with MPACT and Insilico.
  - With reactor state (pin resolved isotopics) provided by MPACT, Shift can yield high fidelity snapshots of flux/power distributions through a cycle.
  - With "on-the-fly" temperature feedback, Shift may be able to provide "validation-like" benchmark results for MPACT with multiphysics coupling.

Foundational development of MPACT and Shift in Phase 1 will allow application to CASL Challenge Problems in Phase 2

RTM Phase 2 Strategy

- Two-pronged approach for code-development activities:
  - **MPACT**: deterministic neutronics for reactor engineering analysis targeting industry-class computing hardware
  - **Shift**: Monte Carlo neutronics for validation and benchmarking + long-range analysis targeting leadership-class computing hardware
- Publish and disseminate RTM-sponsored research that advances the state-of-the-art in reactor neutronics and radiation transport
- Incorporate the most promising research innovations into our code products
- Deploy RTM products to broader community

RTM code strategy has evolved to 2 codes going forward

Phase 2 is focused on 2 neutronics codes and cross section generation

- MPACT – MOC in the plane, low order transport in the axial direction (2D/1D). Pin-resolved transport - resolves every pin, including burnable absorbers and control rods, radially and axially.
- Shift – continuous energy Monte Carlo code for keff or fixed source calculations.
- SCALE/AMPX/ESSM – cross section processing including resonance cross sections

For risk mitigation, Insilico-SPN will be maintained as an alternative neutronics module given its demonstrated capability to perform full-core analyses

Common I/O: neutronics codes are driven by VERAIN – e.g., can run first with MPACT, or Insilico, then with Shift, and compare results using HDF5 output files used in VERAOUT.

Now a glance at the 3 neutronics codes …

RTM L2 Milestones for Phase 2

Year	Category	CP	L1 Milestone Supported	Description
1	Core physics	All BWRs	10, 14, 16, 17	Deterministic neutronics for BWRs: Validation of the planar MOC methodology for BWR subregion transport requirements. (Develop mesh, data models, and geometry that can handle BWR requirements)
	Core physics	All iPWR	2, 3	Development and demonstration of hybrid Monte Carlo methods for full-core PWR and iPWR analysis.
2	Core physics	PCI, RIA	5, 13, 14, 16	Transient neutronics with feedback: Implementation of transient capability with internal TH feedback in MPACT for PWRs
	Core physics	ALL	5, 9	Implementation and validation of photon transport in Shift and MPACT.
3	Core physics	BWR	14, 16, 17	Pin-resolved deterministic neutronics for BWR subregions: Validation of deterministic methods in VERA-CS applied to BWR subregion analysis.
	Core physics	BWR	10	Develop efficient depletion methodology for BWRs including Gadolinium absorbers.
4	Core physics	All	19	Optimization and integration of state-of-the-art nuclear data for multi-group and continuous-energy.
	Core physics	PWR, BWR	19	Deploy in line, fully consistent time-dependent neutronics for VERA-CS suitable for PWRs and BWRs.
5	Core physics	All	19	Provide completed documentation for methods, users, and developers for all VERA-CS neutronics packages and methods.
	Core physics	All	19	Implementation of hybrid, fixed-source Monte Carlo methods for ex-core physics.

RTM Phase 2 Execution Plan

MPACT	Shift
Broaden	
• Extend to iPWRs • Extend to BWRs (with limited scope)	
Deepen	
• Capability to perform transient simulations of realistic full core configurations (i.e., RIA). • Carry out V&V/UQ analyses	• Add TH feedback (Doppler broadening) • Complete depletion • Utilize hybrid methods for improved convergence and diagnostics
Optimize	
• Achieve “reasonable” runtimes on industry-class clusters	• Implement heterogeneous hardware acceleration to take advantage of leadership-class hardware • Reduce CE data footprint

Validation Plans in RTM

- AMA.VAL.P4.01 (2012), "*Review of Experiments for CASL Neutronics Validation*" defined 4 classes of experiments for neutronics validation
  - Critical experiments
  - Reactor physics experiments
  - Post-irradiation examination (PIE) for isotopics
  - Plant operational data

Code	Critical Experiments			Reactor Physics Experiments							Post-Irradiation Examination (PIE)	Plant Data
	Strawbridge -Barry	B&W	ICSBEP	Creole	IPEN	KRITZ	TCA	DIMPLE	VENUS	VVER		
MPACT	TBD	1	TBD	TBD							1	1
Shift	TBD	2	TBD	TBD							TBD	1

1 calculations actively being run
2 analysis of data
3 complete
TBD activity in planning stage

RTM working with PHI to plan validation to experimental data in FY15 and beyond

RTM Risk Mitigation

Category	Risk Description	Risk Mitigation
Technical	Transient neutronics capability is too compute intensive.	Have trigger to implement interoperability with existing industry transient neutronics capability to minimize delay of dependent work; engage computer science expertise if necessary in scrutinizing and implement compute efficiency opportunities.
Technical	Unable to devise compute-efficient, accurate, and robust multi-physics coupling models, algorithms and software implementations, especially for the BWR core simulator.	Perform research on advanced coupling methods as a backup to standard Picard iteration to provide an alternative approach with improved convergence properties.
Programmatic	Overall scope outpaces constrained budget and schedule for the BWR core simulator, where development proves more difficult than planned and results in delays in delivery of capability.	Implement multiple technical paths where possible, proactively engage BWR fuel vendors, IC and SC for requirements definition and review/consultation, and insert decision point milestones for go/no-go or de-scoping. Utilize predictions from industry-based core simulator in interim until CASL capabilities are available.
Technical	Run times for MPACT full-core, multi-cycle depletion with TH-feedback are too high for industry class clusters.	Several efforts are underway to improve MPACT run times, with expected gains of 5-10. If these fail, Moore's Law continues to make computing cheaper and may allow re-definition of "industry class cluster".

End of Phase 2 RTM Goals

- Capability
  - VERA-CS (MPACT) capable of performing full CASL problem progression on industry-class hardware
  - VERA (Shift) capable of performing fully coupled TH-neutronics on leadership-class hardware
- Deployment
  - MPACT and Shift distributed with VERA
  - Full documentation to enable broad community use of the codes
- Industry Impact
  - VERA used by multiple vendors and utilities
- Dissemination
  - Double journal article production rate

Questions?

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A Few Background Slides

- Core Simulator Progression Problems Drive VERA Development
- The Need for Pin-resolved Transport
- Code Coupling
- Initial Physics Coupling Approach – MPACT
- Thermal Hydraulics – COBRA-TF
- Coupled Domain Mapping
- Neutronics Reference Solutions with KENO-VI

Core Simulator Progression Problems Drive VERA Development

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 ✓
- #4 HZP 3x3 Assembly CRD Worth ✓

FY13

- **#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

*** Bold text signifies ability to compare to measured plant data**

The Need for Pin-resolved Transport

Challenge Problems require pin-resolved transport

- CRUD challenge problems require 3D full-core power distribution with pin-resolved transport and neutronic/T-H coupling
- PCI challenge problems require 3D full-core power distribution with pin-resolved transport and neutronic/T-H/structural (clad deformation) coupling
- RIA challenge problem requirements similar to PCI except need transient capability to assess cladding and fuel integrity under up-power maneuver.
- Implications for RTM development:
  - Need to resolve the fuel pins radially (~10-20), axially (~100-200), and azimuthally (~8-16) for each of 40,000 pins.
  - Need coupling to conjugate heat transfer within fuel pin and coolant surface, as well as coupling to structural and materials performance codes within the fuel/clad.
  - Need this as a function of depletion with TH feedback in order to predict the reactor state (isotopics)

Need pin-resolved transport with TH coupling and depletion

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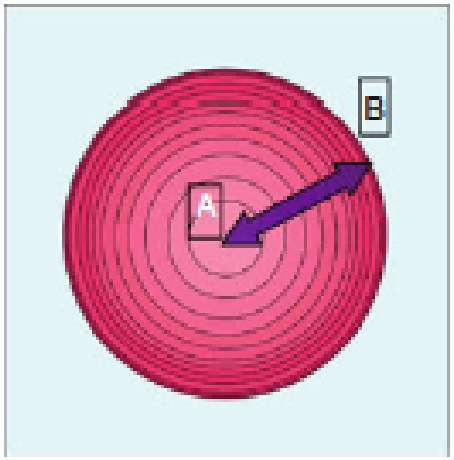
Why pin-resolved transport is needed



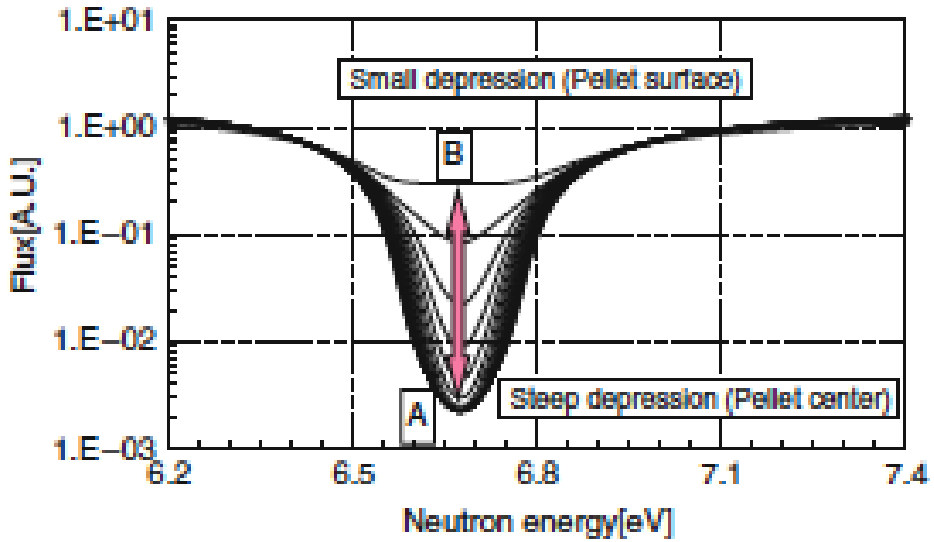


Figure 12 From Cacuci, Handbook of Nuclear Engineering, Ch 9, 2010.

Space dependency of neutron spectrum in a fuel pellet

- The neutron energy spectrum depends sensitively on the fuel temperature. A "harder" (higher energy) spectrum yields more Pu-239 and other isotopics are affected. Pin resolved transport with TH feedback and depletion is essential to get the intra-pin isotopics correct.
- The fuel temperature depends on the TH coupling. It is likely that CFD coupling will be needed to accurately determine intra-pin fuel temperature to address CRUD challenge problems as well as the "rim effect" due to Pu-239 buildup in the periphery of the fuel pin.

Why pin-resolved transport is needed (2)

- The resonance self-shielding varies radially and azimuthally within a fuel pin. This is handled by the resonance model, which can be subgroup or ESSM (extended) in the case of MPACT. This phenomenon is global (Dancoff factor) – distant fuel pins or proximity of reflectors or Gd pins can affect the self-shielding in a pin.
- If the radial dependence of the self-shielding is not treated, Pu isotopics will be in error.
- The self-shielding will also depend on the temperature, so radial and azimuthal variations in temperature must be accounted for.
- Yuxuan Liu's work on extending ESSM can handle radially-dependent self-shielding, including temperature variations, as well as resonance interference. Azimuthal variations are not accounted for at the present time but a similar extension may be possible and will be examined this year.

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Legacy core calculation approach cannot predict flux/power distributions within pins – only pin-average quantities

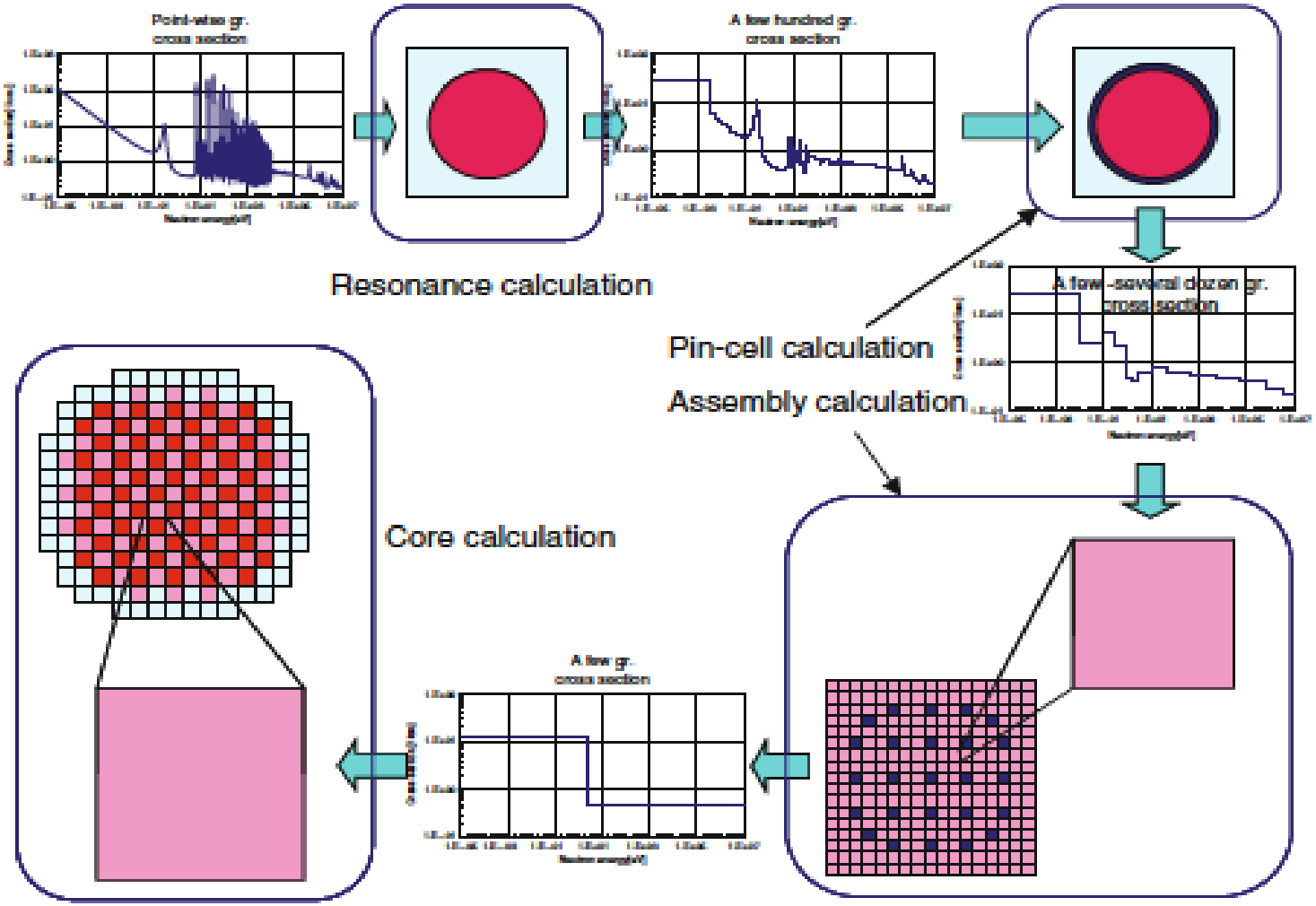
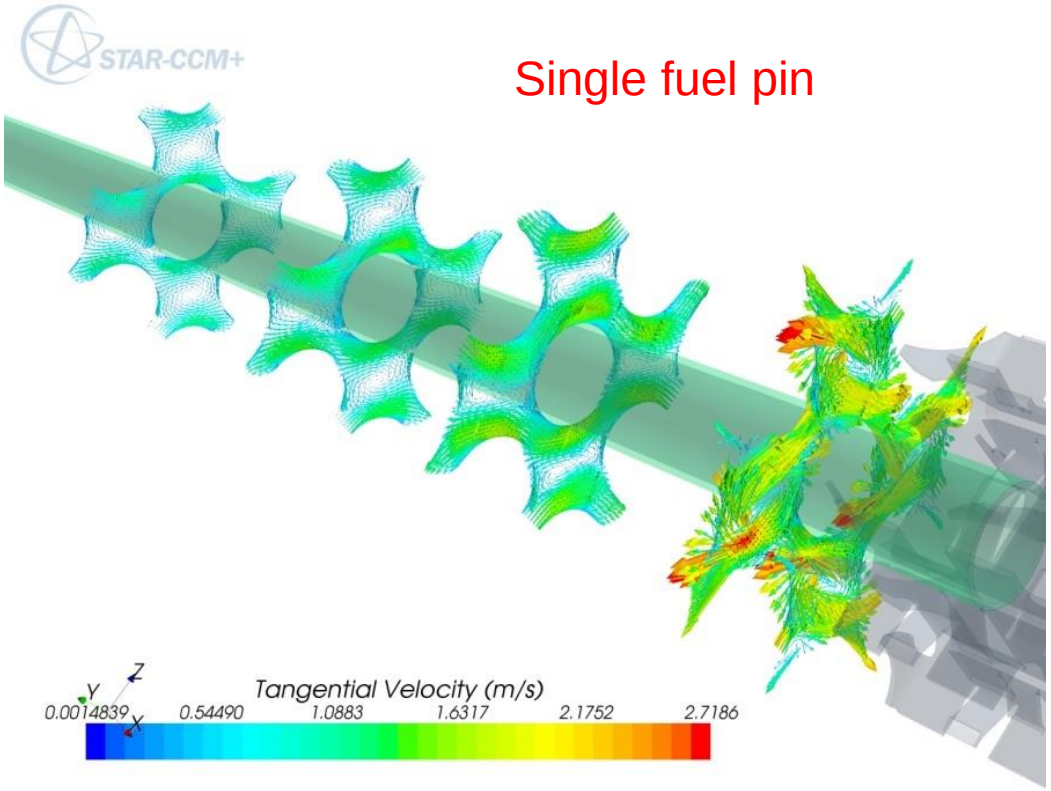
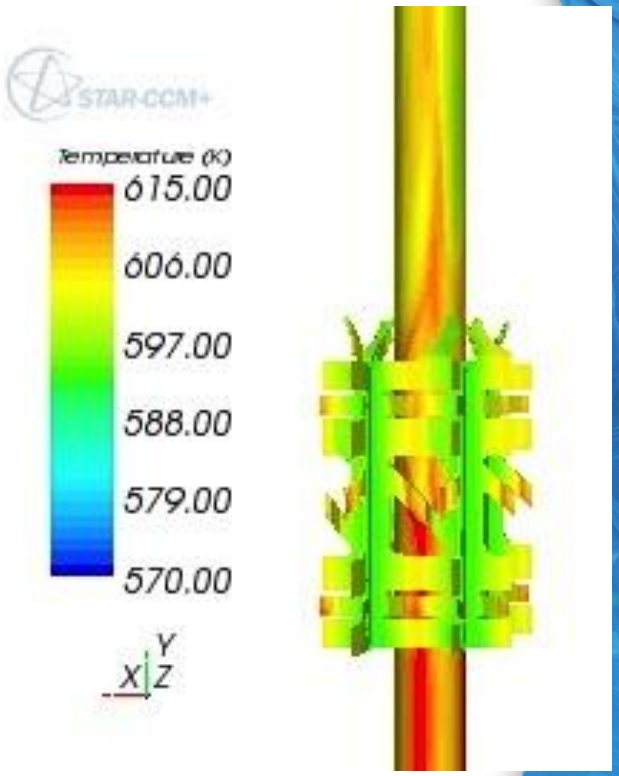


Figure 10
General calculation flow for core analysis

Pin-resolved flux/power distribution not available with legacy methods

Coupled High-Fidelity CFD: need to resolve flow effects due to grid spacers

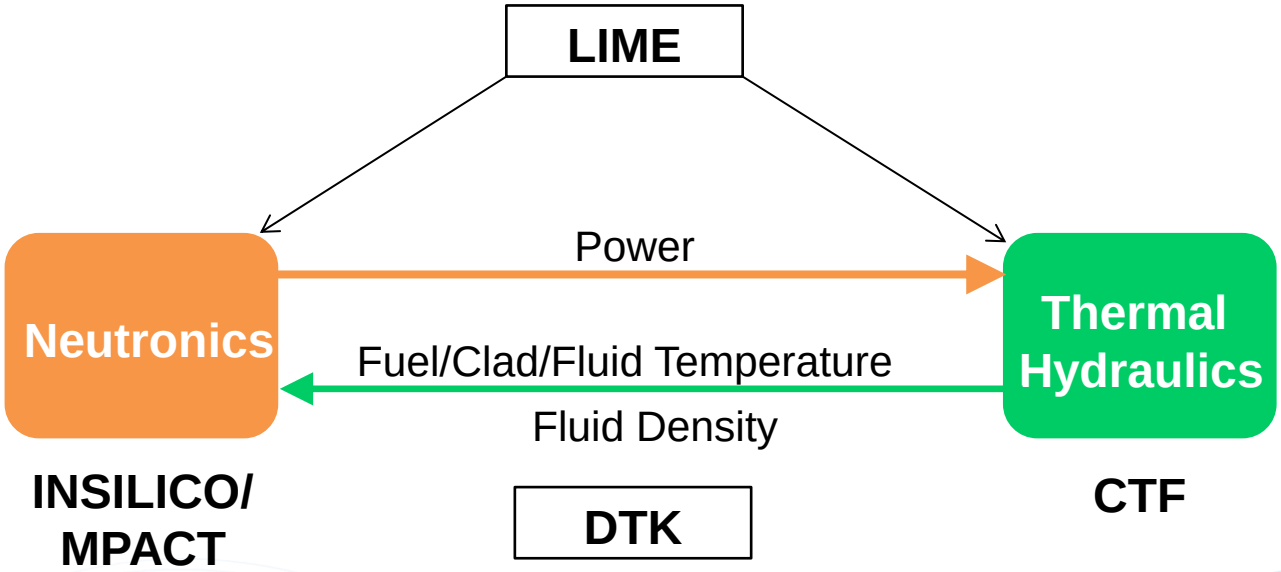




Code Coupling

- **LIME** used as the "manager" to control the iterations and code execution
- **Data Transfer Kit** (DTK) used to pass data between codes in parallel

(both are open source toolkits)



More Details in Coupling Presentation

Initial Physics Coupling Approach - MPACT

- Initial method involves the transfer of the coupled field quantities (power density, temperature, and density) on a "pin cell averaged" basis.
  - Includes an axial discretization.
- Coupling of fields occurs primarily in the active fuel region
  - Below active fuel (inlet) T/H conditions are specified
  - Above active fuel and outside baffle there's no bulk heat generation

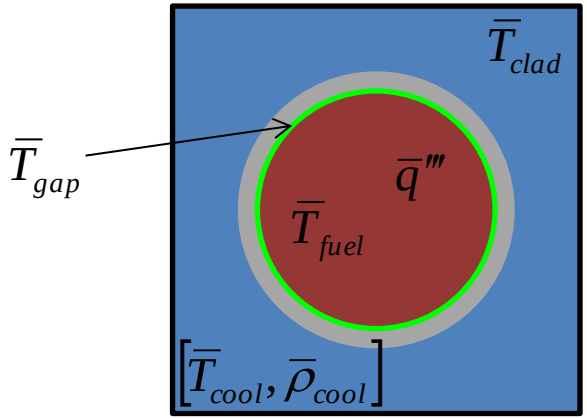


Illustration of a "pin cell"

$\bar{\rho}_{cool}$ - average coolant density

$\bar{T}_{cool}$ - average coolant temperature

$\bar{T}_{clad}$ - average cladding density

$\bar{T}_{gap}$ - average gap temperature

$\bar{T}_{fuel}$ - average fuel temperature

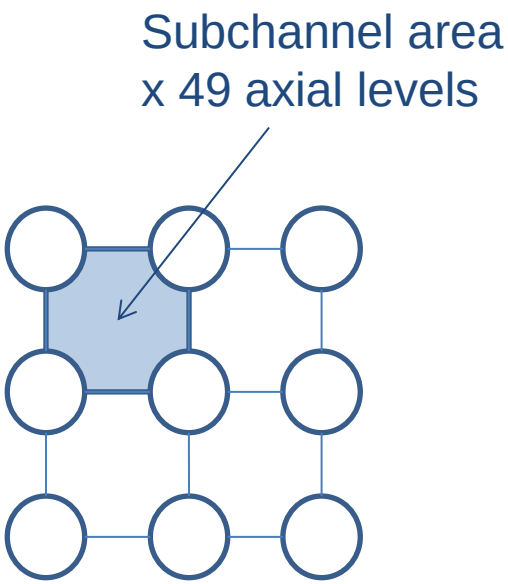
$\bar{q}'''$ - average power density

Coolant (H_2O) Cladding (Zr-alloy)

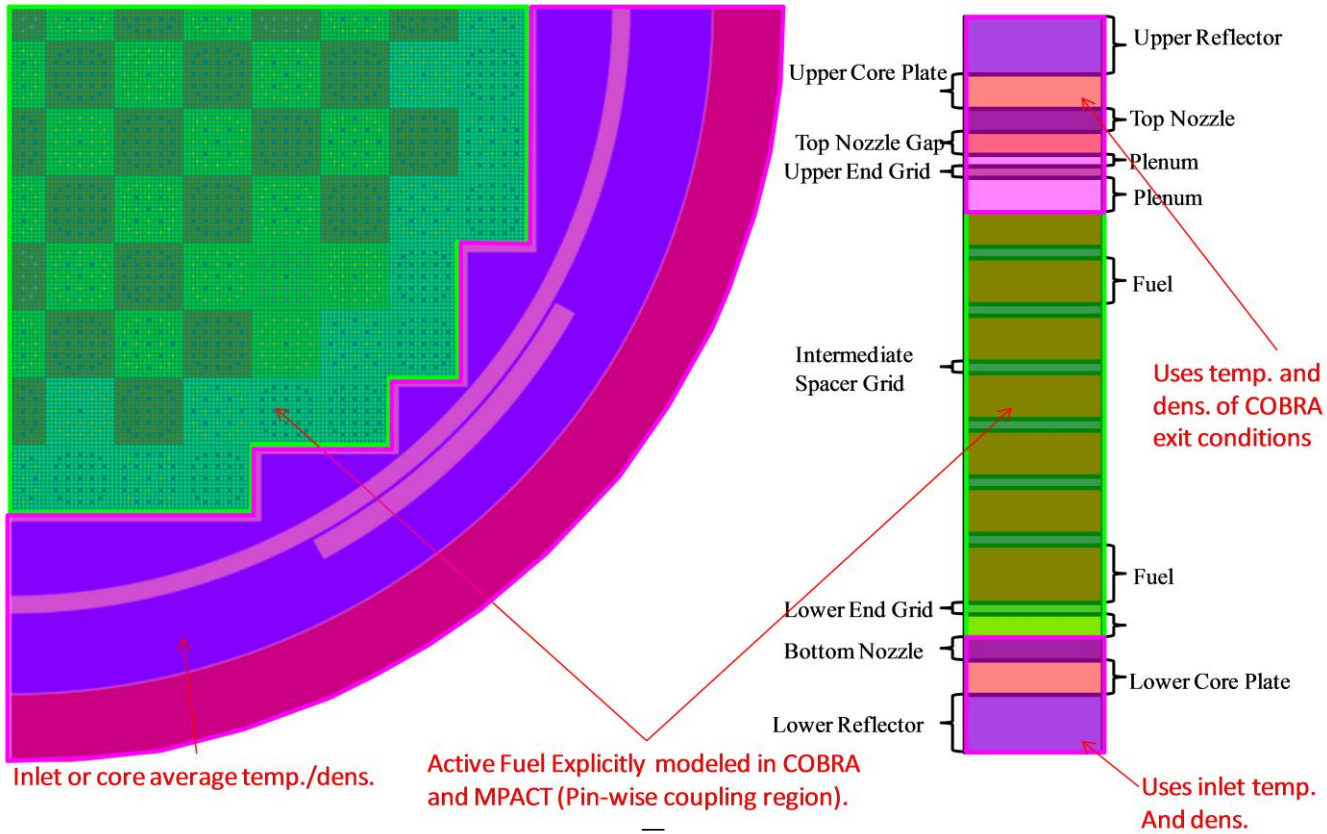
Gap (Helium) Fuel (UO_2)

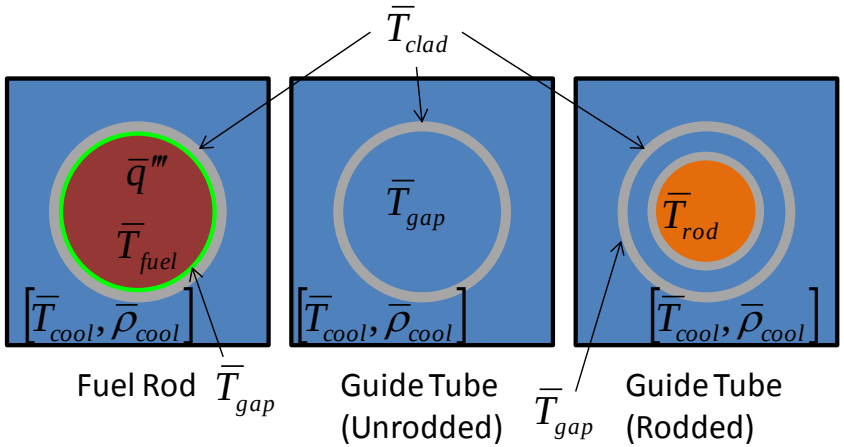
Thermal Hydraulics – COBRA-TF

- Input directly from common input (VERAIn)
- COBRA-TF (CTF) subchannel code from PSU
- Two-fluid, three-field representation of the two-phase flow
  - Continuous vapor (mass, momentum and energy)
  - Continuous liquid (mass, momentum and energy)
  - Entrained liquid drops (mass and momentum)
  - Non-condensable gas mixture (mass)
- Spacer grid models
- Internal pin conduction model
- Built-in material properties
- Parallel Solution (one assembly/core)



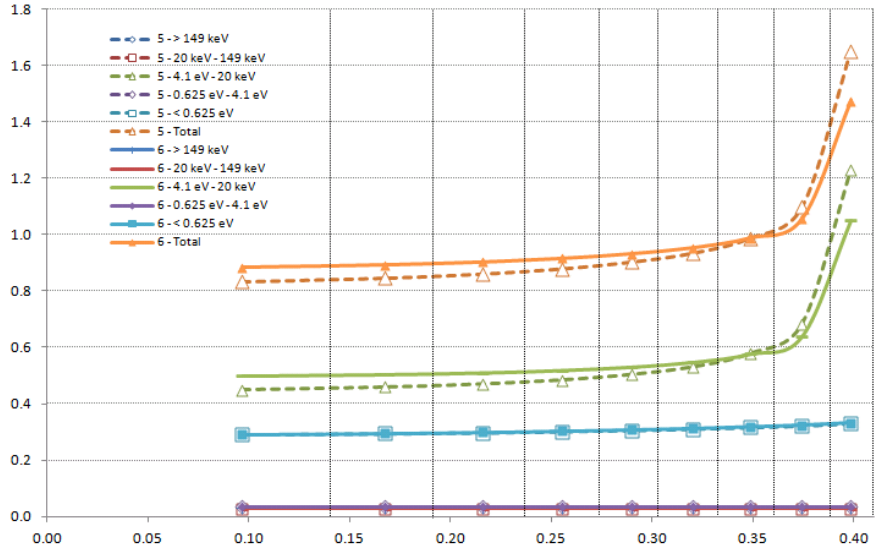
Coupled Domain Mapping



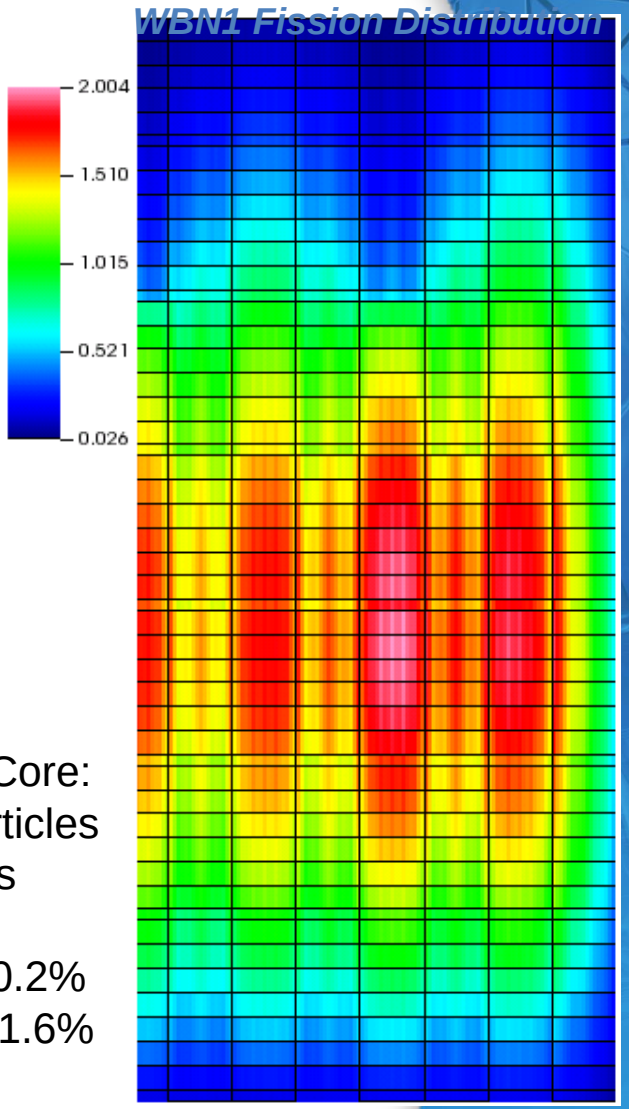


Neutronics Reference Solutions with KENO-VI

- Over 120 continuous-energy Monte Carlo solutions for Watts Bar 1 geometries
  - Pin Cells → Quarter-Core geometries
  - Eigenvalues and Fission rate distributions
- Over 70 CE MC solutions for AP1000 geometries
- Intra-pin temperature-dependent radial fission and capture distributions with energy dependence
- Pin cell and Lattice CE MC depletions (FY14)
- Subset of cases validated against MCNP and measured data



Quarter-Core:
100B particles
180 cores
29 days
Avg σ = 0.2%
Max σ = 1.6%



Center

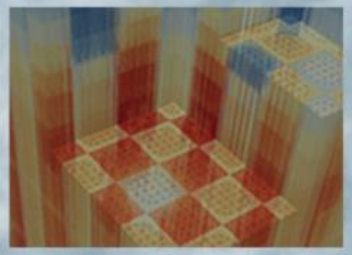
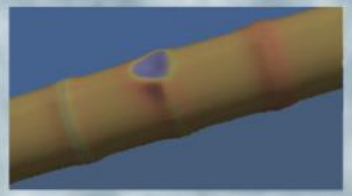
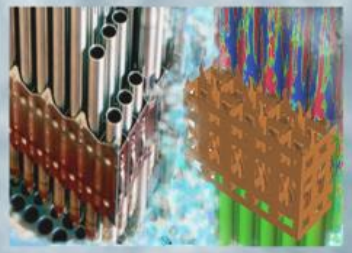
Edge

A DOE Energy Innovation Hub

Technology Deployment and Outreach (TDO)

Dennis Hussey
Rose Montgomery

Joint SC/IC Meeting
Oak Ridge National Laboratory
September 9-10, 2014

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Overview

- Introduction to Technology Deployment and Outreach (TDO)
  - TDO Team
  - Objectives
  - Roles and Responsibilities
    - The post-CASL entity
    - Outreach
    - VERA Release and Support
    - Test Stand deployment
  - Planned Milestones

An increased focus on sustainability and deployment

TDO Team

- Dennis Hussey (EPRI), Lead / Industry Council Executive Director
- Rose Montgomery (TVA), Deputy Lead / Working Groups
- Steve Hess (EPRI), Test Stands
- Matt Sieger (ORNL), Software Quality and Release Management

Close collaboration with others:

- Education Program
- Communications
- Partnerships
- Industry Council

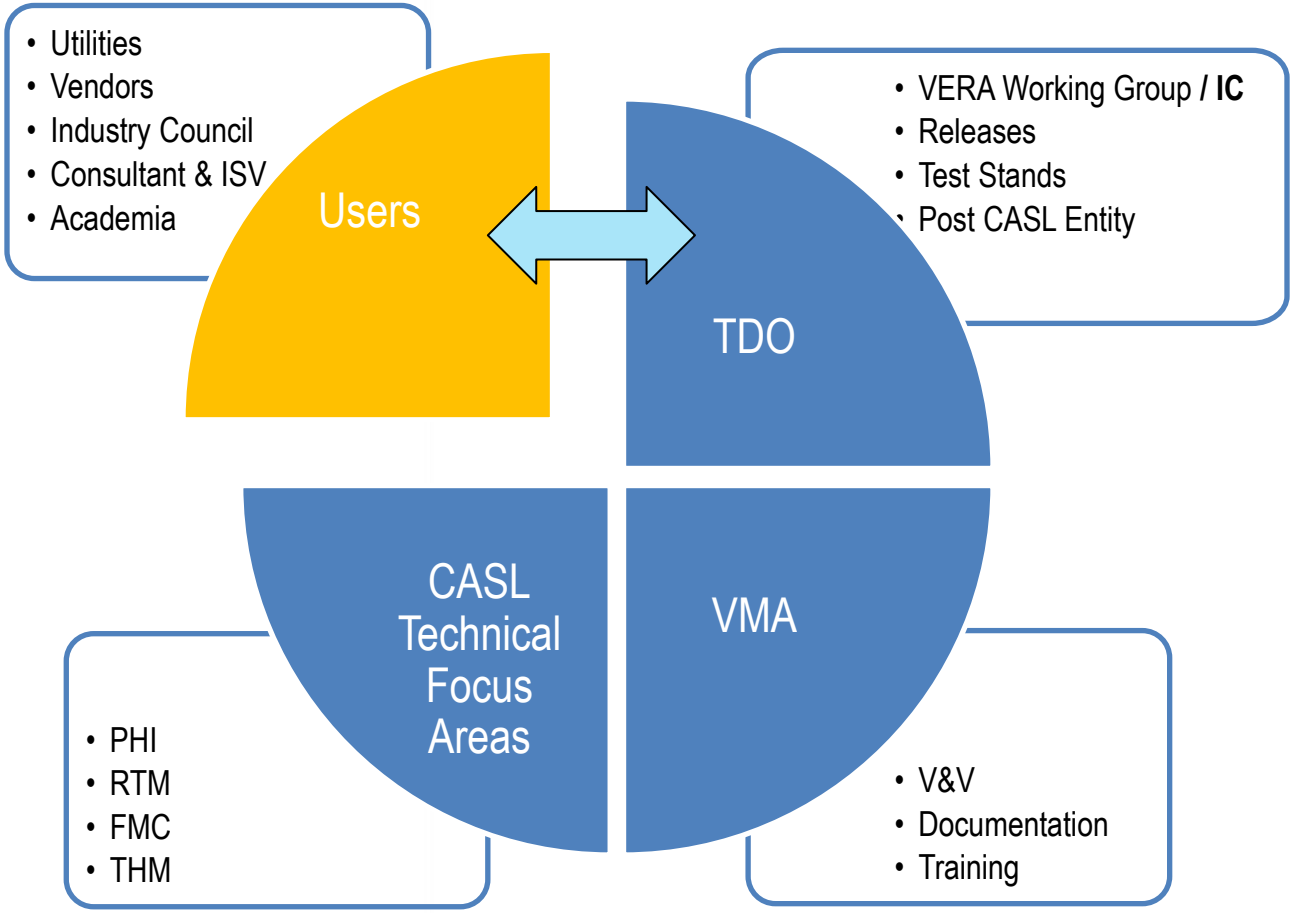
Team combines utility, industry, lab, and academic skillsets

TDO Objectives

- TDO's priority is deployment and sustainability of the CASL technologies
- TDO seeks to ensure CASL technologies are delivered to the nuclear energy community
- Four areas of TDO
  - Evolution of the post-CASL Entity
  - Outreach
  - Release and Support
  - Test Stands

TDO will be the deployment conduit for CASL technology

TDO's Role in CASL



TDO is the liaison to the VERA user community

TDO Responsibilities

TDO

Post CASL Entity
- Investigate options
- Develop business cases
- Evolve the most viable option(s)

Outreach
- User recruitment
- VERA Working Group
- Training
- Workshops and demonstrations

Release and Support
- Entry level tech support, delegate detailed requests
- Release management
- Address gaps in licensing strategy
- Identify/develop VERA candidates for regulatory applications

Test Stand Deployment
- Evolve selection process
- Establish multiple Test Stands
- Derive maximum CASL value
- Establish more VERA Users

Ultimate goals: Establish a user-base for VERA; Establish a vehicle to sustain the CASL technology after Phase 2

Post-CASL Entity

- TDO envisions a long-term sustaining body (called the "post-CASL entity")
  - Responsible for primary VERA distribution and user support
  - Manage the VERA Working group
  - Facilitate VERA training
  - Coordinate further development of the VERA suite of tools
  - Liaison with other ModSim initiatives
- TDO will investigate options for the post-CASL entity in Year 1
  - Accessible to all potential Users (as limited by export control)
  - Capable of providing support to all Users
  - Able to conduct continued outreach activities

Develop options and recommendations in FY15

Post CASL Entity

Business case for Sustainability

- Determine market for CASL tools
  - Investigate potential use cases (risk assessment, safety analysis, margin assessment)
  - Understand plans for use, including regulatory licensing
  - Assess the value associated with the use cases
- Develop revenue model based on market
  - Identify revenue streams (e.g., funded/commercial projects, license fees, user group fees)
  - Use existing experience (RELAP5, ISVs) to develop strategy
- Determine staff and compute resource costs needed to satisfy market needs
- Build business plan for sustaining VERA indefinitely
  - Identify resources for maintenance and future enhancements
  - Specify HPC resources needed

DOE Support may be needed to define post CASL entity requirements

Outreach

Communication with the Nuclear Community

- Nuclear community engagement is necessary for sustainability
- TDO will work with CASL staff to more fully develop communication vehicles
  - Website
  - TechNotes
  - Fact Sheets
  - Journal Articles / Conference Papers
- TDO plans to continue / expand engagements with selected groups
  - PWROG/BWROG
  - INPO Driving to Zero
  - EPRI Fuel Reliability Program
  - NRC (led by Jess Gehin, PHI)
- Initial plan has been vetted by Industry Council

Find Users; Manage Expectations

NRC Engagement

Objective: Inform, discuss, and exchange information with NRC Staff on CASL activities and approaches with key desired outcomes being to:

- Familiarize NRC with CASL R&D and use of advanced M&S for nuclear reactors
- Seek feedback and exchange on scope of work, developments, and approaches
- Work within constraints to avoid conflict of interest issues

February 2014 – Most recent update meeting

- Well-attended by RES and NRR Staff
- Discussion topics – Overview, VERA, Challenge problems. TH, Validation Data, Phase 2

Update Meetings at NRC
October 2010
November 2011
March 2012
November 2012
February 2014

Commissioner Seminars at NRC
January 2012
November 2012

Commissioner Tour/Briefings at ORNL
October 2012 - Ostendorf
January 2012 – Apostolakis
January 2012 – Magwood
March 2014 – Svinicki
April 2014 - Magwood

NRC Participation in DOE Reviews
August 2011
August 2012
August 2013

Other
July 2014 – Attendance at DOE Milestone Briefing
March 2012 – CASL Presentation at NRC RIC
Overviews in Westinghouse Update Meetings

Outreach

Demonstrations, Workshops, Training

- Demonstrations and Workshops will offer potential users the opportunity to work with VERA
  - CASL Industry and Science Councils
  - Selected industry conferences
  - Support for CASL Education Program
- Initial Demonstration will be held at 'Advances in Nuclear Fuel Management' Conference in Hilton Head March 29-April 1, 2015
- Training opportunities will be developed and coordinated with VMA and the Education Program
  - Materials developed will leverage already existing CASL-edu materials
  - Summer school a possibility
  - Delivery vehicles to be investigated

Outreach
VERA Working Group

- Initial draft charter is provided in the proposal
- The WG is expected to serve as an administrative body to enable the sustained use and development of VERA
- The WG is a forum for VERA users to:
  - Receive product information / updates
  - Receive software support for VERA
  - Participate and support VERA's Verification and Validation testing program
  - Provide input into VERA's business, design, functional, and quality requirements
  - Obtain VERA training
- Initially positive feedback from IC

Sustain; Connect; Share; Collaborate

Outreach
VERA Working Group

- The WG hopes to serve as a coordinating group for several DOE advanced ModSim software development projects
  - TDO will reach out to other projects to develop plans for collaboration (e.g., NEAMS, LWRS)
- The WG will be encouraged to engage with the VERA requirements development process
- To establish the WG, TDO will leverage existing VERA subcomponent User Groups
- CASL Industry Council will be encouraged to join

Sustain; Connect; Share; Collaborate

Outreach
VERA Working Group

- Phase 2 expects minimal (possibly zero) dues to start
  - CASL funds are budgeted for support
- Post Phase 2, User fees or VERA fees are expected to sustain the WG
- The WG may develop a fee structure that is based on a market analysis
  - Examples of existing working groups have been identified, and initial studies have been completed
  - Further studies to be completed in year 1
- The WG is a candidate model for the post-CASL entity
- Source of WG operating budget either user-funded or funded collaborative projects
  - Pending study results

The WG is intended to be self-sustaining

Release and Support

- Releases will be focused on providing a useful product to potential CASL users
  - the philosophy is to be aggressive about pushing technology out, with full disclosure regarding the quality and maturity of product
- VERA releases will occur at least annually, with development updates occurring more frequently
- TDO will manage CASL internal VERA release process and release package bundling (software, documentation, etc)

Release process has been demonstrated in Phase 1 with successful results

Release and Support

Support Tracking System

- CASL has set up a dedicated support ticket system to track VERA bugs, issues, support requests, and suggestions submitted by users (CSICAT), support@casl.gov
  - Configured to track three types of tickets:
    - Problems
    - Support requests
    - Suggestions
  - Procedures and contact lists for handling support requests are in place and being used

First Line Technical Support

- For common installation/setup/execution issues, TDO will field requests.
- In-depth requests will be dispositioned by TDO

Release and Support

- TDO will ensure appropriate licensing vehicles exist
- Perceived Gaps
  - Currently only Government Use and Test and Evaluation Licenses are in use
  - Commercial and non-commercial terms are needed
    - Early drafts are provided in the proposal
    - Much more work is needed to
      - Establish terms and conditions acceptable to all partners
      - Establish fee structure
      - Address CASL and external derivative works
  - TDO will work with Partnerships to ensure appropriate standard licensing terms are ready for use
    - At least one External Test Stand will be selected to drive this development

Phase 2 Test Stands

- CASL Test Stands have been very successful
  - Recruits new users
  - Provides opportunity for (relatively) unbiased feedback
  - Exercises the codes in extended areas
  - Offers potential for additional validation
  - Develops User support strategy
- TDO goal is one Test Stand per year
- In Phase 1, Test Stands were piloted by CASL Founding Partners.
- In Phase 2, the focus will turn towards "External" hosts
  - New Phase 2 CASL Partners
  - Non-CASL participants

Test stands will be continued in Phase 2

Test Stand Selection Process

- In Phase 1 a process was developed to select Test Stand topics
  - In Phase 2, the process will be revisited to ensure it fully addresses external hosts
- Selection of External Test Stand hosts in Phase 2 will consider:
  - Fit with CASL milestones
  - Validation potential
  - Expansion of User Group
  - Cost share
- Test Stand participants will progressively require user support
  - Motivates the Working Group and CASL support systems
- Compute resources may be provided by CASL
  - Preference is for host to utilize their own resources or apply for resources using established HPC programs
  - Cloud option a possibility

TDO Planned Milestones

Year	Category	Description
1	Business operations	Establish a business case, identify and evaluate options for the post-CASL entity, determine mode of recruitment, and make recommendation for post-CASL entity
2	Business operations	Select the post-CASL entity
	Working Group	Establish the VERA Working group
	Training	VERA Training Pilot
	Test Stands	External Test Stand (key industry stakeholder)
3	Release	"Unlimited" VERA release only restricted by DOE regulations and US export control laws
5	Business operations	Finalize transition of CASL-supported functions to post-CASL entity (e.g., Give keys to post-CASL entity)
	Release	Final CASL VERA Release

Summary

- TDO will be the liaison between CASL Users and CASL developers
- Early Phase 2 TDO tasks will build the framework for the eventual transition of CASL to the nuclear power community
- Strong collaboration among CASL team, Industry Council, and potential users is needed to realize TDO goal
- Strong outreach to industry, with goal of wide use of VERA by industry

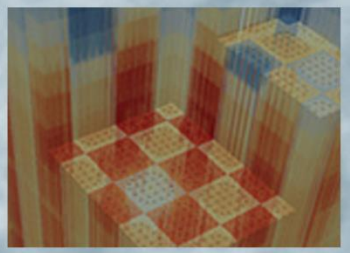
TDO seeks to make CASL products 'used and useful' to the nuclear community

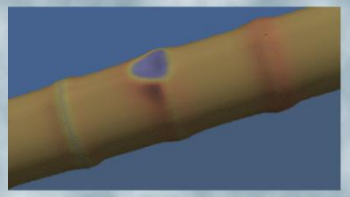
A DOE Energy Innovation Hub

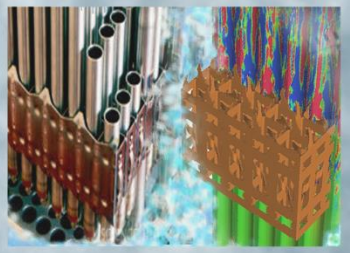
Spotlight on Thermal Hydraulic Focus Area

Mark A. Christon, Lead, LANL
Emilio Baglietto, Deputy Lead, MIT

presented by: Igor A. Bolotnov, NCSU







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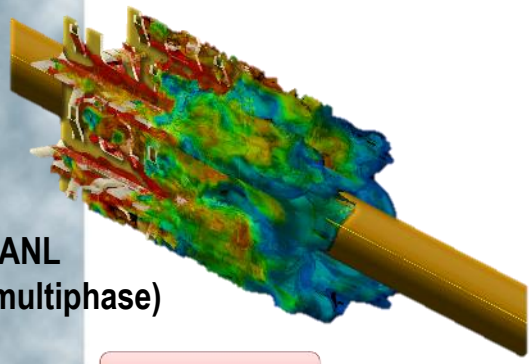
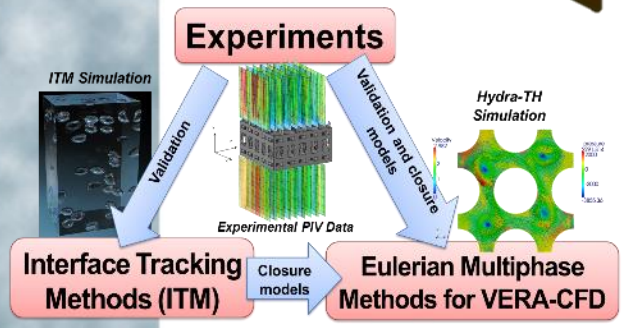
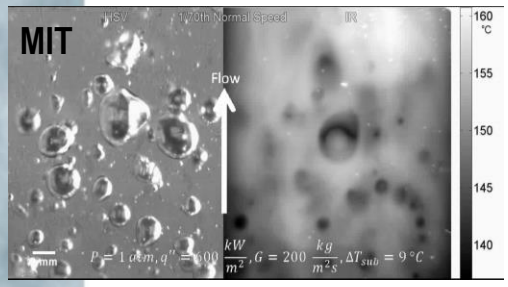
Thermal Hydraulic Methods

Delivers thermal-hydraulic simulation capabilities to VERA



LANL
(multiphase)





- **Computational Fluid Dynamics (CFD):** Deliver scalable, verified and validated CFD tools
- **Closure Modeling (CLS):** Exploit micro-scale simulation results and experimental data for CFD closure models and validation based on new physical understanding
- **Leveraging capabilities** of THM teams to deliver <u>state-of-the-art</u> models and methods for T-H simulation

Advances in THM driven by fidelity requirements for CASL Challenge Problems

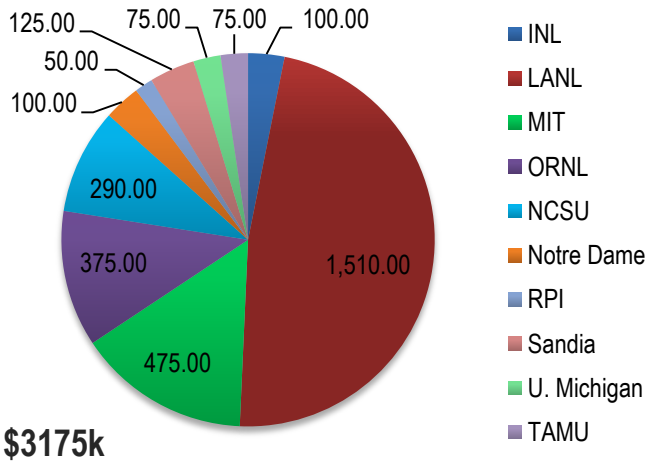
Thermal Hydraulics Methods

FY14 -- Plan of Record PoR-8 and PoR-9

Activities and Priorities

- Priorities (Defined by SLT):
  - Hydra-TH multiphase model functional in realistic geometries
  - Subcooled boiling model development implementation, application
  - Momentum closure (lift/drag) model development, implementation, application
  - Support DNB L1
  - Conjugate heat transfer capability integrated/enabled
  - Full vessel work (includes meshing strategies)
- Activities – FY14 THM Workshop (Hosted at MIT)
- Code Distribution/User Support: > 52 licensed users

Budget



- **Total: $3175k**

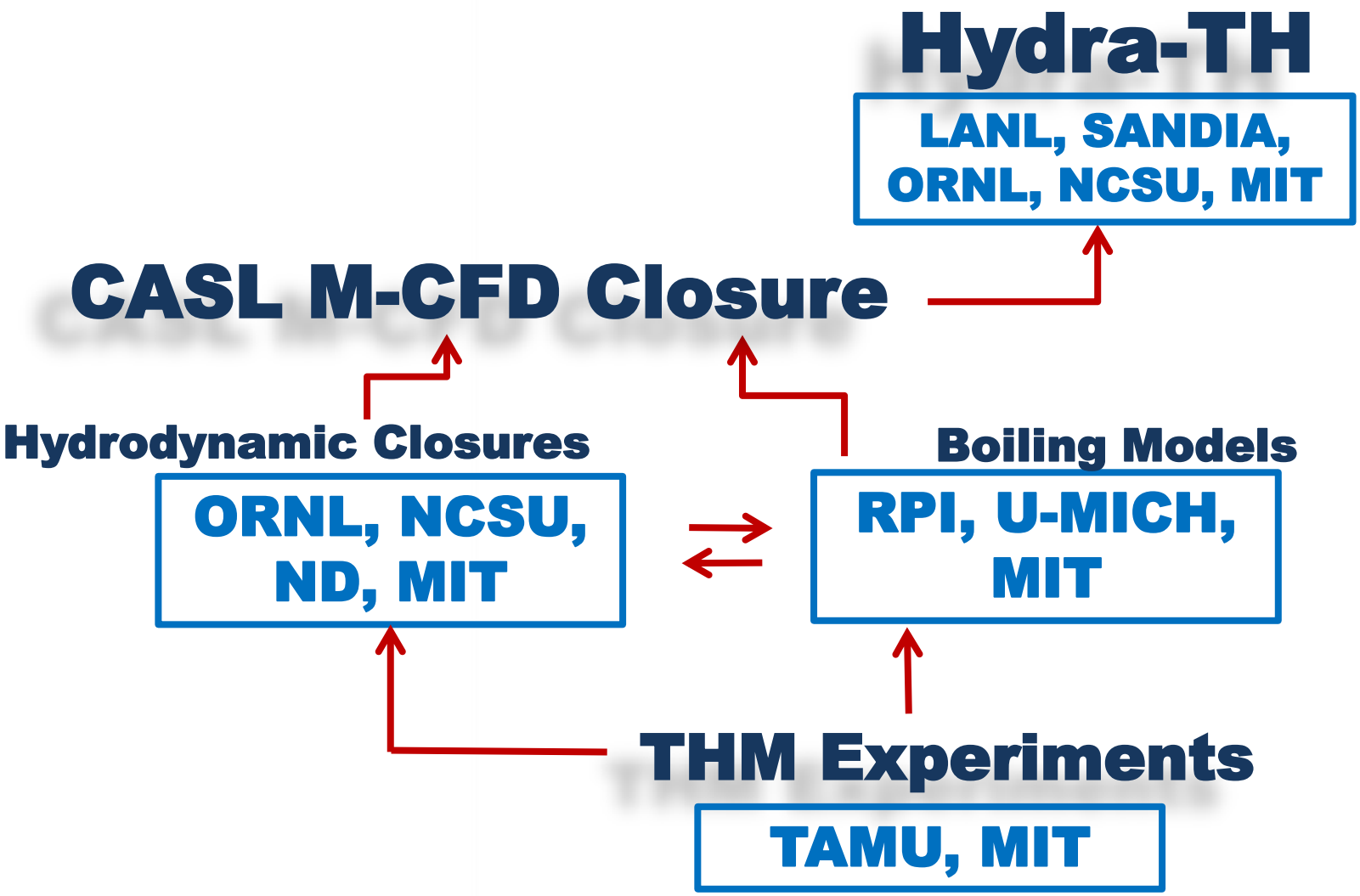
Challenges and Risks

- Challenges:
  - Coordinating efforts among the 10 THM institutions
  - Balancing R&D efforts and code development with V&V activities, user support with limited resources
  - Code delivery with limited resources and manpower
- Risks:
  - Staff retention
  - Impact of user support on development

Milestones

- L2:THM.CFD.P9.01: Single Phase Validation of Hydra-TH for Fuel Applications
- 11 L3 CFD milestones, and 9 L3 CLS milestones supporting the L2 milestone
- THM Workshop focused on coordinating research efforts, organizing requirements for DNS/Experimental data and improving V&V/UQ efforts

The THM Team Roles



2013 Review Findings of Note
(THM specific)

1. Advanced, 3D, high resolution tools may not be necessary for GTRF but tools like this will be needed for FAD – would like to understand strategy for incorporating advanced structural mechanics into VERA
2. **THM is being very aggressive about the complexity of the work it is planning to do – be careful about being realistic about what is accomplishable in Phase 1**
3. While the current focus in VERA is on creating simulations of the quasi-steady state of a reactor, it is not clear whether or not this approach will be sufficient to capture fast transient behaviors as seen in reactor accident conditions.
4. "Figures of Merit" for the validation of the M&S tools were not clear – CASL should work on creating them so it is clear what CASL considers to be "good enough" from a validation perspective
5. Be careful to ensure that "hard wired" challenge-problem-specific capabilities in VERA that only address a single or small set of uses are not created
6. Maintain caution in deployment of Test Stands to ensure that "scope creep" is avoided in dealing with issues not directly aligned with current CASL scope.
7. Consider what it would take and who could host an Education Test Stand

4 year progression leverage

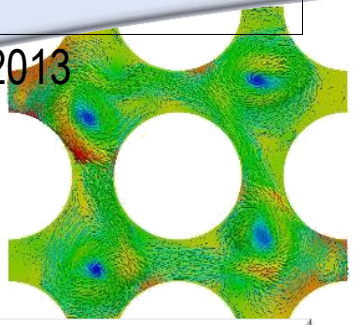
… *accomplishable in Phase 1*

FY2011 - 2012

- Hybrid Parallel Meshing of V5H. 3x3 and 5x5 V5H meshes up to 192M cells
- Development of a priori mesh assessment based on y+
- Runtime turbulence statistics
- Parallel Visualization (ParaView)
- L1 Milestone: Determine sensitivity of structural response to GTRF RMS forces
- Investigate sensitivity of GTRF forces to URANS and LES models
- Validation LES calculations with 5x5 V5H TAMU Data
- Direct integration of Hydra-TH forces using WEC VITRAN code. Less than 1.7% difference compared to STAR-CCM+ "gold standard"
- Development of Hydra-TH Multiphase development roadmap

FY2013

- Hydra-TH Assessment on THM Benchmark Problems
- Development of Hydra-TH V&V/Benchmark Problems and Documents
- General-purpose Steam Property Library (IAPWS-95/97)
- Fully-implicit single-phase
- Initial (anelastic) multiphase flow demonstration
- Integration of asymmetry preserving drag model
- Enthalpy and Internal Energy form of Energy Equation
- Enhanced surface/statistics output
- Direct nightly code integration into VERA
- Addition of ~ 60-70 licensed users

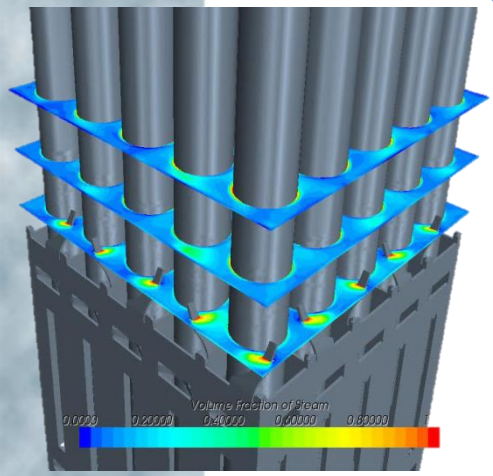


FY2014

- Expose Native CHT Capabilities
- Release porous drag for simplified meshing
- Single-phase validation for fuel applications
- Improved parallel linear algebra
- Enhanced turbulence single/multiphase turbulence models
- Fully-implicit multiphase
- Boiling closure models
- Single/multiphase V&V
- Hydra-Mamba direct coupling
- Expanded "open" Hydra development model

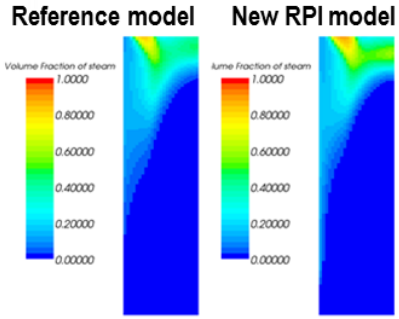
Clear Focus on what can be delivered in Phase 1

The approach:
deliverable vs. innovative

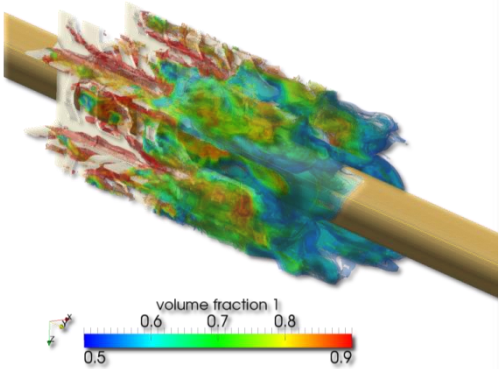


- **Baseline:** *Industry and International Benchmark Experience*

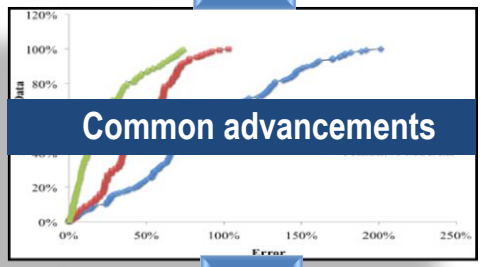
GEN-I



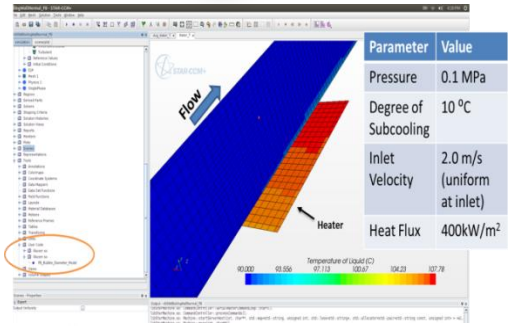
- Incorporates Experience Based Robustness



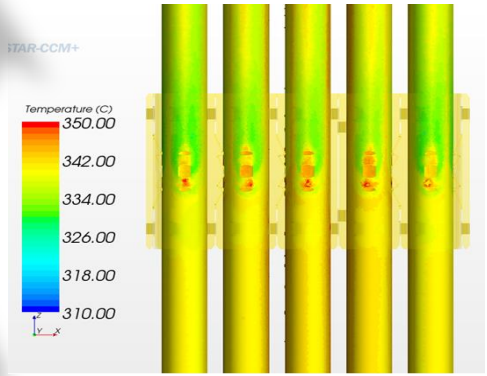
- First Generation Delivery in Hydra-TH



GEN-II



- DNB oriented advanced closures



- Immediately available for testing *(STAR-CCM+)*

THM FY2014 Milestones
Hydra-TH Centric

DOE Reportable:

- **L2:THM.CFD.P9.01:** Single Phase Validation of Hydra-TH for Fuel Applications

Hydra-TH Features/Performance

Development and Distribution Environment:

- **L3:THM.CFD.P9.09:** Hydra-TH release, bug/issue tracking and feature enhancement

New Features, Performance Enhancement:

- **L3:THM.CFD.P8.02:** Expose porous drag capabilities for DNB single-phase "mixing" calculations
- **L3:THM.CFD.P9.02**: Expose native CHT in Hydra-TH for stand-alone rod-bundle calculations
- **L3:THM.CFD.P9.11:** Hydra-Mamba coupling, i.e., Mamba as a sub-grid scale model
- **L3:THM.CFD.P9.03:** Hydra-TH linear algebra improvements and performance optimization

Hydra-TH Phase 1 Delivery

Turbulence Modeling:

- **L3:THM.CFD.P9.06:** Enhanced turbulence model capabilities in Hydra-TH
- **L3:THM.CFD.P9.13:** EARSM turbulence modeling for fuel assembly applications

V&V and Assessment

- **L3:THM.CFD.P9.01:** CFD hexahedral mesh generation for selected problems and Hydra-TH verification
- **L3:THM.CFD.P9.05:** Single/Multiphase CFD assessment, verification and validation

Hydra-TH Multiphase

Multiphase

- **L3:THM.CFD.P9.12**: Demonstration of multiphase boiling flow with Hydra-TH in realistic subchannels with mixing vanes
- **L3:THM.CFD.P9.07:** Advanced turbulence models for multiphase flow (BHR, cascade, etc.)

THM FY2014 Milestones
Closure [Boiling] Centric

Development and Assessment of Closures:

GEN-II

- **L3:THM.CLS.P9.08:** Advanced Subcooled Flow Boiling Models
- **L3:THM.CLS.P9.03:** Advanced momentum closures for multiphase flow
- **L3:THM.CLS.P9.07:** Novel Robust Momentum Closure Approach for Multiphase CFD
- **L3:THM.CLS.P9.06:** Assessment and improvement of heated surface effects treatment for subcooled flow boiling models

GEN-I

- **L3:THM.CLS.P9.04:** Continuous Improvement of a mechanistic subcooled boiling model for PWR assemblies

Dedicated Micro/Meso-scale Experiments:

GEN-II

- **L3:THM.CLS.P9.01:** Experimental Determination of the Effects of (Synthetic) CRUD on Subcooled Boiling

GEN-I GEN-II

- **L3:THM.CLS.P9.05:** High Resolution (PTV)/ Shadowgraphy of near wall bubbly flow

ITM/DNS towards model upscaling:

GEN-I GEN-II

- **L3:THM.CLS.P9.02:** Transient evolution and dispersion of bubbles in a channel and data mining
- **L3:THM.CLS.P8.01:** Perform limited time simulations of single subchannel geometry and 2x2 realistic geometry with spacer grids and mixing vanes

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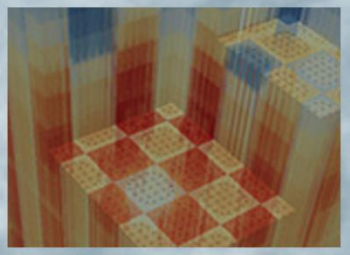
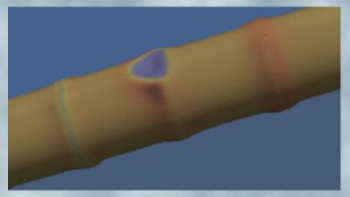
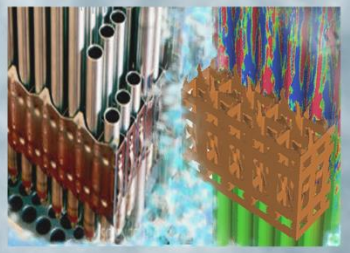
Hydra-TH Year 4 Highlights







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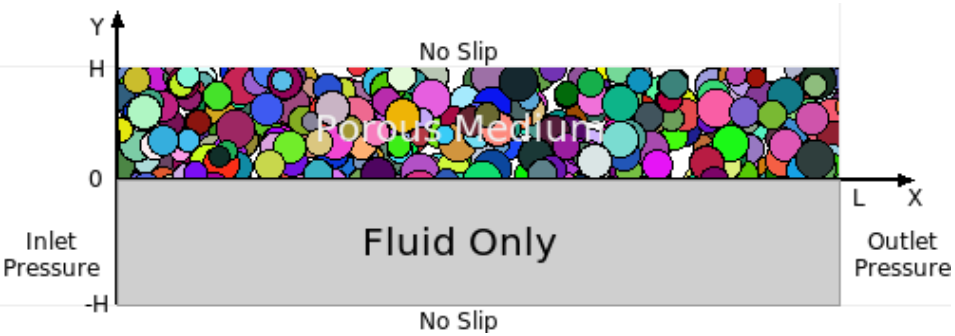
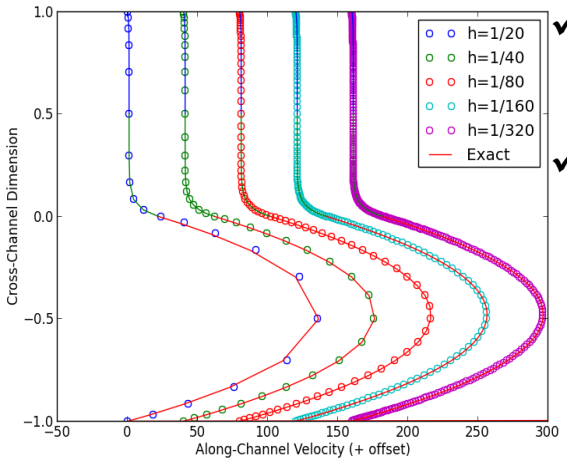
FY14 Science Highlight: Porous Drag Capability in Hydra-TH [Supporting TVA Test Stand]

Milestone Accomplishments

- Check and Expose Porous Drag Capability in Hydra-TH
- Perform and document V&V tests
- Develop and document user test case of 3x3 rod bundle with spacer grid replaced by porous medium

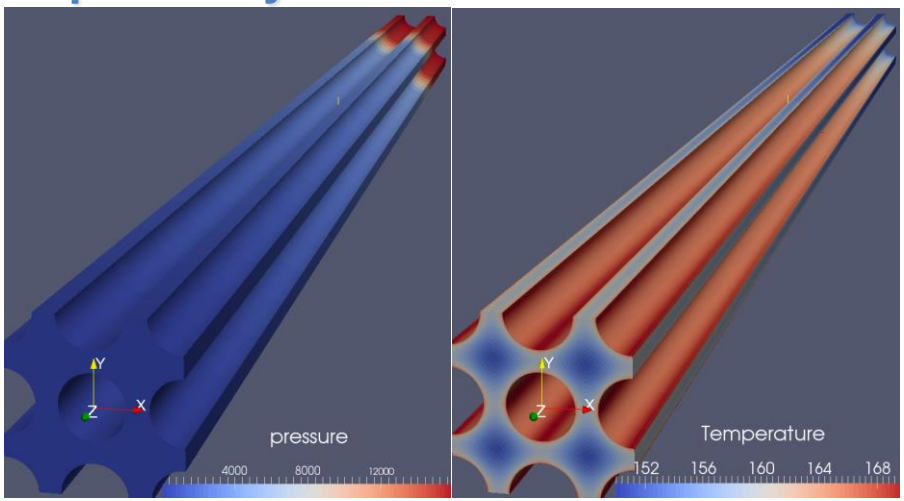
Forced Convection Validation Test

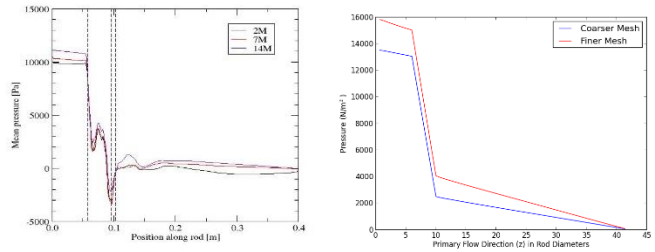




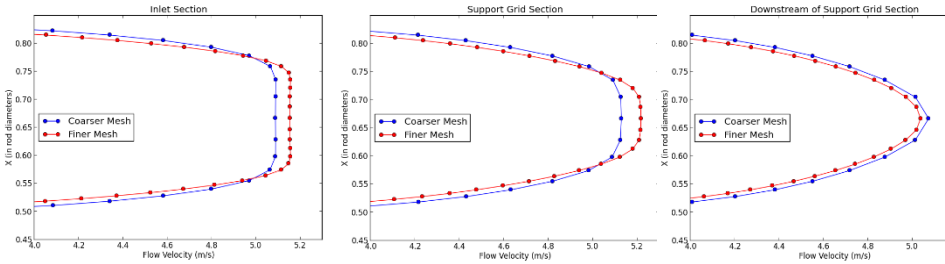
- ✓ Exact Solution Developed and L_2 and L_∞ Error Considered
- ✓ Convergence on Uniform and Stretched Grids using both Semi-Implicit Projection-based time-stepping & fully-implicit time-stepping studied

3x3 Rod Bundle with Spacer Grid Replaced by Porous Medium





Can match LES pressure drop across spacer grid



Velocity Profile Upstream of Porous Medium is Turbulent whereas Downstream Profile is Laminar

Key personnel: B.T. Nadiga & M.A. Christon (LANL)

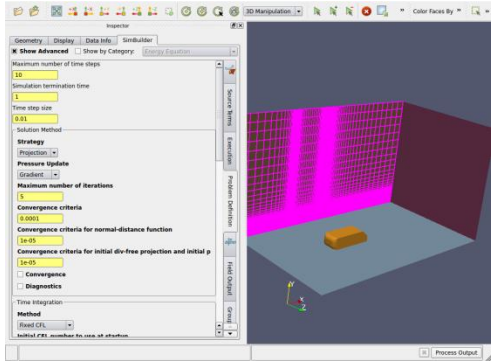
FY14 Science Highlight: Simulation Tools [THM-SBIR Leveraging]

CMB pre-processing tool

- Update on latest developments for creating Hydra input from CMB
- Configurable XML file for specifying Hydra input parameters
- Python script for generating Hydra input file
- Beta users to improve Hydra integration

Contributors:

A. Bauer, Kitware

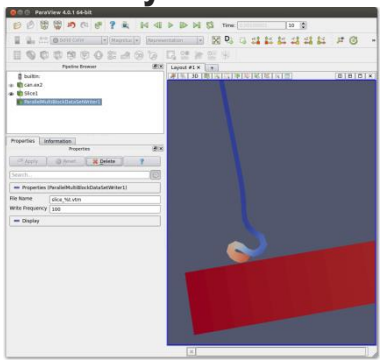


ParaView tutorial

- Introduction to use
- Dealing with large data in parallel
- Connecting to HPC machines
- Python scripting for repeated tasks
- Catalyst for *in situ* analysis and visualization

Contributors:

D. DeMarle, Kitware



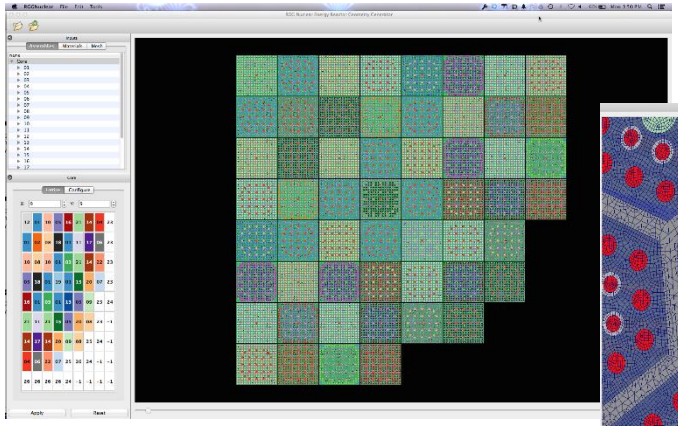
RGG Application Tool

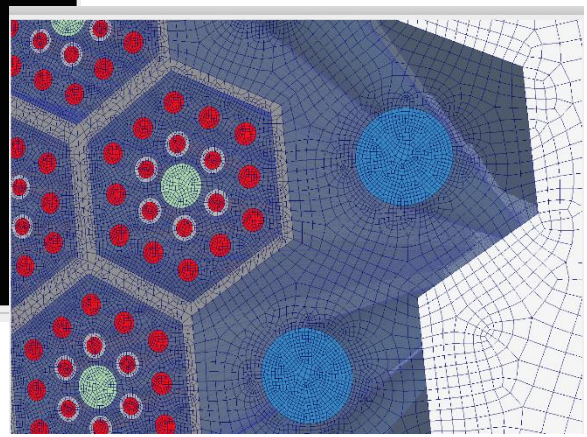
- Pin Editing
- Creating and Modifying Assemblies
- Creating and Modifying Cores
- Integration with MeshKit/RGG Tools
- Mesh Generation and Visualization

Contributors:

R. Jain, Argonne

B. O'Bara, Kitware

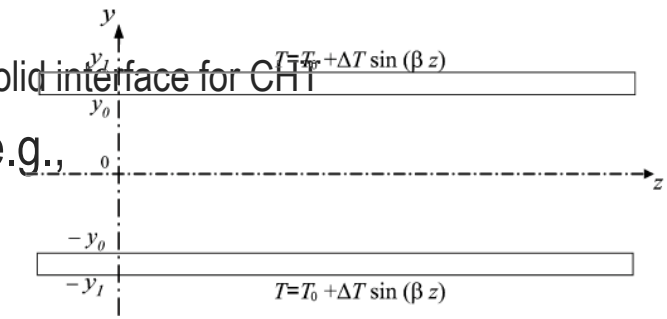


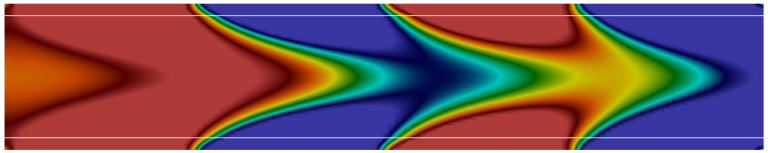


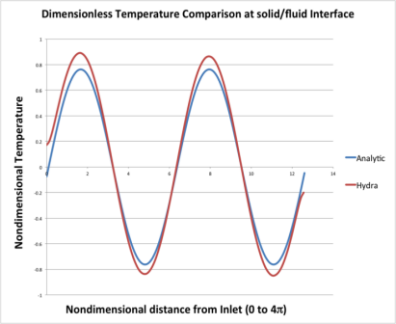
Native Conjugate Heat Transfer Uses Automated Interface Detection for Complex Reactor Geometries

- Conjugate Heat Transfer between fuel and coolant required for TH/Neutronics/Surface coupling
- Automated interface detection segregates solid materials from fluid materials
  - Automatic specification of no-slip/no-penetration BC's, turbulence quantities, etc.
  - Preserves heat flux continuity at the fluid-solid interface
  - Avoids time-consuming, error-prone user identification of fluid-solid interface for CHT
- Hexpress/Hybrid permits meshing multiple volumes, e.g., fluid and solid, in one step with coincident interfaces

Automated interface detection can be applied to arbitrarily complex geometries

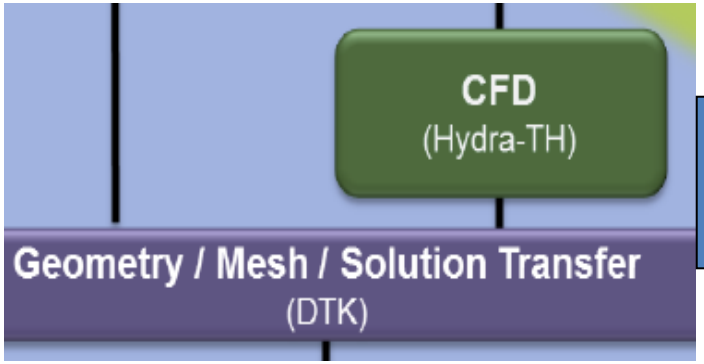




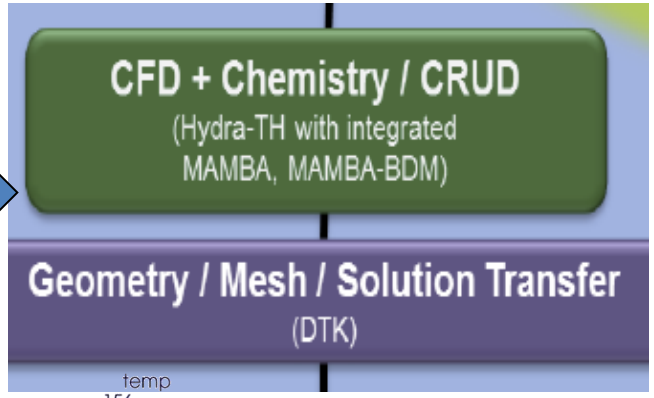


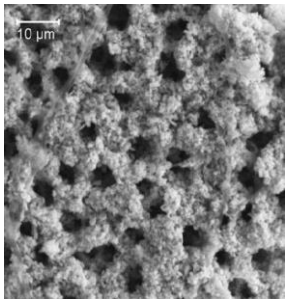
Conjugate forced convection heat transfer in a plane channel: Longitudinal periodic regime (A. Barletta et al., International J. Thermal Sciences 47, 42-51, 2008).

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

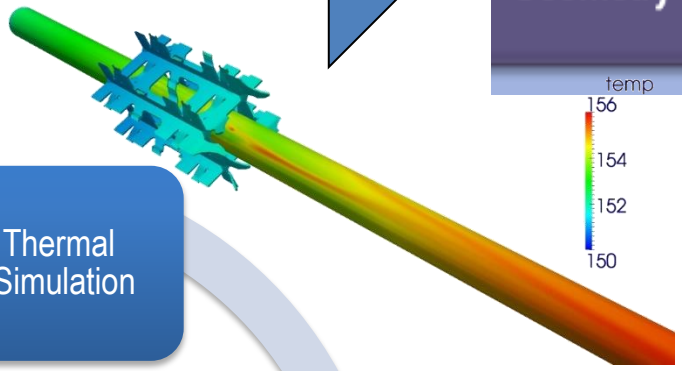


Evolution of Hydra-TH in VERA From End of Phase 1 to Phase 2





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



Fully-Implicit Projection

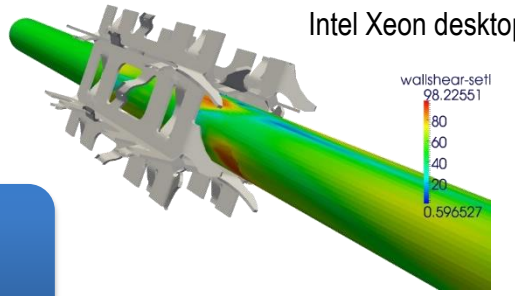
- RNG k-ε model
- Re ~ 4.0×10^5
- $q_w = 10^6$ W/m^2
- 2.4M elements, ~18M DoF
- ~ 4.75 hours on 16-core Intel Xeon desktop

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

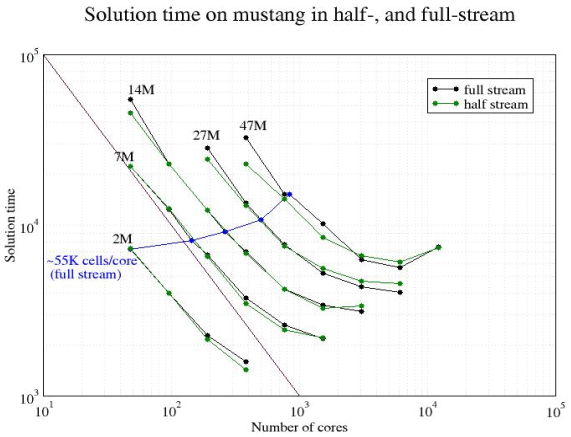
Wall-Shear, Temperature, Heat Flux



Performance Assessment, Memory Improvements and Linear Algebra

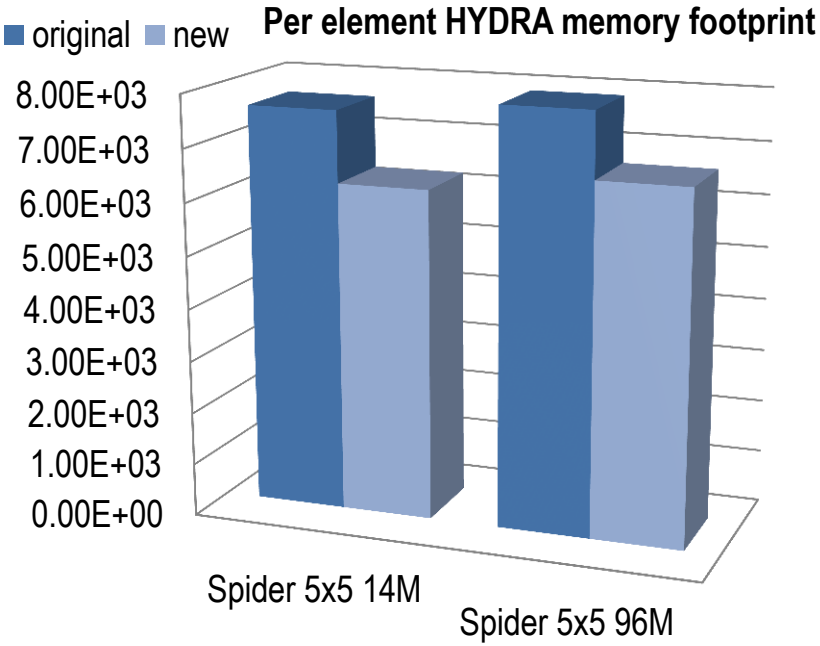
Assessment of computational performance using existing MPI-parallelism on Titan and LANL Turquoise HPC clusters using V5H GTRF problem

- Hydra-TH scales when using 20 – 50,000 elements per core
- No consistent benefit from running Hydra-TH in full stream mode on Titan



Implementation of nvidia AMGX solver for TITAN

New matrix pre-allocation algorithms for Hydra's PETSc linear solvers



PETSc → Trilinos

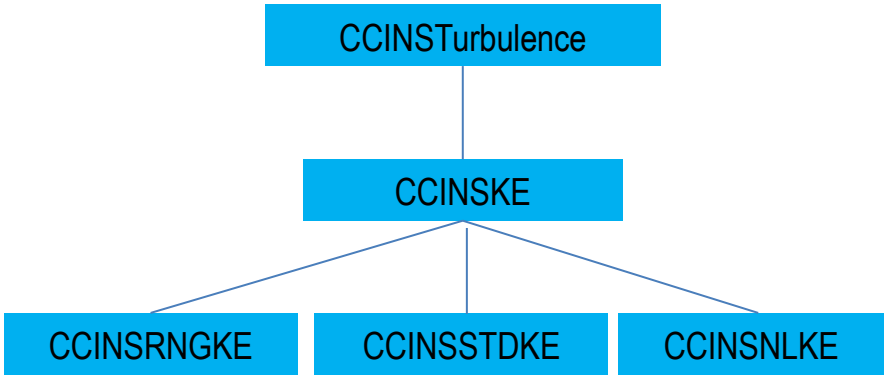
Conversion to Trilinos/ML for PPE

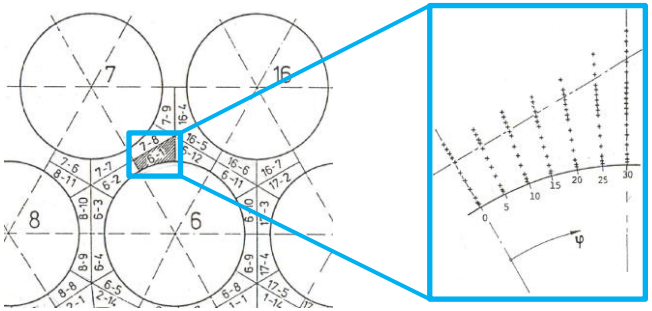
- Required by VERA for Multiphysics Coupling Avoid library incompatibilities in VERA integration
- Follow new releases of ML: maintained under Trilinos
- Implement with: Epetra/Trilinos vector and matrix and Belos/Trilinos solver packages
- Easy-to-use generic wrappers in Hydra linear algebra classes: Minimal change to client code

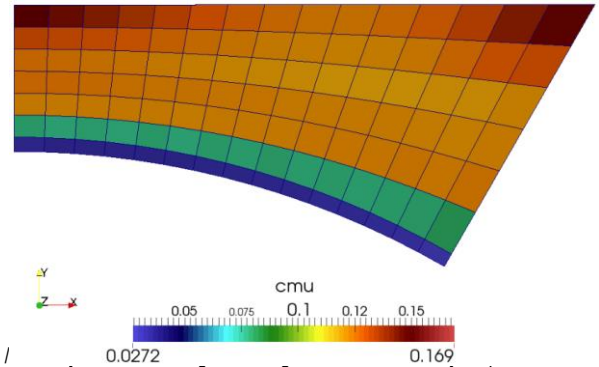
New k-ε models in Hydra-TH

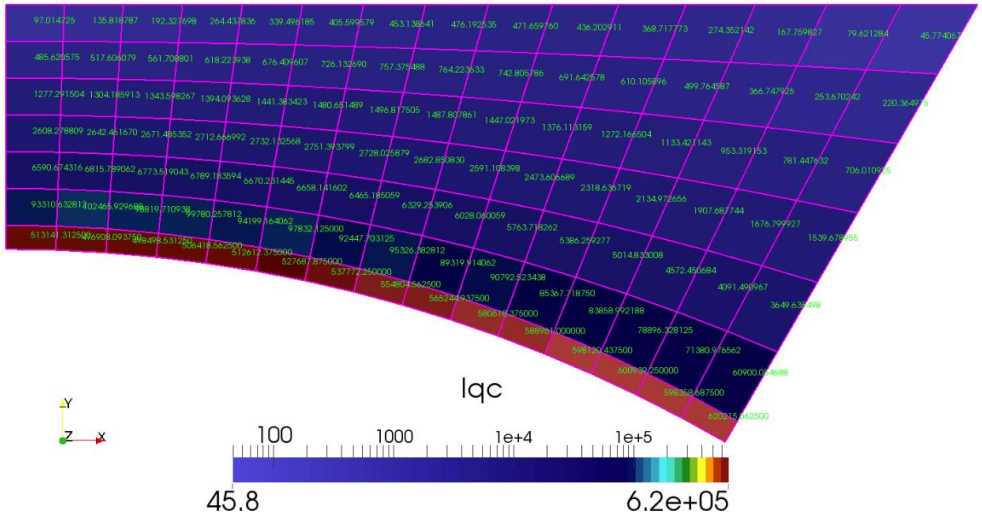
Restructuring permits addition of multiple variants of the k-ε model

- Standard model
- RNG model
- Non-linear model (anisotropic viscosity model)
  - Captures secondary rotational flows damped by other k-ε models



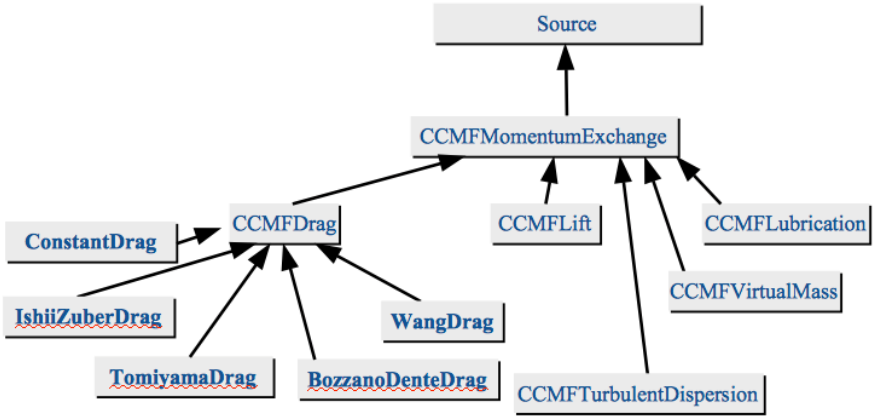






Ratio of Linear to Quadratic Stresses

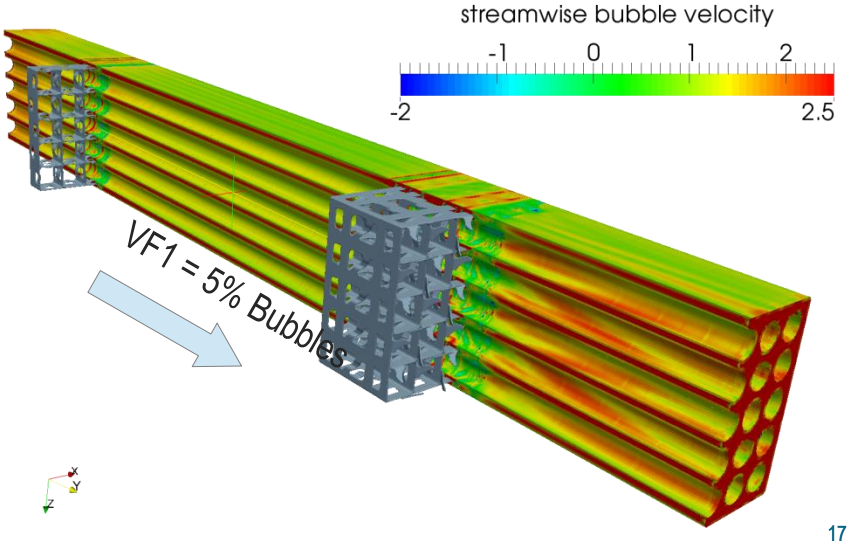
Multiphase Flow in Hydra-TH



- **Generic *N*-field algorithm:** semi-implicit and fully-implicit, skew-symmetry preserving, predictor-corrector algorithm
- **"Expert-user" multiphase capability:** User can specify different closure for any field-pair
- **Scales:** Tested on Titan with 35K CPU cores
- **Momentum exchange:**
  - drag, lift machinery implemented, verified (more closures to come)
  - mass and energy exchange (e.g., vetted THM sub-cooled boiling model) to come

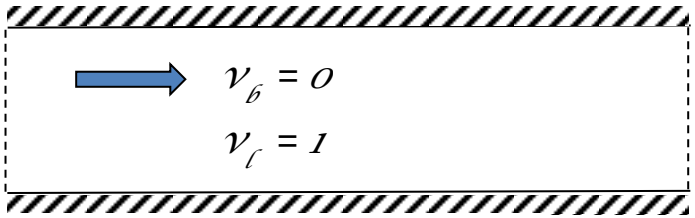
Example calculation

- Two-phase calculation with drag
- V5H 5x5 Spacer – 14M Cells
- Re=28,000 (TAMU Exp. Cond.)
- 100:1 water/air density ratio



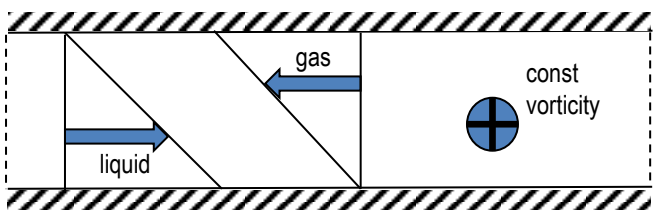
Multiphase Flow in Hydra-TH – Verification

- **Verify drag force anti-symmetry and momentum-conservation to machine precision**
- Drag verification



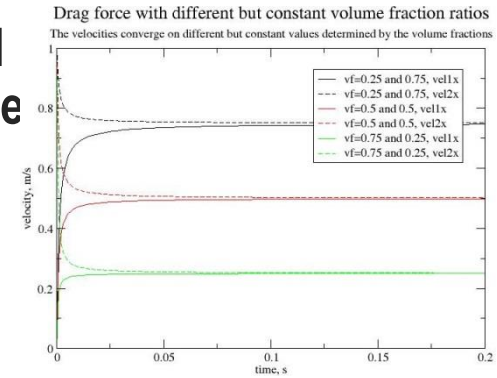
$$\mathbf{F}_d^D = -\frac{3}{8r_d} C_D \alpha_d \rho_c \left|\mathbf{v}_r\right| \mathbf{v}_r$$

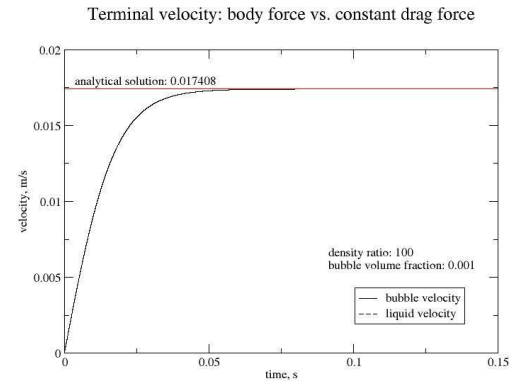
- Lift verification

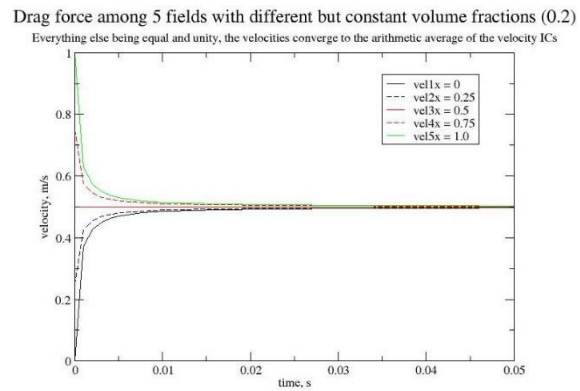


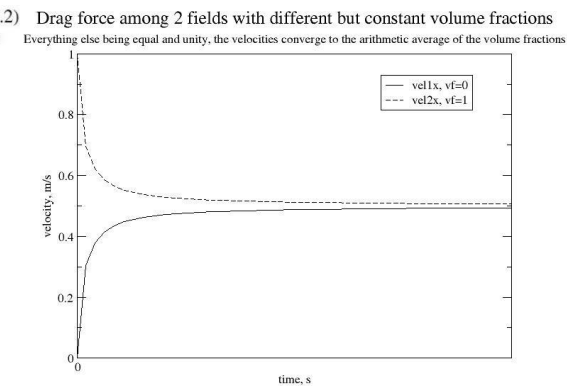
$$\mathbf{F}_d^L = -C_L \alpha_d \rho_c \mathbf{v}_r \times (\nabla \times \mathbf{v}_c)$$

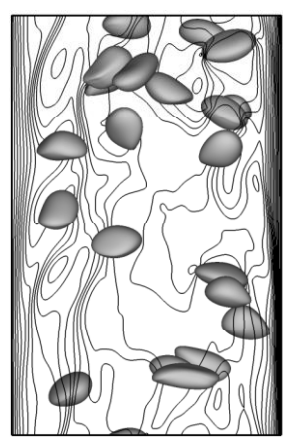
- More complex cases testing lift from:
  - Emilio Baglietto, Star-CCM+
  - Gretar Tryggvason's interface tracking code









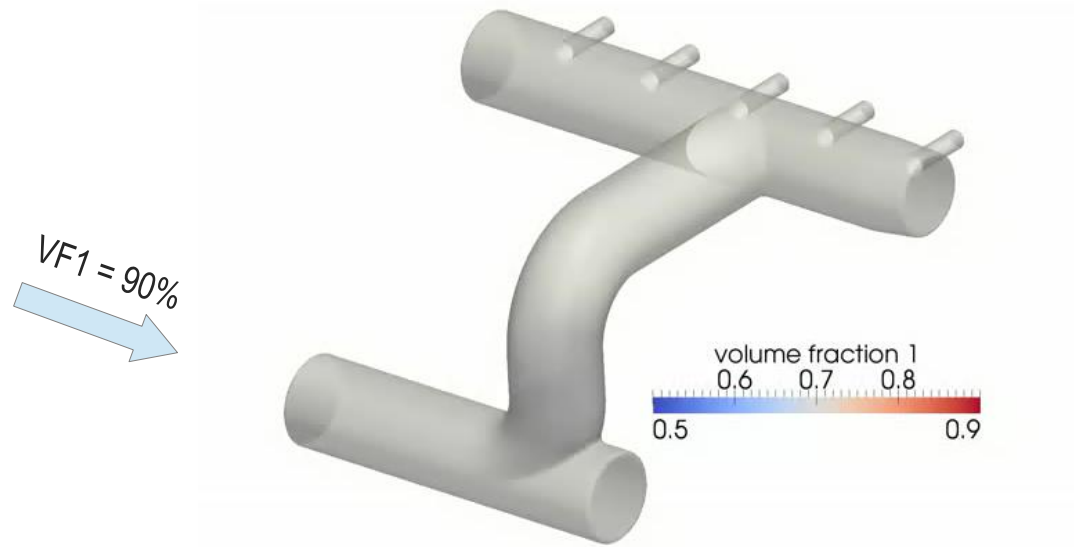


- Vary bubble diameter
- Vary spatial directions
- Vary volume fractions
- Vary number of fields
- Validation: balance of drag and body force results in terminal velocity with analytical solution

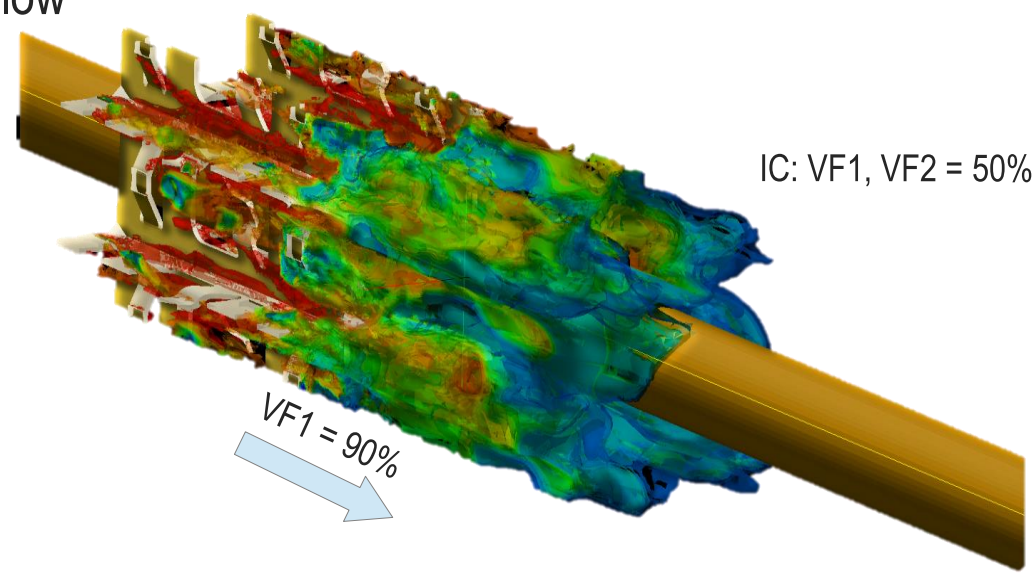
Some Multiphase Flow Calculations

IC: VF1, VF2 = 50%

- Manifold flow
- 2 fields, same densities
- Coupled through single pressure via projection algorithm
- IC: VF1: 50%, VF2: 50%
- BC: VF1 at inlet = 90 %



- V5H GTRF 3x3
- Same conditions as previous pipe flow
- Titan (400 CPU cores)



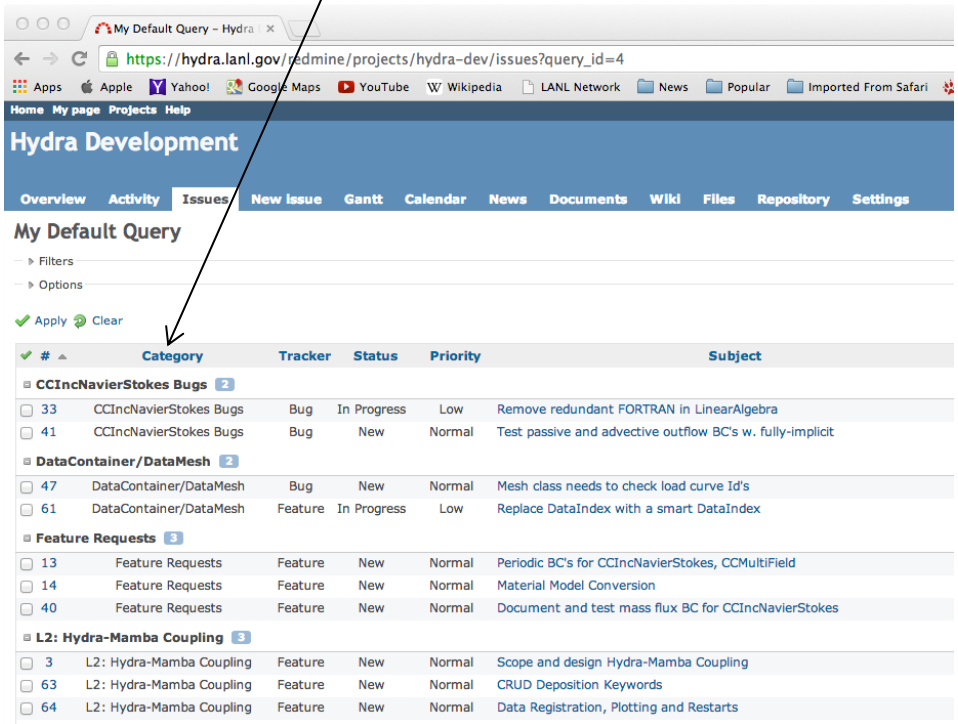
IC: VF1, VF2 = 50%

Scaled to 36,000 cores on Titan,
192 Million element mesh

Upgraded Development Environment – based on methods/practices used by Kitware, DS SIMULIA

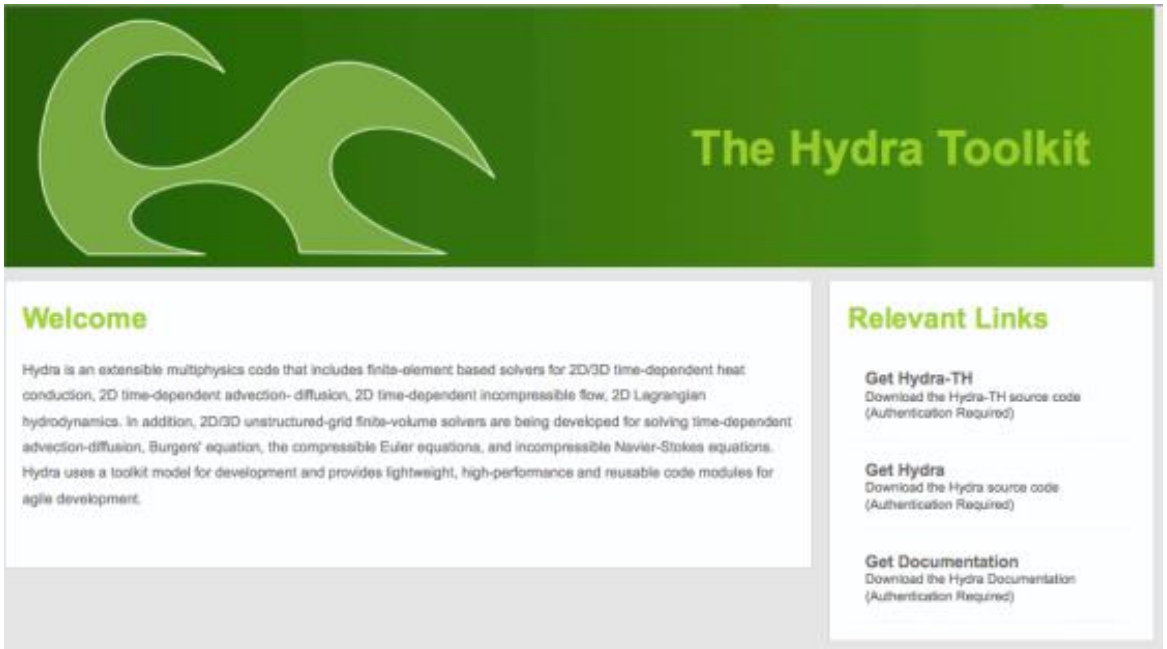
- FY14 saw a rapid expansion in Hydra developers outside LANL
  - Typical LANL process was extremely long (~3 months), required use of VPN which typically doesn't work for non-LANL computers, and resulted in many project delays
- Desirable to have "open-access" to project tracking, repositories, documentation while preserving export controls
  - Model based on environment used by Kitware, and practices by Kitware/DS SIMULIA
  - Using ccs-green machine at LANL on "open" network
  - git for code repositories, Redmine for development process, gerrit for code-reviews, migrating to CTest/CDash
  - New time for adding a developer ~ 3-4 days for Tech Transfer licensing
  - 12 new developers added over the past 6 months

Mapping issues by milestones and other tasks such as bug fixes, features



Hydra-TH Deployment, Support & Impact

- Early deployment of Hydra-TH was requested by a number of users, e.g., Jin Yan at Westinghouse, AMA, Dec., 2012
- Hydra-TH Licenses since January 2013
- User support, code distribution, porting issues have diluted Hydra-TH development efforts in FY13/FY14
- E-mail support: hydra-th-users@lanl.gov
- Downloads: get-hydra.lanl.gov
- Pursuing code distribution via Kitware…



Institution	Seats
AECL (Canada)	3
Aston University (UK)	2
Carnegie-Mellon	2
INL	1
Kitware	5
MIT	8
NASA -- Houston	1
NCSU	7
ORNL	2
Penn State	2
Sandia	3
Texas A&M	2
TVA	2
U. Michigan	3
U. Texas	2
WEC	7
Total	**52**

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

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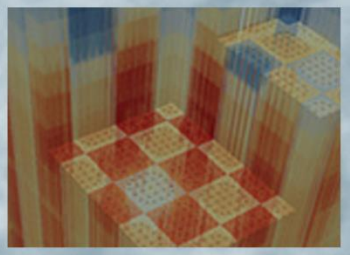
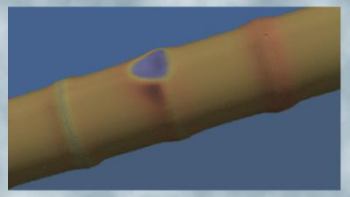
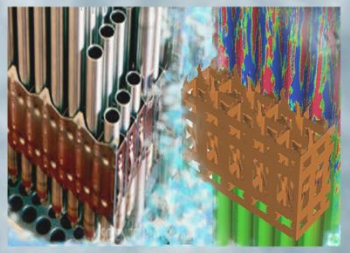
Closure Modeling Year 4 Highlights







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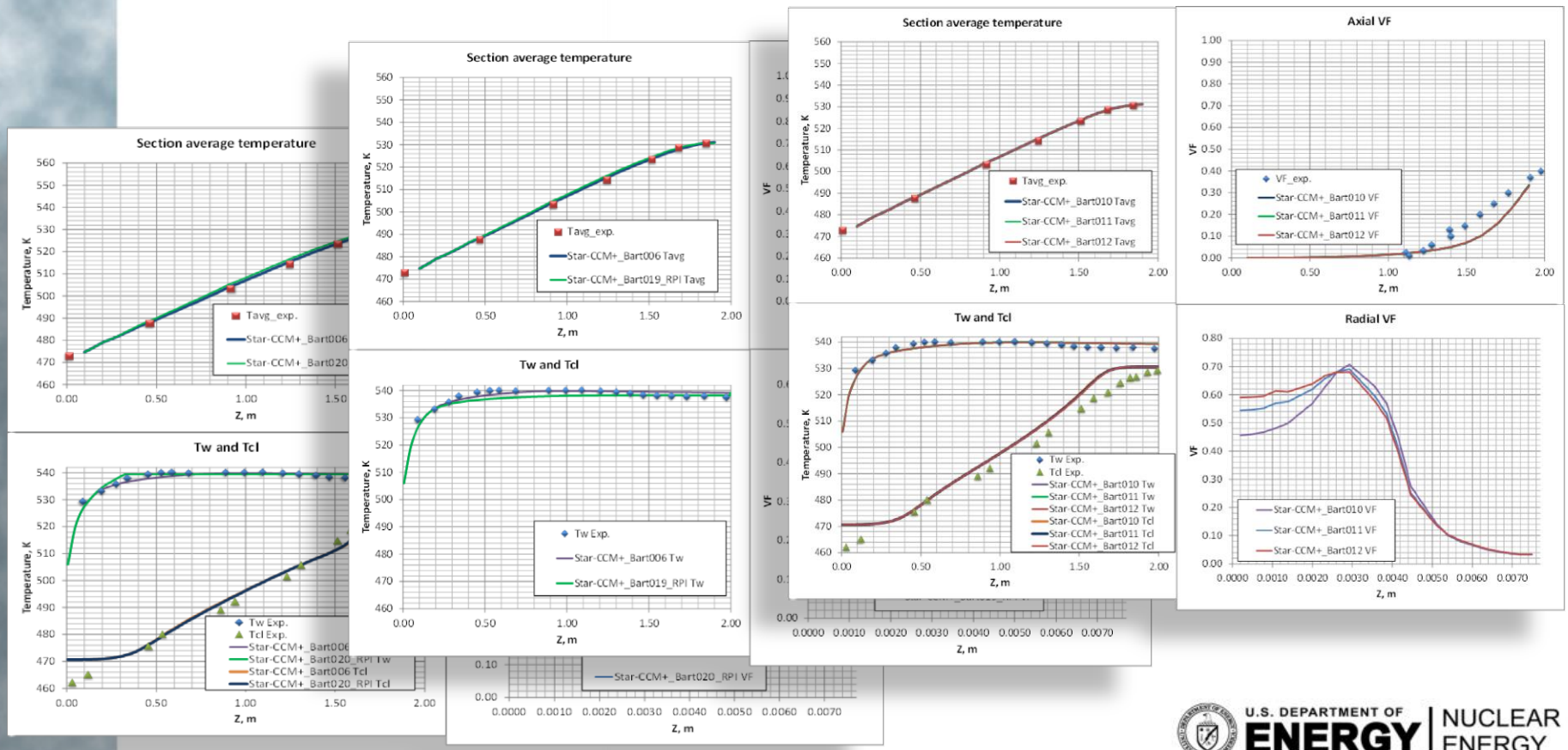
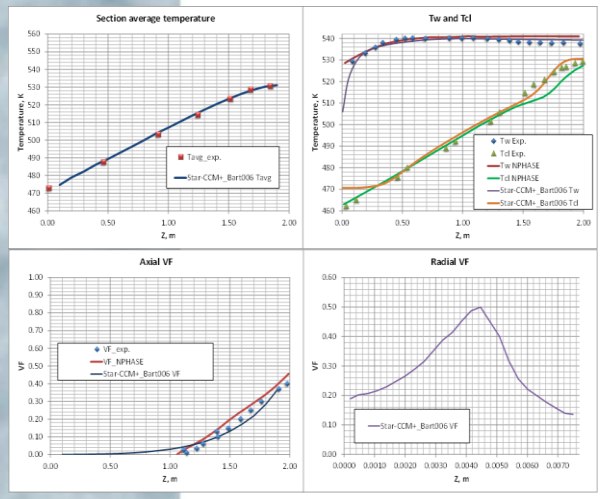
2013 Delivered:
GEN-I Robust Baseline Closure

- Demonstrated Maturity of Assessed Closures
- Demonstrated Portability of Closures (STAR-CCM+ vs. NPHASE)
- Confirmed the findings from PoR-3 V&V Study (closure UQ)
- Baseline for ongoing implementation in Hydra-TH



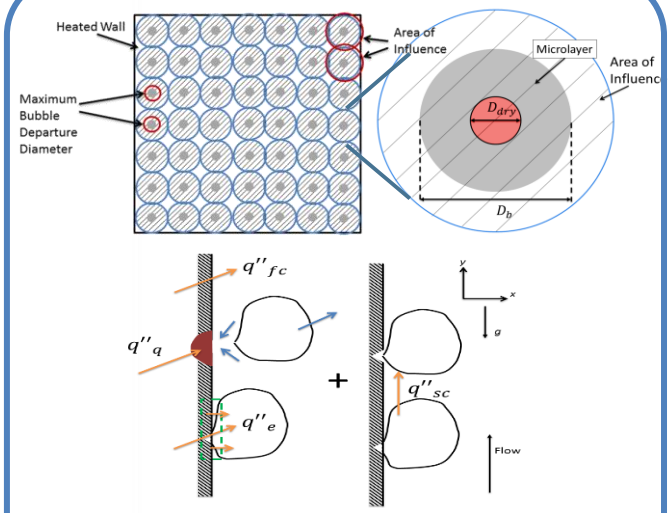
2014 Focus:
GEN-II Boiling → towards DNB

Robust Baseline Closure



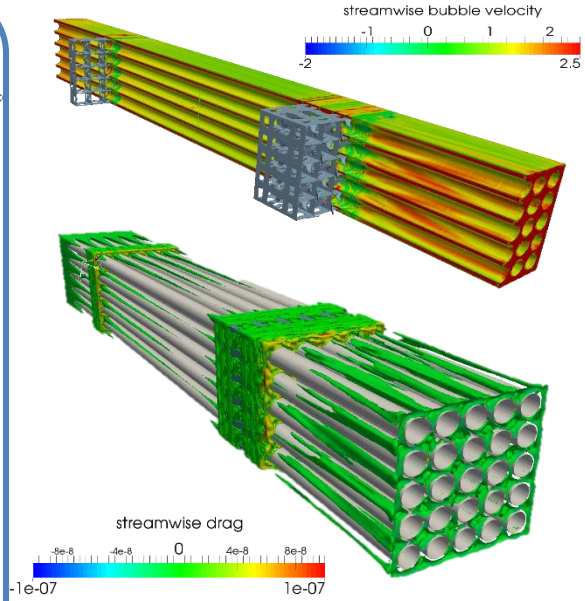
- First Generation Closure in Hydra-TH should leverage existing experience
- Implementation of baseline closure in STAR-CCM+ allows direct comparison to CD-adapco baseline closure results (platform independent)
- Sensitivity of model parameters should confirm PoR-3 studies

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)

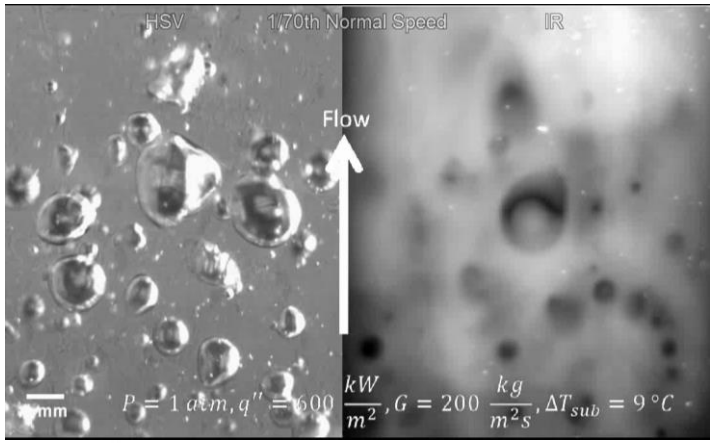
New M-CFD Platform

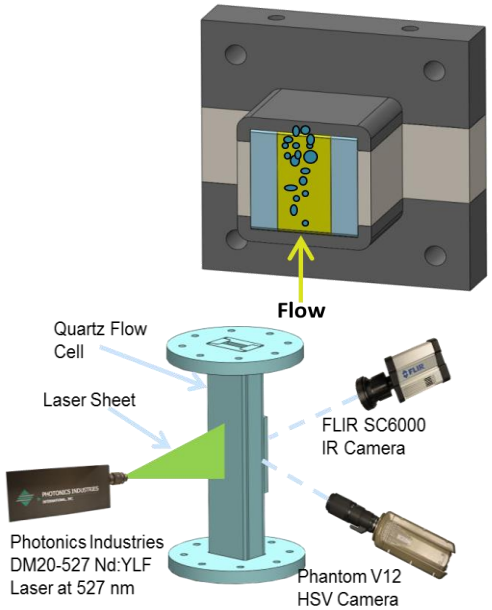


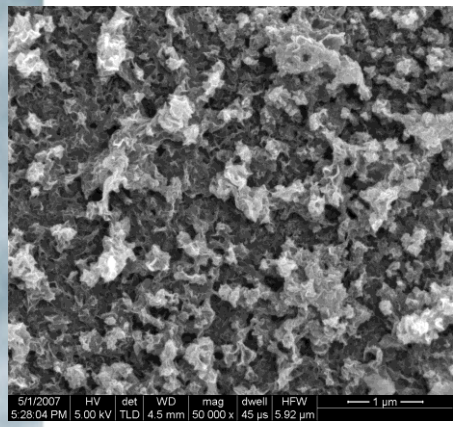
- Hydra-TH baseline multiphase capabilities first shakedown
- Hydra-TH Multiphase implementation targets enhanced applicability towards transient simulations (including fast transients)

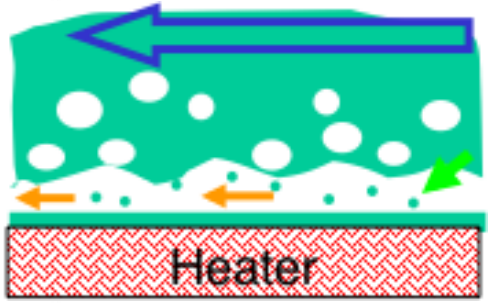
New Physical Understanding: Subgrid Surface Representation

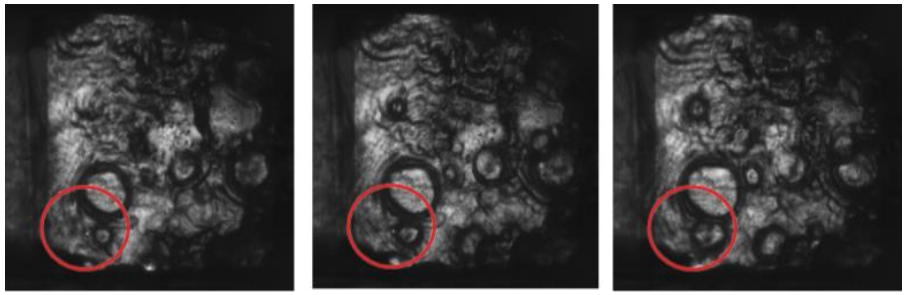
- **Extension to DNB requires physical representation of heater surface**
- **Includes bubbles interaction**









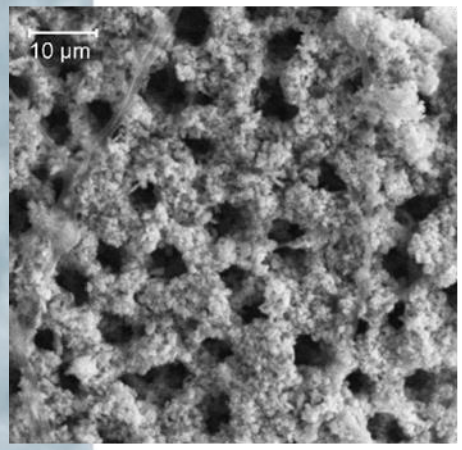


- Platform must include the modeling capabilities
- Experiments/DNS are used for continuing improvement of physical understanding
- Understand/agreement on boiling microhydrodynamics

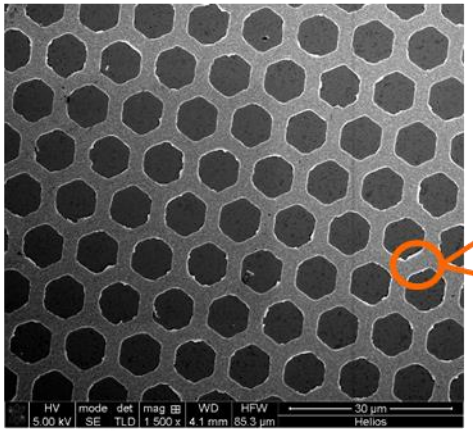
Synthetic CRUD and its Effects on Subcooled Boiling

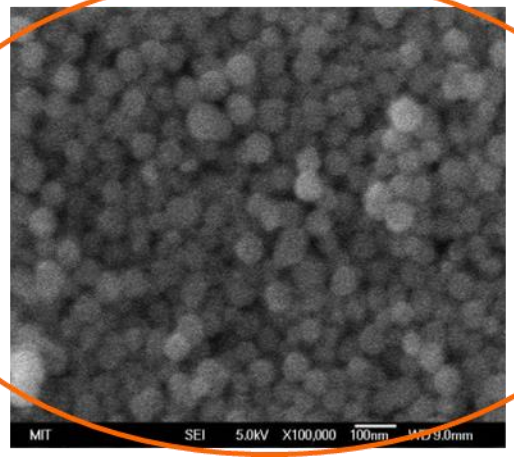
Synthetic CRUD: iron-oxide nanoparticles deposited with layer-by-layer technique, chimney array created by photolithography; laid on sapphire-ITO heaters

Reactor CRUD



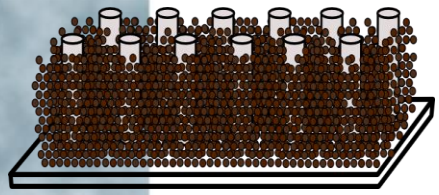
Synthetic CRUD

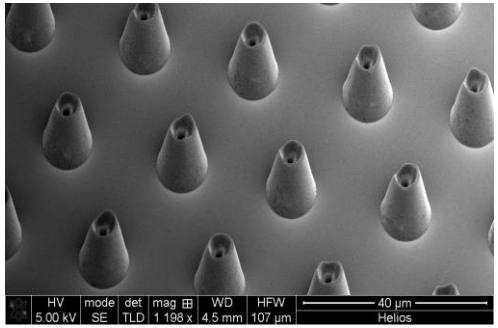




Carolyn Coyle, Jacopo Buongiorno, Thomas McKrell - MIT

- 10µm diameter, 25µm pitch





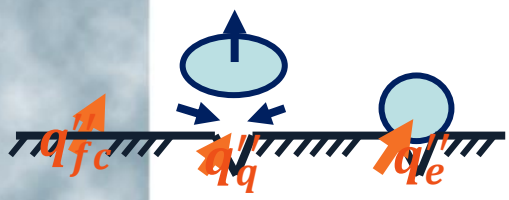
	Reactor CRUD	Synthetic CRUD
Composition	NiO, Fe_3O_4, $NiFe_2O_4$, ZrO_2	Fe_3O_4
Thickness	10-100 µm	5-15 µm
Roughness	R_a ~ 0.5-3.0 µm	R_a < 0.5 µm
Wettability (contact angle)	10-30°	20-40°
Porosity (not including chimneys)	40-50%	40-60%
Pore size	0.1-1.0 µm	0.02-0.2 µm
Chimney size	2-10 µm	5-10 µm
Chimney spacing	5-20 µm	10-100 µm

FY14 Science Highlight

GEN-I

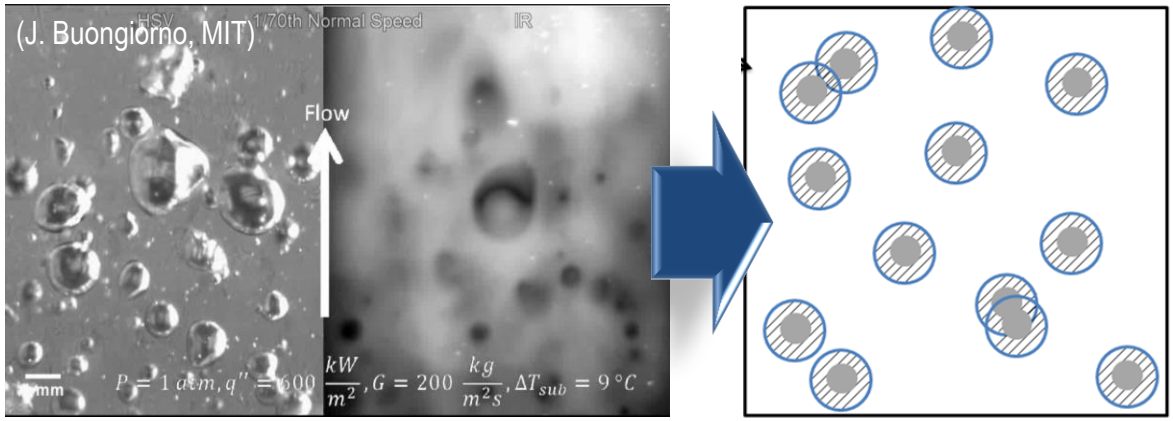
$$q''_{tot} = q''_{fc} + q''_{q} + q''_{e}$$

Convective Quenching Evaporation



- Mechanistic model proposed by Judd and Hwang (1976)
- Adapted by Kurul and Podowski (1990) for wall heat flux partitioning during pool nucleate boiling.
- While limited it is de-facto the only model in M-CFD

GEN-II Heat Partitioning Model

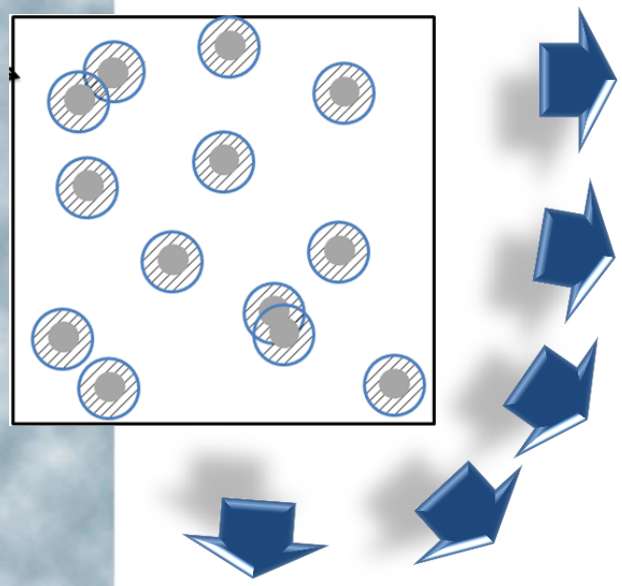


Subgrid Representation of Surface (flow boiling)

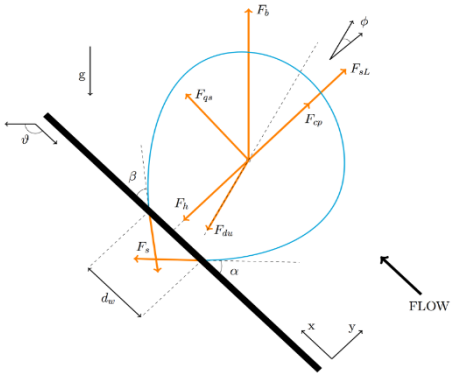
Challenges:

- Extremely complex phenomena, cannot be represented by first principle
- Local characteristic in the CFD solution must be used to drive the SGS Model
- Evolving/incomplete understanding of bubble dynamics
- Generality – e.g. surface characteristics

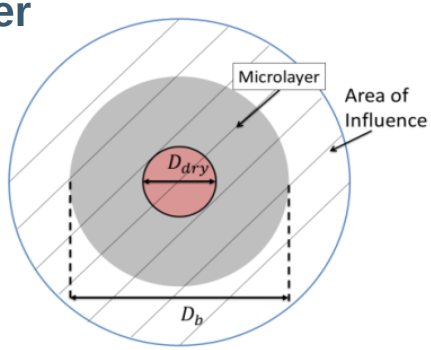
GEN-II Heat Partitioning
Quick Overview



1. Mechanistic Representation of Bubble Lift off and Departure Diameters

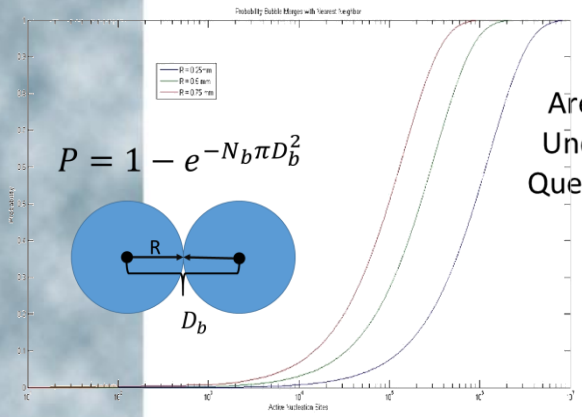


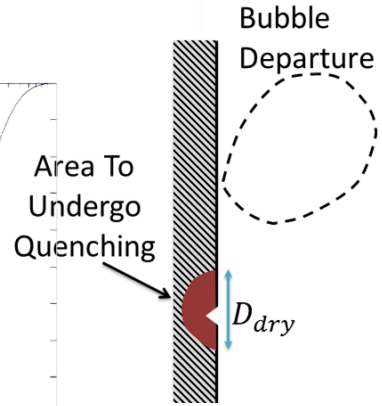
2. Accurate evaluation of evaporation heat flux by modeling effective microlayer

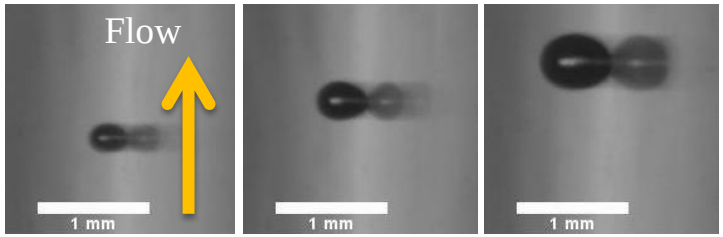


3. Account for sliding bubble effect on heat transfer and nucleation sites

5. Account for bubble interaction on surface





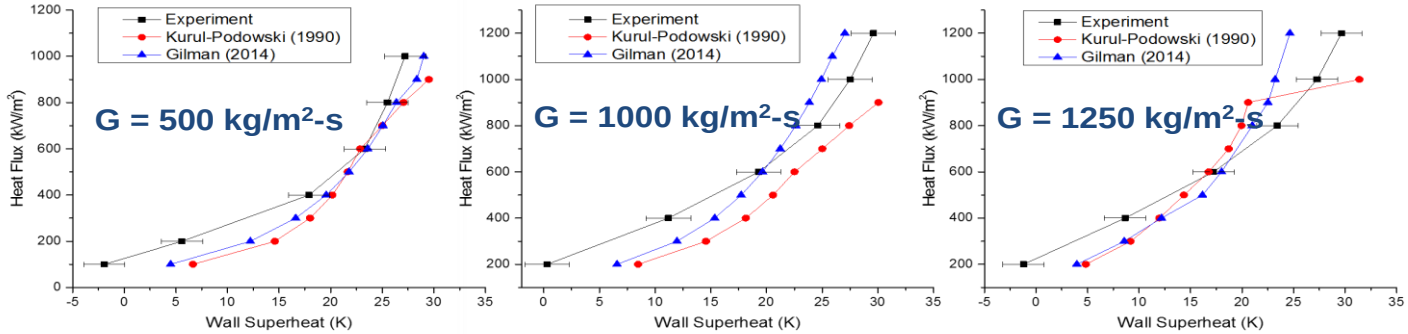


4. Account surface quenching after bubble departure

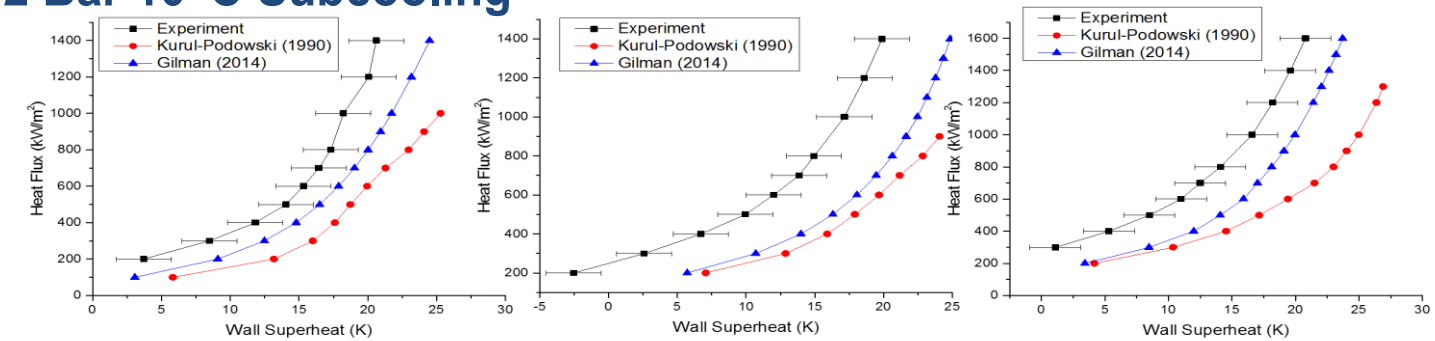
Calibration-free Assessment

extensive small scale CASL database

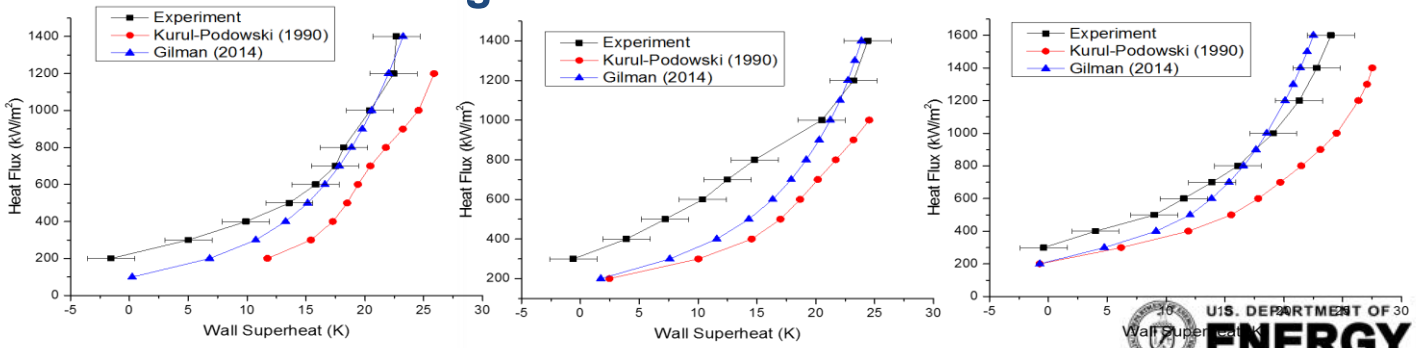
1 Bar 10°C Subcooling



2 Bar 10°C Subcooling



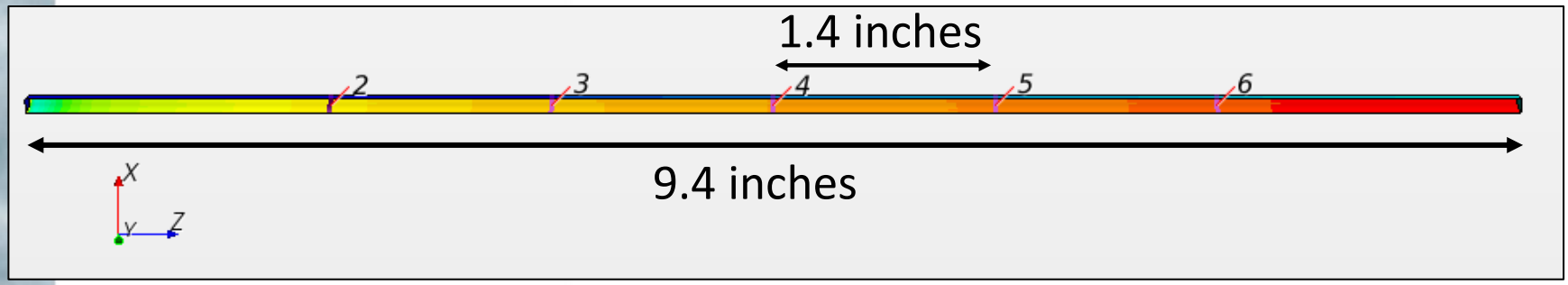
2 Bar 15°C Subcooling



Rohsenow High Pressure Experiment

- P = 2000 psi (137.9 bar)
- Nickel tube 9.4 inches long
- Inner diameter of 0.1805 inches
- Outer wall temperature measurements at 7 locations
- Vertical upflow

Heat Flux [MW/m2]	Inlet ΔT_{sub} [K]	Thermocouple Positions	Experiment ΔT_{sup} [K]	Experiment Error [K]	Gilman (2014) ΔT_{sup} [K]
3.41	130.7	5, 6	2.58	+/- 1.7	0.98
4.07	130.9	2,3,5,6	2.65	+/- 1.7	1.10
4.61	131.0	2-6	3.92	+/- 1.7	1.02
5.11	136.4	2-6	4.14	+/- 1.7	2.36



CLS Overall Review: Year 1-4

- Three fundamental Steps aimed at “delivery” and “science”

Closure Evaluation: physical representation, assessment database, robustness

Closure Model UQ: parameter sensitivity (driving experiments and ITMs), uncertainty evaluation, challenges

Closure Model Implementations: code dependency, portability, extendibility

1

ITM/DNS Refocusing: microscale boiling ITM not sufficiently mature, not applicable for closure development

Isothermal Bubble transport greatly support interpolation/extrapolation of experimental findings

GEN-I vs. GEN-II: necessary to separate closure efforts in two successive generations

2

GEN-I Delivery: Robust First Generation Closure in Hydra-TH should leverage existing experience

GEN-II Improved physical representation: Second Generation Closure should incorporate new physical understanding

Increased synergy with experimental “micro” measurements

Extended applicability

Include modeling toward limiting behavior (CHF)

3

Feedback from THM Science Council Representative for FY14 Efforts Reported at THM Workshop

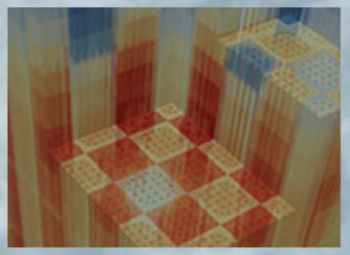
"R. Lahey -- indications after the FY14 THM workshop underline positive advancement and point to an important discussion on the role of CFD codes in the CASL effort. The indications are particularly relevant for the Phase-2 effort.

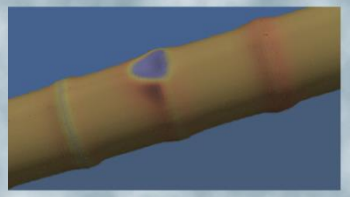
THM Workshop Comments & Recommendations:

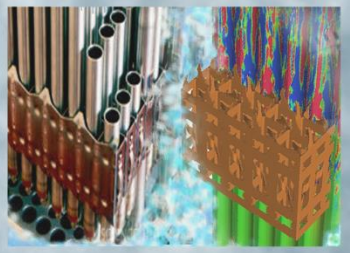
- Solid verification of Hydra-TH methods is a necessary component but should not use large resources, we should move up and refocus the expertise to support development
- **Hydra-TH should not be the only tool for short term deliverables**
  - ✓ leverage commercial codes "where appropriate" to support critical path, application of models
  - ✓ allow the Hydra-TH development to work towards the final goal rather than continuous partial delivery
  - ✓ off-load support effort
- **Very Positively impressed by experimental results, looks to be on track to support model development and demonstration**
- **CLS deliverables seems to be on target, good split between deliverables and future Milestones groundwork**

A DOE Energy Innovation Hub

Phase 2







U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

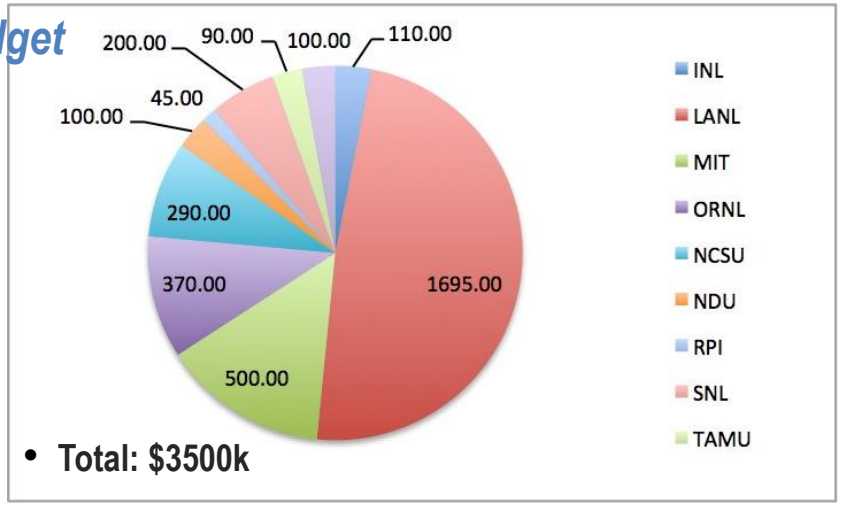
Thermal Hydraulics Methods

FY15 -- Plan of Record PoR-10 and PoR-11

Activities and Priorities

- Priorities (Defined by SLT):
  - Multiphase w. GEN-I model for subcooled boiling
  - Solutal transport, variable density in Hydra-TH
  - Extensions to single/multiphase turbulence models
  - Validation of momentum closure models
  - Enhanced DNB closure modeling
- Activities – FY15 THM Workshop

Budget



- **Total: $3500k**

Challenges and Risks

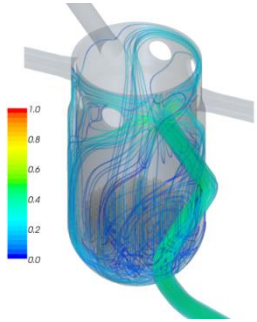
- Challenges:
  - Coordinating efforts among the 10 THM institutions
  - Balancing R&D efforts and code development with V&V activities, user support with limited resources
  - Code delivery with limited resources and manpower
- Risks:
  - Staff retention
  - Impact of user support on development

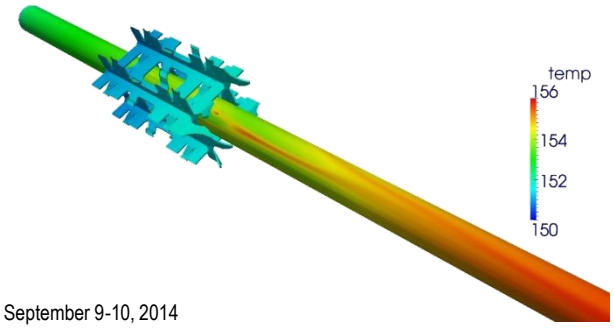
Milestones

- L1: Qualify multiphase CFD capability for bubbly flow regime: Hydra-TH will be used to simulate out-of core fluid experiments targeted at providing validation data for the bubble flow regime, with predictions contrasted to measurements.
- L2: Demonstration of CASL M-CFD Closure Models for Subcooled Boiling and Bubbly Flow
- L3 CFD milestones, and CLS milestones being defined to support the L2 milestone and future L2 in year 2-3
- THM Workshop focused on coordinating research efforts, organizing requirements for DNS/Experimental data and improving V&V/UQ efforts

THM Phase-2 L2 Milestones

Year	Category	CP	L1 Milestone Supported	Description
1	Thermal-Hydraulics	CHF (DNB)	4	Demonstration of CASL M-CFD Closure Models for Subcooled Boiling and Bubbly Flow
2	Thermal-Hydraulics	CHF (DNB), CILC	11, 18	Wall Closure Models for Subcooled Boiling using DNS for Wall Conditions
	Coolant / Corrosion Chemistry	CHF (DNB), CILC, LOCA	12	Advanced Subgrid-Scale Modeling of Corrosion Chemistry and Boron Mixing/Precipitation (CFD-based CILC)
3	Thermal-Hydraulics	CHF (DNB)	18	Demonstration of Gen-II CASL M-CFD Closure Models for the onset of DNB
	Thermal / Solutal Convection	Convective Flow, LOCA	12	Demonstration of Thermal and Solutal Convection for Boron Mixing during ECCS Injection
4	Thermal-Hydraulics	Flow Regimes	15	Investigation of Flow Topology Recognition for M-CFD Closure Models for BWR-like Flow Regimes
	Coolant / Corrosion Chemistry	CHF (DNB), CILC	6, 18	Demonstration of advanced subgrid-scale chemistry model for CRUD deposition
5	Thermal / Solutal Convection	CHF (DNB)	18	Low flow rate boiling in a rod bundle
	Deployment	N/A	19	Hydra-TH User, Theory, V&V/THM Benchmarks Manuals

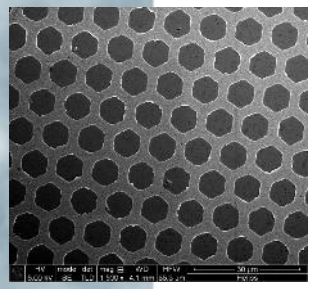




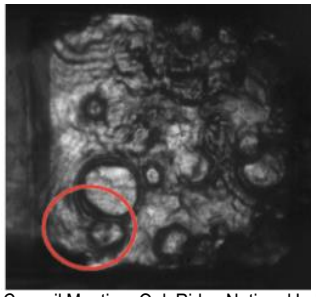
Demonstration of GEN-II M-CFD Closure for onset of DNB

GEN-II

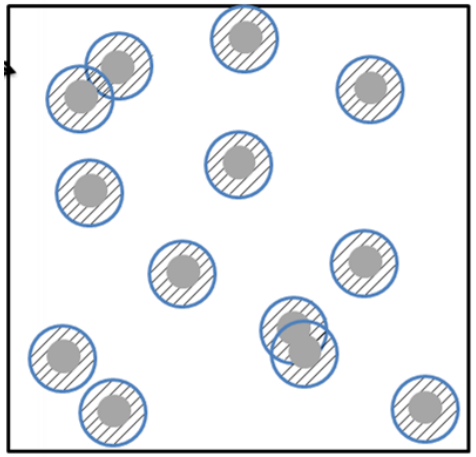
- **Developed and tested a new physically-based wall boiling model in CFD**
  - Captures physical phenomena on heated surface
  - More accurate wall temperature predictions without data fitting
    - Low and High Pressure
- **Developed statistical bubble tracking method**
  - Limiting nucleation site density on the surface
  - Calculates dry area for extension to DNB prediction

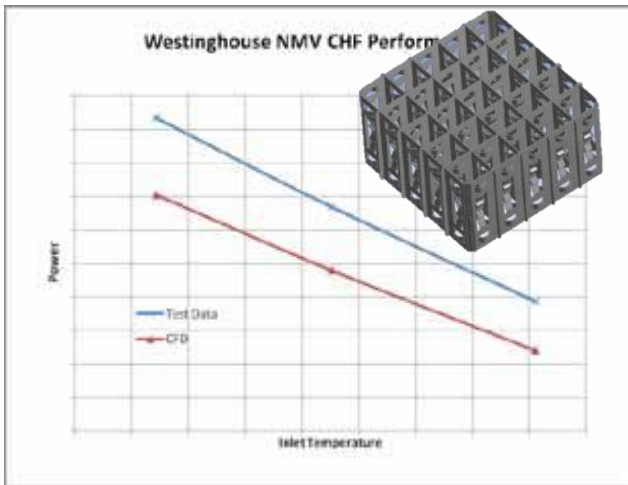


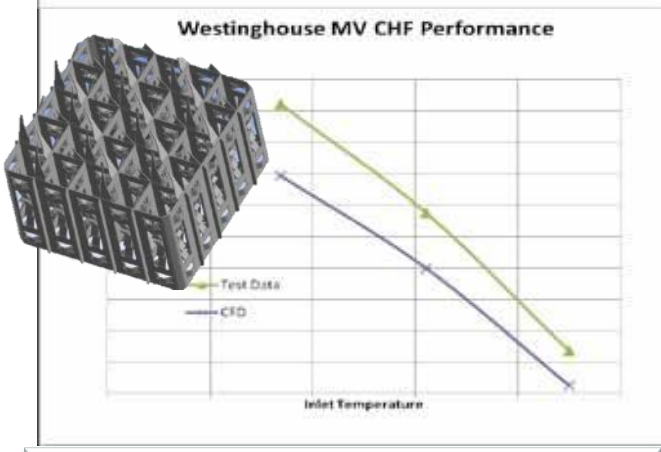
Synthetic CRUD (MIT)



DNB inception - Nam Dinh (NCSU)





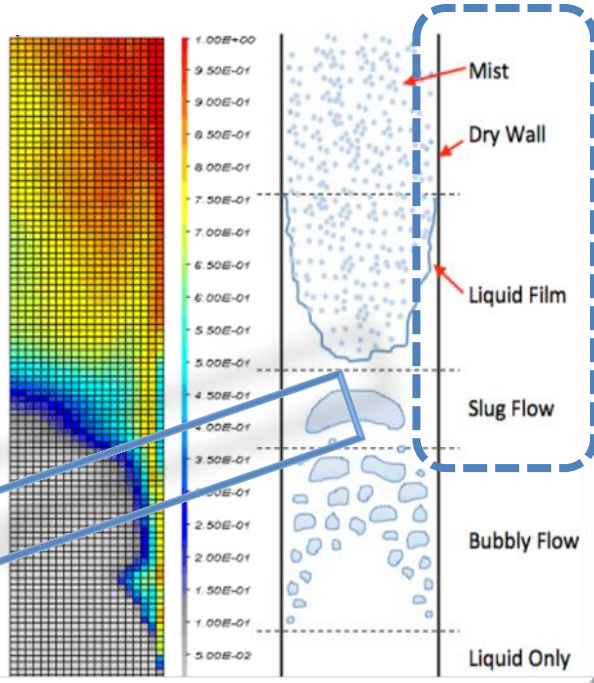


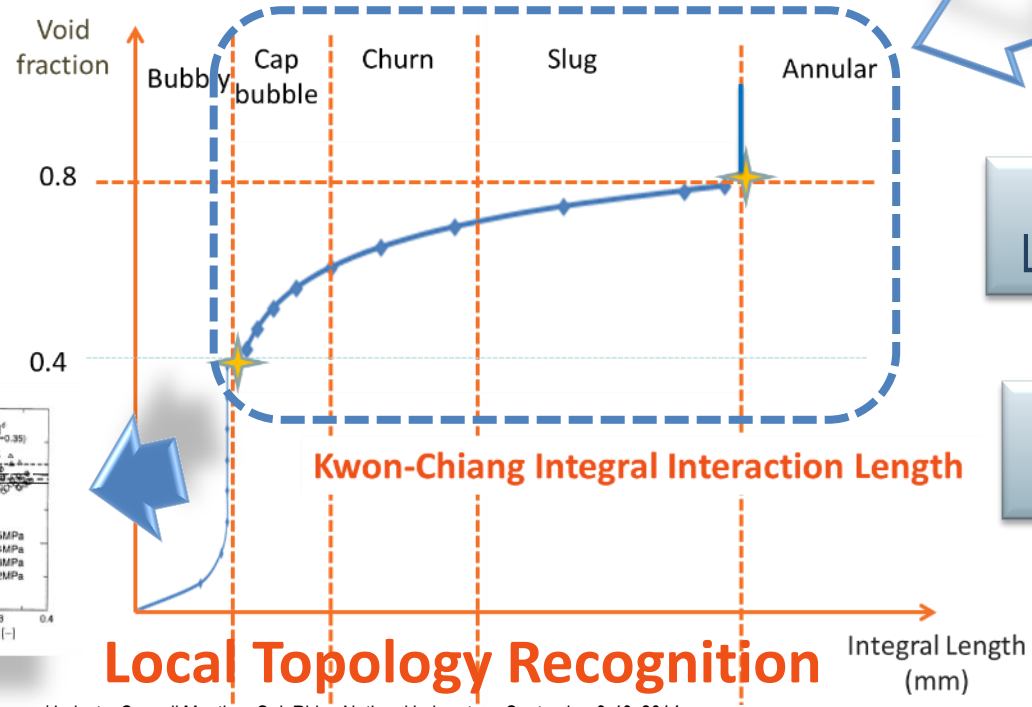
Current State of the Art

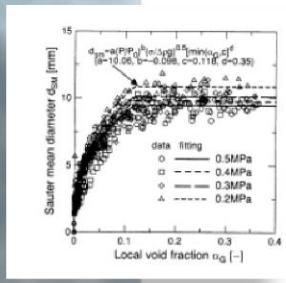
Jin Yan -ISACC-2013, Xian, China

Extension to BWR Application

- ***Local Topology Recognition*** applies adequate closure on a cell-by-cell basis
- ***Algebraic Length Scale*** for robust "fuel" applications
- **Extendible** to off-core via population balance approaches
- **FY14 activities** for accelerated delivery demonstrate promising potential



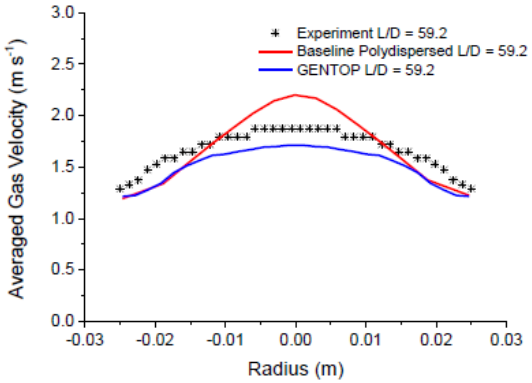


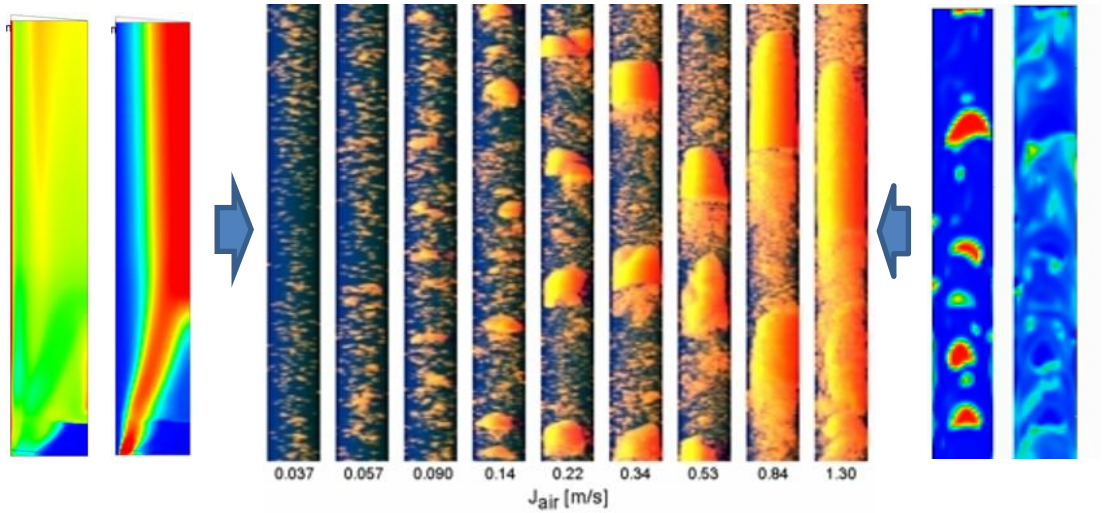


A fundamental distinction:
Local topology vs flow regime

Confidence based on experience and validation

Extension to BWR Application



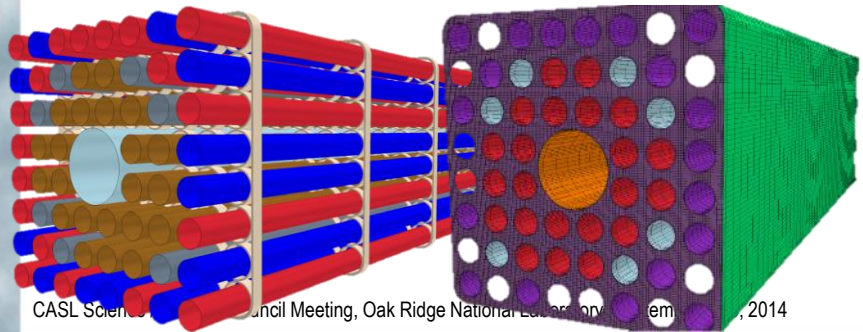


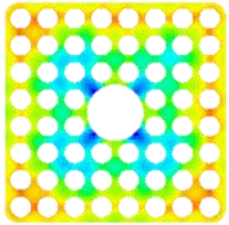
Comparative analysis of high void fraction regimes using an averaging Euler-Euler multi-fluid approach and a generalized two-phase flow (GENTOP) concept. Montoya, G.; Baglietto, E.; Lucas, D.; Eckhard, E.; Höhne, T.

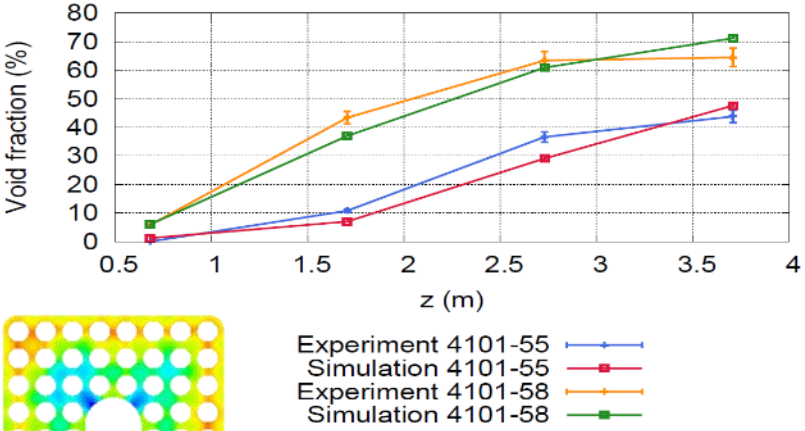
Winner – ICONE22 Student Competition

NUPEC BWR Full-size Bundle Test (BFBT)

- Provides robust validation of closures predictive capabilities

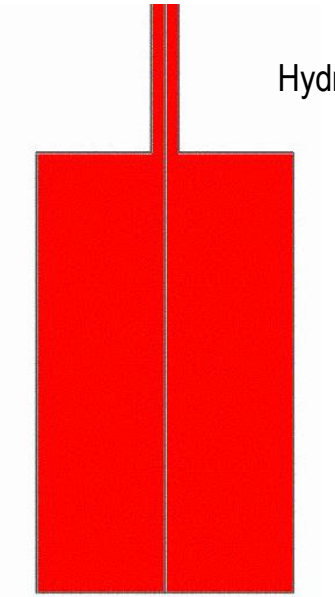


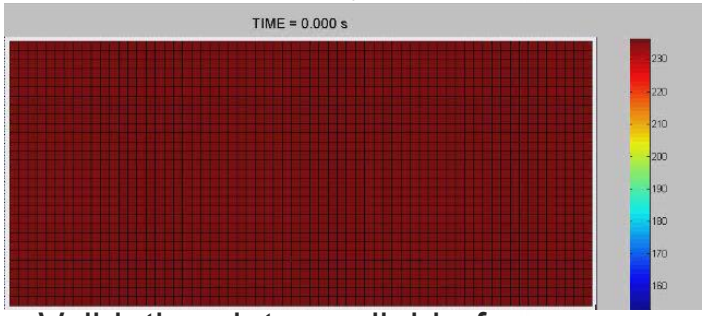




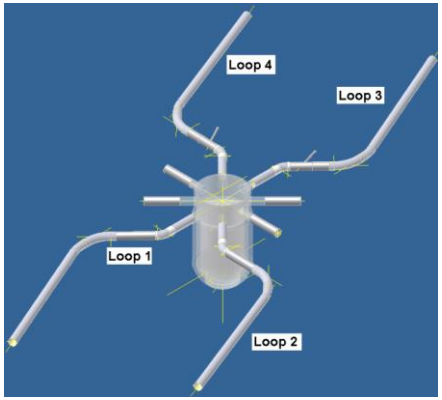
Convective Flow Challenge Problems

- Thermal and concentration driven flows
  - Prevalent industry methods are 1-D and cannot capture 3-D mixing effects
- Exercise the transient capabilities of Hydra-TH in 3-D
  - Projection methods are well known for their ability to accurately capture transient buoyancy-driven flows (e.g., see IJNMF Special Issue, 2002)
- Available experimental data:
  - ROCOM, Rossendorf/Germany
  - PKL, AREVA/Germany
  - BOMIX-I and II, KAERI/Korea
  - VALL-02, Vattenfall/Sweden
  - VVER, Gidopress/Russia
  - Gavrilas et al., Maryland/USA



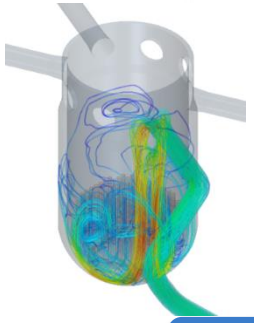


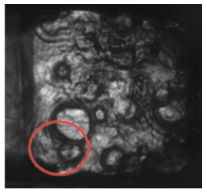
ROCOM Test Facility

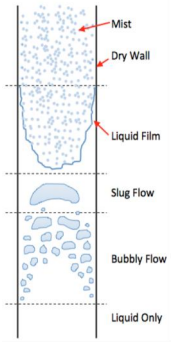


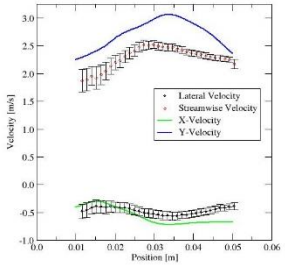
- Validation data available from many sources, but may be augmented by high-resolution U. Mich. experiments

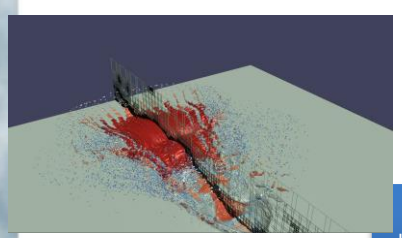
Phase-2 End-State

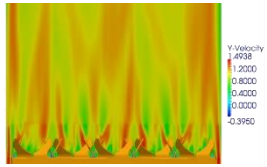


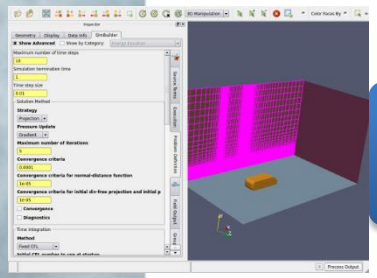


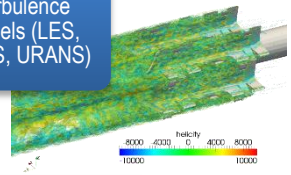


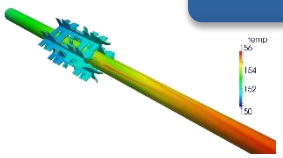












Thermal/Solutal Convection

Advanced Closure Models: GEN-I, GEN-II, …

Extensions for BWR flow regimes (topology recognition)

In-Situ Parallel Visualization

Documented V&V

Computational Model Builder

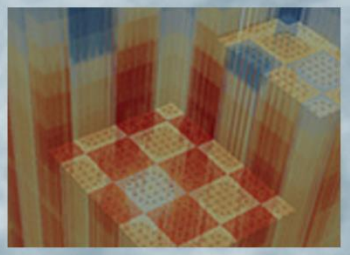
Advanced Turbulence Models (LES, RANS, URANS)

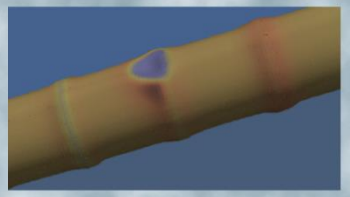
Scalable, Open, Advanced Architectures

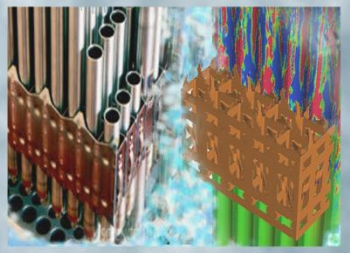
VERA CFD (Hydra-TH)

Surface Chemistry

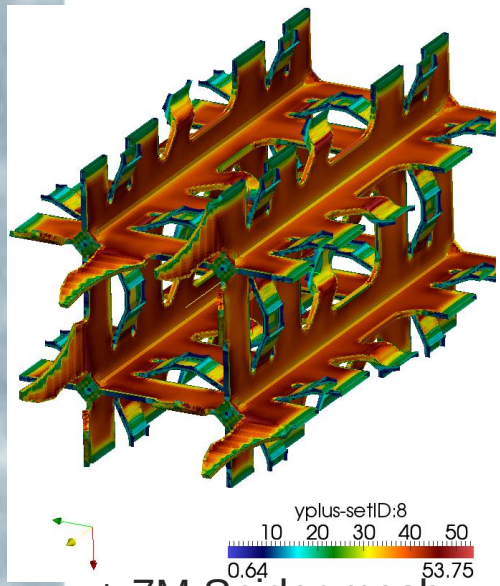
Backup Slides



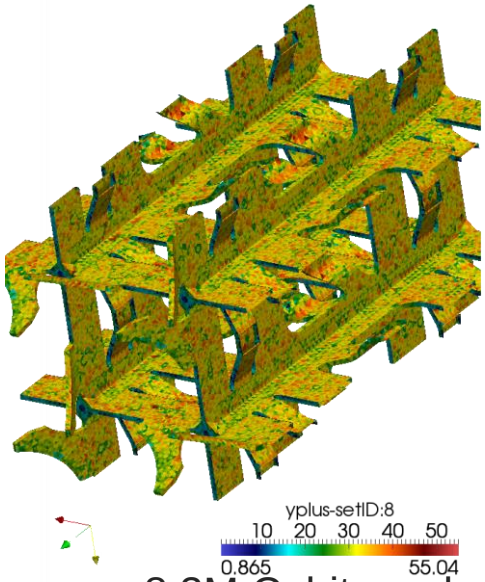




A Quantitative "A Priori" Mesh Assessment Methodology has been Developed for GTRF



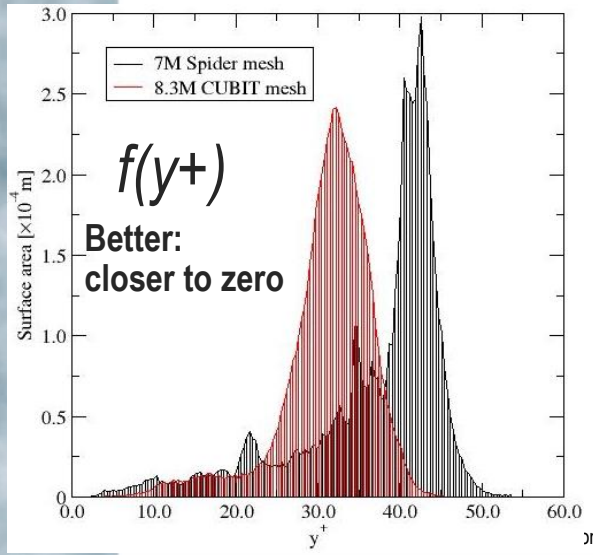
y+ 7M Spider mesh

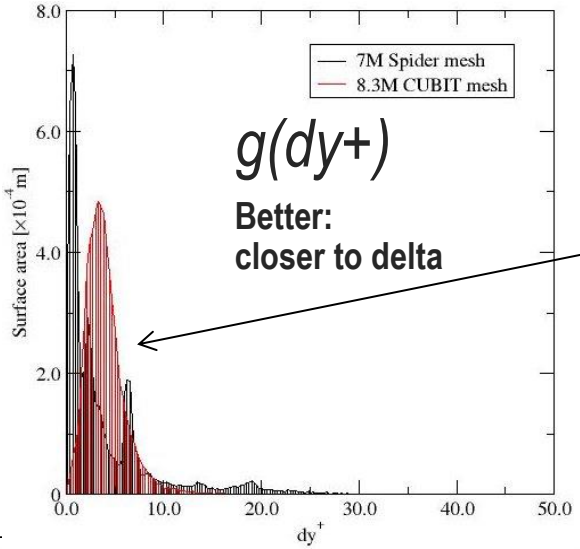


y+ 8.3M Cubit mesh

$$y^+ = \frac{y}{\nu}\sqrt{\frac{\tau_w}{\rho}}$$

- *How well is the boundary layer resolved?*
- *How good is the mesh quality at walls?*

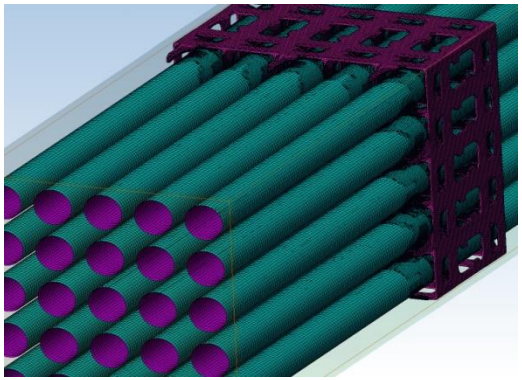




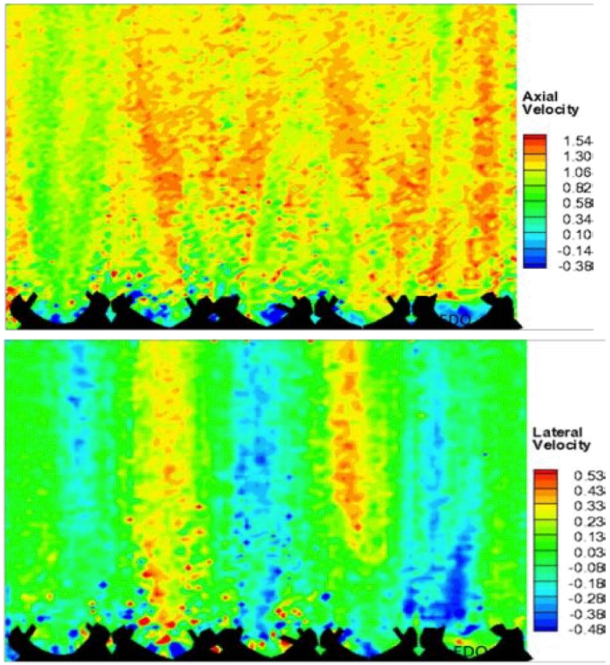
Total Variation Metric

- **Cubit spike shifted to right**
- **Poor uniformity near walls**
- **May lead to non-physical perturbations in boundary layers**

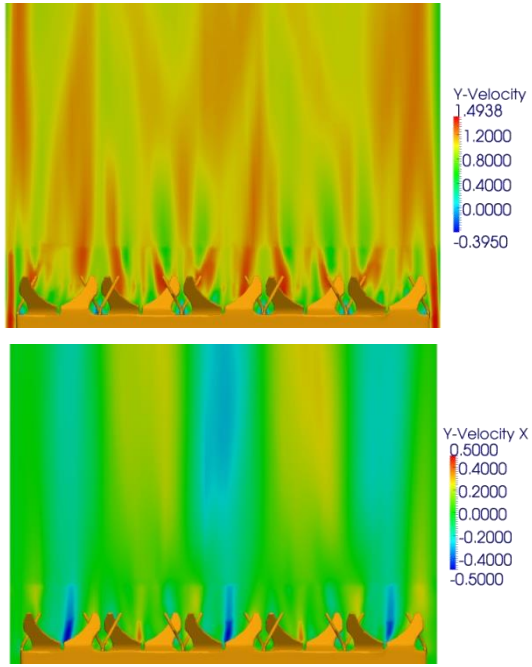
5x5 V5H study shows good agreement with experimental data



- Predicted mean peak velocities within 5% of experiments

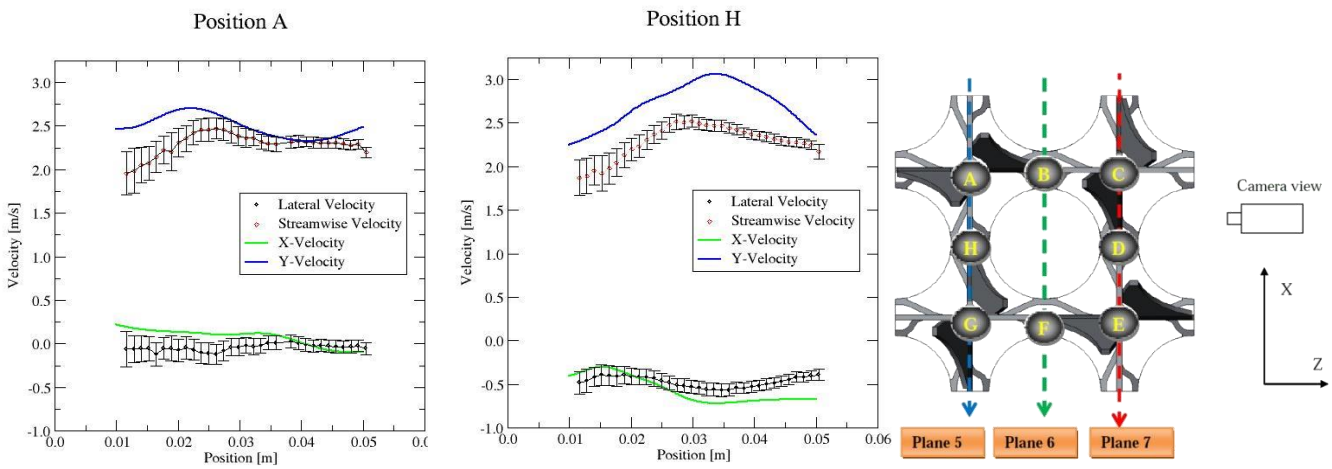


Texas A&M experiments



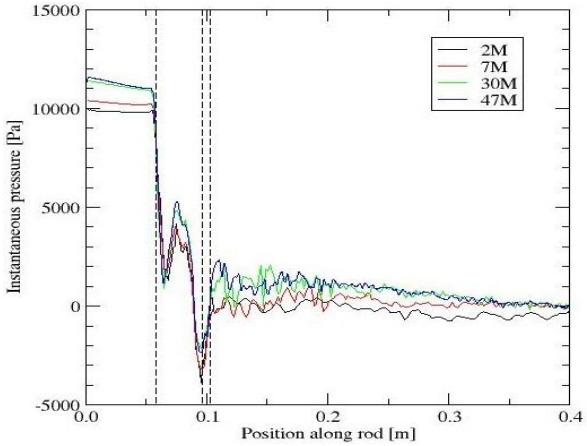
Hydra-TH calculations

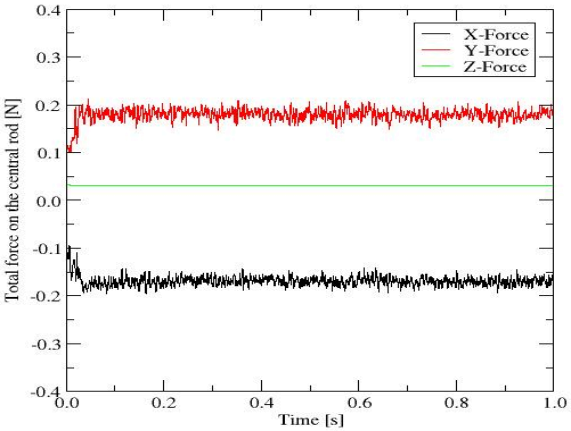
- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)

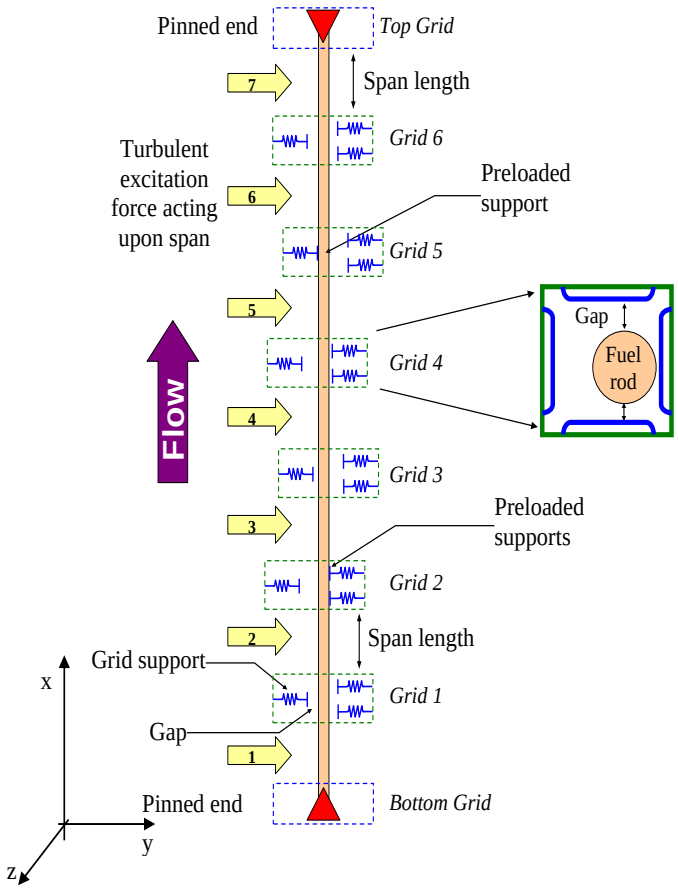


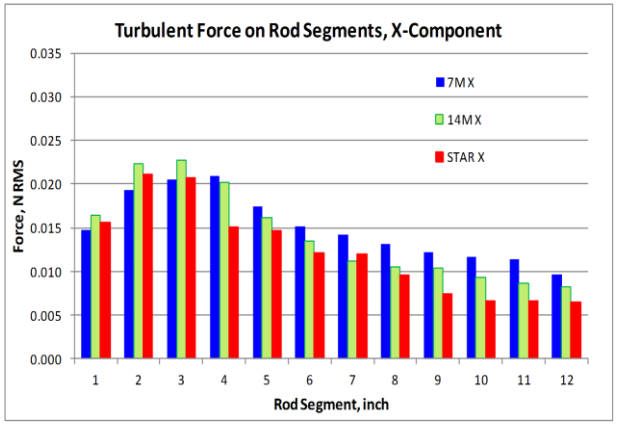
Large-Eddy Simulations Used to Drive Modal Dynamics and Wear Work Rate Calculations using VITRAN

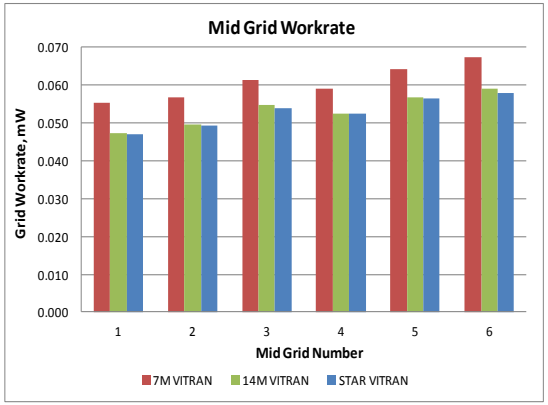
- Pressure Profiles and Rod Forces are extracted from Hydra-TH for the 3x3 Rod Bundle
- The data are used as input to VITRAN to compute rod acceleration/displacement
- 7 to 14M meshes required for reasonable fidelity in design analysis ~ 8 – 24 hour calculations









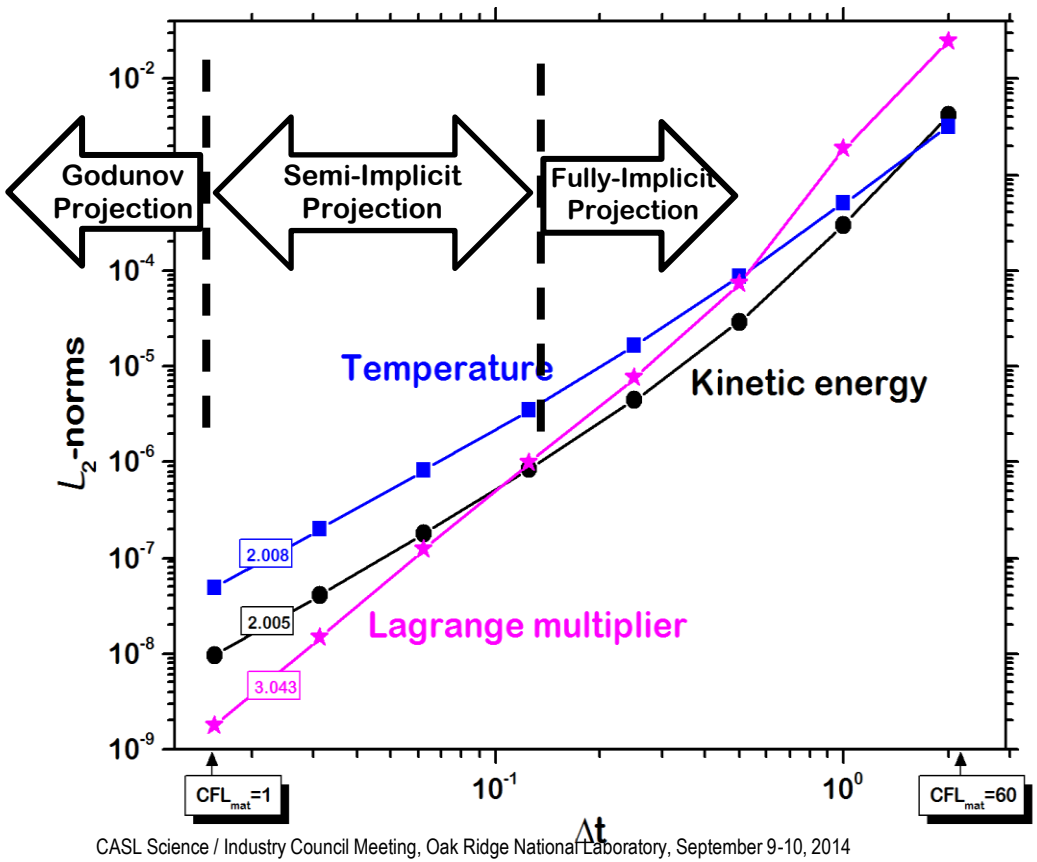


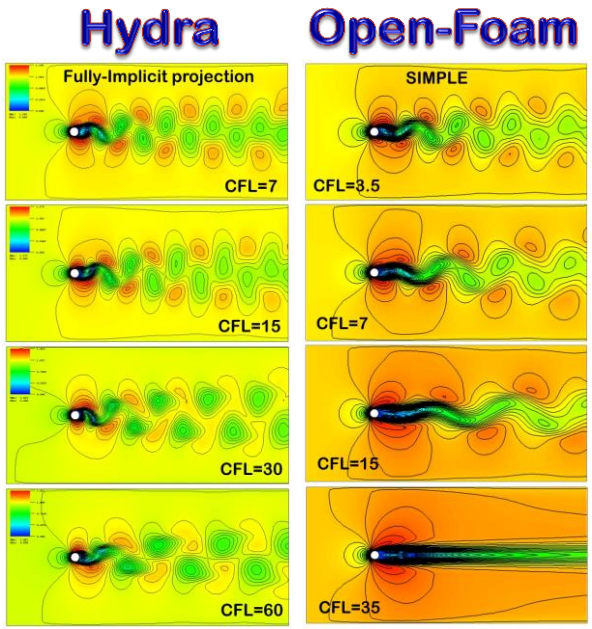
2% difference between CCM+ and Hydra-TH wear work-rates

Force time history data is used for subsequent rod dynamic analysis, e.g., with VITRAN

Fully-Implicit Algorithms based on Projection Methods

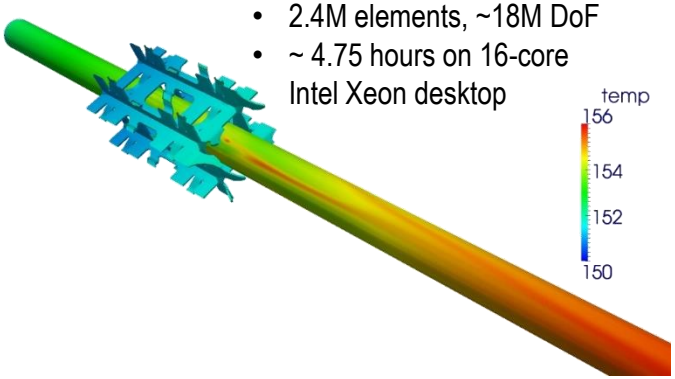
- Projection method acts a physically-based preconditioner providing an approximate factorization of the discrete Navier-Stokes Equations
- Nonlinear Krylov acceleration (N KA) for fully-implicit algorithms implemented for single/multiphase





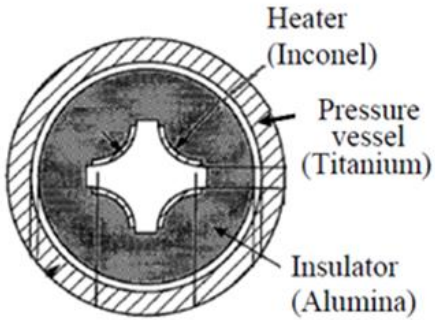
Fully-Implicit Projection:

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

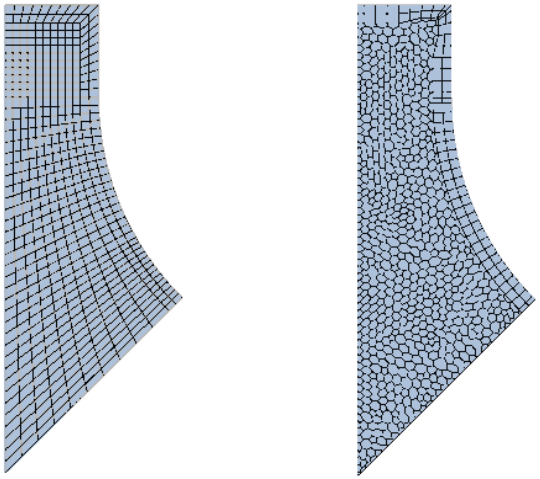


Validation of boiling models – PSBT mesh sensitivity

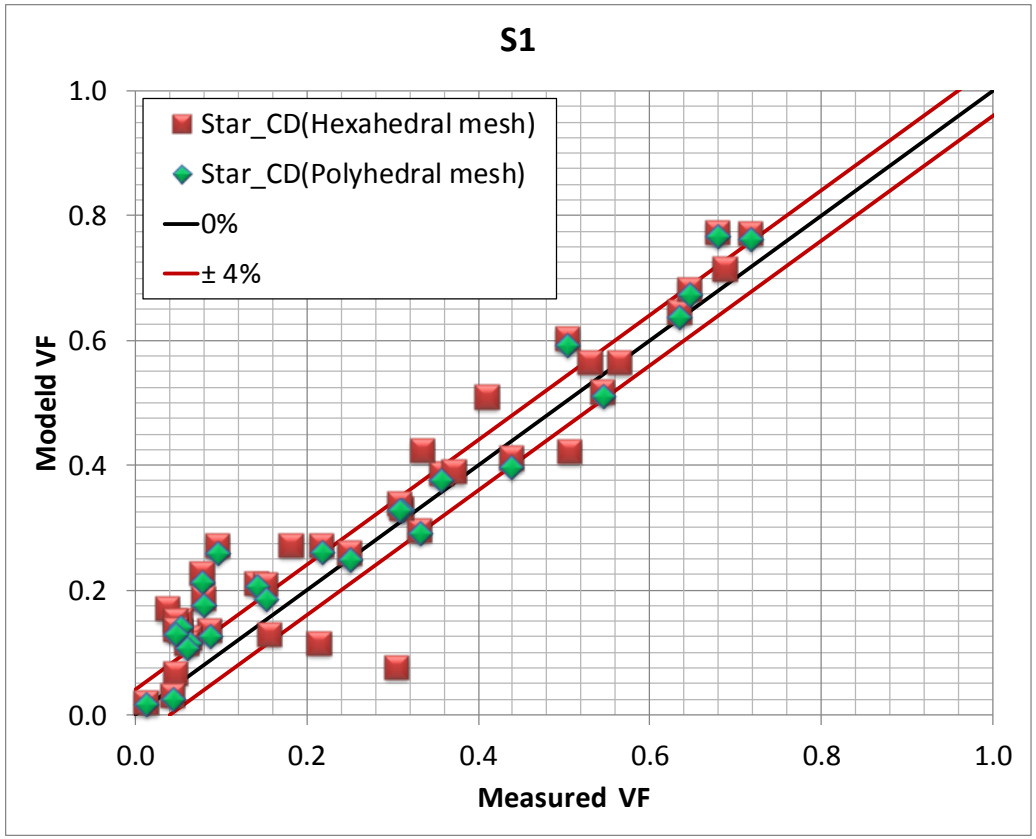
- PSBT Subchannel data



Central (Typical) Subchannel
S1



Hexahedral vs Polyhedral mesh type



Mesh type does not affect the prediction of void fraction, however it does affect the convergence robustness

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Challenge Problem Progress

Science / Industry Council Meeting

September 9, 2014

Overall Challenge Problem Integrator:

Zeses Karoutas

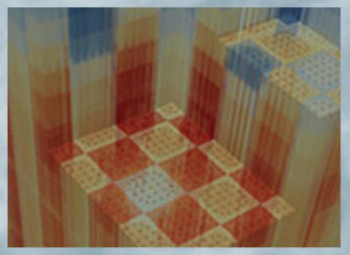
Challenge Problem Integrators:

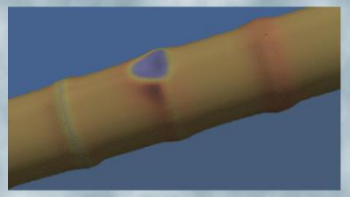
Jeff Secker, Brian Wirth,

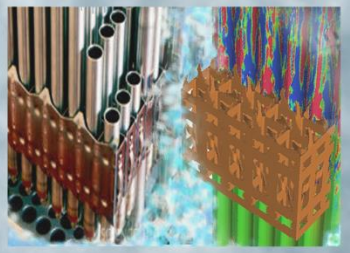
Rob Montgomery, Yixing Sung,

Gregg Swindlehurst

Presenter: Jeff Secker





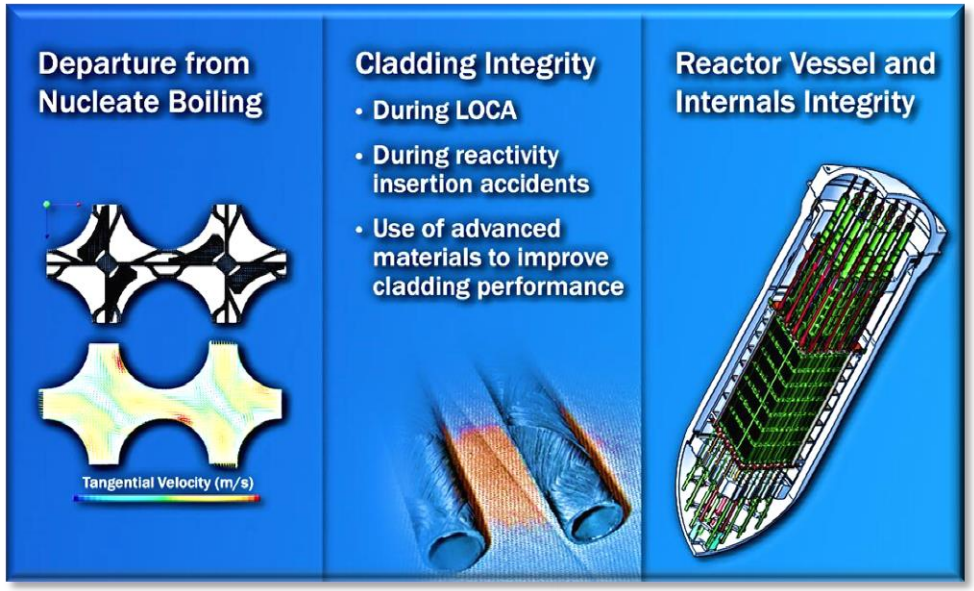


U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Outline

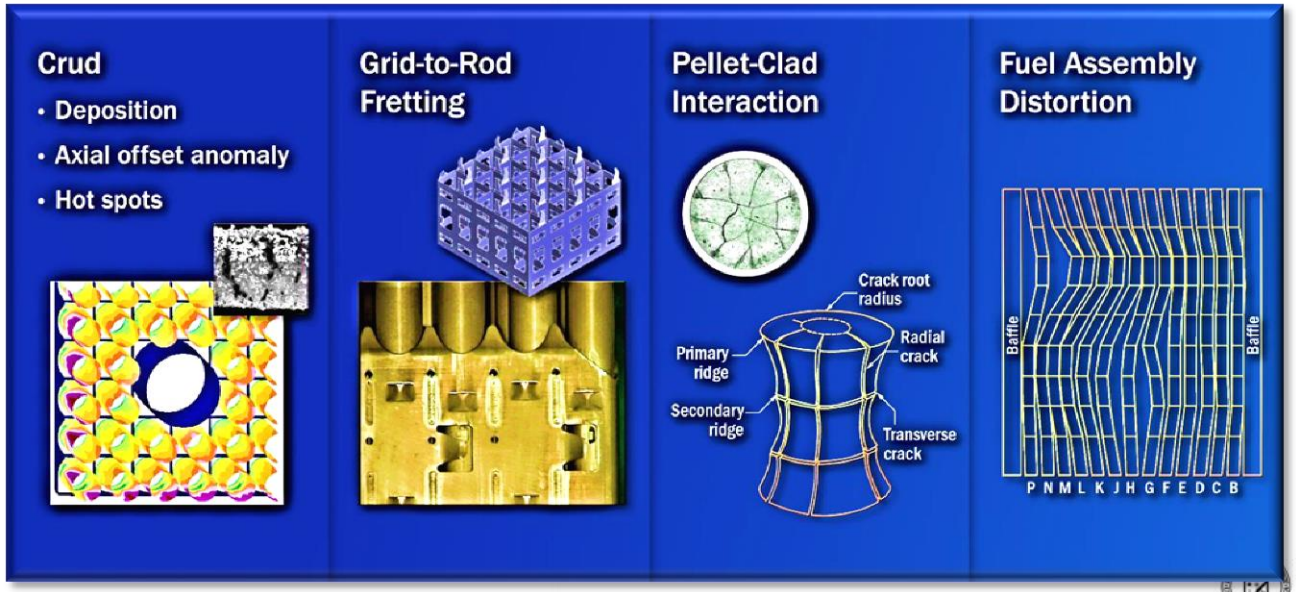
- CASL Challenge Problems
- CASL VERA Tools
- High Level CASL Plan to Address Challenge Problems
- Challenge Problem Progress from Challenge Problem Integrators (CPIs):
  - CRUD — Jeff Secker
  - PCI — Rob Montgomery
  - DNB — Yixing Sung
  - RIA & LOCA — Gregg Swindlehurst
  - GTRF — Brian Wirth
- Overall Challenge Problem Progress

CASL Challenge Problems

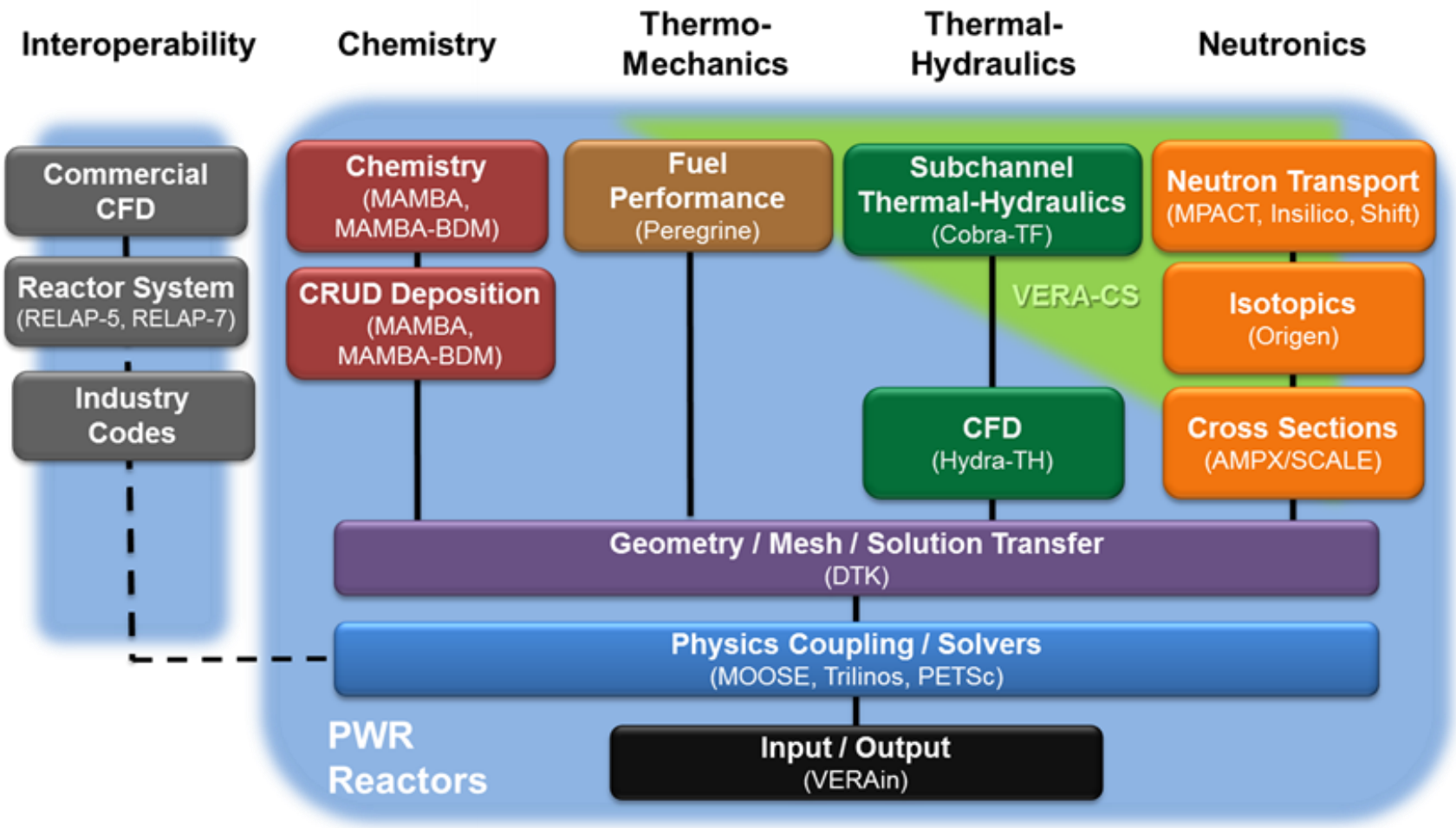


CASL is committed to delivering simulation capabilities for

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



VERA, Virtual Environment for Reactor Applications



High Level CASL Plan to Address Challenge Problems

PCI*

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

CRUD*

- **CIPS:** Predict Boron Uptake with **MAMBA2D and COBRA-TF**
- **CILC**: Predict Crud thk & corrosion with **MAMBA3D and HYDRA-TH**

VERA-CS*

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

RIA*

- Predict PCMI Margin using **MPACT** and **PEREGRINE2D**

LOCA*

- Predict PCT – Oxidation Margin using **PEREGRINE2D** & System Code **RELAP5 or W COBRA-TRAC**

DNB*

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

GTRF*

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

For Each Challenge Problem Apply DAKOTA using Coupled Tools for UQ

CP	Baseline Objectives
CRUD (CIPS / CILC)	• Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD vulnerable assembly and pin in PWR configuration; generate quantities relevant to CRUD initiation and growth. • Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness. • Model boron uptake from reactor coolant into CRUD on fuel rods. • Predict CIPS by calculating CRUD formation, boron uptake, resulting axial power shape • Predict CILC using higher fidelity 3D models around fuel rod
Structural (GTRF / FAD)	• Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting. • Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration. • Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods. • Calculate fuel rod material wear

CP	Baseline Objectives
DNB	• Initial modeling of DNB with multi-physics subchannel tools. • Improved modeling of DNB with CFD tools
Cladding Integrity (PCI / RIA / LOCA)	• Initial modeling of peak clad temperature, cladding oxidation, and embrittlement, and fuel performance during operational transients and design basis accidents
Lifetime Extension	• Model reactor vessel fluence and material property changes that result in material degradation and limit vessel performance.

Challenge Problem Progress from CPIs

- Description of Challenge Problem
- Current Industry Practice
- Path Forward
- Accomplishments in Phase 1
- Innovations
- Validation
- What is Success in Phase 1

Overall Challenge Problem Progress

	Development	Innovation	Validation
Operational			
CRUD-induced power shift (CIPS)			
CRUD-induced localized corrosion (CILC)			
Grid-to-rod fretting failure (GTRF)			
Pellet-clad interaction (PCI)			
Fuel assembly distortion (FAD)			
Safety			
Departure from nucleate boiling (DNB)			
Cladding integrity during (LOCA)			
Cladding integrity during (RIA)			
Reactor vessel integrity **	**LWRS**		
Reactor internals integrity **	**LWRS**		

Significant Progress

Planning & Scoping

Good Progress

Not Started

Success in Phase 2 for PWR Challenge Problems

- Perform CIPs analyses with VERA with full core depletion for all rods in core and compare to BOA and Vogtle and Seabrook data
  - Zoom in and perform CILC analyses for limiting Seabrook assembly
- Perform DNB RIA analysis with VERA and compare to data
- Develop preliminary CFD method to predict DNB
- Benchmark VERA tools to available RIA and LOCA test data
- Perform RIA and LOCA analyses using Peregrine for typical plants
- Perform core wide PCI analysis and zoom in for MPS PCI leaker for a plant with PCI leakers
- Utilize fretting wear test data and other data to complete wear model
- Implement material wear and growth models and CFD excitation forces into VITRAN and compare to wear data in field

Utilize DAKOTA for above to support validation

A DOE Energy Innovation Hub

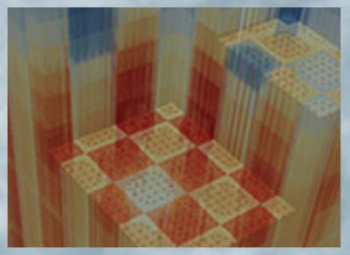
Crud Challenge Problem Progress

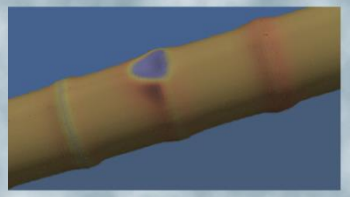
Science / Industry Council Meeting

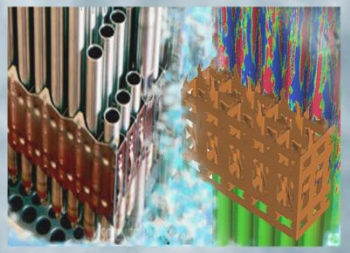
September 9, 2014

Jeff Secker

Westinghouse Electric Co.







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Crud Challenge Problem

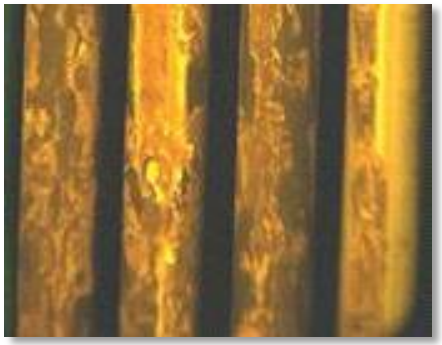
- Description of Crud Challenge Problem
- Current Industry Practice
- Path Forward
- Accomplishments in Phase 1
- Innovations
- Validation
- Definition of Success in Phase 1 and Phase 2 plans

Crud Challenge Problem Charter – CASL-I-2013-0033-000

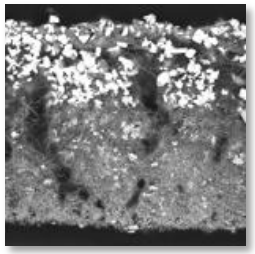
Crud Challenge Problem Implementation Plan – CASL-I-2013-0032-000

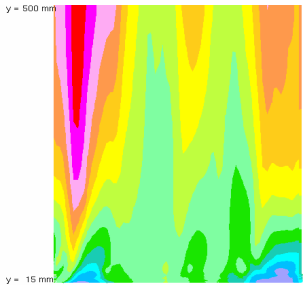
Crud Induced Power Shift (CIPS) and Crud Induced Localized Corrosion (CILC)

- CIPS - Deviation in axial power shape caused by corrosion product deposits on fuel rods
  - Subcooled boiling in porous crud layer concentrates boric acid, lithium hydroxide in crud
  - Boron (neutron absorber) compunds will precipitate in crud when concentrated sufficiently
  - Causes unexpected shift in axial power distribution, affects core reactivity, shutdown margin, and axial power distribution control
  - Affects fuel management and thermal margin in many plants
- CILC –
  - Hot spots on fuel caused by local variations in heat transfer lead to localized sub-cooled boiling
  - Excessive boiling with high crud concentrations in coolant can lead to thick crud deposits, crud dryout, and accelerated cladding corrosion
  - Result: Fuel leaker



CRUD deposits





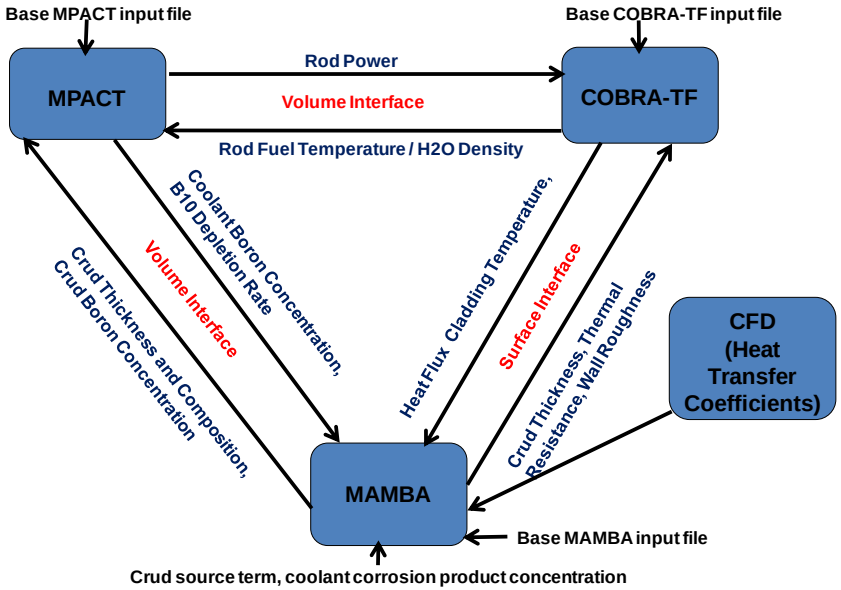
Industry costs for CIPS/CILC estimated at

> $215M to date

Current Industry Approach to Crud Modeling

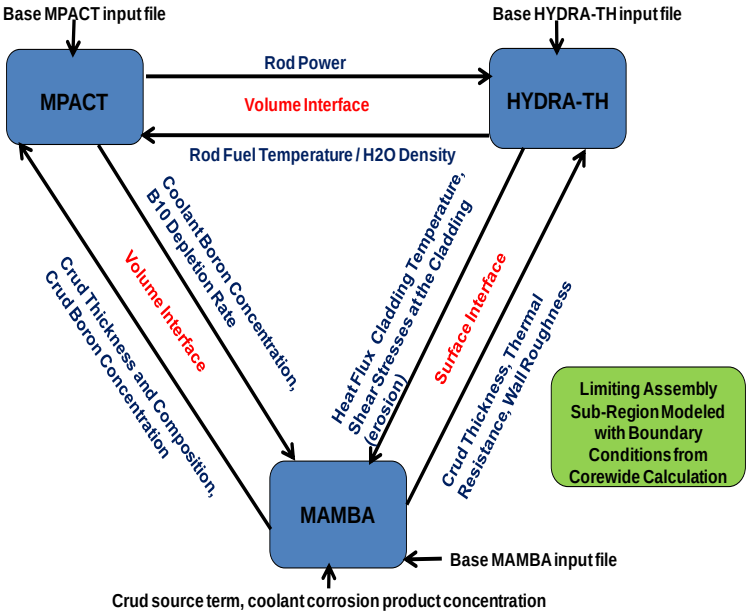
- Current tools: CIPS
  - ANC neutronics code (2 group nodal method) provides ¼ assembly averaged core power distributions to:
  - VIPRE sub-channel model (¼ assembly resolution) which calculates core thermal-hydraulic condition for input to:
  - BOA code (crud, boron deposition on ¼ assembly average basis)
  - No feedback between codes
    - Boron deposition affects local power, local power affects sub-cooled boiling, sub-cooled boiling affects crud and boron deposition
- Current tools: CILC
  - Advanced BOA – rod by rod model for selected single assembly
  - CFD thermal/hydraulics used for heat transfer coefficient variation – 20 radial segments for each rod
    - Stand alone model for single grid span within assembly to capture grid and mixing vane effects on flow and heat transfer
    - Not specific to core being modeled

Model Needs for CIPS



- 3D, quarter core, pin-resolved transport neutronics
  - Boron and crud feedback
  - Provide power distribution to T-H
- 3D, quarter core sub-channel core T-H model
  - Calculate sub-channel T-H conditions and clean surface sub-cooled boiling rate
  - Use crud thermal resistance and surface roughness from crud model
  - Pass local coolant temperature, heat flux, heat transfer coefficients, pressure, cladding temperature, flow to crud code and coolant density to neutronics code
- 3D, quarter core, crud/chemistry model
  - Calculate crud composition and mass/thickness deposited on cladding
  - Calculate sub-cooled boiling rate when crud is present
  - Determine mass and distribution of boron deposited in crud
  - Determine erosion of crud
  - Pass crud and boron number densities to neutronics code

Model Needs for CILC



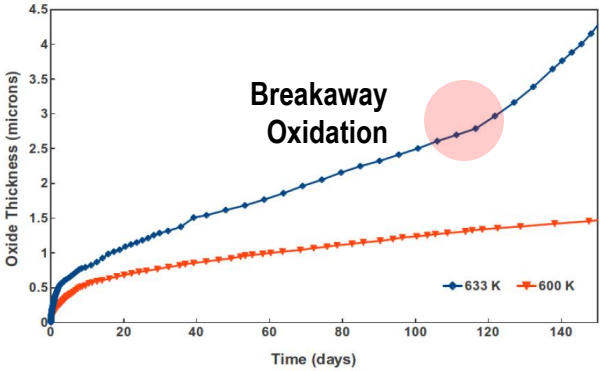
- Model at risk sub-region of core based on CIPS model results
  - 3D, portion of assembly, boundary conditions from CIPS calculation
- Neutronics – pin resolved transport
  - Vary azimuthal and radial power within rod
  - Feedback from crud and boron deposited
  - Pellet power distribution to T-H or fuel performance code
- CFD based T-H Model
  - For azimuthal/axial variation in local T-H conditions
  - Input to crud/chemistry model
  - Calculates cladding temperature – provides input to fuel performance model
- Crud/Chemistry Model
  - Calculate local (azimuthal/axially varying) crud composition and mass/thickness deposited on cladding
  - Calculate sub-cooled boiling rate when crud is present
  - Determine mass and distribution of boron deposited in crud
  - Determine erosion of crud
  - Pass crud and boron number densities to neutronics code, thermal resistance to T-H
- Fuel Performance code
  - Cladding corrosion based on cladding temperature and local chemistry at cladding surface

Phase 1 Crud Accomplishments

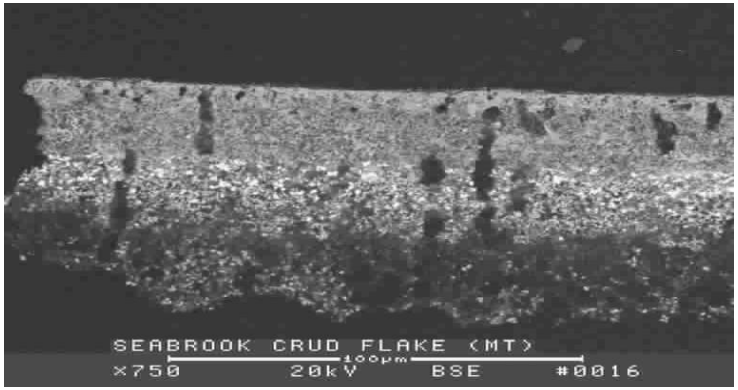
- Coupled ANC/VIPRE/BOA industry tools and applied to Watts Bar 1 Cycles 1-3 and Vogtle 1 Cycles 11-14
  - CASL-2011-0125-000-CI, CASL-CI-2012-0091-000
- Developed advanced crud codes MAMBA and MAMBA BDM (micro-scale)
  - CASL-I-2012-0030-000
- Applied coupled CFD (STAR-CCM+) / MAMBA to single rod and 4x4 rod array
  - CASL-I-2012-0045-000
- Coupled COBRA-TF subchannel code with MAMBA for CIPS modeling
  - 5x5 Seabrook Cycle 5 rod array modeled – CASL-I-2013-0191-000
- Improved STAR-CCM+ / MAMBA coupling
  - 5x5 Seabrook Cycle 5 rod array modeled - CASL-U-2013-0224-000
- Westinghouse updated ANC/VIPRE/BOA linkage with new EPRI BOA 3.1 version - CASL-CI-2014-0035-000
- HYDRA / MAMBA linkage underway with MAMBA embedded in HYDRA
- COBRA/MAMBA linkage to be updated with MAMBA embedded in COBRA
- Planned: Neutronics (MPACT) coupling with sub-channel T-H (COBRA) and crud/chemistry (MAMBA) as well as CFD T-H (HYDRA) and crud/chemistry (MAMBA)

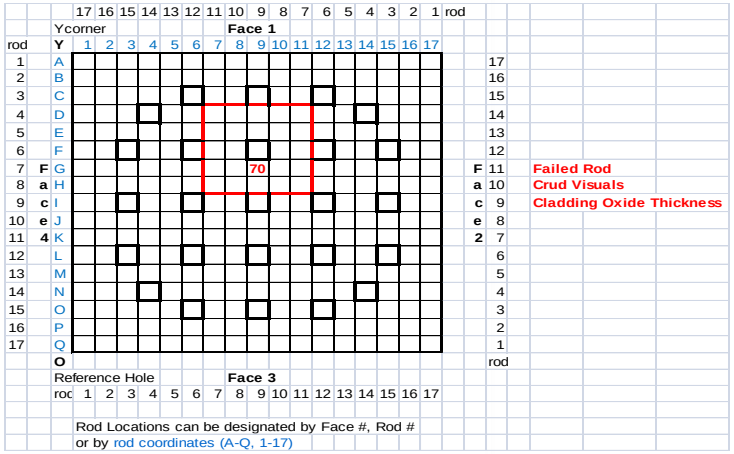
Advanced CASL Models for Crud – MAMBA, MAMBA-BDM

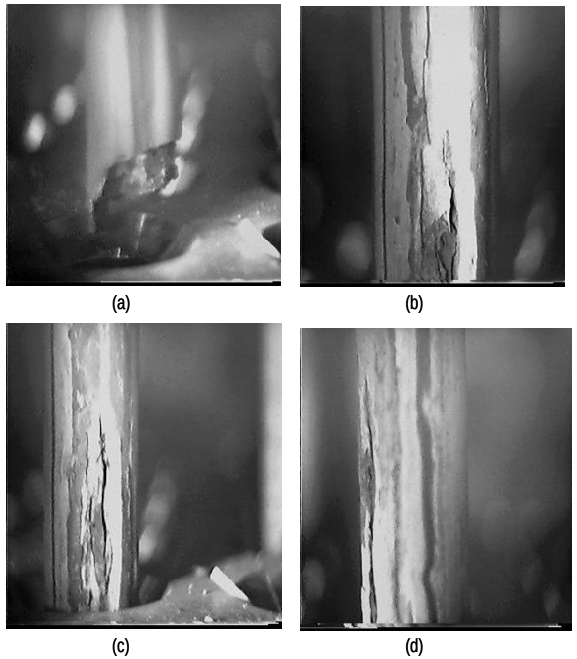
- Non-linear, time-dependent 3D heat transport equation determines internal crud temperature distribution including sub-cooled boiling and crud porosity evolution
- Mass transport models for concentration of soluble species via boiling flow, concentration gradient diffusion, and vaporization
- Chemistry models for crud deposition and boron precipitation
- Crud erosion model
- Improved thermodynamics for crud and precipitates
- Previous coupling with STAR-CCM (T-H CFD) improved, initial coupling with COBRA-TF (TH) implemented, coupling with HYDRA (CFD), underway, future coupling with MPACT (neutronics) planned
- MAMBA-BDM
  - new clad corrosion model with crud



Validation - Seabrook Cycle 5 with CIPS/CILC 5x5 Rod Array







Assemblies with failures were some of the highest powered assemblies/rods throughout the cycle

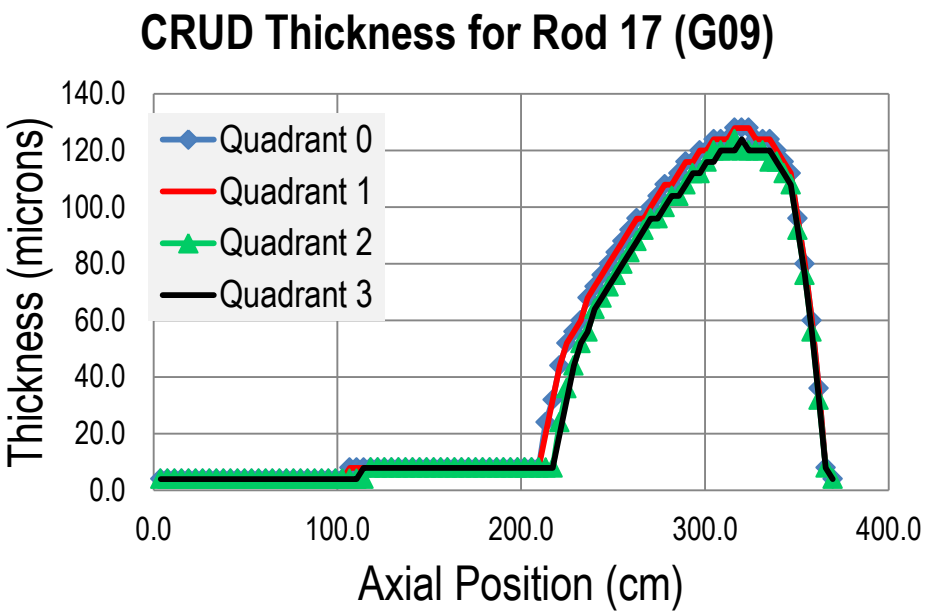
Predicted Crud and Boron Distribution – 5x5

	7	8	9	10	11
D	9.9	9.6	10.7	9.6	10.0
E	9.8	10.0	10.2	10.0	9.9
F	10.9	10.2	2.2	10.2	11.0
G	10.1	10.2	10.4	10.2	10.0
H	10.4	10.1	11.3	10.1	10.4

Seabrook Assembly G70 Rods D7-H11 predicted crud mass (grams)

	7	8	9	10	11
D	106.3	102.1	116.3	102.2	107.3
E	105.0	106.8	108.8	107.3	105.5
F	119.0	109.5	8.2	109.4	119.5
G	107.9	110.2	112.7	110.1	107.3
H	112.7	108.9	123.8	108.6	111.9

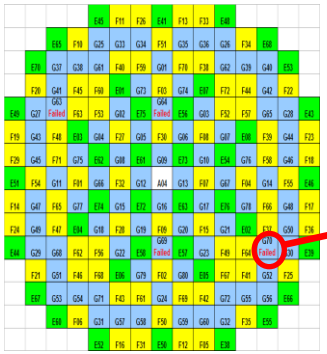
Seabrook Assembly G70 Rods D7-H11 predicted boron mass (milligrams) deposited in crud

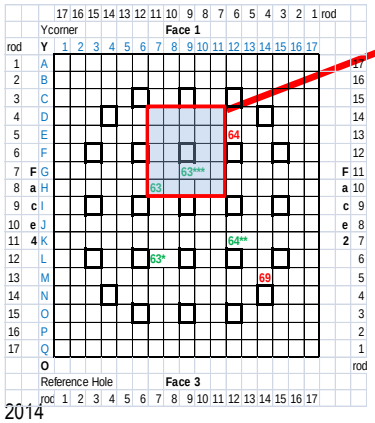


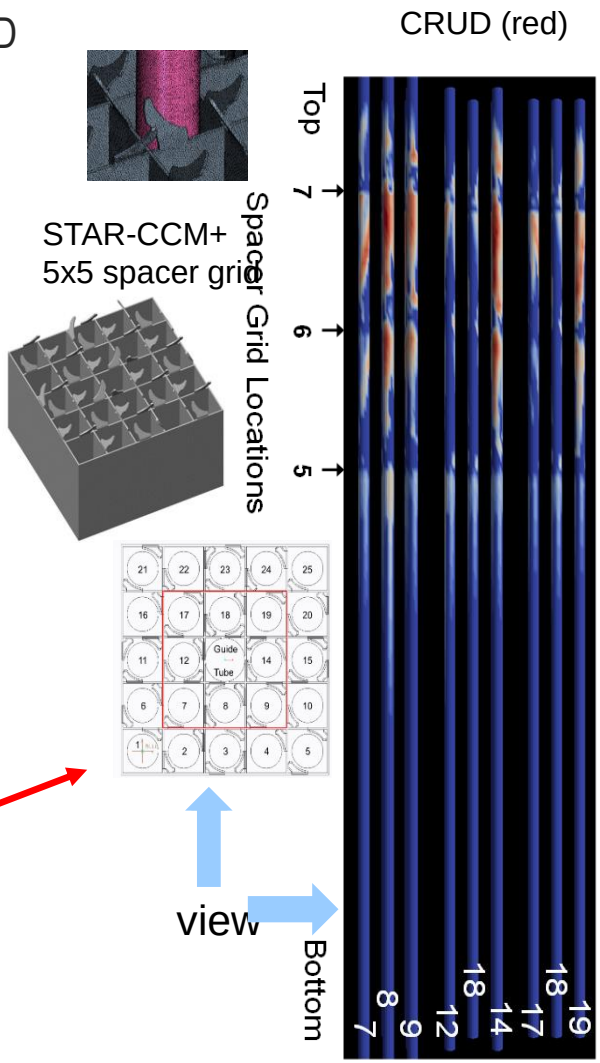
Simulation of Seabrook 1 Cycle 5 CRUD Formation using Coupled STAR-CCM+ and MAMBA3D

CASL's high-fidelity CRUD simulation capability using STAR-CCM+ and MAMBA3D has been used to simulation the formation of CRUD in Cycle 5 at the Seabrook 1 PWR

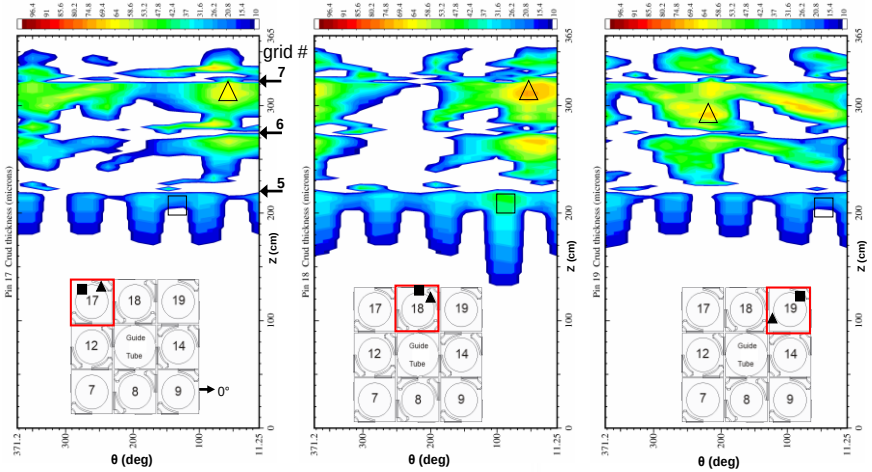
- 5-rod by 5-rod array for which qualitative and quantitative data is available was selected for analysis
- First high-fidelity, two-way coupled CFD/CRUD simulation of an industrial relevant plant cycle
- Input power provided by industry simulations
- Showed that <u>both</u> axial and azimuthal thermal hydraulic effects dramatically affect CRUD deposition patterns
- Showed that azimuthal power variations have very little impact on CRUD deposition patterns
- Axial and azimuthal CRUD deposition patterns were consistent with plant data

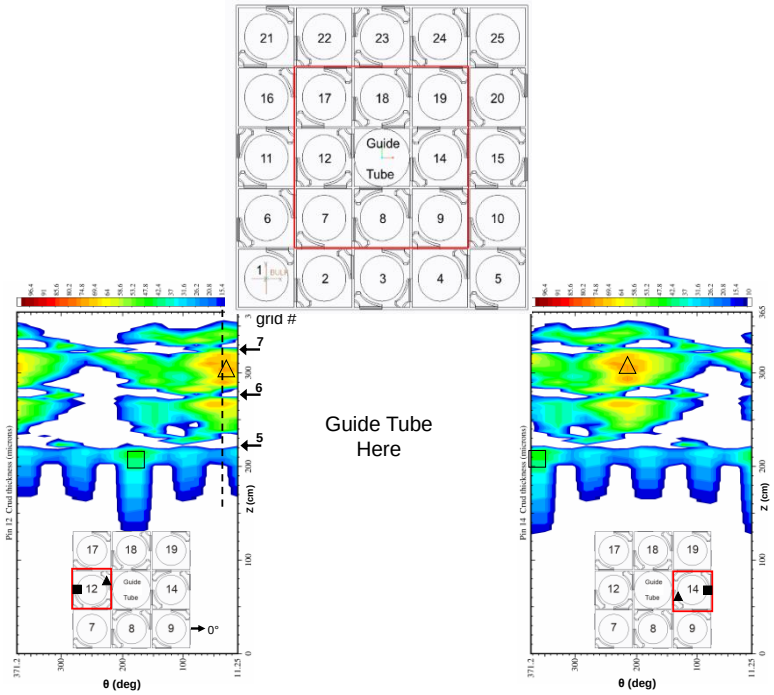






MAMBA Computed Crud Thickness at 502 days





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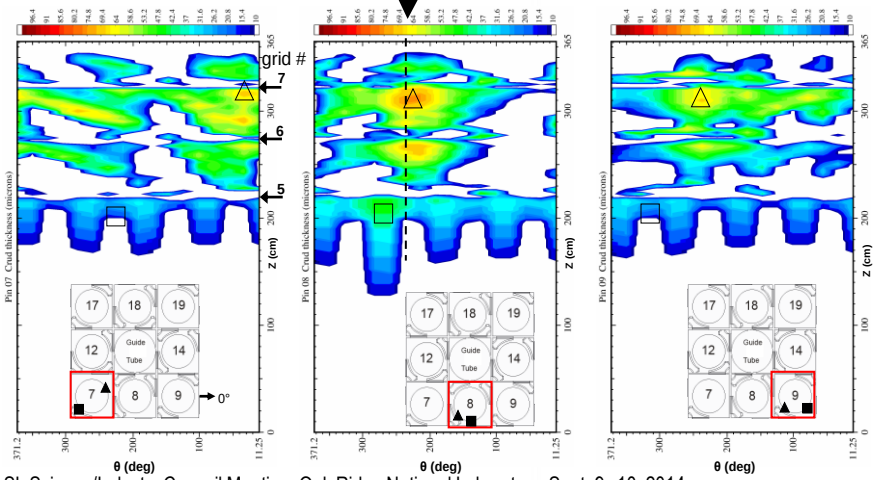
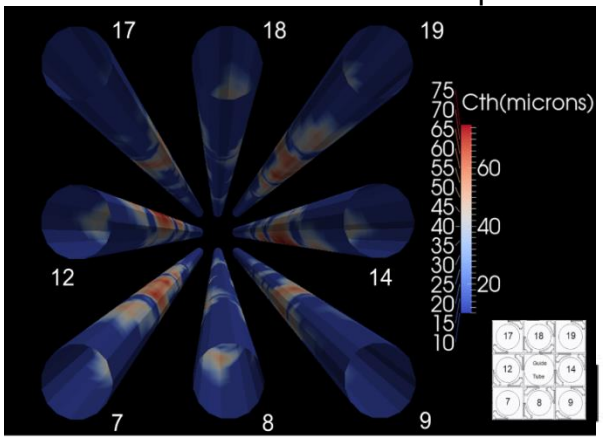
1D profile slice on next slide

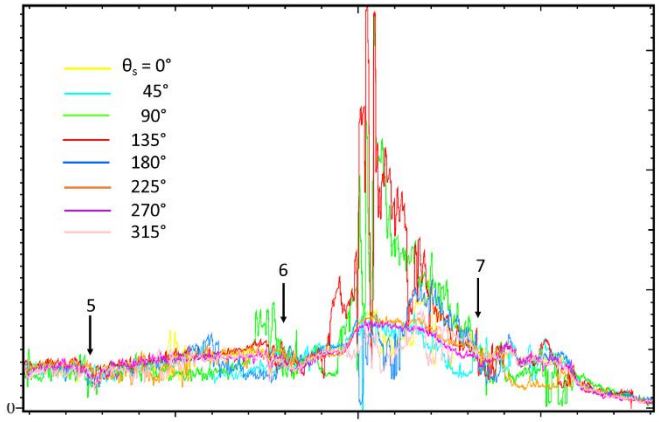


CRUD (red) 3D Top view

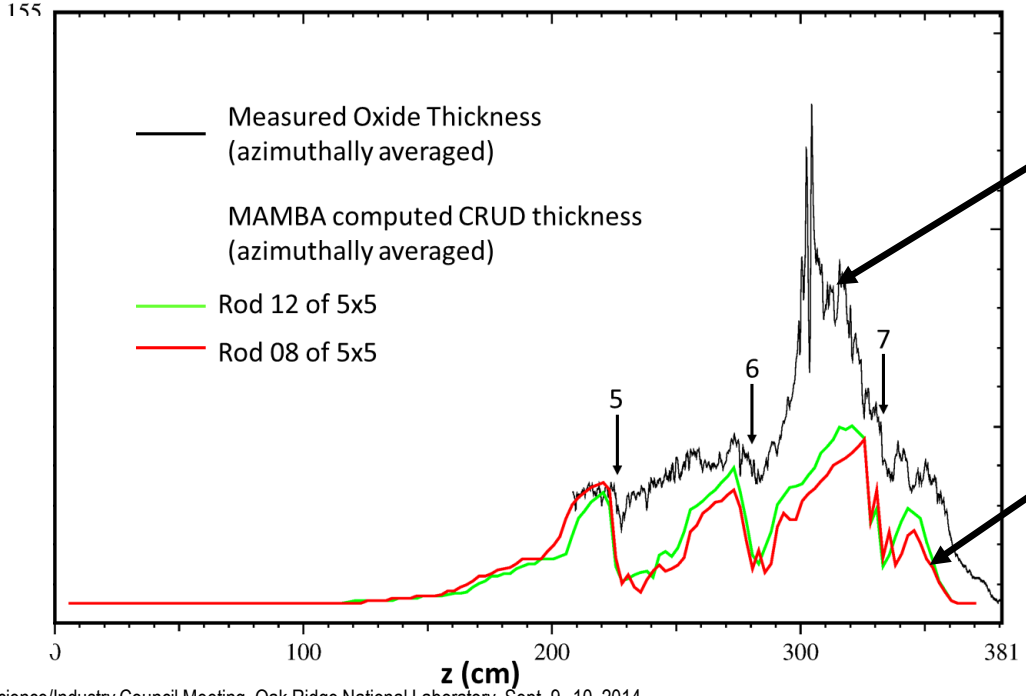


Comparisons with Seabrook Cycle 5 oxide data

Measured Oxide Thickness for FA G70 Rod G09



Average Oxide/CRUD Thickness for FA G70 Rod G09

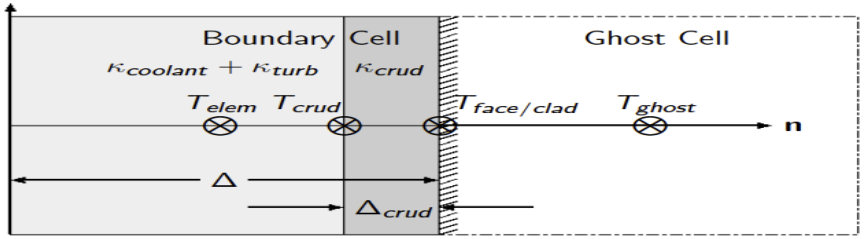


Average of azimuthal data plotted in black

MAMBA computed crud thickness plotted in color

Current Crud Efforts

- New thermodynamic correlations added to MAMBA for several boron phases including Bonaccordite
- 1D MAMBA version developed and validated against 3D MAMBA
- Interface specification for coupling 1D MAMBA with HYDRA and COBRA has been defined and implemented, library delivered to LANL HYDRA team



- Improved MAMBA/STAR-CCM+ coupled simulation of Seabrook 5x5 rod array underway with LANL and U. Michigan
- MAMBA surrogate model to be added into COBRA based on HYDRA lessons learned in anticipation of embedding MAMBA as a library for CIPS analysis
- CASL interaction with EPRI P-TAC continues
- Demonstration of coupled CFD/Crud for a portion of an assembly
  - FY14.CASL.012

Crud - Definition of Success

- Phase 1 - Implement higher fidelity CASL neutronics and T-H models and extend crud models to 3D, couple codes, calibrate and assess compared to available crud validation data; Use advanced linked codes to improve current industry codes/methods

Phase 2 Plans

- Apply coupled MPACT/COBRA/MAMBA to cores with CIPS history
- Complete VUQ on CIPS models
- Apply coupled MPACT/HYDRA/MAMBA to fuel assemblies with CILC history
- Complete VUQ on CILC models
- Validation Data:
  - CIPS cores - measured axial power distribution behavior, crud locations from visual exams (Vogtle 1, Seabrook, other cores)
  - CILC failures – location and time of failure, crud scrape data (Seabrook)

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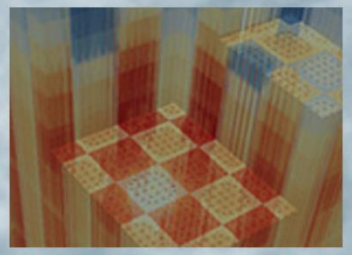
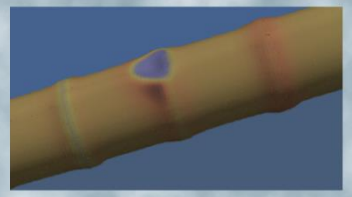
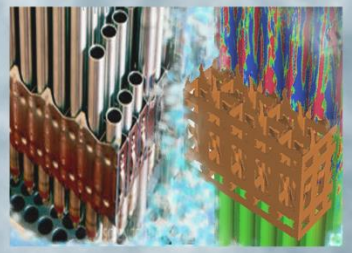
DNB Challenge Problem

Yixing Sung, DNB Challenge Problem Integrator

Presenter: Jeff Secker







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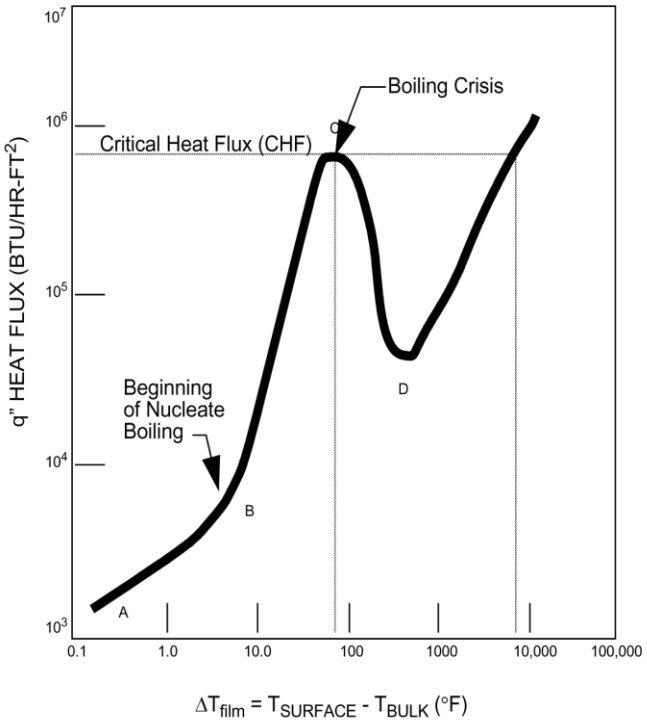
Challenge Problem Progress DNB

- Description of Challenge Problem
- Current Industry Practice
- Path Forward
- Accomplishments in Phase 1
- Innovations
- Validation
- What is Success in Phase 1

Departure from Nucleate Boiling (DNB)

- DNB also referred to as Critical Heat Flux (CHF)
- Local clad surface dryout causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow)
- One of safety and regulatory acceptance criteria for PWR (DNB) and BWR (dryout)
- CASL objectives and path forward defined in Charter and Implementation Plan
  - CASL-I-2013-0110-001 (Charter)
  - CASL-X-2013-0277 (Implementation)
  - Focus on PWR (DNB) in the first 5 years (Phase I)

Boiling Curve

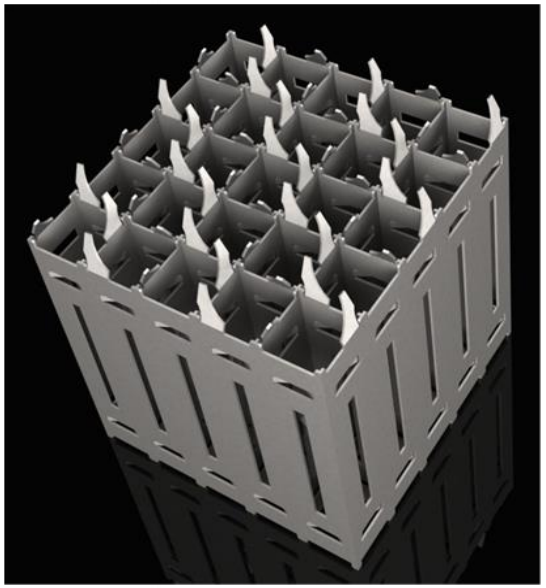


Critical Steps of Industry Practice & Current CASL Focus (Highlighted)

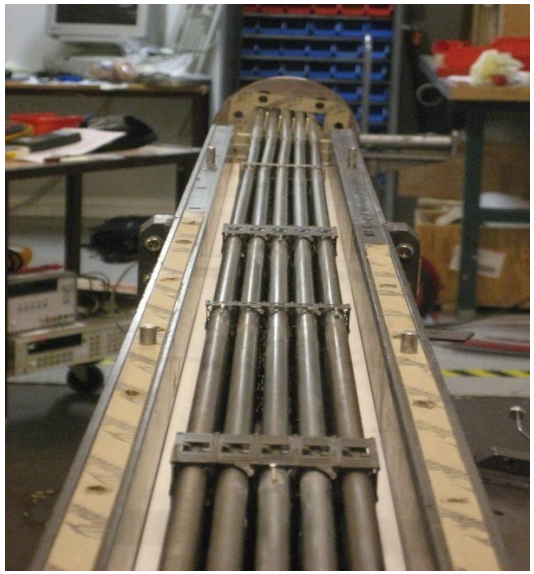
Fuel Hardware Design

Small Scale Testing (5x5 bundle) → Subchannel Code Predictions → DNB Correlation → Licensing Approval → Non-LOCA Accident Analysis

Plant Design Conditions



Mixing Vane Grid Spacer



Rod Bundle Test

CASL Path Forward – Address Modeling & Simulation (M&S) Needs for Industry

- Fuel hardware design improvement
  - Higher fidelity of M&S capabilities (multi-phase) to predict fluid and fuel surface conditions and effects of fuel design features (e.g., grid spacer)
  - Applications of advanced data assimilation and uncertainty quantification methods on test design, data collection and analysis
  - Control and optimization of fuel cladding surface morphology and properties during reactor operation

- Margin quantification in accident analysis
  - Multi-scale and multi-physics M&S capabilities
  - Technical basis for DNB-related fuel failure (e.g., DNB during Reactivity Insertion Accident (RIA))

CASL Phase I DNB CP Deliverables

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Yr1

Developed Hydra-TH M-CFD code utilizing fully-implicit, parallel solver and closure relationships developed using experimental data and DNS

Yr2

Enhanced computational performance of VERA/COBRA-TF (CTF) subchannel code via improved solver with parallelization

Yr3

Collected rod bundle DNB and mixing test data, provided reference solutions of industry T/H codes, applied CTF to predict thermal-hydraulic behaviors and rod responses during RIA transient

Yr4

Developed initial Hydra-TH modeling of subchannel turbulent mixing in rod bundles with grid spacers, compared CTF predictions with rod bundle test data, and developed CTF subchannel models of fuel assembly and reactor core

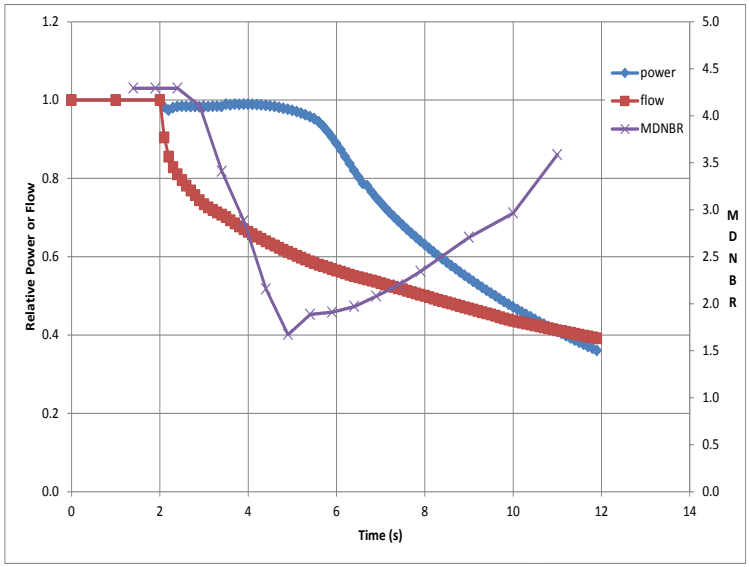
Yr5

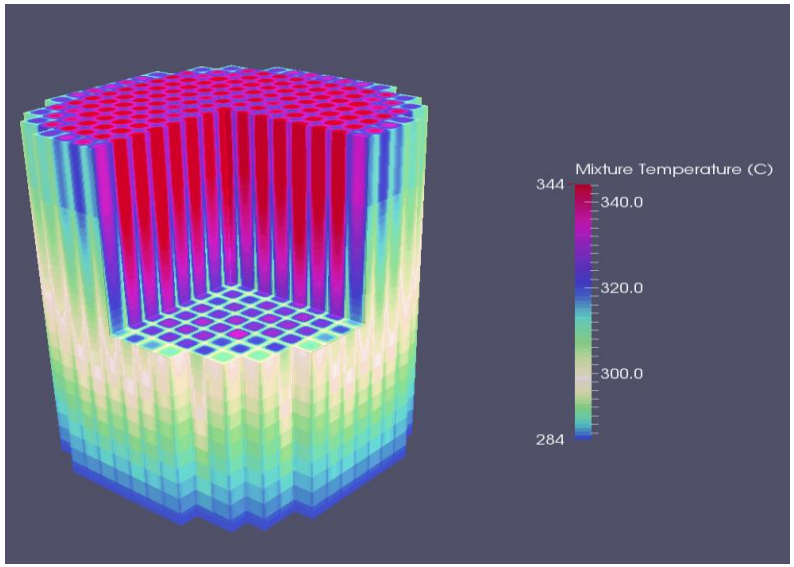
Complete CTF full core modeling and simulation of DNB limiting events, Hydra-TH simulation of rod bundle mixing tests, 2-phase CFD simulation using industry code, and UQ of turbulent mixing model

CASL VERA Applications
(Black – Completed, Red – Report by 08/31)

- COBRA-TF (CTF) subchannel code
  - Rod bundle mixing and DNB test simulations
  - RIA experiment simulation
  - Reactor core modeling under DNB limiting conditions (LOF, Steamline Break and RIA)
- Hydra-TH CFD code
  - Rod bundle model and execution on industry computer
  - Rod bundle single-phase mixing initial study
- VUQ study initiated on code and CP applications
  - Rod bundle turbulent mixing model calibration
- Results demonstrate VERA advancement and capability improvements

CTF Simulation of Loss of Flow Transient

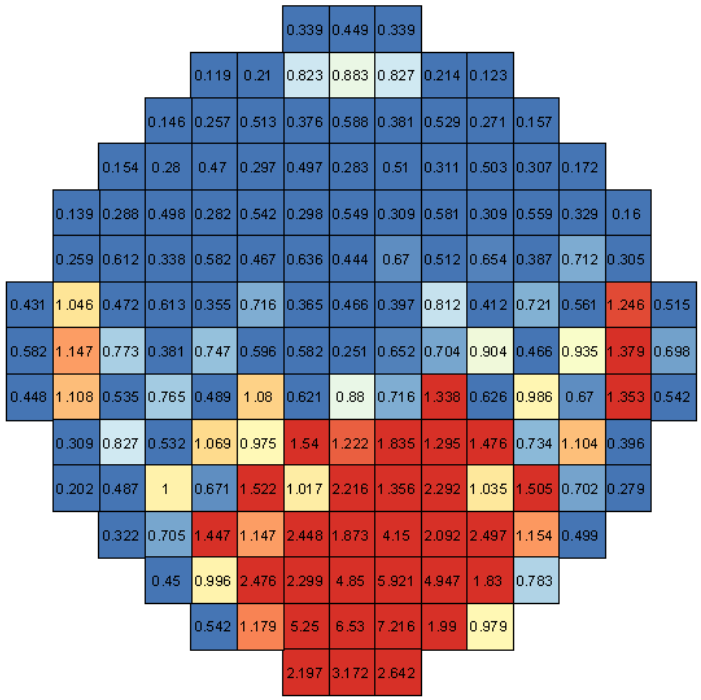


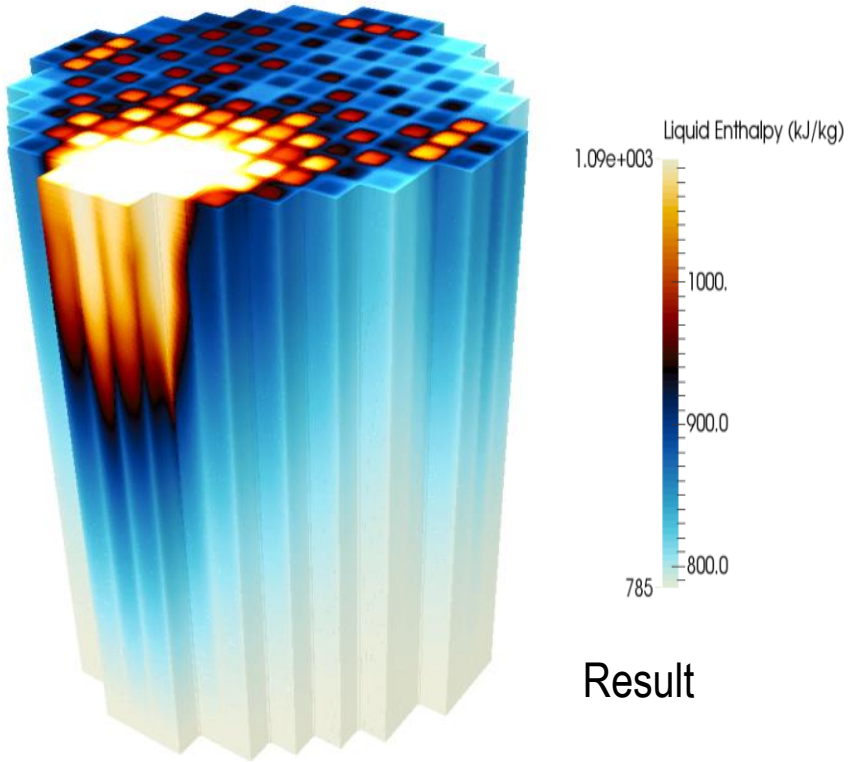


- PWR DNB event – Complete loss of coolant flow
- Power distribution input without VERA neutronic coupling
- Large model of reactor core simulating transient response
- 56288 channels x 151 axial nodes = 8.5M control volumes
- Minimum DNBR occurred at about 5 seconds

CTF Simulation of Low Flow Steamline Break

Input

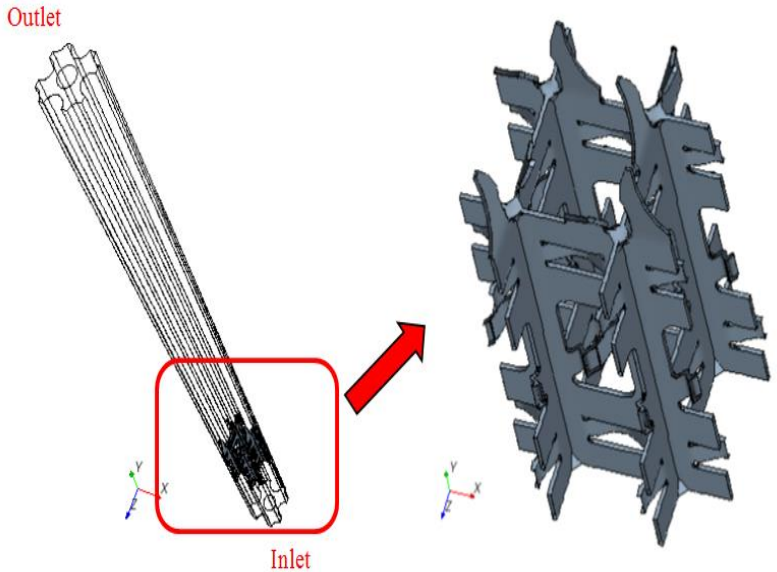




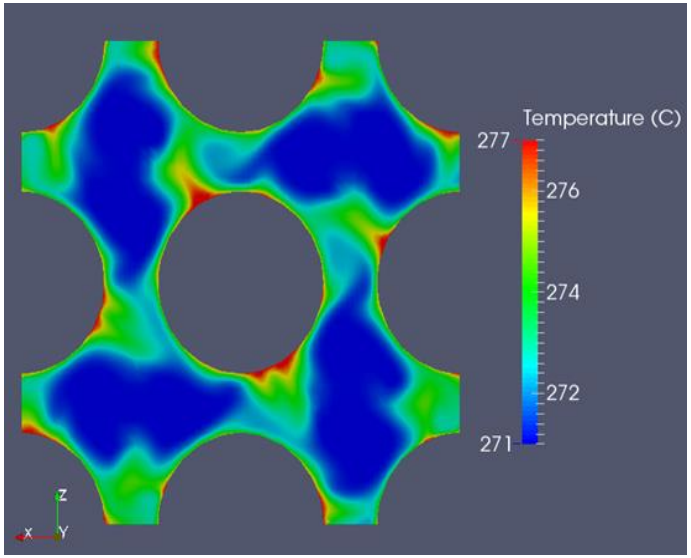
Result

- PWR DNB event - steamline break without offsite power
- Large model of reactor core simulating asymmetric distributions
- 56288 channels x 151 axial nodes = 8.5M control volumes
- Simulation of DNB limiting time step (low pressure/low flow)
- High void predictions in hot channels without VERA neutronic coupling

Hydra-TH Rod Bundle M&S on WEC Computer Platform



Geometric Model



Hydra-TH Prediction

- Establish process for application (mesh generation, result visualization)
- Learning and training of younger engineers
- Benchmark with existing CFD results and test data

Validation Activities

- Data collection
  - Test data from industry to guide VERA development and initial validation (e.g., CASL-I-2013-0035)
  - New test data being generated from special effect tests at universities (MIT, Texas A&M, NCSU, and etc.)
  - Additional data from industry continue to be identified and collected for CASL
- VERA code validation in progress (e.g., DAKOTA/COBR-TF)
- VUQ study of DNB CP initiated
  - Mini-PIRT
  - Turbulent mixing model calibration
- More DNB CP validation planned under VMA in Phase 2
  - Support code PCMM
  - Support development of VUQ process to address CP
  - Application of VUQ process to DNB CP

Success in Phase 1

- Minimum level in DNB CP charter will be met
  - VERA T/H codes and VUQ applied to improve test and fuel designs
  - VERA T/H subchannel code applied to reactor DNBR margin predictions
- Strive to achieve partial success of Desirable Level by the end of Phase 1
  - VERA high fidelity T/H code (CFD Hydra-TH) with VUQ capability applied to fuel design and thermal analysis
- Pursue complete success of Desirable Level and Ultimate End Game in Phase 2
  - Coupled VERA-CS code system with kinetic and VUQ capabilities
  - Application of multi-physics and high fidelity modeling and simulation and VUQ capabilities to resolve DNBR margin prediction as an unknown barrier in safety analysis

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Pellet-Cladding Interaction (PCI) Challenge Problem Status Update

Brian Wirth (UTK), on behalf of:

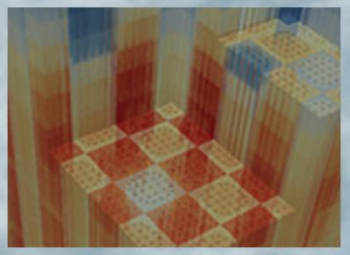
Robert Montgomery

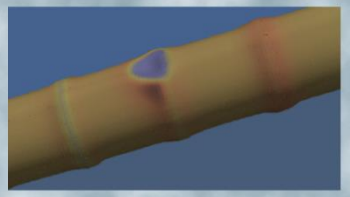
Pacific Northwest National Laboratory

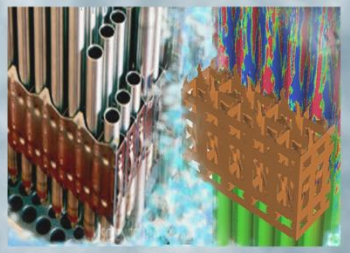
CASL IC/SC Meeting

September 9, 2014

Oak Ridge National Laboratory







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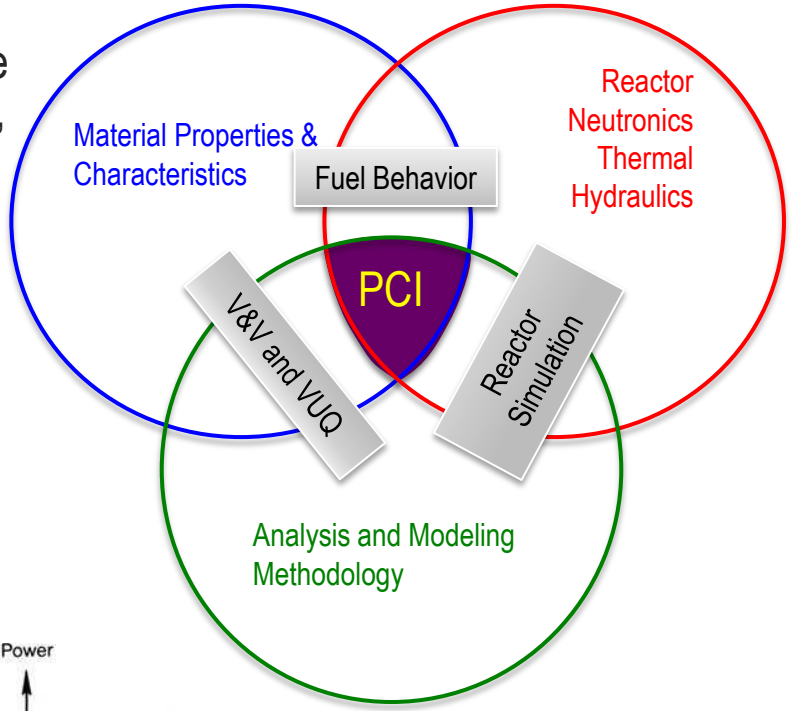
PCI Challenge Problem Review

- Description of Challenge Problem
- Current Industry Practice
- Path Forward
- Accomplishments in Phase 1
- Validation Strategy
- What is Success in Phase 1

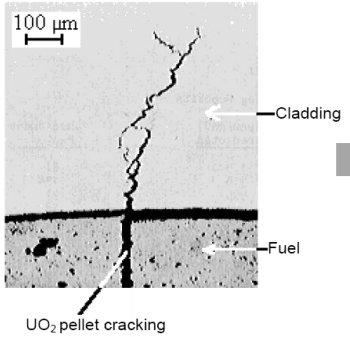
PCI: Why it is important?

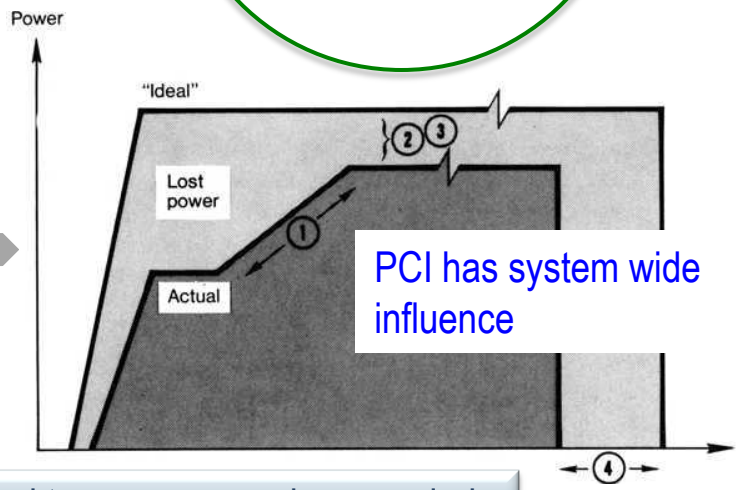
- PCI failure potential limits reactor performance associated with power uprates, higher burnup, fuel rod manufacturing quality and operating flexibility during power changes
- Requires new 3D multi-physics simulation capability to reduce uncertainties in assessing PCI failure conditions during normal operation and in the presence of anomalies



PCI is possible in many rods and assemblies

PCI is controlled by local effects





PCI has system wide influence

3D fuel performance modeling is critical to assess complex, coupled physics and multi-scale processes for PCI fuel failures

Current Industry Practices for Mitigating PCI Failures

- Power ramp rate restrictions during restart following a refueling outage or mid-cycle power maneuver
- Limitations on extent of low power operation with return to full power (important for the new paradigm of grid reliability)
- Restrictions on core loading patterns to minimize power peaking
- Fuel design changes to address key mechanisms of SCC
- EPRI PCI Guidelines from “Zero by 10” initiative outlines PCI Risk Assessment Procedure (PRAP)

Costs ($100 M/yr) associated with lost power generation, fuel development, and process restrictions

Desired Industry Path Forward

- Increase confidence in PCI failure potential assessments
  - Account for uncertainties in fuel performance parameters using improved mechanistic material models
  - Improve representation of non-uniform (non axi-symmetric) effects not included in current modeling approaches
  - Take advantage of improved neutronics simulations to reduce uncertainties in local power and burnup
  - Reduce empiricism in current methods used to assess cladding failure
- Improve core-wide PCI failure assessment process

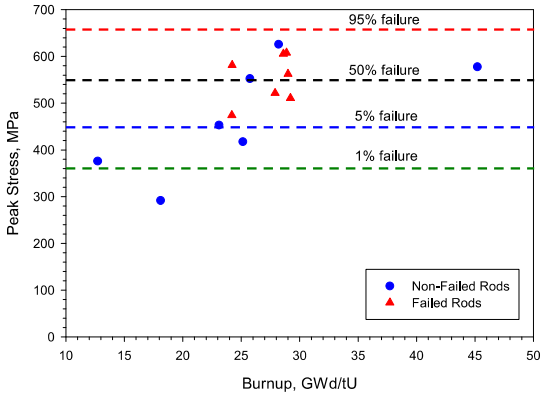
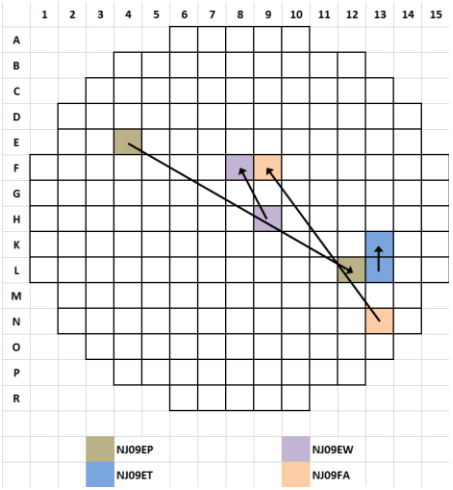
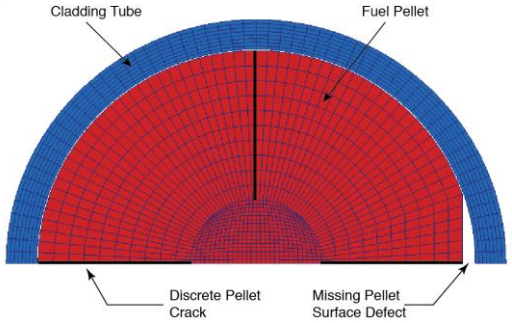
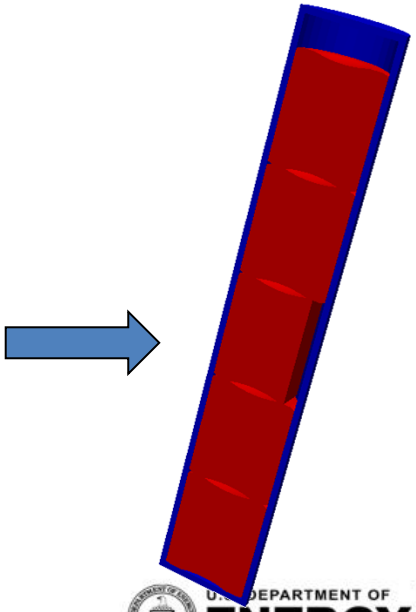


Figure 12. Stress-Based Failure Probability Levels







PCI M&S Capabilities Required

- Core-wide neutronics for local fission density and neutron flux that considers depletion, time dependent effects, and local reactivity perturbations (control rod movement)
- Subchannel thermal hydraulics for clad to coolant heat transfer conditions
- Full core fuel rod behavior modeling using reduced dimension (2-D) representation – Figure of Merit (FOM) calculation
- Local effects fuel rod simulation (3-D) accounting for non-uniformities, improved mechanistic material and behavior models

Reactor Simulation

Fuel Behavior

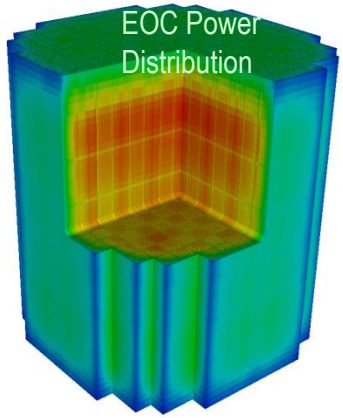
V&V and VUQ

Core-wide to local effects bridging

Accomplishments in Phase 1

- Peregrine development for 2-D and 3-D modeling for both full-length and local effects geometry (L1:CASL.P9.01)
- Lower-length scale material modeling of cladding
  - Visco-plastic self consistent model (VPSC) for thermal and irradiation creep and growth (L2:MPO.P9.03)
  - Dislocation density crystal plasticity model for Zr-cladding fracture (L3:MPO.CLAD.P9.02)
  - Corrosion and hydriding behavior of Zr-alloys (L3:MPO.CLAD.P8.01)
- Peregrine integration into VERA-CS (Tiamat) for multi-rod/multi-assembly simulations (L1:CASL.P9.03)
- Development of depletion capabilities within MPACT neutronics code (L3:RTM.PRT.P9.02)
- EPRI Test Stand focus on PCI modeling
  - Initial focus on fuel performance modeling with Peregrine (L4:AMA.EPRITestStand.P8.01)

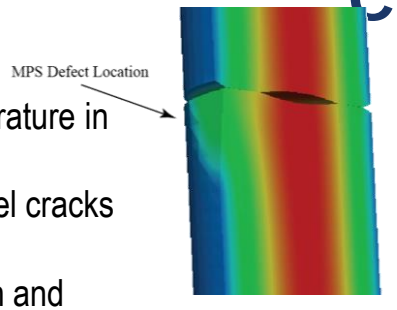
Cladding deformation and stress contour around MPS defect (displacements x20)



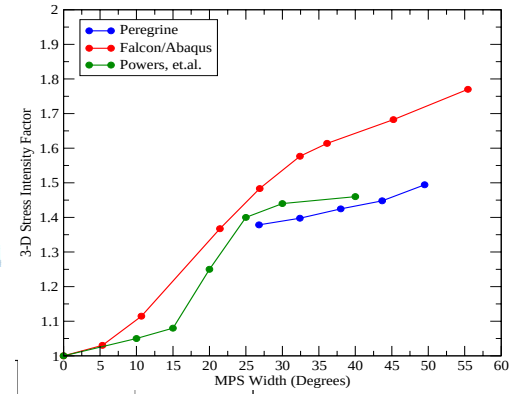
Peregrine/Bison-CASL: Assessment of 3-D Modeling Capabilities for the PCI Challenge Problem

Objective and Approach

- Calculate localized cladding stress and temperature in the vicinity of pellet cracks or MPS defects
- Include 2-D and 3-D geometric modeling of fuel cracks and MPS defects
- Compare to results published by EPRI (Falcon and ABAQUS), and AREVA (ANSYS)



Temperature Contour



TEAM:

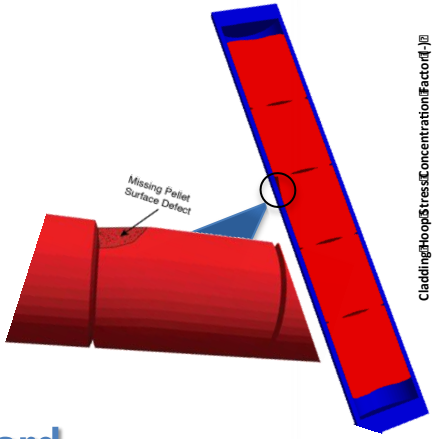
Pacific Northwest NATIONAL LABORATORY

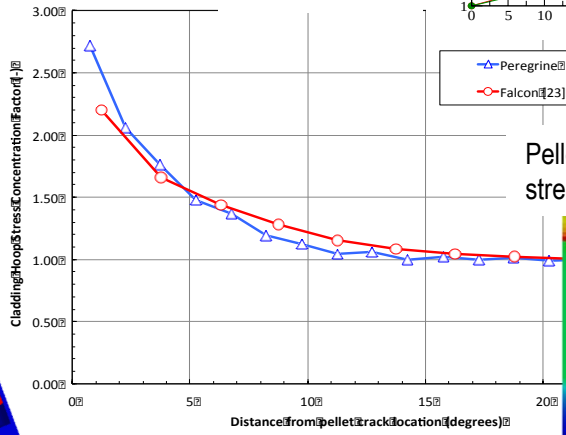
UF

ANATECH CORP.

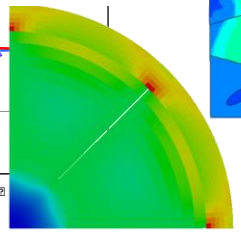
NC STATE UNIVERSITY

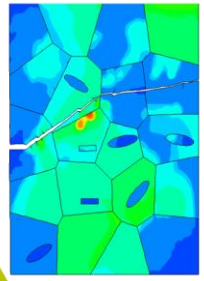
INL Idaho National Laboratory





Pellet and cladding stress contour





Dislocation density contour

Path Forward

- Implement robust 3-D mechanical contact algorithm
- Implicit model for fracture behavior of the ceramic UO_2 pellet
- Interface with a fission product chemistry and reaction model for initiation and propagation of cladding cracks by SCC

Assessment

- 2-D PCMI modeling is consistent with current state of the art in fuel behavior modeling for PCI
- Impact of MPS defect size on stress concentration factors similar to Falcon and general-purpose structural analysis codes
- Dislocation-density crystal plasticity model coupled with microstructural features is able to characterize crack growth evolution unique to Zr-alloys

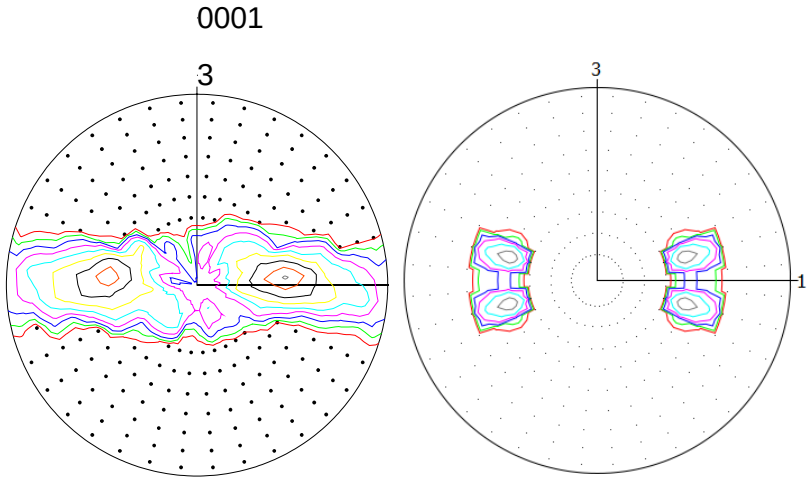
(L1:CASL.P9.01)

Using VPSC (Vulture) to Model Plastic Deformation

Use of physics-based VPSC allows for explicit consideration of anisotropy and texture, which are not aspects of current empirical models.

A 4 grain texture is constructed from full texture of cladding tube by imposing the same Kern factors (projection of c-axes along tube main directions)

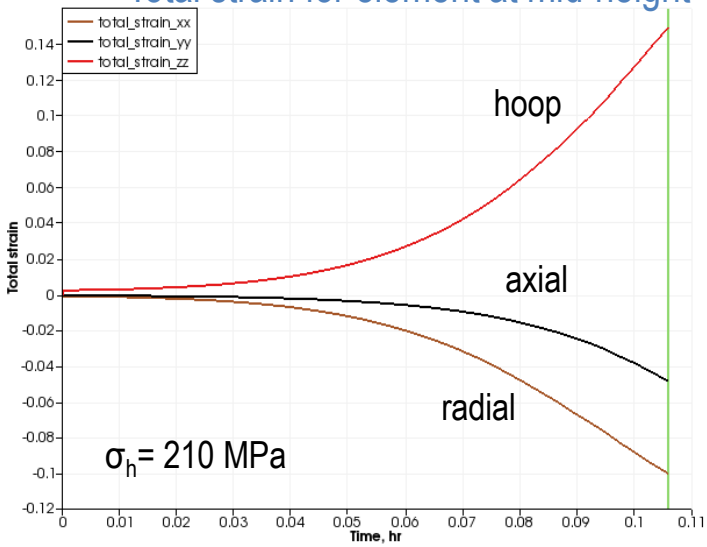
Predictions are within 10% of those obtained using the 1944 grain texture

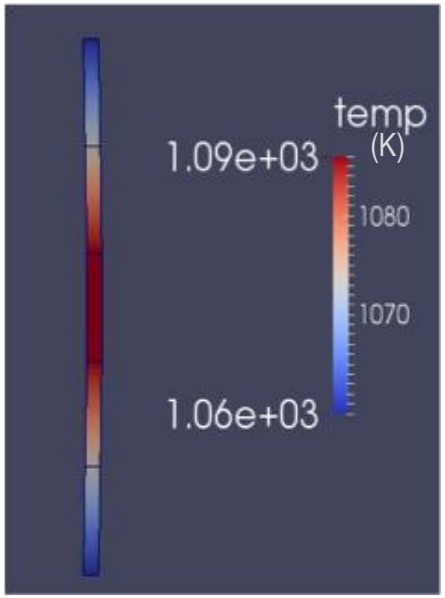


1944 grains

4-grain texture representation speeds VPSC-PEREGRINE interface by ~3 orders of magnitude

Pressurized tube analysis.
Total strain for element at mid-height



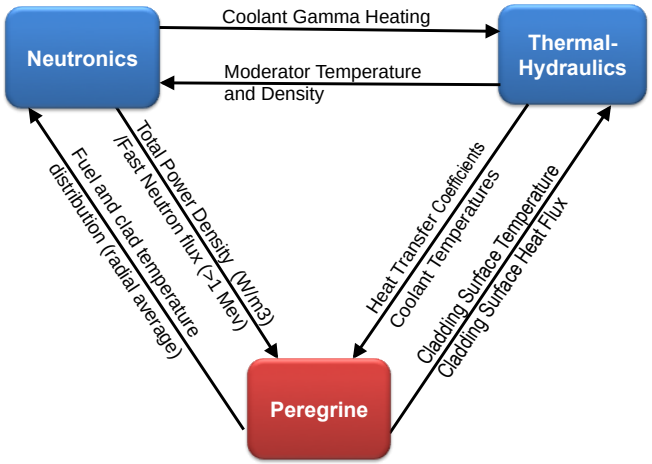


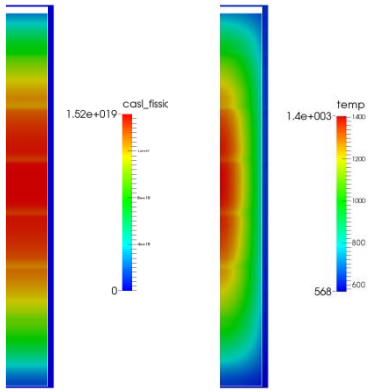
Preliminary demonstration of Peregrine-VPSC using constitutive model allowing for creep, growth and plastic deformation to be solved simultaneously.

(L2:MPO.P9.03)

Multi-rod/multi-assembly simulations with VERA-CS and Peregrine

- **PCI** – Neutronics-TH-Fuel Performance
  - Approach: Tiamat coupling of Insilico-CTF-Peregrine
- Challenges
  - Stable ramping from zero to full power
  - Conserving quantities through data transfers
  - Software integration
- Successfully performed single assembly calculations and on track for L1 reportable milestone completion for multiple assemblies
- Provides coupled temperature effect on x-sections and the ability to perform Figure of Merit calculations
  - Results to date are encouraging





Insilico Fission Rate

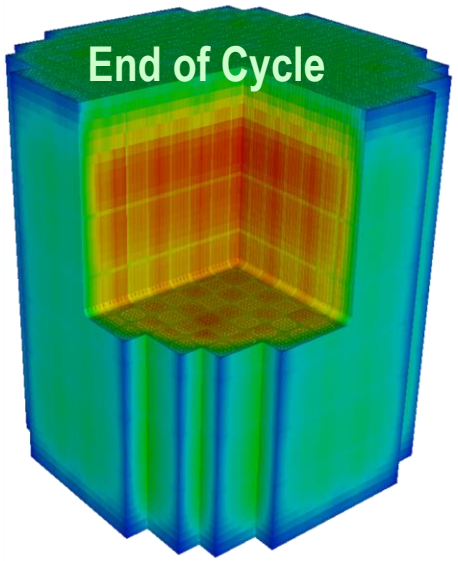
Peregrine Fuel Temperature

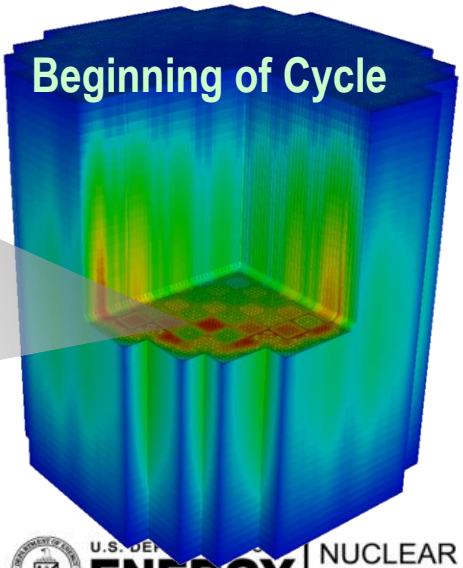
First Steps to Core-Wide Fuel Performance Calculations

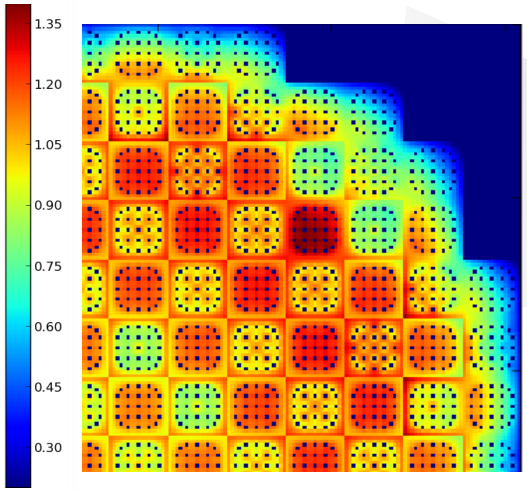
(L1:CASL.P9.03)

Full Core Depletion with MPACT

- Simulation of WBNPP Cycle 1 was performed with MPACT at 100% power for 400 Effective Full Power Days (EFPD)
  - Neglected variations from 100% power
  - Internal TH feedback (assembly axial energy balance without cross-flow + 1D fuel temperature)
  - Critical boron search
- Pin-resolved power is important for modeling fuel behavior leading to PCI as a function irradiation conditions
  - Further work needed to provide flux and power maps at power levels <100 % with xenon effects included





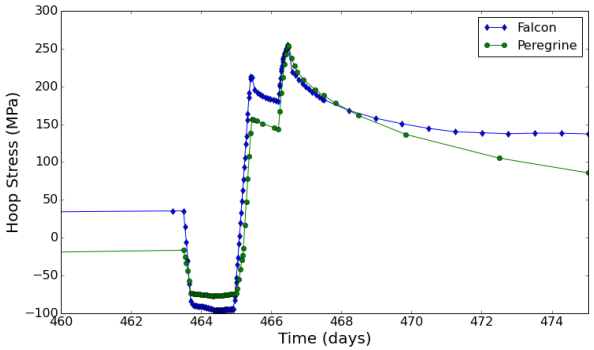


(L3:RTM.PRT.P9.02)

Lessons Learned from EPRI Test Stand Experience

- Maturity level of VERA components needs evolution to facilitate user experience base
  - Wide variety of proficiency with advanced M&S tool sets (scripting, pre/post processing, etc…)
  - Robustness of physics suite to address problems relevant to industry
- Peregrine comparisons to EPRI code results are encouraging
  - General agreement in observed trends
  - Differences in procedures for problem initialization and approaches to apply forcing functions (e.g. power)
  - Impact of potential material model differences were observed
- Validation/experience of Peregrine needs expansion to more broadly cover user application needs
- User interface, documentation, and training improvements were identified

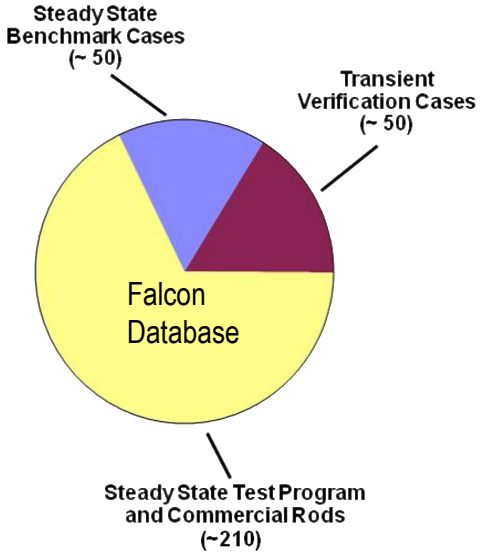
New EPRI HPC Platform
~500 core/8 teraflop machine

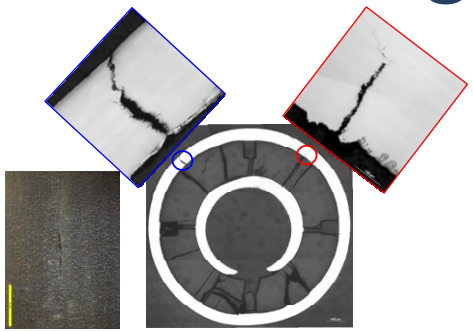


(L4:AMA.EPRITestStand.P8.01)

PCI Challenge Problem Validation Strategy

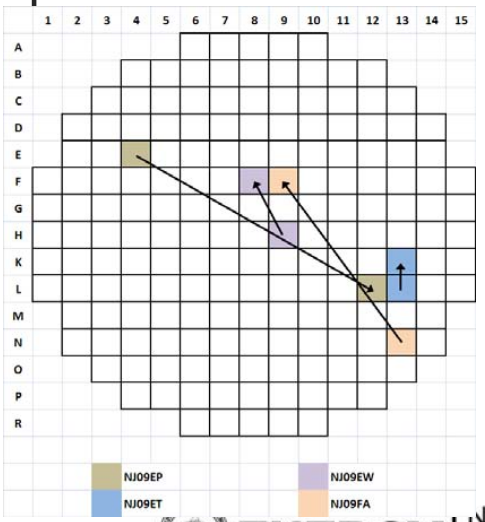
- Peregrine validation is following a rigorous approach based on industry experience (engineering scale effects)



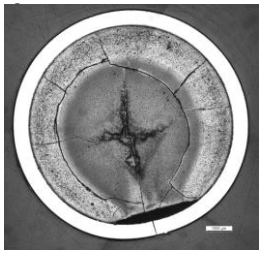


C. Anghel, et.al "An Out-of-Pile Method to Investigate Iodine-induced SCC of Irradiated Cladding" Top Fuel 2009 Paris, France, September 6-10, 2009.

- Separate effects testing and characterization will be used to validate material behavior/properties at the microscale

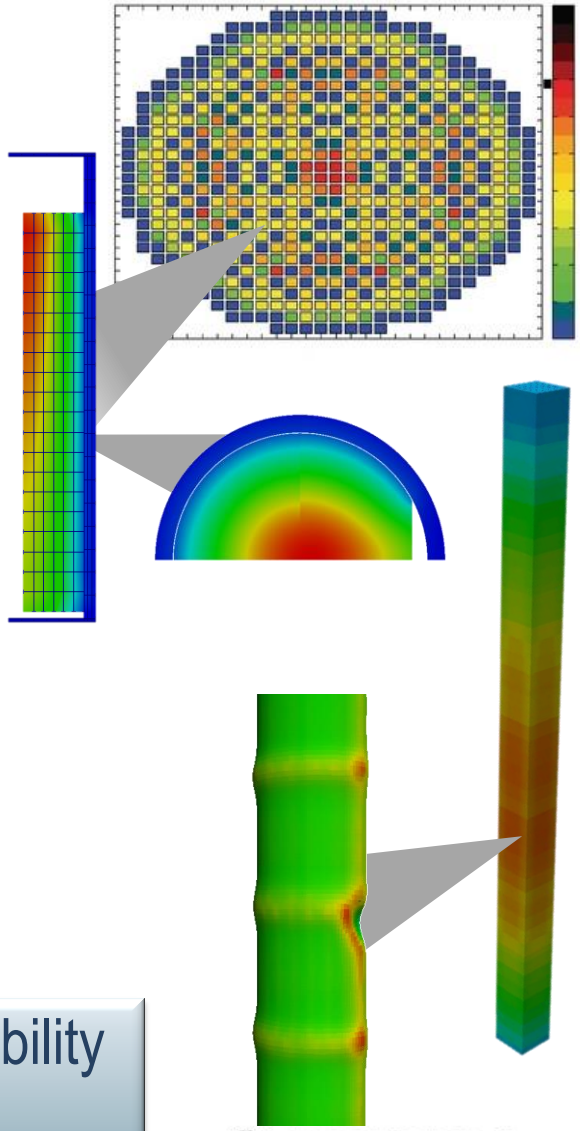


- Occurrences of MPS defect failures in commercial fuel will be used to validate coupled approach



Measures of Success

- Minimal: Use coupled neutronics/thermal-hydraulics/fuel performance to calculate axi-symmetric cladding stress distribution throughout the core.
  - Compare to empirical failure threshold stress (e.g. XEDOR/Powerplex)
- Acceptable: Use coupled neutronics/thermal-hydraulics/fuel performance to calculate local cladding stress concentrations in core region of interest
  - Requires separate 3-D local region standalone calculation
  - Compare to empirical failure threshold stress (e.g FALCON/SIMULATE)

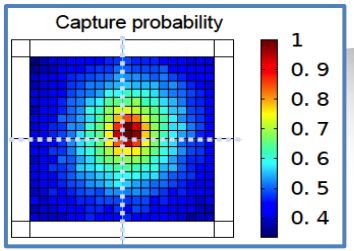


Goal: Methodology for PCI Failure Probability Assessment

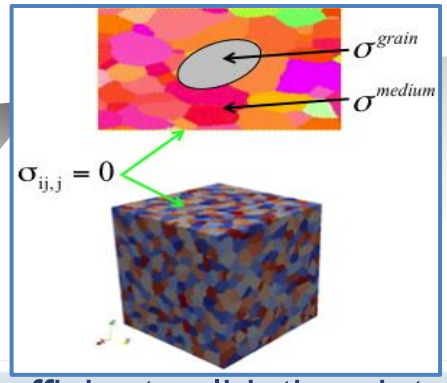
Measures of Success (con't)

- Ultimate End Game:
  - Reliably calculate PCI failure potential for specific core loading patterns and operating strategies
  - Define impact of material defects and material properties/characteristics on PCI failure potential
  - Define impact of plant operating strategy and fuel design on PCI failure potential

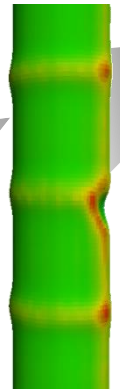
Atomistic simulation for defect behavior, including mobility and interaction with dislocations

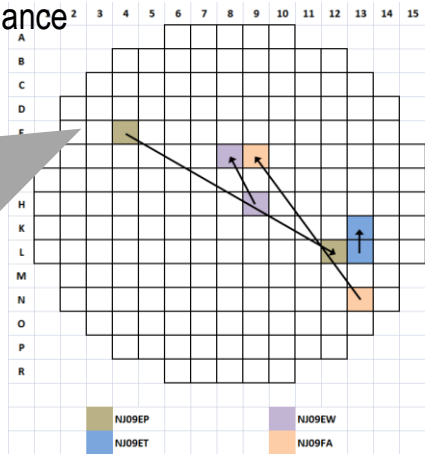


Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)



Peregrine engineering scale fuel performance





Challenge will be sufficient validation data to provide high level of confidence

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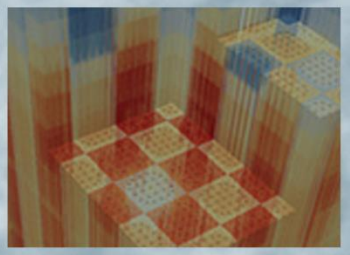
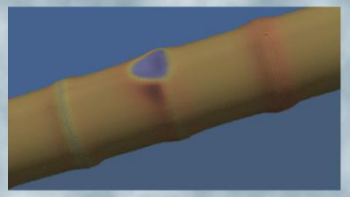
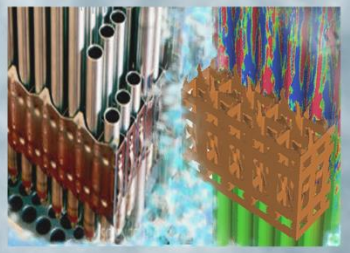
GTRF Challenge Problem Progress

Brian Wirth, Zeses Karoutas







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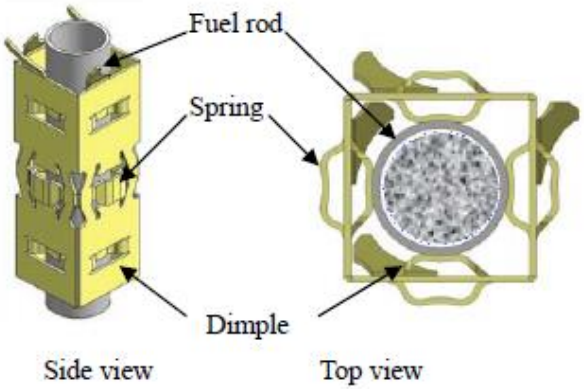
Grid-to-rod fretting failure (GTRF)

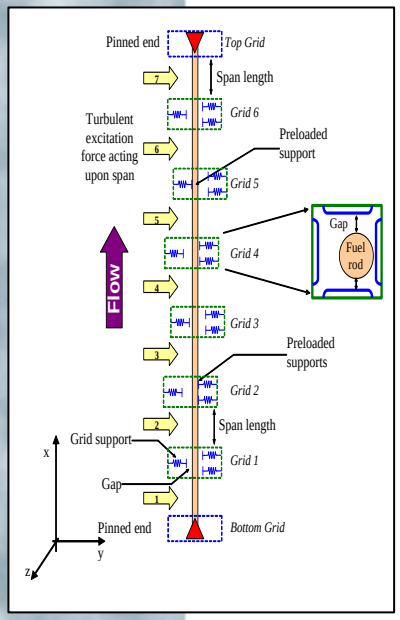
- Clad failure that occurs as a consequence of high cycle vibrational contact between spacer grid (spring, dimple) and fuel rod
- Leading cause of PWR fuel leakers (reliability & performance issue)
- Power uprates and increasing fuel burnup could exacerbate GTRF failures
- Important components of GTRF:

  - Development of gap between spacer grid and clad (due to thermal expansion, thermal/irradiation creep, spring relaxation, oxidation stress & growth);
  - Flow induced vibration;
  - Contact and abrasion/wear; and
  - Full length rod vibration and wear depth



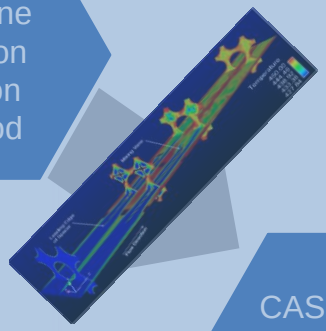
Industry practice & Evolution of CASL GTRF approach --- January 2012

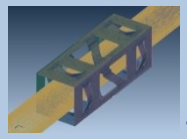
WEC VITRAN Methodology*



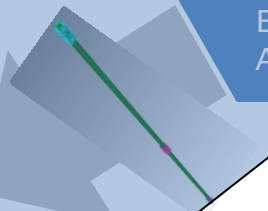
- Point contact at wear site
- 1D model
- PSD excitation force and 1D flow correlation

CFD to Determine Excitation Force on Fuel Rod

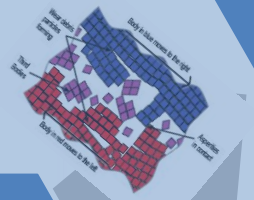


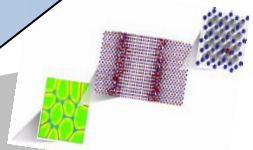


3D Structural Finite Element Analysis



CASL/VERA Development of GTRF Capabilities





GTRF Wear Mechanisms
Time varying material degradation, contact conditions

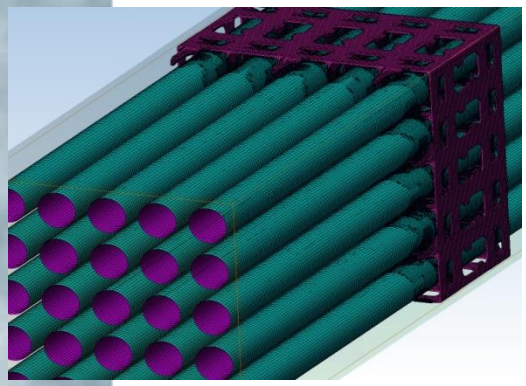
Integrate with Validation and Uncertainty Quantification

Constitutive Models:
Capturing thermal creep, irradiation creep and growth, and hydriding

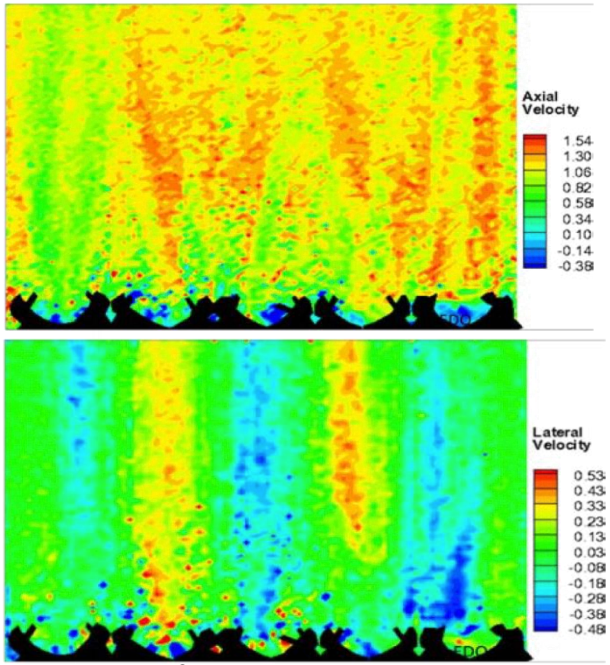
- Single crystal and polycrystal modeling of creep and dislocation mechanisms in irradiation environment
- Molecular statics, molecular dynamics, and accelerated molecular dynamics modeling of clad microstructure involving interaction of both interstitials and vacancies with edge dislocations
- Pair potential development to simulate chemistry and mechanical response

* Lu, Karoutas and Sham, *JOM* **63** (2011) 53-58

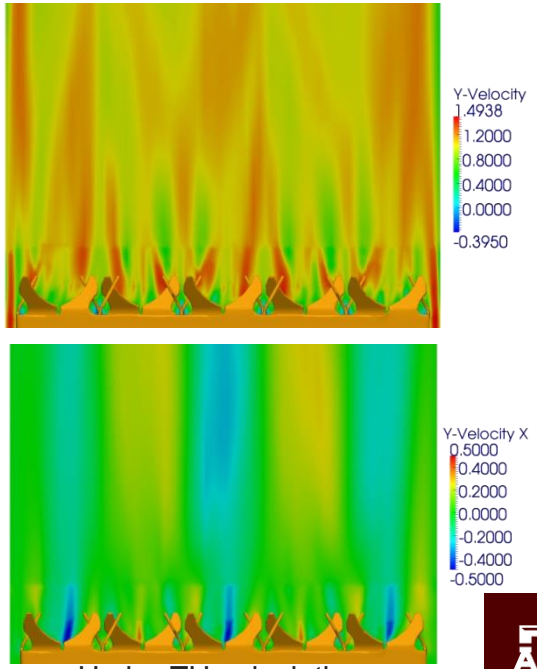
5x5 V5H study shows good agreement with experimental data



- Predicted mean peak velocities within 5% of experiments

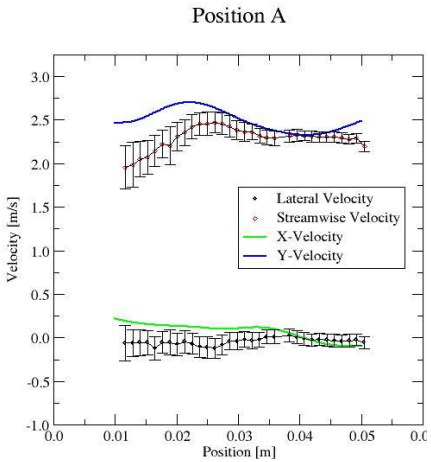


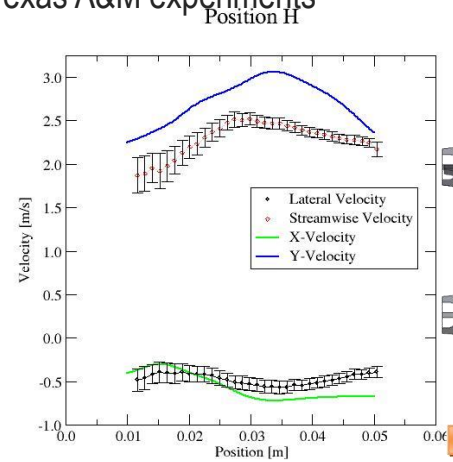
Texas A&M experiments

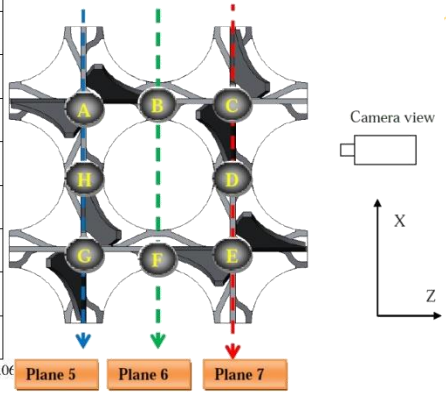


Hydra-TH calculations

- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)



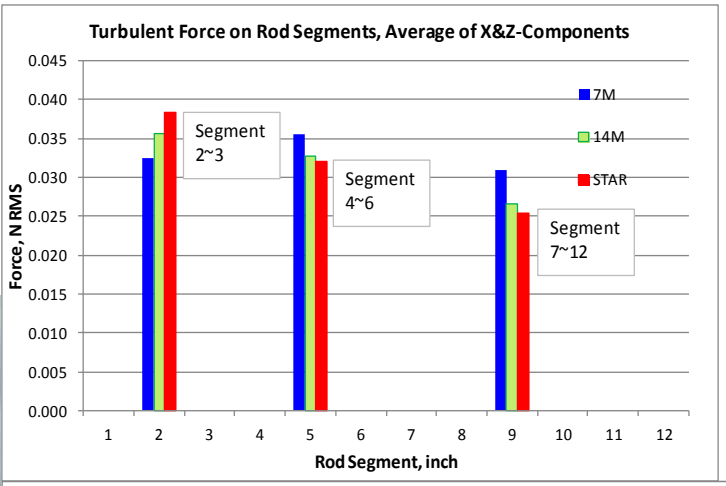


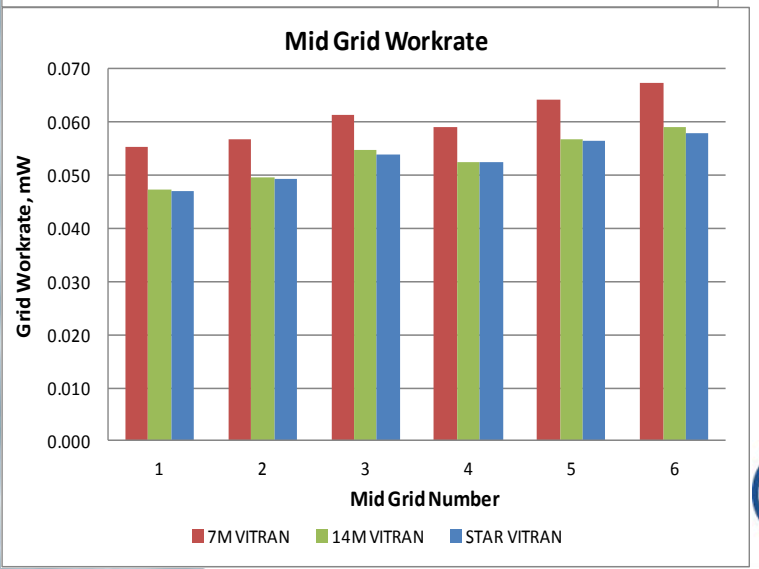


TEAM: Mark Christon, Jozsef Bakosi, Roger Lu, Y. Hassan

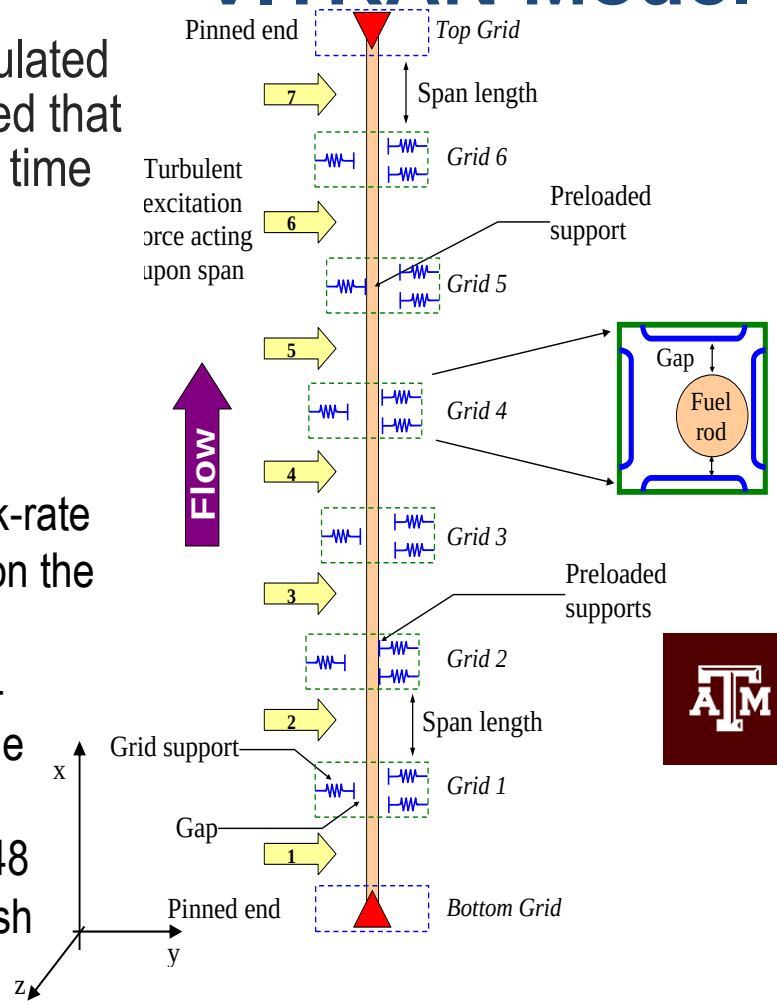
Input Turbulent Forces and VITRAN Model

- Three lumped forces are used to replace the forces calculated at every one inch segment along each span. It is assumed that the lumped forces are not correlated to each other in the time domain.



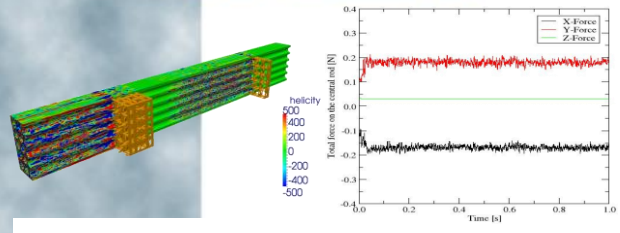


The computed work-rate differences based on the Hydra-TH results computed with a 14 million mesh and the STAR-CCM+ data computed using a 48 million element mesh differ by less 2%

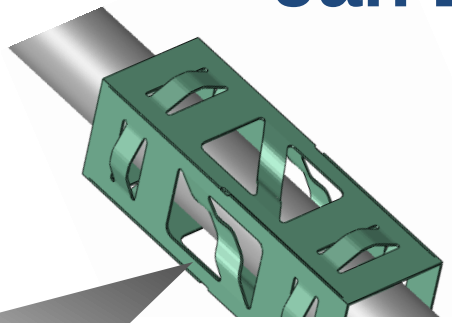


TEAM: Mark Christon, Jozsef Bakosi, Roger Lu,

CASL Approach to GTRF – Jan 2013



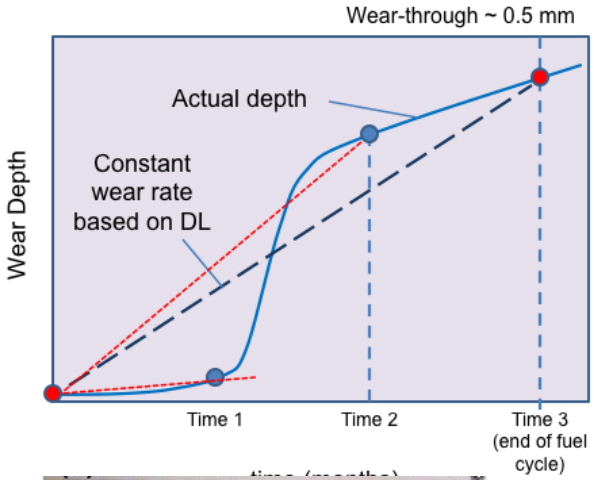
CFD Pressure Load History (Hydra-TH & limited fluid-structure interaction sims)

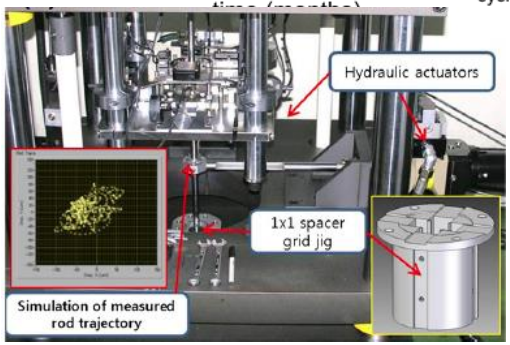


Structural mechanics thru interoperability with ISVs

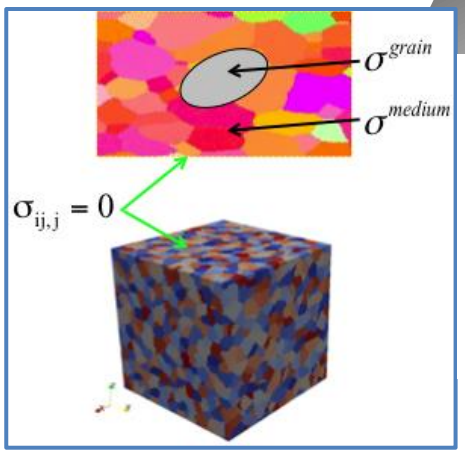
TEAM: Dave Parks, Ken Kamrin, Michael Demkowicz, Sam Sham, Peter Blau. Jun Qu, Roger Lu, Michael Thouless, Wei Lu,

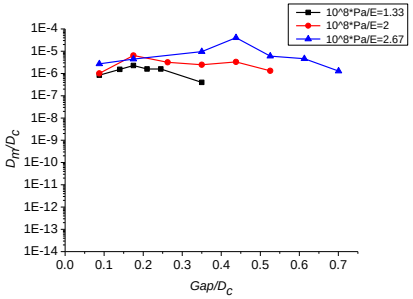
Wear model Consisting of incubation, oxide and substrate controlled stages in the wear history.





ORNL controlled fretting wear measurements





Grid-rod gap evolution, mechanical property evolution & parameteric studies of gap size/rod stiffness on wear shapes

Engineering Wear Model development

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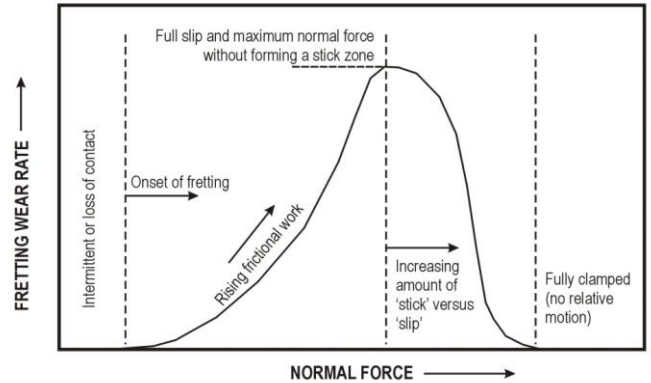
Factors like Normal Force, Frequency and Amplitude of Sliding Contact Affect GTRF

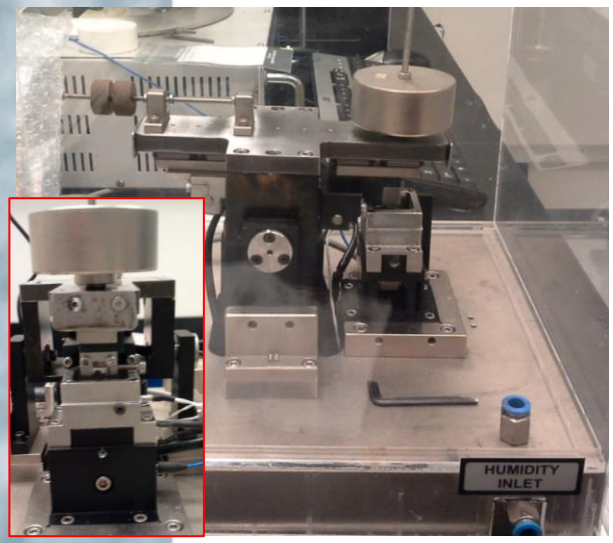


If normal force is either too high or two low, fretting is reduced or stopped.

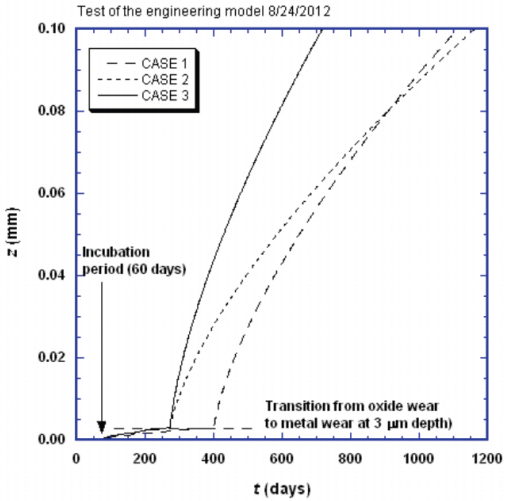
Use lab tests to evaluate effects of water flow rate & temperature, and to verify the model, which will be 'trained' against literature/ field data

$$ZrO_2\ thick. = K_{waterflow} \frac{\mu_{ZrO2}\, P_{rec}\, (2X_{rec})\, f_{rec}\, T_1}{A_1} \left(\frac{V_{w\text{-}lab\text{-}ZrO2}}{\mu'_{ZrO2}\, P_{lab}\, (2X_{lab})\, f_{lab}\, t_1} \right)$$

$$Z_t = K_{waterflow} \frac{\mu_{Zr}\, P_{rec}\, (2X_{rec})\, f_{rec}\, (t\text{-}T_1)}{A_t} \left(\frac{V_{w\text{-}lab\text{-}Zr}}{\mu'_{Zr}\, P_{lab}\, (2X_{lab})\, f_{lab}\, t_2} \right)$$



TR282 fretting wear testing at ORNL suitable for friction/wear testing under water conditions, ball on disk or tube on tube – provide laboratory data for engineering wear model validation



(μ) Friction coefficient

(P_{rec}) Normal force during time t

(X_{eff}) amplitude of oscillation

(f) oscillation frequency

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* P.J. Blau, *Wear* (2014) http://dx.doi.org/10.1016/j.wear.2014.02.016

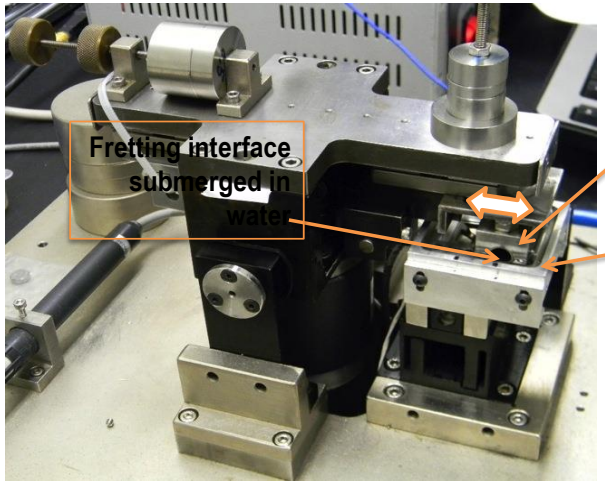
Fretting wear test: facility & measurements

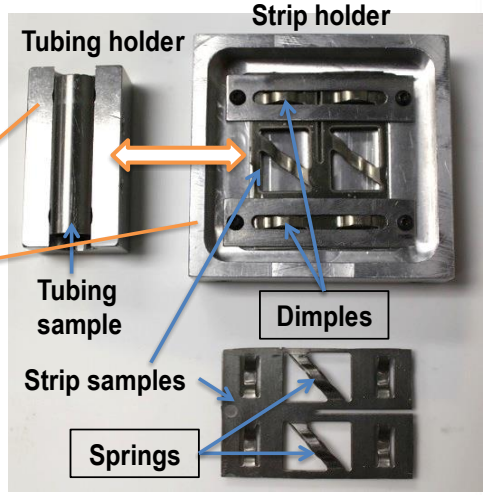
FY14.CASL.005 – L2.MPO.P9.01

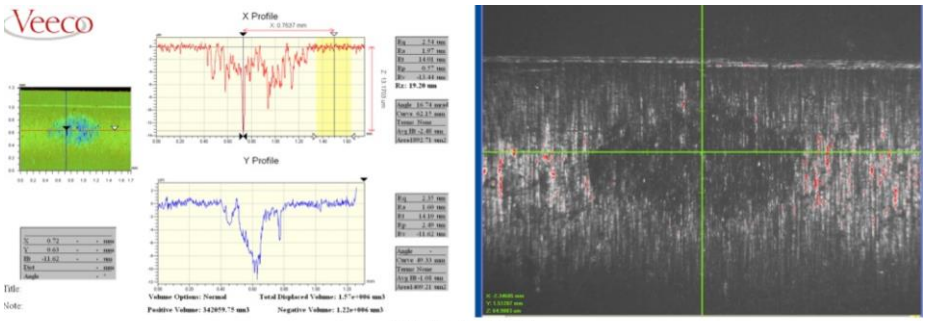
- Commercial sliding tribometer modified into a fretting machine, with contact loads in range from 0.1 to 0.5 N (tube-spring) and 0.5 to 2.5 N (Tube – dimple), 25 Hz and 0.2 mm amplitude in water --- generating data relevant to GTRF phenomena & benchmarking Engineering Wear model

- Zirconium alloy tubes and grid strap provided by Westinghouse, and heat treated to pre-oxidize – thus, specimens measured in as-received versus pre-oxidized conditions

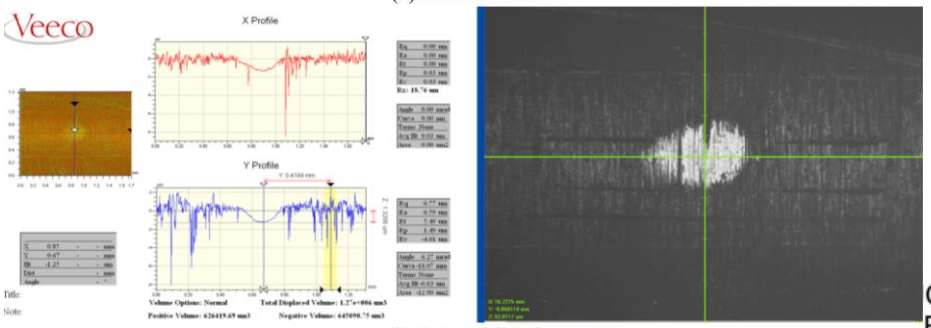
- Initial measurements showed significant reduction (~15X) of the wear volume in the pre-oxidized specimens







(a) As-received



(b) Pre-oxidized

TEAM: Roger Lu, Jun Qu, T.S. Byun, Lance Snead

Fretting wear test results

- **The wear depth and wear coefficient results obtained in ORNL bench fretting tests are within the range of literature data – except Tube-Dimple at 2.5N**
- **Reasonable to good repeatability.**
- **Pre-oxidation reduces the wear depth by >10X and wear coefficient by >>>50X!**

Tube-Dimple: 0.5 N

		Max wear depth (µm)	Wear volume ($x10^{-3}$ mm^3)	Wear coefficient ($x10^{-15}$ Pa^{-1})
As-received	Test 1	17.3	6.3	17.5
	Test 2	21.5	10.1	27.9
	Ave	19.4	8.2	22.7
Pre-oxidized	Test 1	1.1	0.09	0.26
	Test 2	1.7	0.11	0.31
	Ave	1.4	0.10	0.28
Ratio (As-received/ Pre-oxidized)		14.4X	80X	80X

Tube-Spring: 0.1 N

	Max wear depth (µm)	Wear volume ($x10^{-3}$ mm^3)	Wear coefficient ($x10^{-15}$ Pa^{-1})
Test 1	11.9	1.0	11.1
Test 2	13.3	1.3	14.3
Ave	12.6	1.1	12.7
Test 1	0.8	0.03	0.31
Test 2	0.8	0.02	0.20
Ave	0.8	0.02	0.25
d/ Pre-oxidized)	15.8X	51X	51X

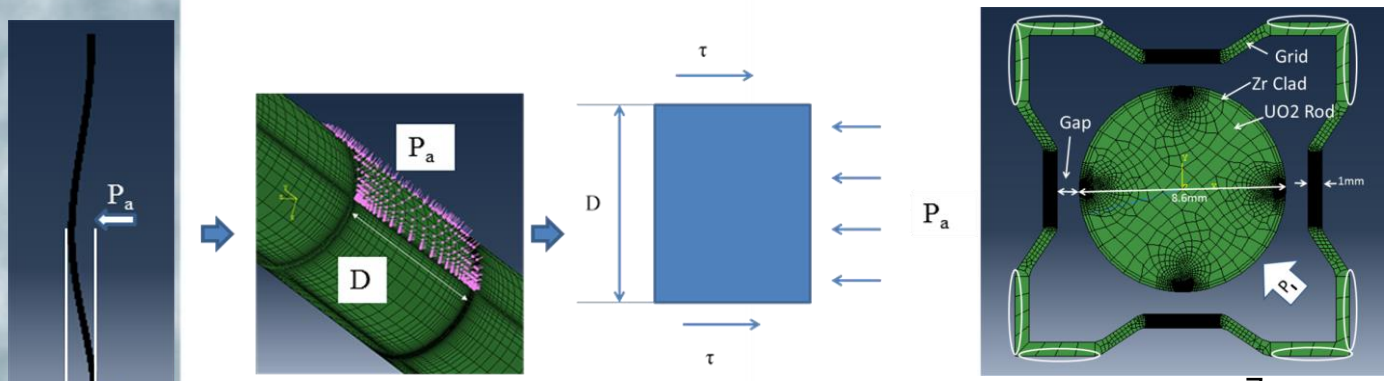
Tube-Dimple: 2.5 N

		Max wear depth (µm)	Wear volume ($x10^{-3}$ mm^3)	Wear coefficient ($x10^{-15}$ Pa^{-1})
As-received	Test 1	92.4	179.0	497.2
	Test 2	82.6	127.0	352.8
	Ave	87.5	153.0	425.0
Pre-oxidized	Test 1	1.6	0.13	0.37
	Test 2	1.3	0.14	0.39
	Ave	1.4	0.14	0.38
Ratio (As-received/ Pre-oxidized)		60.9X	1107X	1107X

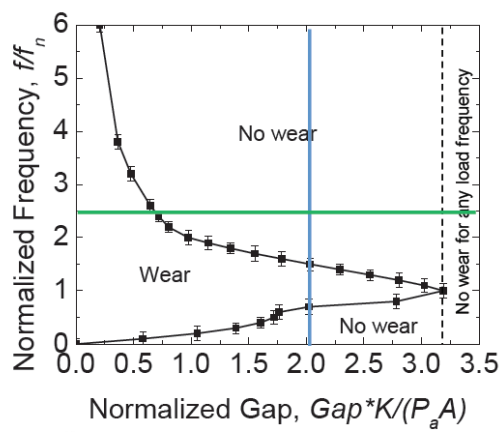
Tube-Spring: 0.5 N

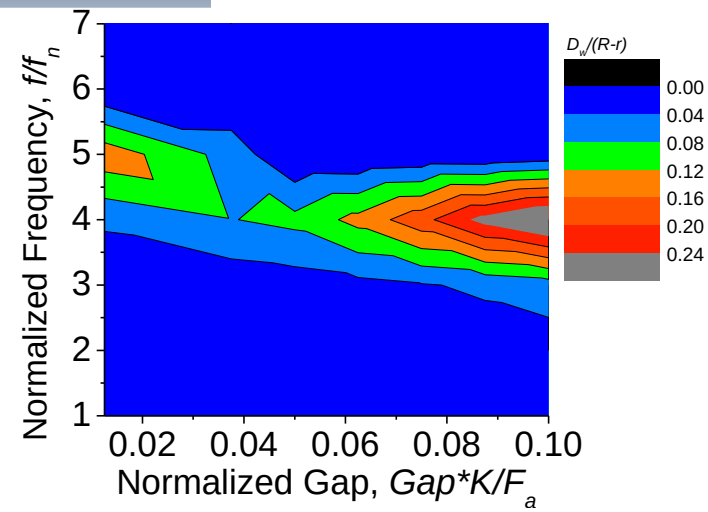
	Max wear depth (µm)	Wear volume ($x10^{-3}$ mm^3)	Wear coefficient ($x10^{-15}$ Pa^{-1})
Test 1	14.7	5.5	60.6
Test 2	12.6	3.4	37.8
Ave	13.7	4.5	49.2
Test 1	0.8	0.01	0.12
Test 2	0.9	0.03	0.35
Ave	0.9	0.02	0.23
ved/ Pre-oxidized)	16.1X	211X	211X

Parametric variation of key GTRF assumptions within 3D single cell grid (e.g., creep mechanisms*, rod stiffness & gap size)



- Rod stiffness, gap & load frequency affects vibration and wear
- The wear rate reaches a peak value at a certain gap.
- Moving towards 'wear map' show the overall dependence on grid-tc rod gap and load frequency





* Wang, Hu, Lu and Thouless, *JNM* **4333** (2013) 188-198

Summary

- FY13 & FY14 saw transition of GTRF approach within MPO, shift away from full-scale, coupled fluid-structure interactions activities to emphasize engineering wear model development and laboratory data to refine that model -- in addition to smaller-scale, University activities to provide base physics and pragmatic evaluation of FSI and structural mechanics activities using ISV codes

- Phase 1 success within CASL on GTRF is engineering wear model + pragmatic structural mechanics assessments (e.g., creep models in ABAQUS, influence of gap), in addition to CFD analysis of turbulent excitation forces

- Path forward: Phase 2 work will focus on wrapping up a validated engineering wear model benchmarked to additional laboratory (evaluating different wear regimes of fretting vs. impact loads), VIPER and reactor data, plus limited structural mechanics assessments (e.g., gap development effects) using ISVs

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Status of LOCA and RIA Challenge Problems

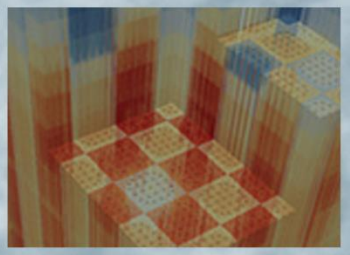
Gregg Swindelhurst

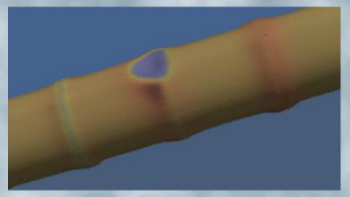
Challenge Problem Integrator

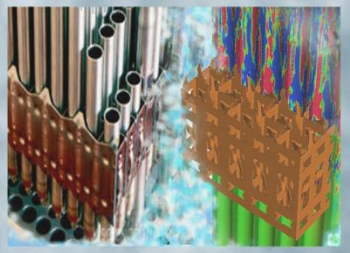
Presented by

Paul Turinsky

Chief Scientist







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LOCA & RIA Challenge Problem Progress

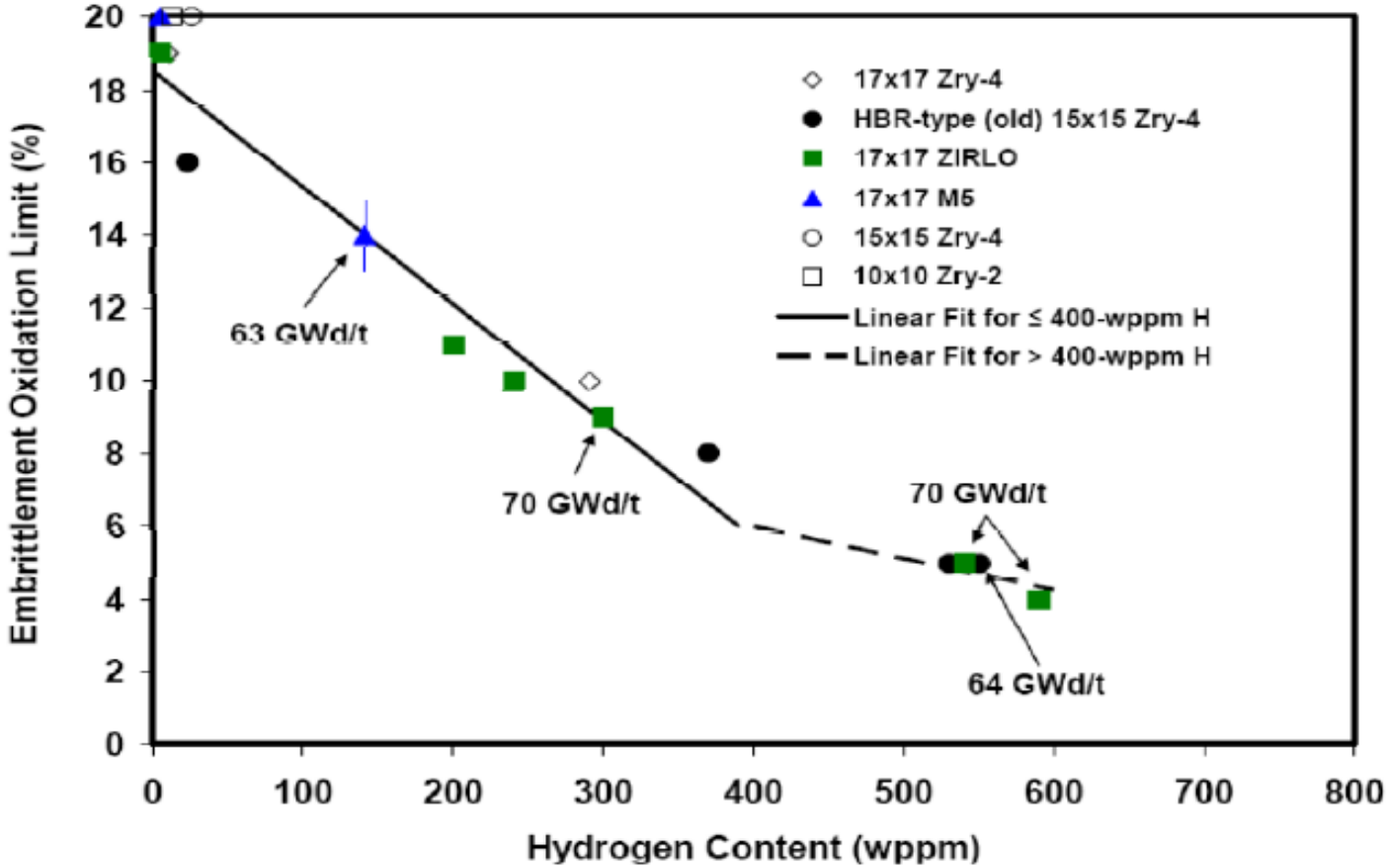
LOCA remains a technical and regulatory challenge to the industry

- 10 CFR 50.46c rulemaking to include higher burnup effects currently in public comment period
- Fuel and reload core design impact [loss of margin]
- History of emerging issues and high cost of LOCA code development and reanalysis

Reactivity initiated accident (RIA) also being revisited by NRC to address higher burnup effects

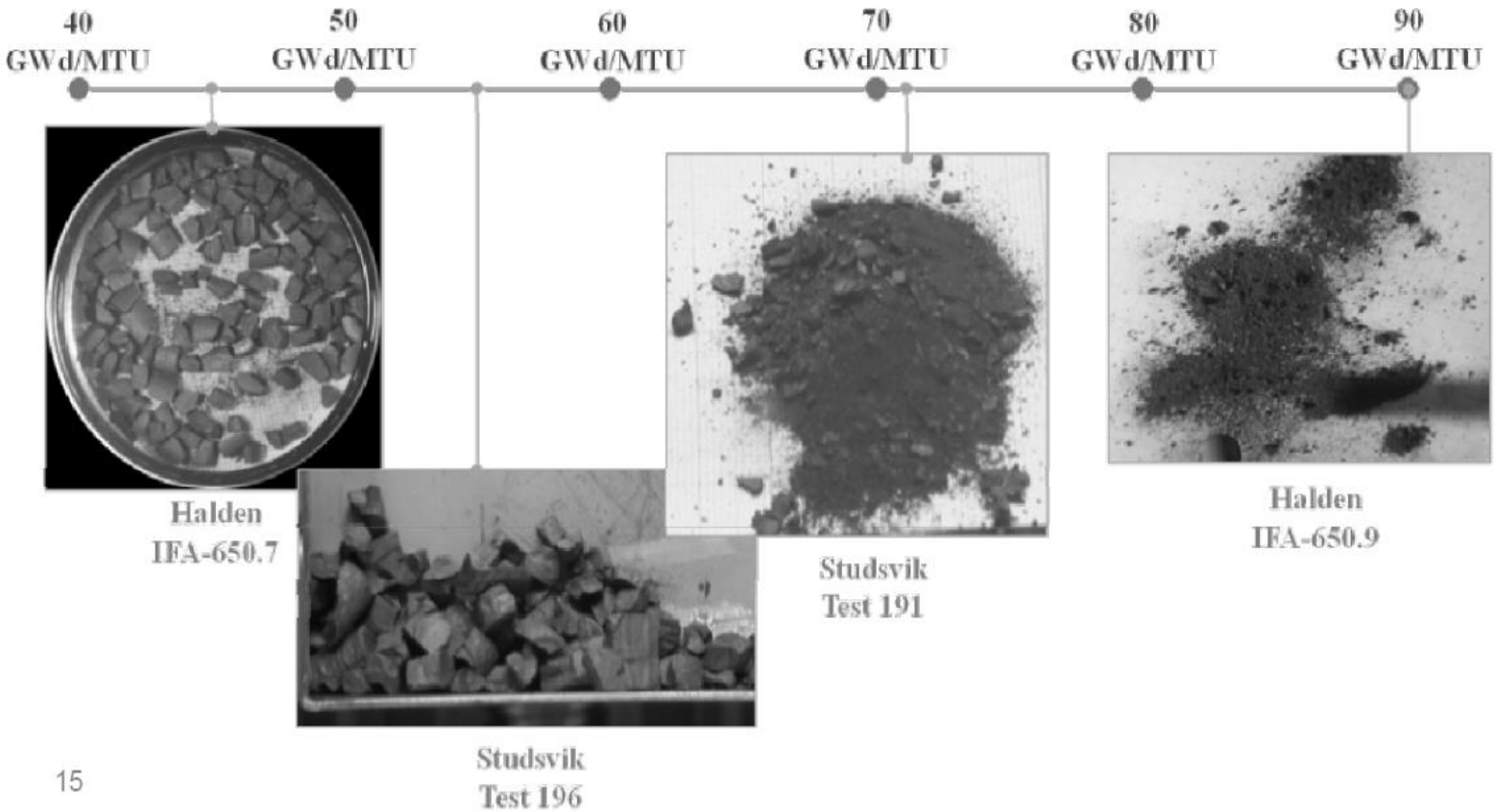
- Final revised acceptance criteria expected late 2014 or 2015 [loss of margin]

LOCA & RIA Challenge Problem Progress



NRC-funded LOCA testing program at ANL showed need to reduce 17% cladding oxidation limit due to pre-existing hydrogen pickup in cladding [DG-1263]

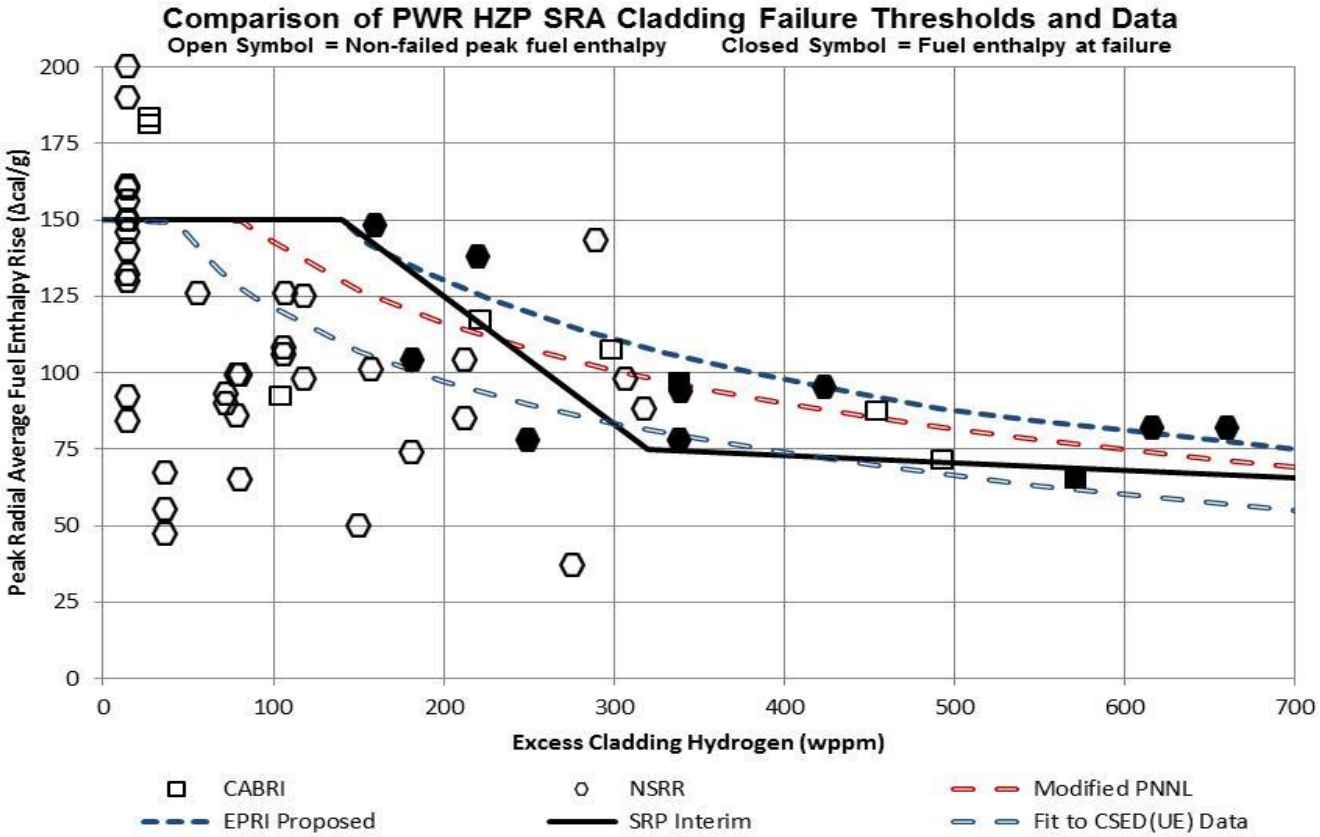
LOCA & RIA Challenge Problem Progress



Post-LOCA fuel fragmentation vs. burnup shows a threshold between 55 and 70 GWd/MTU [NRC presentation at 3/13/2014 public meeting]

Note CASL will not attempt to model post-cladding failure behavior

LOCA & RIA Challenge Problem Progress



Reduction in RIA fuel enthalpy limit of 280 cal/gm due to higher burnup fuel effects [NRC presentation at AREVA 5/2014]

LOCA & RIA Challenge Problem Progress

CASL Path Forward for LOCA

- CASL to focus on fuel rod behavior during LOCA
- Peregrine transient fuel rod thermal-mechanical code
  - Higher-fidelity fuel rod modeling capability for LOCA
  - System thermal-hydraulic LOCA boundary conditions from WEC WCOBRA/TRAC or RELAP5

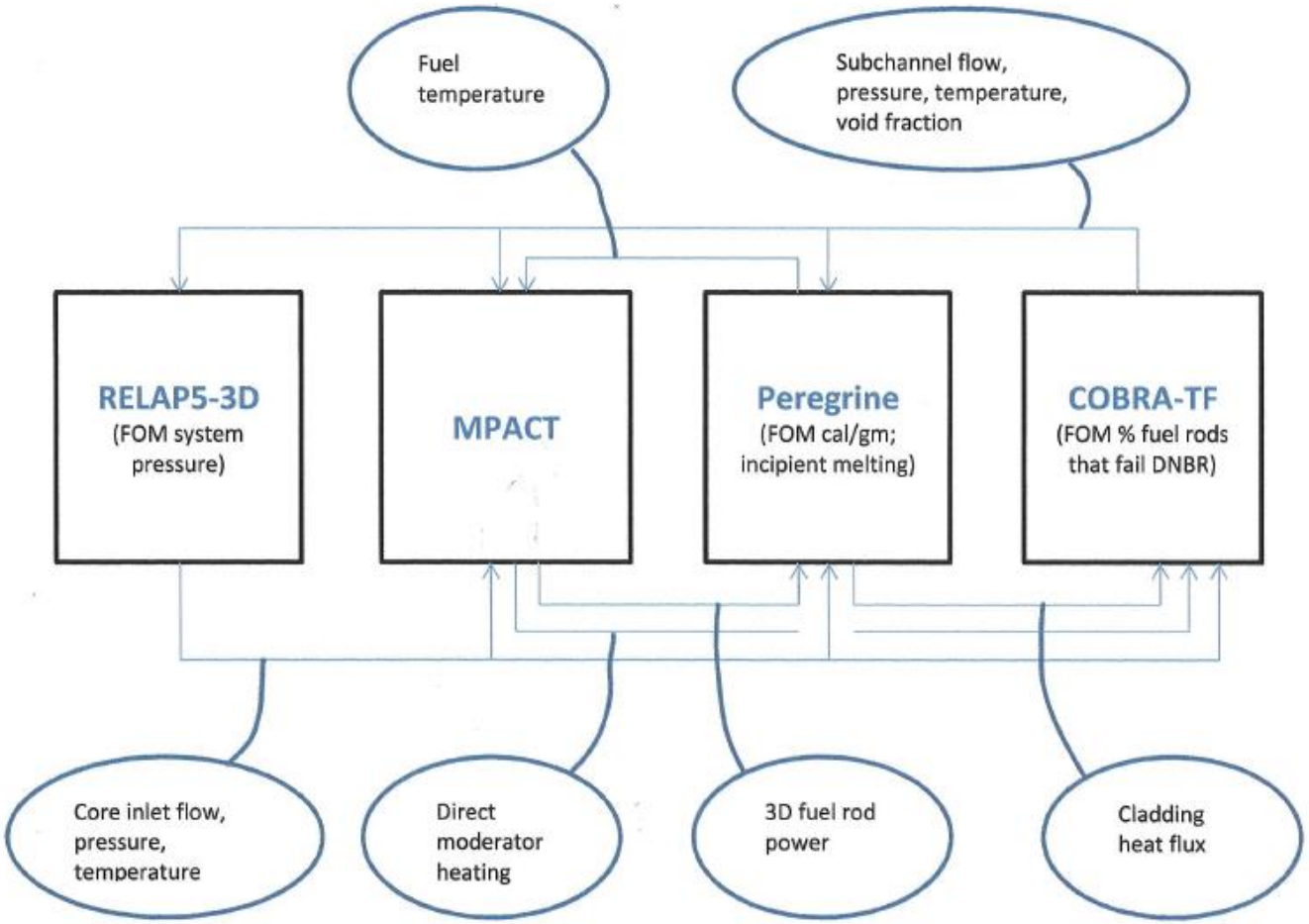
CASL Path Forward for RIA

- CASL to achieve tightly-coupled multi-physics modeling of RIA

Goals: Address technical and regulatory issues and increase analytical margin

LOCA & RIA Challenge Problem Progress

VERA RIA Coupling

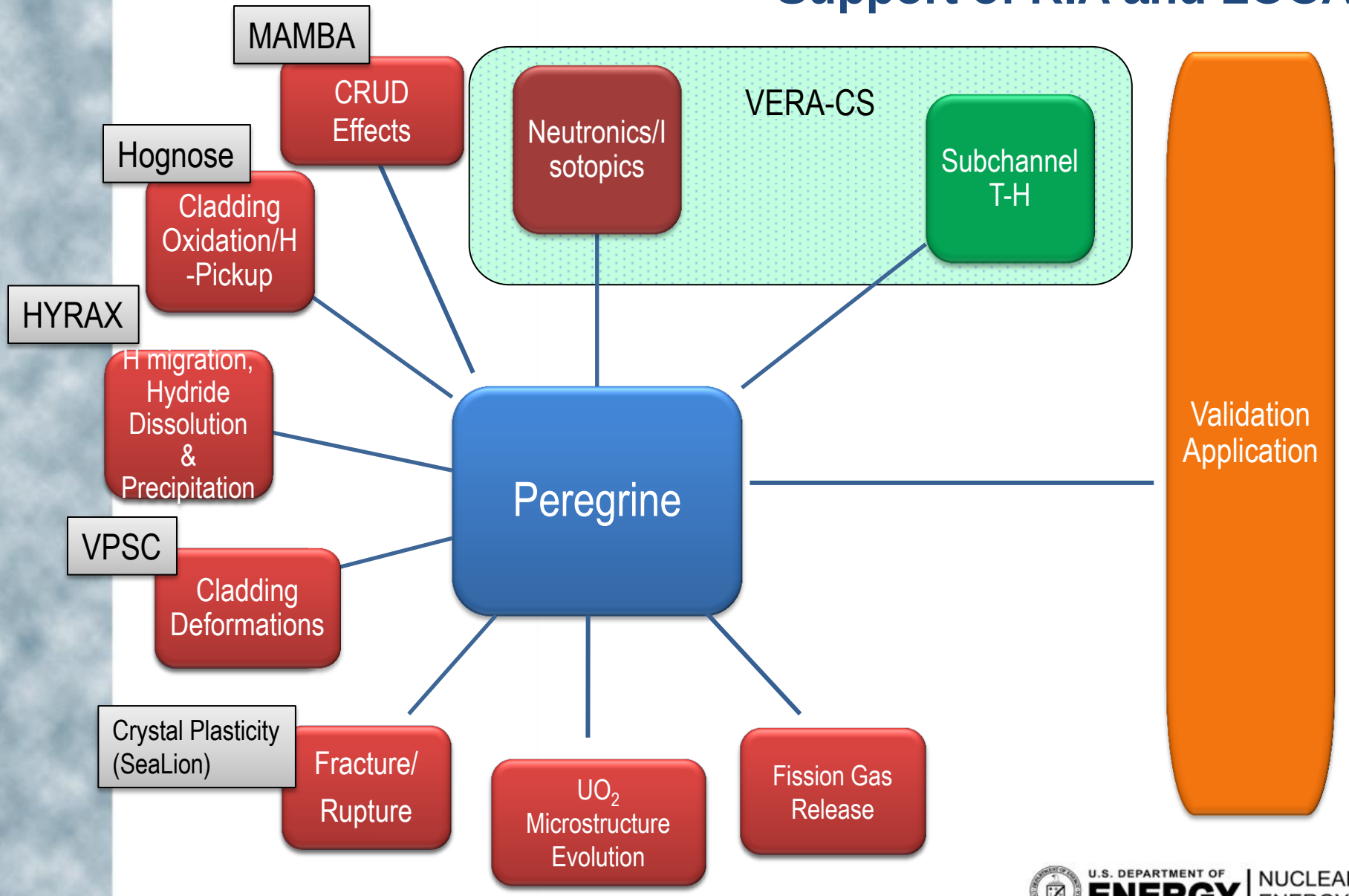


LOCA & RIA Challenge Problem Progress

Accomplishments to Date

- RIA and LOCA Charters and Implementation Plans completed
- Peregrine fuel rod initial conditions modeling
  - Cladding corrosion and hydrogen pickup completed
  - Material properties vs. exposure completed
  - RIA test case and LOCA cladding ballooning modeling (by 9/30/2014)
- COBRA-TF subchannel T/H development
  - Whole core models
  - RIA demo problem completed
- MPACT transient neutronics development
  - Transient capability completed
  - SPERT reactor RIA test validation (by 9/30/2014)
- MPACT coupled to COBRA-TF completed

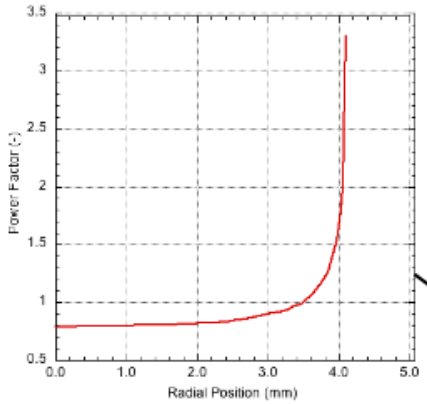
Peregrine Fuel Performance Modeling in Support of RIA and LOCA



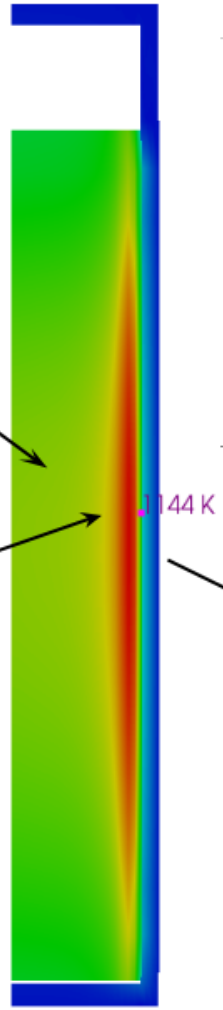
Peregrine Transient Modeling of RIA Demonstration

Temperature Contour at 0.5 seconds

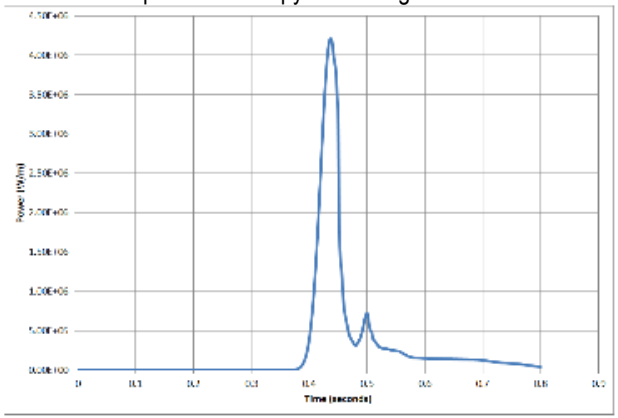
Pellet Burnup - 75 GWd/tU



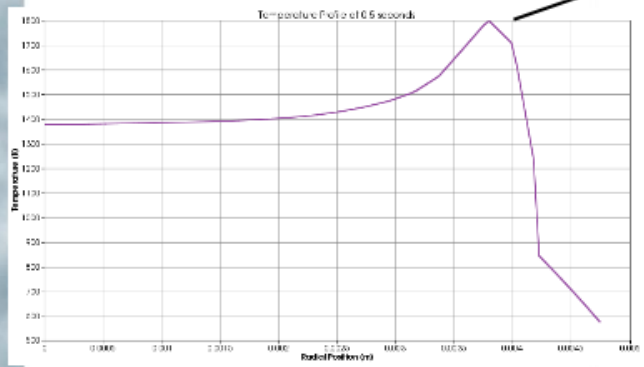
Pellet Radial Power Factor Distribution



Deposited Enthalpy ~120 cal/gm

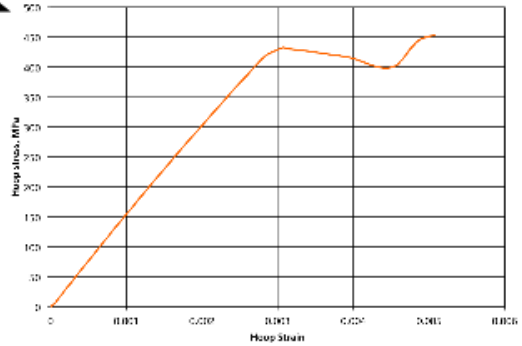


Fuel Rod Average Linear Power Time History



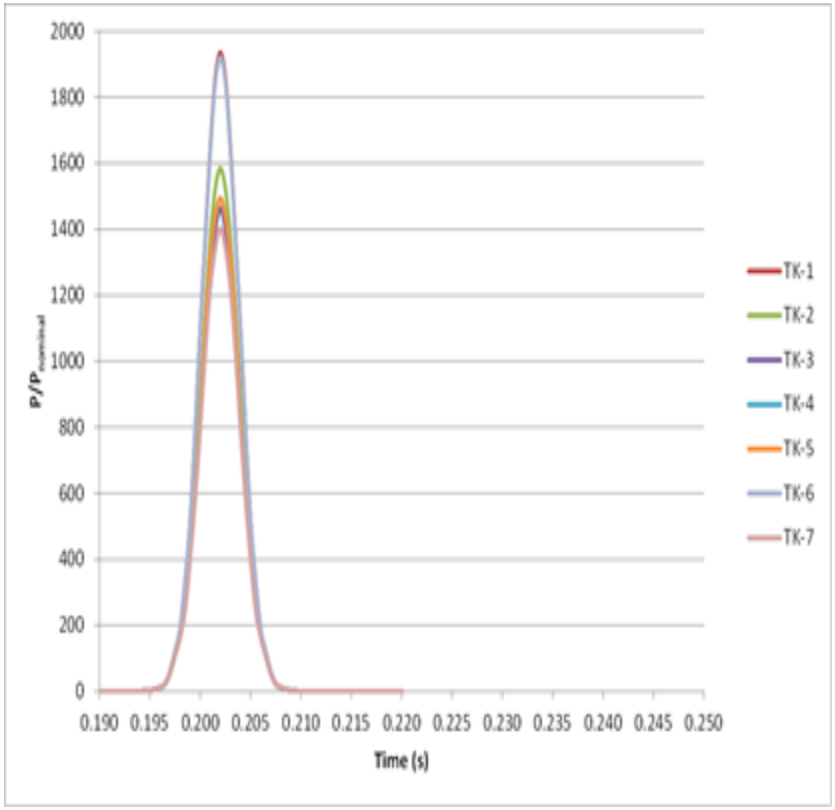
Radial Temperature Distribution at 0.5 secs

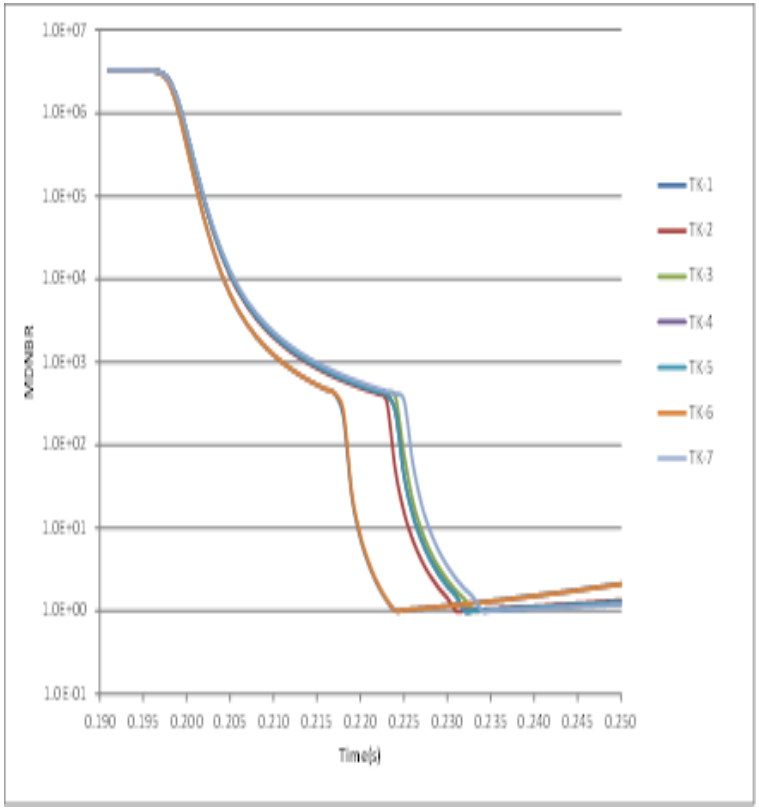
Fast Fluence ~ 1.2×10^{23} n/cm^2-s



Cladding Stress and Strain Response

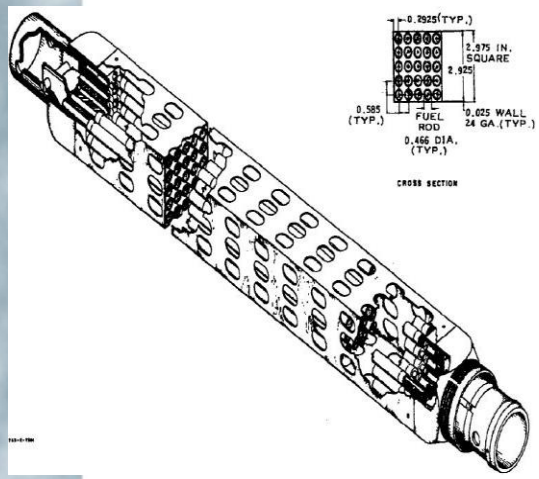
COBRA-TF RIA Demonstration

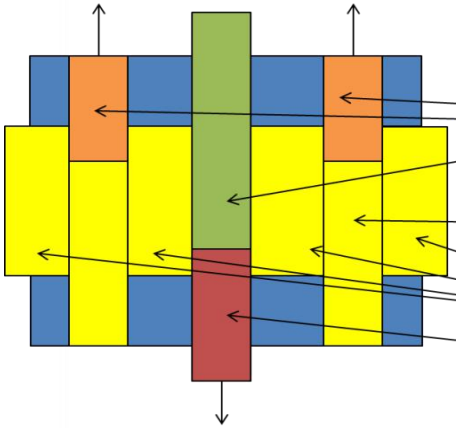


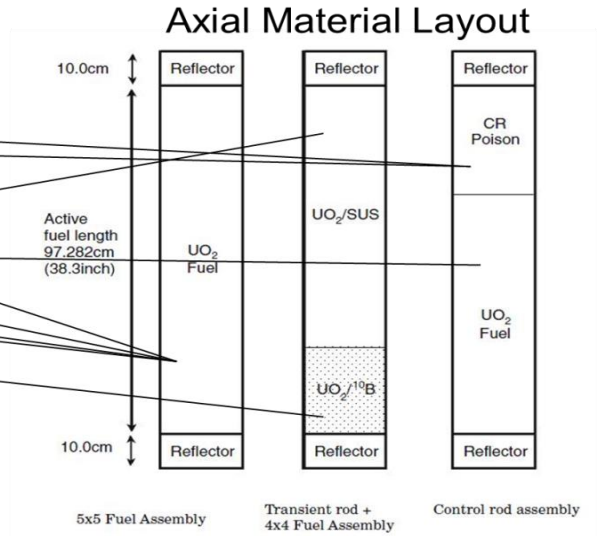


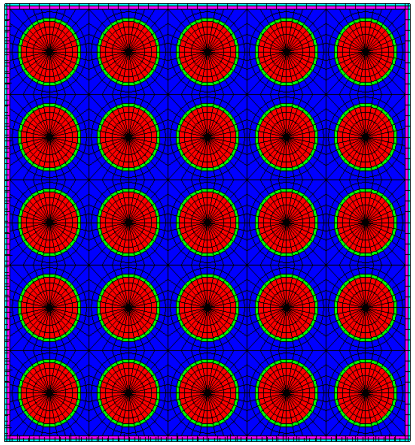
DNBR predictions for Japanese NSRR RIA TK test series

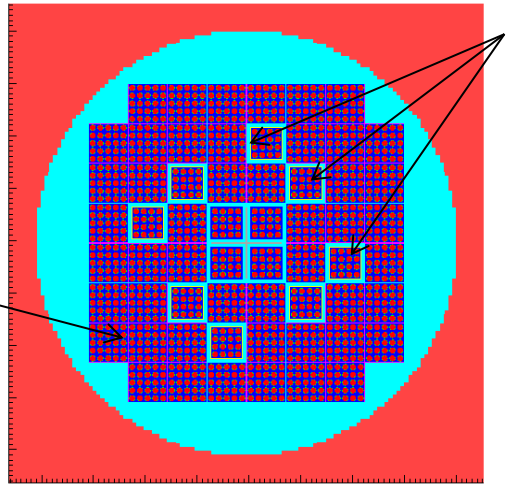
MPACT SPERT RIA Model











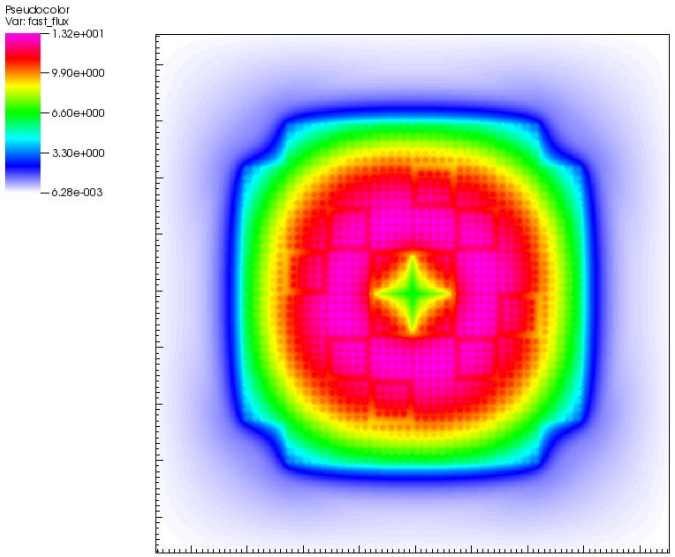
Control Rod Positions

5x5 Fuel Rod Assembly

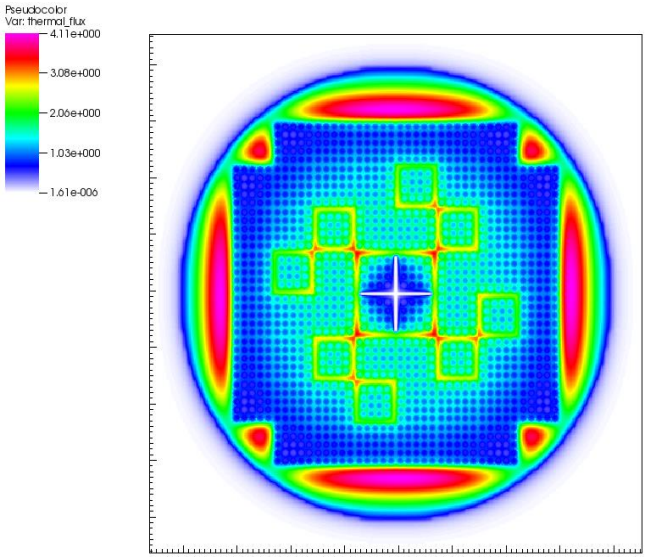
Middle of Active Core

MPACT Steady-State SPERT RIA Results

MPACT Fast Flux



MPACT Thermal Flux



Comparison of Critical Condition w/ KENO-CE

Case	Temperature (F)	C.R. Position(cm)	MPACT	KENO-CE
CZP	70	36.957	0.99411	0.99999 ±0.00082
HZP	550	71.755	0.99690	1.00242 ±0.00079

LOCA & RIA Challenge Problem Progress

Future RIA Validation Activities

MPACT

- SPERT reactor RIA tests
- WEC RAVE PWR rod ejection (code-to-code)

Peregrine

- CABRI and NSRR RIA fuel rod tests

COBRA-TF

- CHF tests (DNB CP)
- NSRR and future CABRI RIA fuel rod tests

LOCA & RIA Challenge Problem Progress

Future Peregrine LOCA Validation Activities

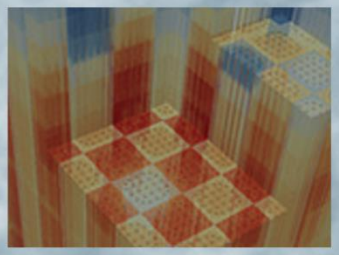
- Post-DNB PBF Test PCM-2
- Post-DNB TREAT Tests FRF-1 and FRF-2
- ORNL THTF Blowdown Tests
- PSU RBHT Reflood Tests
- FLECHT-SEASET Reflood Tests
- ANL Cladding Embrittlement Tests
- NUREG-0630 Swelling and Rupture Tests
- ANL Swelling and Rupture Tests
- Halden Swelling and Rupture Tests
- Studsvik Swelling and Rupture Tests
- Halden Fragmentation and Relocation Tests
- Studsvik Fragmentation and Relocation Tests

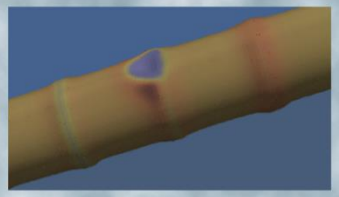
A DOE Energy Innovation Hub

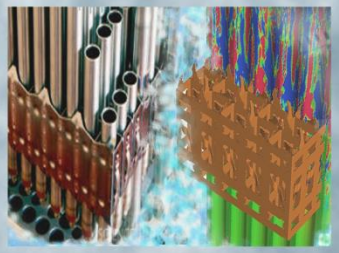
CASL's Phase 2 Workscope

Rose Montgomery
Deputy Lead, TDO

Paul Turinsky
Chief Scientist







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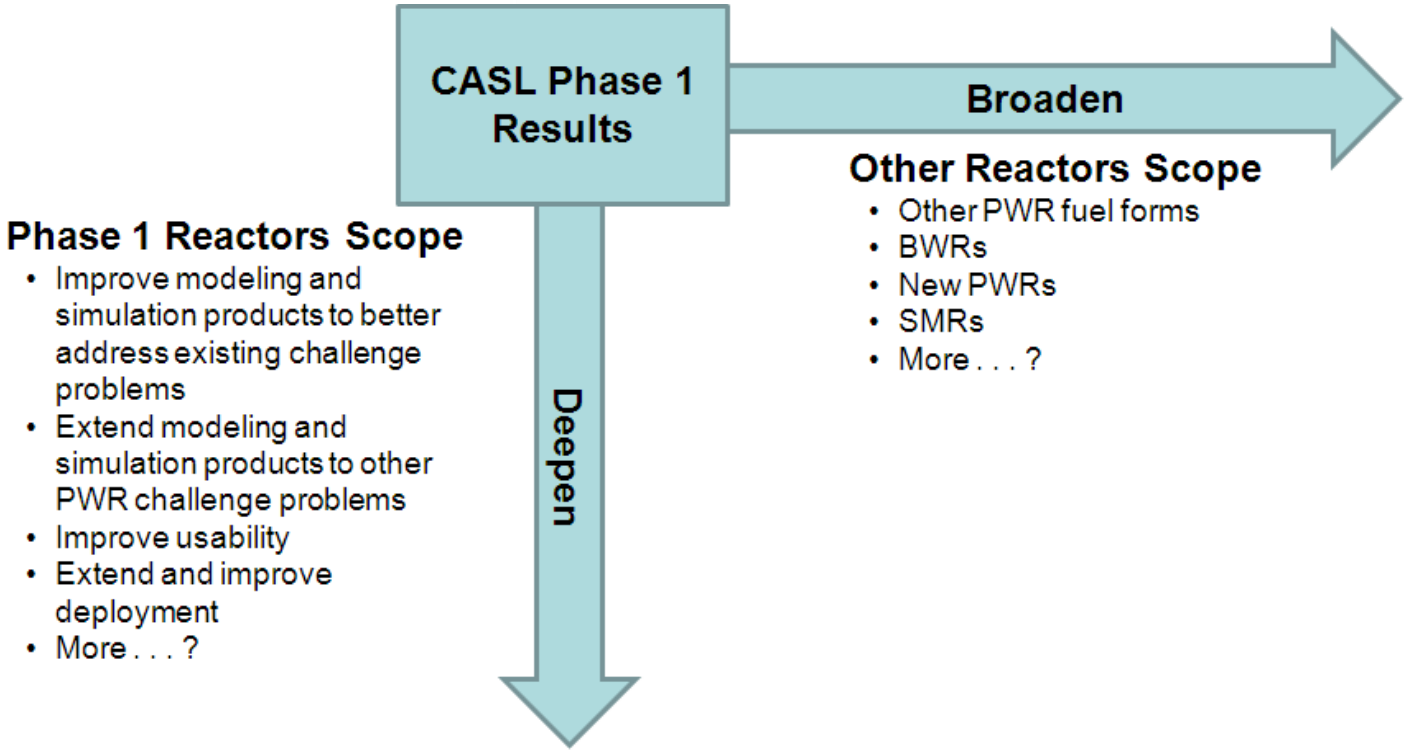
Overview of CASL's Direction

- Phase 1 CASL R&D targets PWRs and steady state conditions to build a versatile capability.
- In Phase 2, CASL seeks to broaden and deepen the Phase 1 technology.
- Phase 2 will continue the successful *Challenge Problem* strategy to target simulation capability for the R&D effort.

Deepening & Broadening

There are many possibilities with regard to how to deepen and broaden during Phase 2



If approved, CASL will transition to Phase 2 in 2015

Guiding Principles for Phase 2

- **CASL's overarching Phase 2 criteria**:
  1. **Enhance** the maturity level of VERA's predictive fidelity to allow industry to incorporate and build upon CASL's capabilities for industrial usage;
  2. **Broaden** the applicability of the capabilities developed in Phase 1 so that they can be applied to a wider class of LWR types; and
  3. **Deepen** the capabilities developed in Phase 1 and their applicability to new challenge problems.

Selection of CPs
(see Section 3 & Appendix B.2)

- To converge on an optimum scope, CASL used a 3-step process:
  1. ***The team suggested CPs*** and (where necessary) prepared "mini-charters" that described the challenge, its safety relevance, and higher fidelity path forward to ensure cross-team understanding of the scope;
  2. The pool of candidate CPs (28 in total) was categorized, and ***a survey was created*** to better understand the views and priorities of stakeholders;
  3. Based on the survey results, and given CASL's guiding principles, the ***SLT reduced the selections to what was believed possible*** given resource and time constraints. The selections were vetted through the CASL BOD.

Selection of CPs

Step 1: Suggest Challenge Problems

- **Many relevant and challenging topics of study were suggested, including both new CPs and continued research on the Phase 1 CPs. These included:**

Driver	Challenge Problem or Capability		
PWR	CIPS, CILC Increased Depth	Fuel Performance (with PCI)	GTRF Increased Depth
	DNB Increased Depth	RIA Increased Depth	LOCA Increased Depth
	Boron Precip (fibrous debris)	Other NSSS and fuel arrays	Core Simulator Extension
BWR	Extend Core Simulator	Fuel Performance	CRUD/CILC
	MELLA+, ATWS	Bypass Flow	Channel Bow
	Dryout	Shadow Corrosion	Stability
SMR	Core Simulator (geometry extension only)	Extension of Phase I PWR CPs	
	Natural Convection (also applies to PWR, BWR)	Boron Precipitation (with fibrous debris)	
Structural	Fuel Assembly Distortion (PWR & SMR)	Fuel Assembly In-Core Response during Steady-State, Transient and Seismic/LOCA Events	
Accident Tolerant Fuel	Mechanical simulation of SiC ceramic matrix composite and supporting materials models	Fuel cycle impacts of proposed concepts	
	Coolant flow effects of proposed concepts	Effects of modified coolant flow and heat transfer on CRUD/chemistry for proposed concepts	

Mini-Charters

Challenge Problem Charter

CONTENTS

1. CHALLENGE PROBLEM DESCRIPTION
   1.1 Background
   1.2 Significance
2. CURRENT INDUSTRY PRACTICE
   2.1 Present Solutions: Science and Engineering Basis
   2.2 Modeling and Simulation Role
3. DESIRED PATH FORWARD
   3.1 Solutions Needed for Reduced Uncertainty and Increased Confidence
   3.2 Modeling and Simulation Needs
4. DIFFICULTY OF IMPLEMENTATION
   4.1 Synergy with Phase I Development
   4.1 Key Challenges to Overcome
REFERENCES

- **12 Mini-charters were prepared to support the review process for the Phase 2 scope selection.**
- **Already existing charters used for Phase 1 CPs.**
- **Ensured cross-team understanding of the proposed R&D**

1. PWR Boron precipitation,
2. other NSSS and fuel arrays;
3. BWR Core Simulator;
4. BWR CRUD/CILC;
5. MELLLA+/ATWS;
6. Dryout;
7. BWR Stability;
8. SMR Core Simulator;
9. Natural Convection;
10. FAD/Seismic mechanical simulation of fuel in core;
11. ATF SiC mechanical simulations;
12. Fuel cycle impacts of ATF; Coolant flow effects of selected ATF; Effects of modified coolant flow due to selected ATF on CRUD/chemistry

Selection of CPs

Step 2: Survey

- The survey included a wide range of stakeholders to ensure selection of CPs that are industry-relevant, innovative science, programmatically aligned, and of interest to the investigators.
- It was possible to be more open because the opportunity was not competitive.
- The survey framework is general enough to be useful to others; was presented at the All-Hub meeting.
- 30 survey participants included a wide range of stakeholders; supplementary discussions were also held with others (e.g., NRC)

Includes representatives of the PWROG

CASL Partnership:	CASL Industry Council:	INPO Driving to Zero:	Specialists/ Management:
• Electric Power Research Institute (EPRI)	• ANSYS	• Exelon	• Constellation
• Idaho National Lab (INL)	• AREVA	• American Electric Power (AEP)	• Westinghouse
• Los Alamos National Lab (LANL)	• CD-Adapco	• Southern Nuclear Operating Company, Inc.	• DOE Accident Tolerant Fuels
• Massachusetts Institute of Technology (MIT)	• EdF	• Dominion	• AREVA
• North Carolina State University (NCSU)	• EPRI	• South Carolina Electric & Gas	• Global Nuclear Fuels
• Oak Ridge National Lab (ORNL)	• Exelon	•Arizona Public Service Company (APS)	
• Pacific Northwest National Lab (PNNL)	• Global Nuclear Fuels (GNF)		
• Sandia National Lab (SNL)	• mPower		
• Tennessee Valley Authority (TVA)	• NuScale		
• University of Tennessee - Knoxville (UTK)	• TVA		
• Westinghouse (WEC)	• WEC		

A wide range of stakeholder viewpoints

Selection of CPs

Step 2: Survey

- **Surveyed institutions ranked each proposed CP based on specific criteria:**

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

Selection of CPs

Step 2: Survey

- **The results were evaluated using the mean score in each category**
  - Because the mean can be misleading in this type of survey, the scores were
    reviewed to determine if there was a majority agreement
    (i.e., at least 50% scored it the same)
    - **agreement was denoted with a ☺.**
  - Industry participant responses were contrasted with other respondent responses in the category of Industry Impact.
  - The "programmatic" category was graphed against the "innovation" scores as an indication of the relative risk and reward associated with the various CPs.
- **The full report is available on the CASL SharePoint:**
  CASL-U-2014-0037-000
- **A summary is provided in the renewal proposal in Appendix B.2**

Survey results indicated broad agreement across stakeholders

Overall Survey Results

The top ten CPs for CASL included:

1. PWR increased fuel performance depth ☺
2. PWR DNB ☺
3. PWR LOCA
4. PWR CIPS/CILC ☺
5. BWR fuel performance
6. PWR boron precipitation (with fibrous debris)
7. PWR RIA
8. BWR core simulator
9. BWR dryout
10. SMR natural convection

The top ten CPs for the CASL Industry Council included:

1. PWR increased fuel performance depth
2. PWR DNB
3. SMR natural convection
4. GTRF
5. SMR Core Simulator (geometry extension only)
6. BWR Core Simulator
7. Fuel Assembly Distortion
8. PWR RIA
9. BWR fuel performance
10. PWR CIPS/CILC

Survey results indicated broad agreement across stakeholders

CASL top CPs relative to Industry Impact:

1. PWR Fuel Performance (with PCI) Increased Depth ☺
2. BWR Fuel Performance ☺
3. Natural Convection (also applications to PWR, BWR) ☺
4. BWR Extend Core Simulator ☺
5. DNB Increased Depth ☺
6. PWR - Boron Precipitation (with fibrous debris) ☺
7. Fuel assembly Distortion ☺
8. PWR CIPS, CILC Increased Depth ☺
9. RIA Increased Depth ☺
10. LOCA Increased Depth ☺

The top average Industry Impact scores from all industry participants:

1. PWR Fuel Performance (with PCI) Increased Depth
2. Natural Convection (also applications to PWR, BWR)
3. DNB Increased Depth
4. GTRF Increased Depth
5. SMR Core Simulator (geometry extension only)
6. BWR Extend Core Simulator
7. RIA Increased Depth
8. BWR Fuel Performance
9. Fuel assembly Distortion
10. PWR - Boron Precipitation (with fibrous debris)

Red indicates appeared in top 10 for both CASL and industry respondents

Survey Score Summary

Indicates that the score isn't representative of a majority opinion

Includes non-CASL respondents

		(a)	(b)	(c)		Overall Rating (a+b+c)/3		
	Institution Interest (Normalized mean)	Programmatic (Normalized mean)	Science/Engineering Innovation (Normalized mean)	Industry Impact (Normalized mean)	Industry Impact, All industry (Normalized mean)	(d) CASL	(e) Industry Council	points diff (d-e)
PWR								
CIPS, CILC Increased Depth	0.83	0.91	0.73	0.70	0.65	0.78	0.76	-2
Fuel Performance (with PCI) Increased Depth	0.88	0.82	0.86	0.95	0.88	0.88	0.68	-19
GTRF Increased Depth	0.33	0.41	0.64	0.50	0.72	0.52	0.79	28
DNB Increased Depth	0.75	0.77	0.88	0.80	0.75	0.82	0.85	3
RIA Increased Depth	0.67	0.68	0.82	0.70	0.69	0.73	0.69	-4
LOCA Increased Depth	0.63	0.77	0.88	0.70	0.63	0.78	0.62	-16
Boron Precipitation w/fibrous debris	0.63	0.73	0.78	0.75	0.65	0.75	0.52	-23
Demonstration of other NSSS and fuel arrays	0.54	0.59	0.36	0.65	0.64	0.53	0.60	7
BWR								
Extend Core Simulator	0.48	0.73	0.50	0.81	0.70	0.68	0.64	-4
Fuel Performance (doesn't include a BWR Core Simulator)	0.67	0.68	0.73	0.85	0.67	0.75	0.60	-16
CRUD/CILC	0.55	0.68	0.64	0.55	0.38	0.62	0.52	-10
MELLA+, ATWS	0.38	0.25	0.50	0.56	0.56	0.44	0.50	6
Bypass Flow	0.18	0.17	0.22	0.39	0.17	0.26	0.31	4
Channel Bow	0.30	0.50	0.50	0.57	0.44	0.52	0.37	-15
Dryout	0.46	0.50	0.86	0.67	0.63	0.68	0.45	-22

Survey Score Summary

Indicates that the score isn't representative of a majority opinion

Includes non-CASL respondents

		(a)	(b)	(c)		Overall Rating (a+b+c)/3		
	Institution Interest (Normalized mean)	Programmatic (Normalized mean)	Science/Engineering Innovation (Normalized mean)	Industry Impact (Normalized mean)	Industry Impact, All industry (Normalized mean)	(d) CASL	(e) Industry Council	points diff (d-e)
Shadow Corrosion	0.36	0.28	0.44	0.44	0.33	0.39	0.42	3
Stability	0.39	0.30	0.60	0.61	0.57	0.50	0.48	-3
SMR								
Core Simulator (geometry extension only)	0.33	0.80	0.25	0.61	0.71	0.55	0.64	9
Extension of Phase I PWR CPs	0.42	0.68	0.36	0.50	0.64	0.52	0.52	1
Natural Convection (also applications to PWR, BWR)	0.54	0.58	0.55	0.81	0.81	0.64	0.80	15
Boron Precipitation w/fibrous debris	0.52	0.32	0.58	0.35	0.21	0.41	0.18	-23
Structural								
Fuel assembly Distortion (likely applicable to PWR & SMR)	0.50	0.35	0.58	0.72	0.67	0.55	0.62	7
Seismic (likely applicable to PWR, BWR, SMR)	0.30	0.36	0.45	0.50	0.56	0.44	0.49	6
Mechanical Simulation of Fuel Assembly In-Core Response during Steady-State, Transient and Seismic/LOCA Events (likely applicable to PWR, BWR, SMR)	0.38	0.47	0.39	0.56	0.64	0.47	0.65	17
Accident Tolerant Fuel Problem								
Mechanical simulation of SiC ceramic matrix composite, including development of supporting materials models	0.34	0.30	0.70	0.22	0.38	0.41	0.47	7

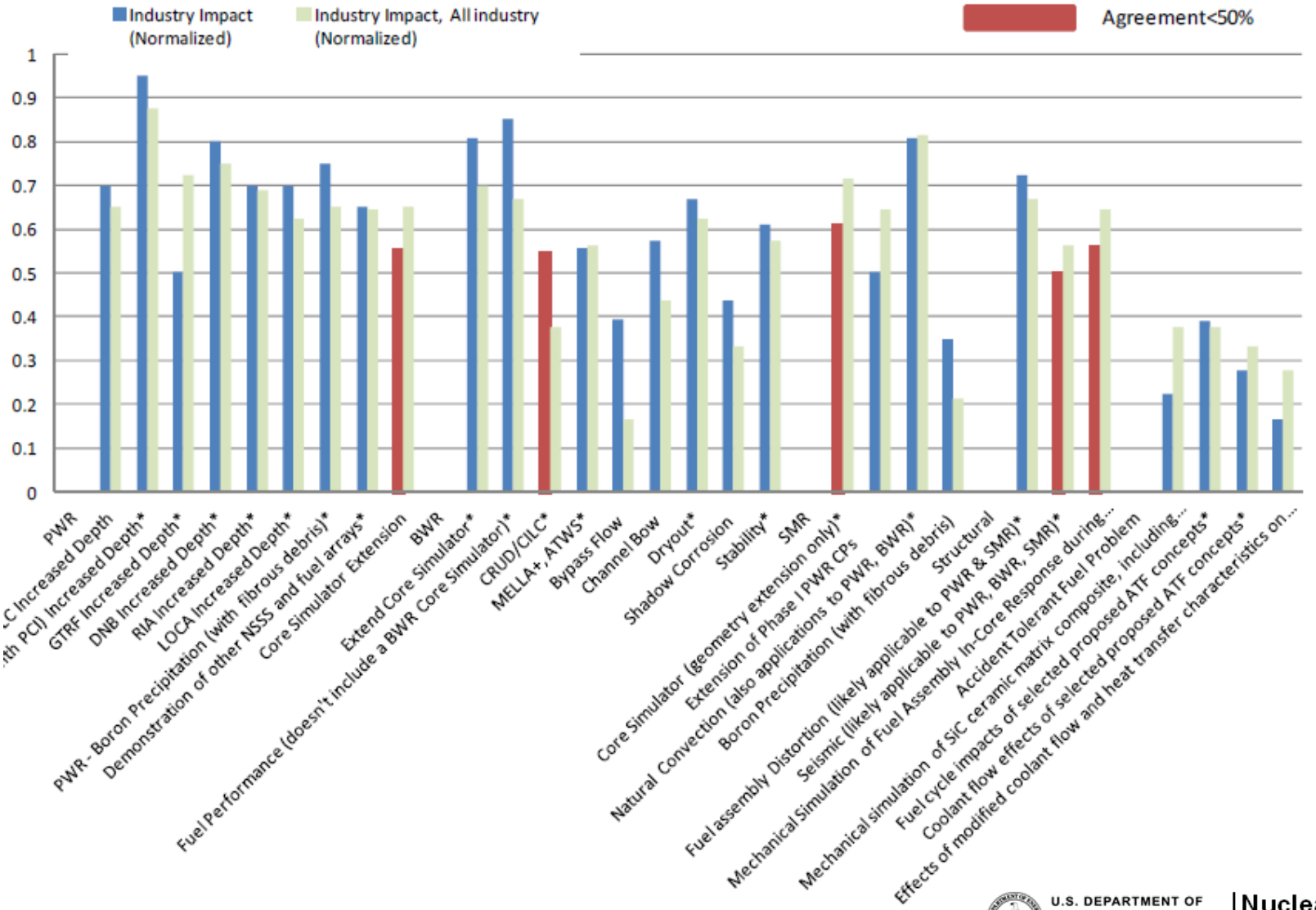
Survey Score Summary

Indicates that the score isn't representative of a majority opinion

Includes non-CASL respondents

		(a)	(b)	(c)		Overall Rating (a+b+c)/3		
	Institution Interest (Normalized mean)	Programmatic (Normalized mean)	Science/Engineering Innovation (Normalized mean)	Industry Impact (Normalized mean)	Industry Impact, All industry (Normalized mean)	(d) CASL	(e) Industry Council	points diff (d-e)
Fuel cycle impacts of selected proposed ATF concepts	0.46	0.45	0.50	0.39	0.38	0.45	0.48	4
Coolant flow effects of selected proposed ATF concepts	0.29	0.40	0.40	0.28	0.33	0.36	0.38	2
Effects of modified coolant flow and heat transfer characteristics on CRUD/chemistry for selected ATF concepts	0.46	0.30	0.45	0.17	0.28	0.31	0.44	14

Industry Impact Scores, CASL vs. Industry Council



Example of Risk-Reward Plot

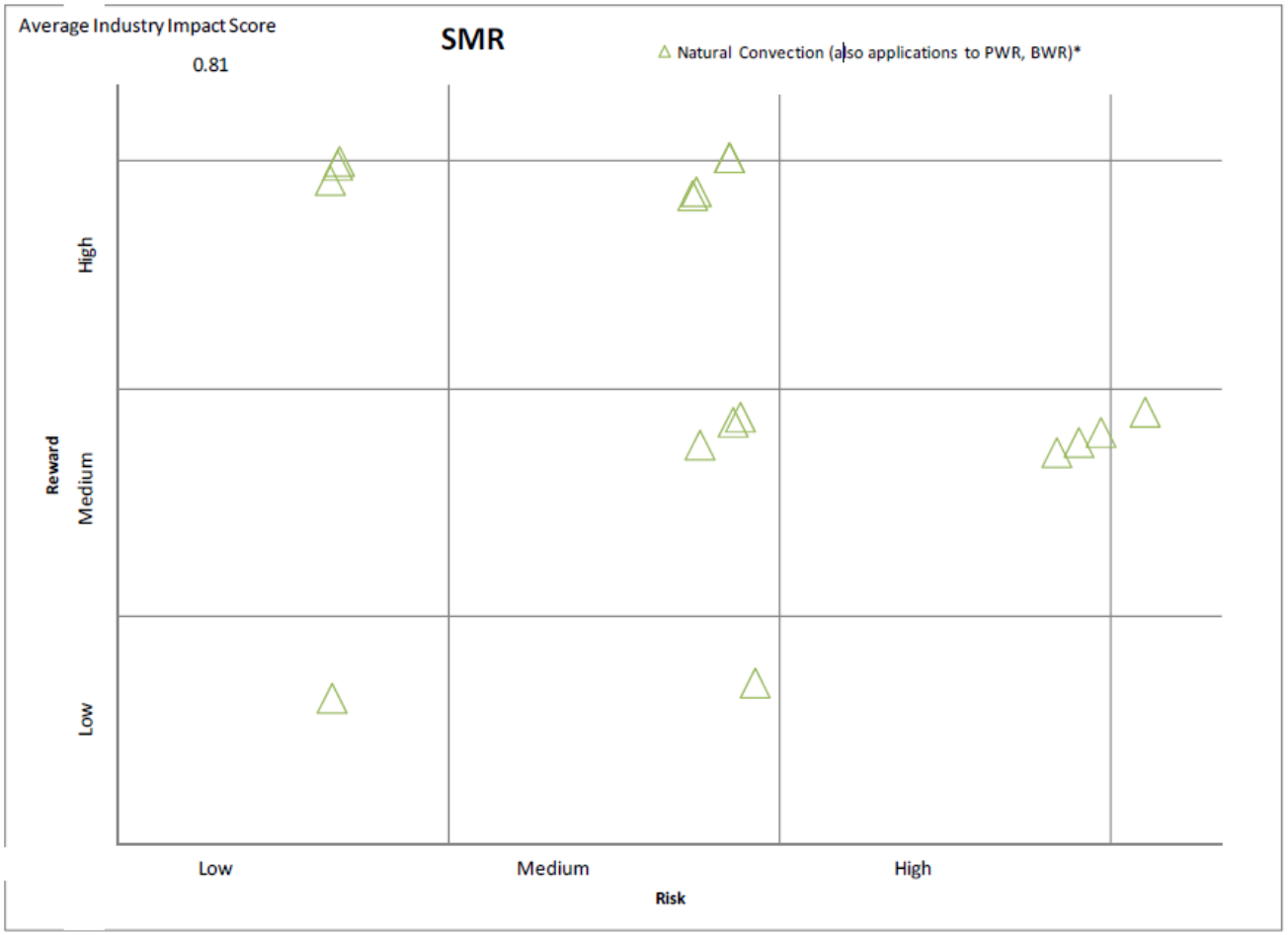


Figure 24 Risk versus Reward, SMR Natural Convection

Based on "innovation" and "programmatic" scores

Recommendations from the Survey

- Based on the survey top ratings and risk-reward results, the following top five CPs were recommended to SLT for Phase 2 deepening of CASL's toolset:
    1. PWR fuel performance
    2. PWR DNB
    3. PWR CIPS/CILC
    4. PWR RIA
    5. PWR boron precipitation (deepening of CASL chemistry tools)
- Also based on the survey results, the following CPs were recommended to SLT for broadening of CASL's toolset:
    1. 1. SMR natural convection
    2. 2. BWR core simulator
    3. 3. BWR fuel performance

Final selections made by CASL SLT

Recommendations from the Survey

- Also, the following proposed CPs should be implemented in Phase 2 as milestone tasks:
    1. SMR Core Simulator (geometry extension only)
    2. Demonstration of other NSSS and fuel arrays
- Additionally, based on the Industry recommendation and risk versus reward results, the CASL team should consider PWR mechanical and fuel assembly distortion tools a priority.

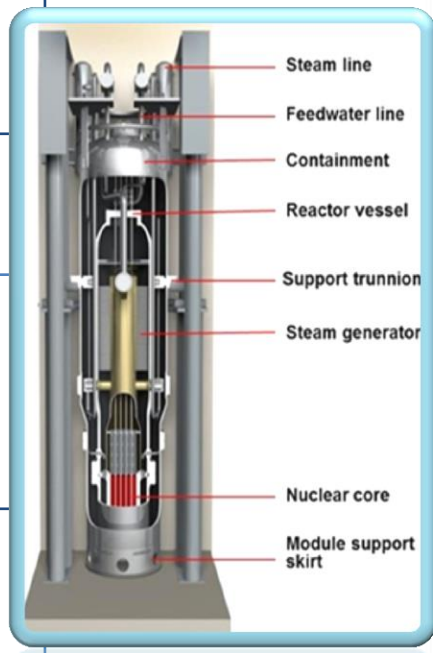
Interoperability with an external structural code to be provided

Selected Phase 2 Challenge Problems

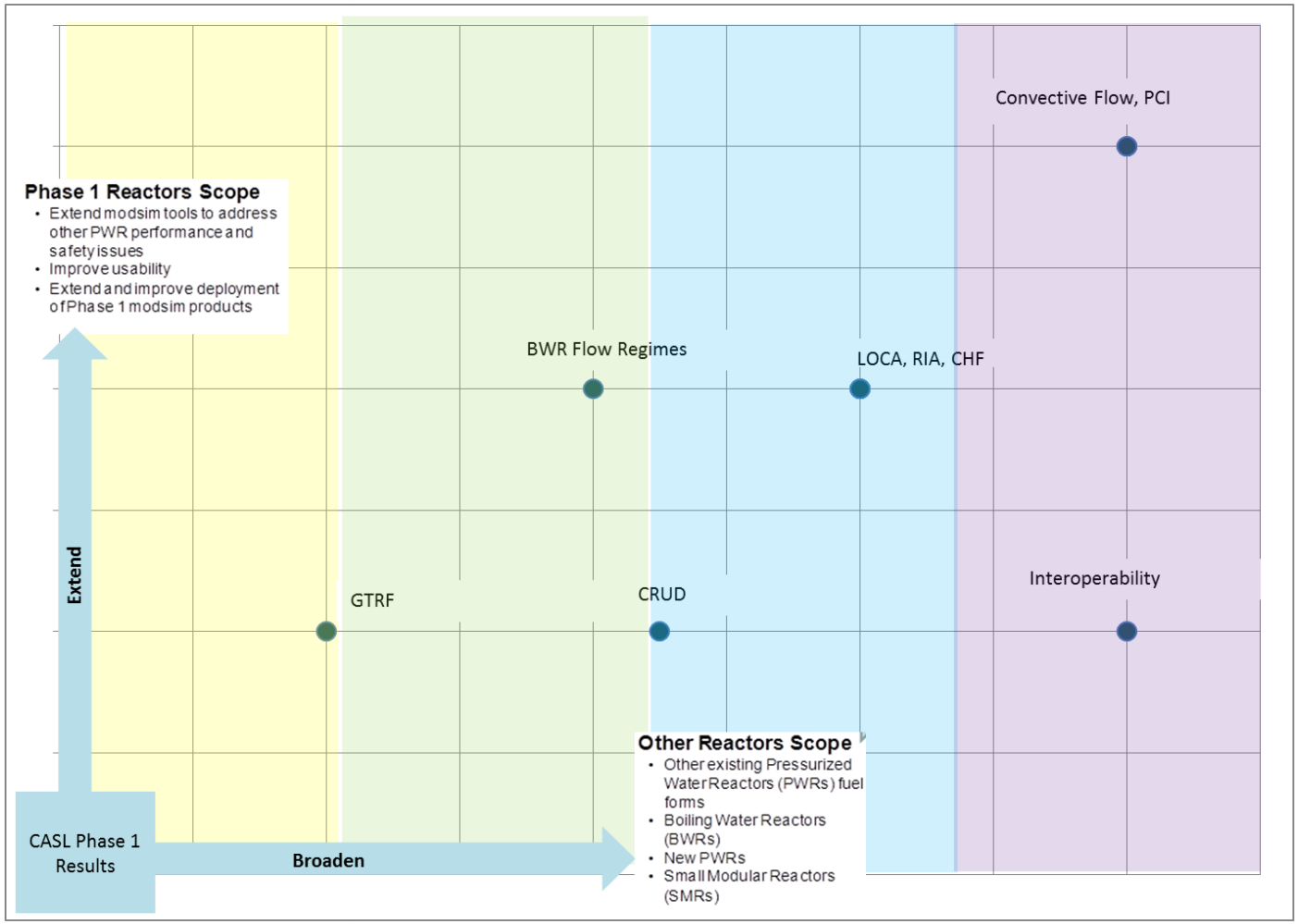
BWRs

Category	Phase 2 New Challenge Problems	Phase 1 CPs targeted for Phase 2 Deepening
Thermal-Hydraulics	Convective Flow (thermal and solutal) iPWR CHF (DNB) BWR Flow Regimes	CHF (DNB)
Cladding Performance	BWR PCI iPWR PCI BWR RIA BWR LOCA	PCI RIA LOCA
Coolant / Corrosion Chemistry	iPWR CRUD (CIPS & CILC)	CRUD (CIPS & CILC)
VERA Core Simulator	Supporting: All BWR and iPWR CPs	Supporting: CRUD (CIPS & CILC) PCI DNB RIA
Interoperability	Supporting: GTRF, FAD LOCA, RIA	

iPWRs



Where at Regarding Deepening & Broadening?



Planned VERA Capability Enhancements in Phase 2 (see Section 3.4 & Appendix B.3)

Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
1	• VERA-CS for PWR multi-cycle simulation • VERA-CS + MAMBA for PWR CIPS • MAMBA with improved CRUD source terms • VERA-CS & Shift for iPWRs • Hydra-TH for subcooled boiling & bubbly flow regime • Peregrine-3D for PCI • Shift with hybrid MC for PWR & iPWR • VERA interoperability with external CFD	Hydra-TH + MAMBA VERA-CS + MAMBA VERA + External CFD	PWR/iPWR CIPS PWR PCI PWR DNB
2	• VERA-C + Peregrine for PWR PCI • VERA-CS + MAMBA & Hydra-TH + MAMBA for PWR CILC • Peregrine + MAMBA for cladding corrosion • CTF enhancements for BWR simulation • MPACT with kinetics to support RIA • MPACT & Shift with photon transport • Hydra-TH + MAMBA advanced subgrid model for CRUD, corrosion chemistry & boron mixing/precipitation	VERA-CS + Peregrine +MAMBA Hydra-TH + MAMBA + Peregrine	PWR/iPWR CILC PWR PCI PWR RIA PWR LOCA BWR Flow Regimes
3	• Peregrine + Hydra-TH + Structural for PWR GTRF • Peregrine for PWR LOCA cladding integrity • VERA-CS for BWR subregion • Hydra-TH for onset of DNB • Hydra-TH for thermal/solutal convective flows with boron mixing • MPACT with depletion for BWR core subregion	VERA + External Structural Mechanics	PWR DNB PWR GTRF PWR LOCA Convective Flows
4	• VERA-CS + Peregrine & Hydra-TH + Peregrine for PWR RIA • VERA-C + Peregrine for BWR PCI • Optimization & integration of group & continuous nuclear data • Hydra-TH flow topology recognition for closure models for BWR-like flow regimes	VERA + External Systems Code Update as needed for new code capabilities	PWR CIPS/CILC PWR RIA BWR PCI BWR Flow Regimes
5	• Hydra-TH + Peregrine for BWR RIA • Peregrine for BWR LOCA cladding integrity • Shift with hybrid, fixed-source Monte Carlo methods for ex-core physics • Hydra-TH for low flow rate boiling in a rod bundle for iPWR	Update as needed for new code capabilities	BWR RIA BWR LOCA iPWR DNB

Note coupling only refers to physics modules, i.e. does not address Dakota

Planned VERA Capability Enhancements in Phase 2

Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
1	• VERA-CS for PWR multi-cycle simulation • VERA-CS + MAMBA for PWR CIPS • MAMBA with improved CRUD source terms • VERA-CS & Shift for iPWRs • Hydra-TH for subcooled boiling & bubbly flow regime • Peregrine-3D for PCI • Shift with hybrid MC for PWR & iPWR • VERA interoperability with external CFD	Hydra-TH + MAMBA VERA-CS + MAMBA VERA + External CFD	PWR/iPWR CIPS PWR PCI PWR DNB

Planned VERA Capability Enhancements in Phase 2

Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
2	• VERA-C + Peregrine for PWR PCI • VERA-CS + MAMBA & Hydra-TH + MAMBA for PWR CILC • Peregrine + MAMBA for cladding corrosion • CTF enhancements for BWR simulation • MPACT with kinetics to support RIA • MPACT & Shift with photon transport • Hydra-TH + MAMBA advanced subgrid model for CRUD, corrosion chemistry & boron mixing/precipitation	VERA-CS + Peregrine +MAMBA Hydra-TH + MAMBA + Peregrine	PWR/iPWR CILC PWR PCI PWR RIA PWR LOCA BWR Flow Regimes

Planned VERA Capability Enhancements in Phase 2

Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
3	• Peregrine + Hydra-TH + Structural for PWR GTRF • Peregrine for PWR LOCA cladding integrity • VERA-CS for BWR subregion • Hydra-TH for onset of DNB • Hydra-TH for thermal/solutal convective flows with boron mixing • MPACT with depletion for BWR core subregion	VERA + External Structural Mechanics	PWR DNB PWR GTRF PWR LOCA Convective Flows

Planned VERA Capability Enhancements in Phase 2

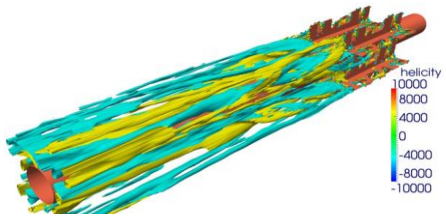
Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
4	• VERA-CS + Peregrine & Hydra-TH + Peregrine for PWR RIA • VERA-C + Peregrine for BWR PCI • Optimization & integration of group & continuous nuclear data • Hydra-TH flow topology recognition for closure models for BWR-like flow regimes	VERA + External Systems Code Update as needed for new code capabilities	PWR CIPS/CILC PWR RIA BWR PCI BWR Flow Regimes

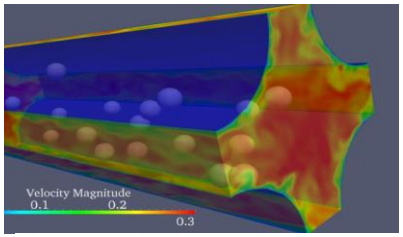
Planned VERA Capability Enhancements in Phase 2

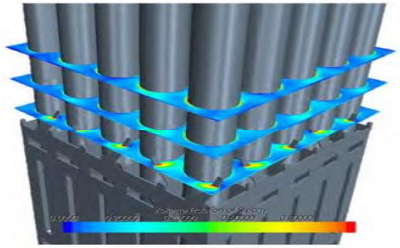
Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
5	• Hydra-TH + Peregrine for BWR RIA • Peregrine for BWR LOCA cladding integrity • Shift with hybrid, fixed-source Monte Carlo methods for ex-core physics • Hydra-TH for low flow rate boiling in a rod bundle for iPWR	Update as needed for new code capabilities	BWR RIA BWR LOCA iPWR DNB

Phase 2 Challenge Problems – Thermal Hydraulic Category

- Develop and incorporate in Hydra-TH Generation 2 closure models and treatment of cladding surface roughness,
- Broaden Hydra-TH to model convective flow, including thermally-driven convection and solutal-driven convective flows relevant to flow conditions occurring during stages of certain LWR accidents and iPWR normal operations;
- Expand Hydra-TH capabilities to lay foundation to model flow regimes beyond bubbly flow relevant to BWR normal operations and certain LWR accidents;
- Apply Hydra-TH to DNB conditions for natural circulation flow conditions in iPWRs;
- Complete VUQ analysis.

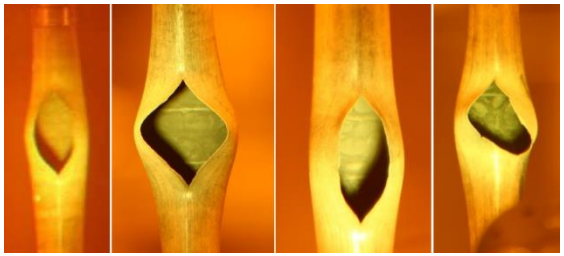


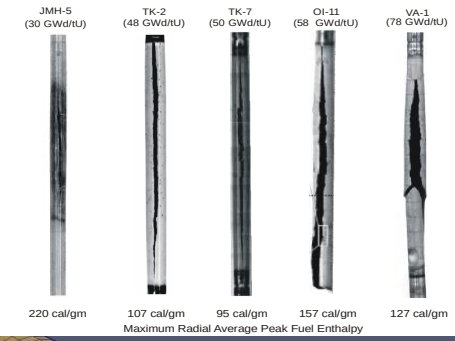


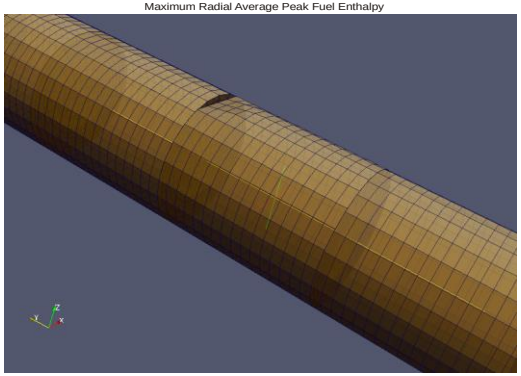


Phase 2 Challenge Problems – Cladding Performance Category

- Enhance fidelity of Peregrine physics models (e.g., pellet cracking, fission product release, microstructure evolution, swelling, cladding stress corrosion cracking, pellet-cladding surface interaction, deformation, growth and creep),
- Expand validation scope, and complete UQ analysis for PWRs.
- Expand Peregrine capabilities to address BWRs and iPWRs, addressing BWR cladding alloy and liner, as well as accounting for the differing thermal-hydraulic conditions.

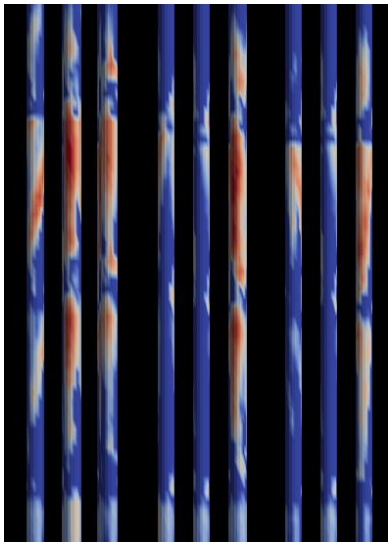


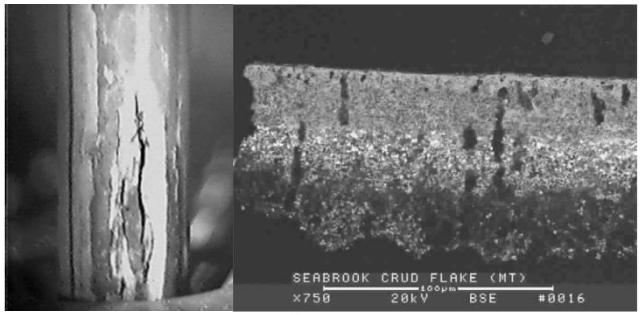




Phase 2 Challenge Problems – Coolant/Corrosion Chemistry Category

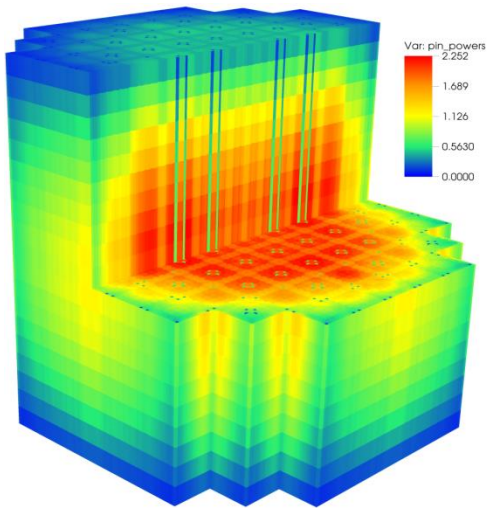
- Develop MAMBA corrosion product source model,
- Improve cladding corrosion models,
- Expand VUQ analysis for PWRs.
- Show applicability of MAMBA to iPWRs.

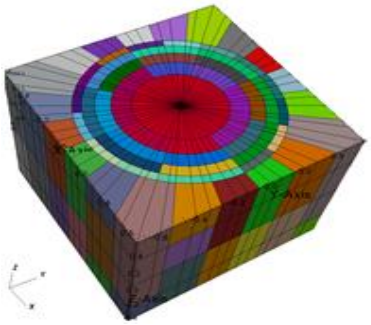




Phase 2 Challenge Problems – VERA Core Simulator

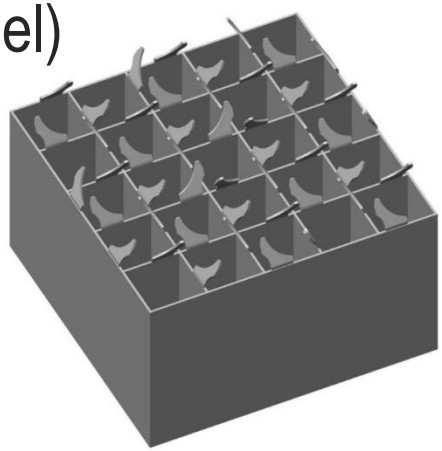
- Add BWR capability
  - Geometric features
  - Selected flow regimes
  - Improved multiphysics solution methods
- Demonstrate applicability to iPWR
- Enhance kinetics capability for application to accident scenarios
- Improve computational efficiency.
- Expand validation scope for PWRs.
- As required, develop Monte Carlo code to support verification of MPACT and other deterministic transport codes.

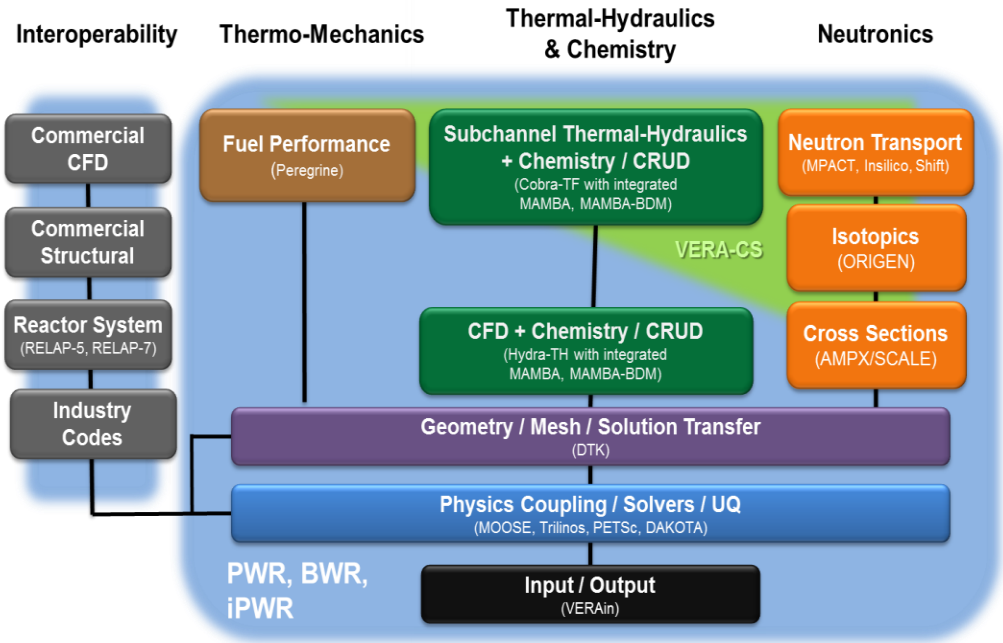




Phase 2 Challenge Problems – Interoperability Category

- Add ability to support usage of ISV capabilities in conjunction with VERA.
- Improve interoperability with plant systems code.
- Finalize work on GTRF (e.g. cladding wear model) and validate, to enable and demonstrate interoperability with structural analysis code





Roadmap for Phase 2

- Level 1 milestones provide a roadmap of the major objectives.
- Supporting Level 2 milestones are developed by focus areas (presented later).
- See Section 3.3 & Appendix B.3

ear	Category	CP	No.	Milestone Description
1	Coolant / Corrosion Chemistry	CIPS / CILC	1	Qualify core-wide PWR CIPS capability with corrosion product treatment: Add corrosion product source term and mass balance to MAMBA, and utilize in VERA-CS to simulate multi-cycles of a PWR that experienced CIPS.
	Core Physics	PWR CPs	2	Qualify multi-cycle PWR core simulator capability: Using VERA-CS simulate first and reload cycles of the Watts Bar Unit 1, with predictions compared to plant measurements with regard to in-core, ex-core and selected startup physics test measurements.
	Core Physics	PCI / RIA / LOCA	3	Demonstrate iPWR core simulator capability: Utilizing VERA-CS, establish an iPWR core model and simulate cycle depletion.
	Thermal-Hydraulics	CHF (DNB) Convective flow	4	Qualify multiphase CFD capability for bubbly flow regime: Hydra-TH will be used to simulate out-of-core fluid experiments targeted at providing validation data for the bubble flow regime, with predictions contrasted to measurements.
2	Cladding Performance	PCI / RIA / LOCA	5	Demonstrate core subregion & core-wide PWR PCI capability: Utilizing VERA-CS with Peregrine-2D, complete PWR multi-cycle core depletion for core maneuver to identify PCI limiting fuel rods; utilizing Peregrine-3D complete PCI analysis for limiting fuel rods.
	Coolant / Corrosion Chemistry	CIPS / CILC	6	Quality CFD-based PWR CILC capability for a subregion: Using the results of the Year 1 CIPS L1 milestone to identify CILC limiting fuel rods and associated powers, CILC analysis will be completed using Hydra-TH with embedded MAMBA coupled to Peregrine.
	Deployment	N/A	7	Create Working Group for CASL software: To support the release to external users, a Working Group will be formed, members recruited, charter written, and first meeting held in conjunction with training on selected usages of VERA.
3	Cladding Performance	GTRF	8	Demonstrate GTRF analysis methodology components: Using the fuel rod mechanical/material modeling of Peregrine, finalized rod wear model, Hydra-TH predicted turbulent pressure forces, and assumed gap opening, demonstrates interoperability capability of VERA with a structural mechanics code. Stretch goal: extend Peregrine to treat the change in spacer grid straps geometry and material properties to capture cladding-grip strap gap formation and impact on wear.
	Cladding Performance	LOCA	9	Demonstrate PWR LOCA fuel performance capability: Use Peregrine to predict the extent of clad ballooning and oxidation, as a function of initial fuel rod state (e.g. hydrogen pickup) using LOCA system transient code generated boundary conditions.
	Core Physics	All BWR	10	Establish BWR core simulator capability for core subregion: Use VERA-CS to simulate a subregion (i.e. one or more fuel assemblies) of a BWR core. Stretch goal: simulate full core.
	Thermal-Hydraulics	DNB	11	Qualify prediction of onset of DNB using M-CFD: Hydra-TH will be used to simulate out-of-core fluid experiments targeted at providing validation data for the onset of DNB, for a range of powers and coolant inlet enthalpy, flow and pressure.
	Thermal-Hydraulics	Convective flow	12	Qualify thermal/solutal convective fluid flow CFD capability: Hydra-TH will be modified via incorporation of appropriate turbulence model and boron solution/dissolution chemistry model and used to predict first thermal convective fluid flow and subsequently thermal/solutal convective fluid flow, with predictions contrasted to validation data where available.
4	Cladding Performance	RIA	13	Demonstrate core-wide PWR RIA capability to simulate ejected rod accident: VERA-CS with neutron kinetics and Peregrine-2D will be used to simulate a PWR ejected rod accident to identify RIA limiting fuel rods; utilizing Peregrine-3D complete RIA analysis for limiting fuel rod(s).
	Cladding Performance	PCI / RIA / LOCA	14	Demonstrate BWR PCI capabilities: Utilizing VERA-CS with Peregrine-2D coupled, complete BWR core subregion depletion from which a maneuver will be completed to identify PCI limiting fuel rods; utilizing Peregrine-3D complete PCI analysis for limiting fuel rod(s).
	Thermal-Hydraulics	BWR Flow Regimes	15	Demonstrate capability to simulate using M-CFD the flow regimes that exist during normal operations of a BWR. Hydra-TH will need to be modified to incorporate the appropriate closure relationships associated with each flow regime and recognize the flow topology in order to utilize the appropriate closure models, including addressing flow regime transitions.
5	Cladding Performance	RIA	16	Demonstrate BWR RIA capabilities: Utilizing Peregrine-3D complete RIA analysis for assumed limiting fuel rod(s).
	Cladding Performance	LOCA	17	Demonstrate BWR LOCA fuel performance capability: Use Peregrine to predict the extent of clad ballooning and oxidation, as a function of initial fuel rod state (e.g. hydrogen pickup) using LOCA system transient code generated boundary conditions.
	Thermal-Hydraulics	CHF (DNB)	18	Demonstrate prediction of onset of DNB using M-CFD for low flow conditions indicative of iPWRs and PWRs during post-trip loss of offsite power event.
	Deployment	N/A	19	Finalize transition of CASL-supported functions to post-CASL entity: Establish post-CASL entity and assist it to manage software release, distribution, training, and the bug fix and enhancement processes.

L1 Milestones

Year	Category	CP	No.	Milestone Description
1	Coolant / Corrosion Chemistry	CIPS / CILC	1	Qualify core-wide PWR CIPS capability with corrosion product treatment: Add corrosion product source term and mass balance to MAMBA, and utilize in VERA-CS to simulate multi-cycles of a PWR that experienced CIPS.
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L1 Milestones

Year	Category	CP	No.	Milestone Description
2	Cladding Performance	PCI / RIA / LOCA	5	Demonstrate core subregion & core-wide PWR PCI capability: Utilizing VERA-CS with Peregrine-2D, complete PWR multi-cycle core depletion for core maneuver to identify PCI limiting fuel rods; utilizing Peregrine-3D complete PCI analysis for limiting fuel rods.
	Coolant / Corrosion Chemistry	CIPS / CILC	6	Quality CFD-based PWR CILC capability for a subregion: Using the results of the Year 1 CIPS L1 milestone to identify CILC limiting fuel rods and associated powers, CILC analysis will be completed using Hydra-TH with embedded MAMBA coupled to Peregrine.
	Deployment	N/A	7	Create Working Group for CASL software: To support the release to external users, a Working Group will be formed, members recruited, charter written, and first meeting held in conjunction with training on selected usages of VERA.

L1 Milestones

Year	Category	CP	No.	Milestone Description
3	Cladding Performance	GTRF	8	Demonstrate GTRF analysis methodology components: Using the fuel rod mechanical/material modeling of Peregrine, finalized rod wear model, Hydra-TH predicted turbulent pressure forces, and assumed gap opening, demonstrates interoperability capability of VERA with a structural mechanics code. Stretch goal: extend Peregrine to treat the change in spacer grid straps geometry and material properties to capture cladding-grip strap gap formation and impact on wear.
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	Core Physics	All BWR	10	Establish BWR core simulator capability for core subregion: Use VERA-CS to simulate a subregion (i.e. one or more fuel assemblies) of a BWR core. Stretch goal: simulate full core.
	Thermal-Hydraulics	DNB	11	Qualify prediction of onset of DNB using M-CFD: Hydra-TH will be used to simulate out-of-core fluid experiments targeted at providing validation data for the onset of DNB, for a range of powers and coolant inlet enthalpy, flow and pressure.
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L1 Milestones

Year	Category	CP	No.	Milestone Description
4	Cladding Performance	RIA	13	Demonstrate core-wide PWR RIA capability to simulate ejected rod accident: VERA-CS with neutron kinetics and Peregrine-2D will be used to simulate a PWR ejected rod accident to identify RIA limiting fuel rods; utilizing Peregrine-3D complete RIA analysis for limiting fuel rod(s).
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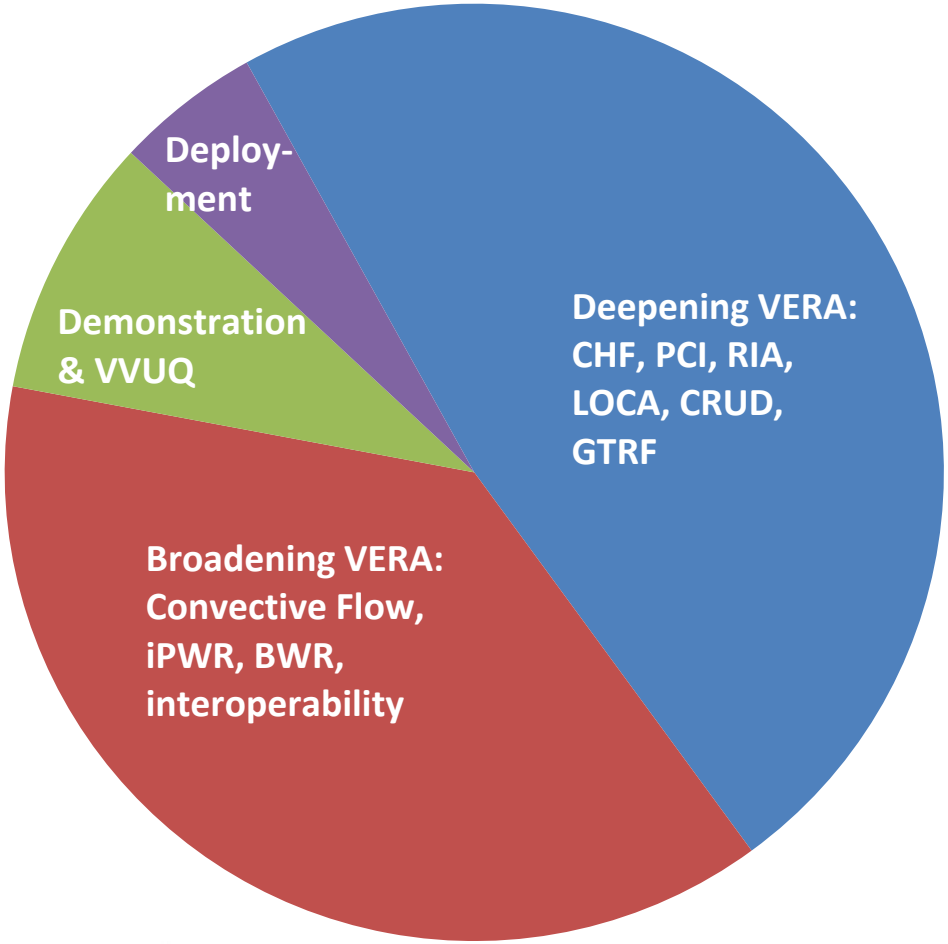
L1 Milestones

Year	Category	CP	No.	Milestone Description
5	Cladding Performance	RIA	16	Demonstrate BWR RIA capabilities: Utilizing Peregrine-3D complete RIA analysis for assumed limiting fuel rod(s).
	Cladding Performance	LOCA	17	Demonstrate BWR LOCA fuel performance capability: Use Peregrine to predict the extent of clad ballooning and oxidation, as a function of initial fuel rod state (e.g. hydrogen pickup) using LOCA system transient code generated boundary conditions.
	Thermal-Hydraulics	CHF (DNB)	18	Demonstrate prediction of onset of DNB using M-CFD for low flow conditions indicative of iPWRs and PWRs during post-trip loss of offsite power event.
	Deployment	N/A	19	Finalize transition of CASL-supported functions to post-CASL entity: Establish post-CASL entity and assist it to manage software release, distribution, training, and the bug fix and enhancement processes.

Target End State Capabilities

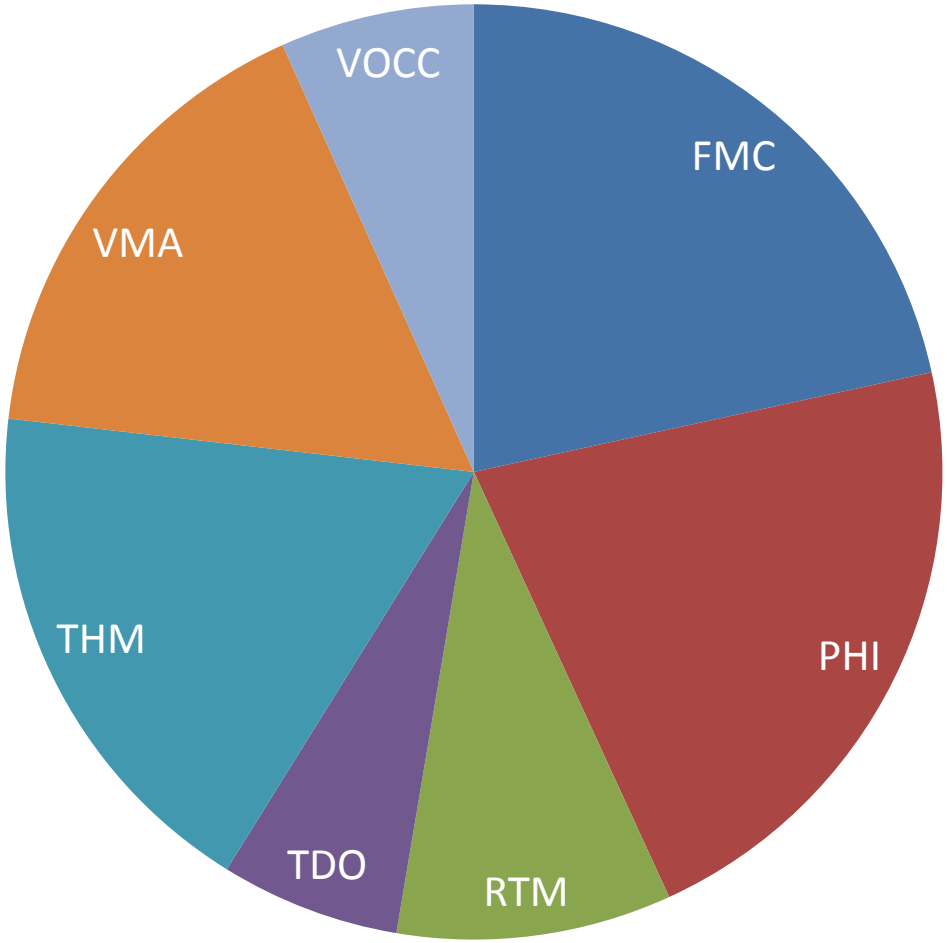
- VERA-CS
  - PWR & iPWR full-core, pin resolved, depletion & transient capability
  - BWR sub-core (stretch full-core), pin resolved, depletion capability
- PCI: PWR, iPWR and BWR capability
- CRUD: PWR & iPWR capability
- GTRF: PWR & iPWR pin behavior (stretch gap opening), wear, fluid forces & interoperability (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
- VUQ: Capabilities integration

Resource Allocations



Estimated resource allocation for deepening, broadening, VVUQ, and deployment for Phase 2

Resource Allocations



Estimated resource allocation by WBS for Phase 2 FY15.

Summary

- Phase 2 scope proposed was based on a rigorous selection process;
- Scope offers broadened VERA applicability and deepened capabilities;
- An optimized R&D plan has been developed with supporting detailed roadmaps.
- Risks have been considered and mitigating activities have been established.

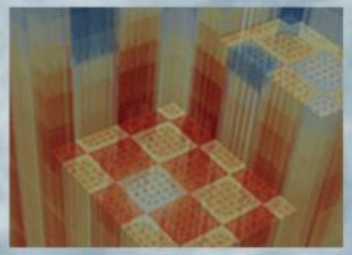
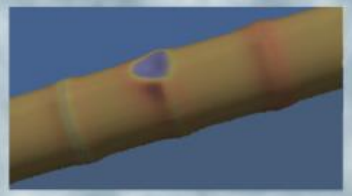
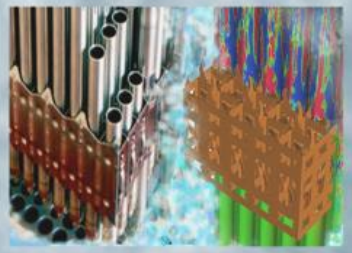
R&D work scope proposed for Phase 2
is **impactful**, **challenging** & **achievable**

CASL
A DOE Energy Innovation Hub

Welcome to the Industry Council

Industry Council Chairman: Dennis Hussey (EPRI)

CASL Industry Council Meeting
Oak Ridge National Laboratories
September 9-10, 2014

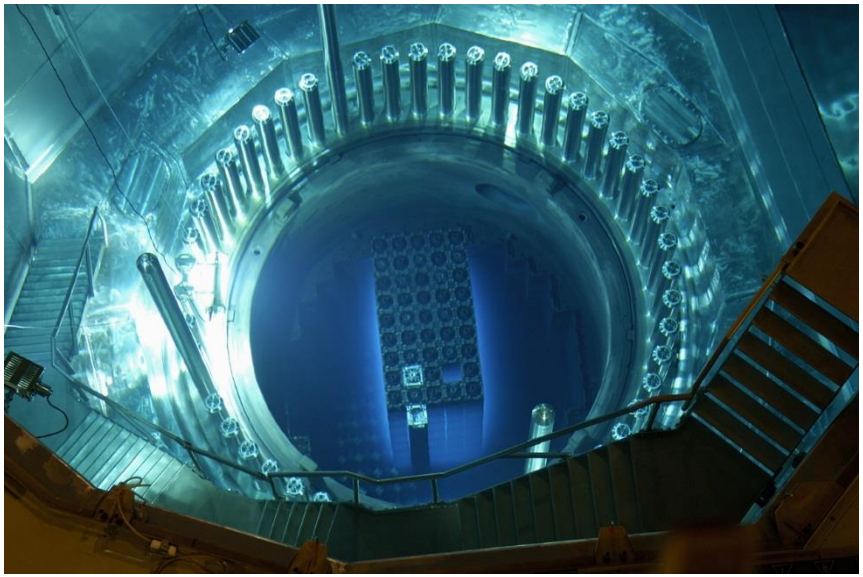
U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Industry Council

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

Objectives and Strategies

- Early, continuous, and frequent interface and engagement of end-users and technology providers
- Critical review of CASL plans and products
- Optimum deployment and applications of periodic VERA releases
- Identification of strategic collaborations between industry and CASL Focus Areas



Outcomes and Impact

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

Industry Council Membership

Owner/ Operators of Nuclear Plants	Fuel and/or 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	B&W Power Generation	EPRI	Dassault Systemes	NVIDIA	
Exelon	NuScale	Rolls Royce	GSE Systems		
TVA	WEC	Studsvik Scandpower			

Agenda (Wednesday, Sept 10)

Time (EDT)	Topic	Speaker
8:30	Welcome and Introductions	Dennis Hussey
9:00	Test Stands – EPRI Test Stand Presentation – SMR modeling highlights – Future Test Stands	Steve Hess Brenden Mervin Kelly Kenner Steve Hess
10:15	Break	
10:30	Phase 2 Industry Council Planning	Dennis Hussey
11:15	VERA User Group	Rose Montgomery
11:45	Working Lunch – Thoughts on Phase 2 (2015-2020) Scope	Doug Kothe
12:45	Vendor Perspective on CASL	Chris Lewis

Actions from March/June IC Meetings

Owner	Action	Due Date	Status
IC	Phase 2 Technical Scope - what's missing, complete matrix by March 14th. Action Complete	March 14, 2014	Complete
Turinsky/Feldman	Provide IC with list of Phase 1 Challenge Problem Charters and Implementation Plans.	April 15, 2014	Complete
Turinsky	Provide IC with list of Phase 2 Mini-Charters.	April 15, 2014	
Gehin/Feldman	Gehin send NRC Meeting Minutes and Attendee List to Feldman. Feldman distribute to IC.	April 15, 2014	Minutes complete In Progress
IC	Provide CASL with your feedback on the Value Proposition. Feldman to request input via email.	April 15, 2014	Complete
Kothe/Turinsky	Work with SMR vendors to identify specific scope.	April 15, 2014	
Banta/Feldman	Banta send Feldman QA plan. Feldman send QA plan to IC.	April 15, 2014	Complete
Feldman/Hussey	Work with Kurt Flaig - CASL presentation to PWROG Analysis Subcommittee.	April 30, 2014	In Progress
Hussey	Discussions with IC on IC evolution.	September 12, 2014	This meeting
Banta/Hussey	Evaluate the existing CASL metrics and determine if CASL should develop metrics based on user base (number of published reports, number of users, etc).	September 12, 2014	In Progress

Actions from March Industry Council Meeting

Action Item—Provide IC with list of Phase 2 Mini-Charters

- **CASL-U-2014-0078-000** – ATF - CASL CP Charter Accident Tolerant and Advanced Fuel Systems - DRAFT.pdf
- **CASL-U-2014-0079-000** – CASL CP Charter for Seismic_FAD - DRAFT.pdf
- **CASL-U-2014-0080-000** – CASL CP miniCharter for Multi-NSSS and Fuel Arrays - DRAFT.pdf
- **CASL-U-2014-0085-000** – CASL Fuel Performance CP Charter-Phase2_v011314 - DRAFT.pdf
- **CASL-U-2014-0086-000** – CASL_CP_Charter_BAP_011414_final - DRAFT.pdf
- **CASL-U-2014-0087-000** – CASL_CP_Charter_MELLLA+_rev5 - DRAFT.pdf
- **CASL-U-2014-0088-000** – CASL_CP_Charter_natural_convection_MAC - DRAFT.pdf

Note: The first two mini-charters are **not** part of the Phase 2 scope, and will not be distributed

Highlights Documents On CASL Website

CASL Website (www.casl.gov)

The following reports are on CASL website in R&D – Publications

- MPO
  - Kendrick, B., C. Stanek, M. Short, *MAMBA (MPO Advanced Model for Boron Analysis), Development for CASL: Update and Applications*," EPRI-PTAC Meeting, February 27, 2014, San Antonio, TX, 2014. (see www.casl.gov for link)
- PHI/Westinghouse
  - Franceschini, F., B. Oelrich Jr., J. Gehin, "Simulation of AP1000 First Core with VERA," *Nuclear Engineering International*, pp. 33-35, May 2014.
- RTM
  - Davidson, G., T. Evans, J. Jarrell, R. Slaybaugh, C. Baker, "Massively Parallel, Three-Dimensional Transport Solutions for the k-eigenvalue Problem," *Nuclear Science and Engineering*, Vol. 177, Number 2, pp. 111-125, June 2014. (ANS Nuclear Science and Engineering subscription required).

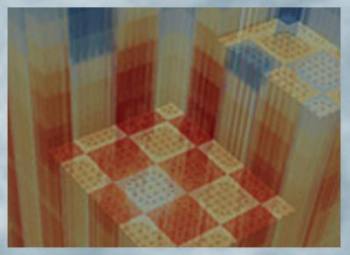
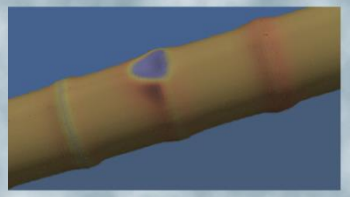
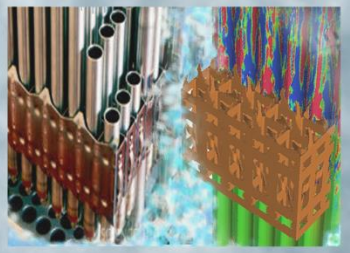
Winter 2015 Meeting

- Webcast planned
- Expect updates on
  - Phase 2 Initiation and Progress
  - Test Stands with expanded partners
- Date to be determined
  - Expect December/January

A DOE Energy Innovation Hub

Test Stand Update to Industry / Science Councils

Stephen M. Hess – AMA Deputy Lead
10 September 2014
Oak Ridge, TN

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2014 Test Stand Milestones

- Significant portion of AMA FY-2014 focus on Test Stand applications and support.
- Key related milestones:

Milestone ID	Milestone Description	Date
L2.AMA.P8.01	Experience with use of VERA in Industry Test Stands (L2 – DOE Reportable) Complete	3/31/14
AMA.VDT.P8.01	Complete Simulations of AP1000 HZP Conditions Complete	1/31/14
AMA.VDT.P8.02	Establish EPRI Test Stand Complete	3/31/14
AMA.VDT.P8.03	Establish TVA Test Stand Complete	3/31/14
L2.AMA.P9.01	Experience with use of VERA in Industry Test Stands (L2)	9/30/14

Experience with Test Stands

- PI: Stephen Hess (EPRI)
- DoE reportable L2 milestone
- Milestone documents experiences obtained to date by CASL industrial partners from execution of their respective Test Stands
  - Zero Power Physics Test (ZPPT) simulations of AP-1000 reactor performed using VERA-CS (Westinghouse Test Stand)
  - Applicable experiences to date from the EPRI Test Stand using Peregrine
  - Planning for TVA Test Stands
- Report CASL-U-2014-0036-000: issued for unrestricted release

Positive industry experiences with significant feedback to enhance future deployments

Westinghouse Test Stand

- Relevant and engaging application of VERA to an advanced PWR first-core
- Remarkable agreement with Monte-Carlo generated results
  - Critical boron and rod worth (excellent agreement)
  - Reactivity coefficients (some discrepancies)
  - Power distribution (very good agreement)
- Positive and useful experience for Westinghouse personnel
- Main recommendations related to expanding capabilities (coupling, depletion) and mitigating computational resources / runtime requirements
- Ongoing analysis effort using MPACT (2D/1D) capabilities

Current Test Stand Status

- EPRI:
  - Completed Test Stand milestone 1 August 2014
  - Results documented in report CASL-I-2014-0121-000-a (currently in process of review for unrestricted access)
  - Details to be provided in this session (Brenden Mervin)
- TVA:
  - Modeling and assessment of Lower Plenum Flow Anomaly (LPFA) phenomenon
    - Work in progress
    - Update to IC presented during June webcast
  - Application of VERA-CS to iPWR SMR initial core design
    - Work in progress
    - Details to be provided in this session (Kelly Kenner)

TVA LPFA Test Stand Update

- Started with trying to run the UT-C mesh without success
  - Not clear if this is a mesh issue, a Hydra-TH issue, or operator error. Would have preferred to start with a smaller problem.
  - Westinghouse having similar issues with their large mesh.
- Smaller trial problems (with our geometry) and coarser mesh generation has been problematic
  - No mesh engine provided with VERA.
  - Steep learning curve with recommended mesh engines.
  - Some are not capable of creating very large meshes.
  - Hardware is not configured for mesh generation.
  - Only one mesh format can be input to Hydra-TH.
- We have tripped over several small Hydra-TH quirks
- TVA Titan allocation approved and export control determination completed (9/2/2014). Ready to run.

Conclusions to Date

- Test Stands have served as useful initial applications of CASL developed methods / tools
- Feedback from AMA discussions with Science Council liaisons (May 2014):
  - Westinghouse Test Stand work characterized as “impressive”
  - EPRI Test Stand demonstrated need for enhancements in internal CASL communications and closer interactions between code developers and end users
  - The challenge will be when CASL reaches outside it’s core partners to get unbiased input from the broader community on the usefulness of VERA – provided recommendation that this outreach needs to happen early in the Phase 2 effort

Future Test Stands

Future Test Stands

- Renewal proposal identified Test Stands as a critical element to transfer CASL developed technology to nuclear stakeholders
  - Key to successful early adoption and use of CASL tools
  - Will be managed by TDO
    - Steve Hess on point for Test Stand interactions
    - CASL Deputy Director to provide executive sponsorship
- Initial engagements with CASL SLT on potential Test Stand applications early in Phase 2:
  - AREVA
  - M-Power
  - Nuscale

TDO will work with IC to identify high value applications and deployment partners

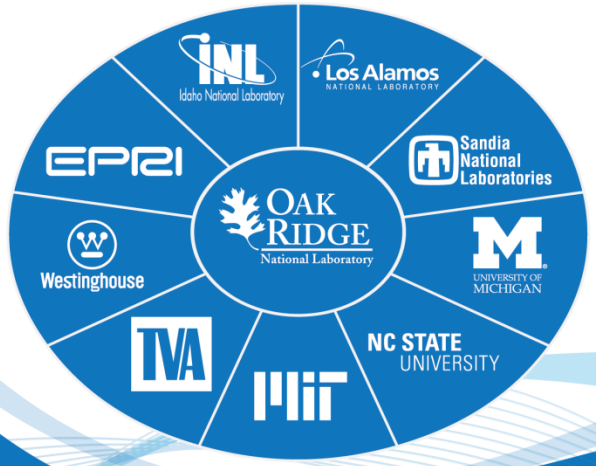
THE UNIVERSITY of TENNESSEE UT KNOXVILLE

TVA

iPWR Modeling with VERA

Kelly Kenner, UTK

09/10/2014



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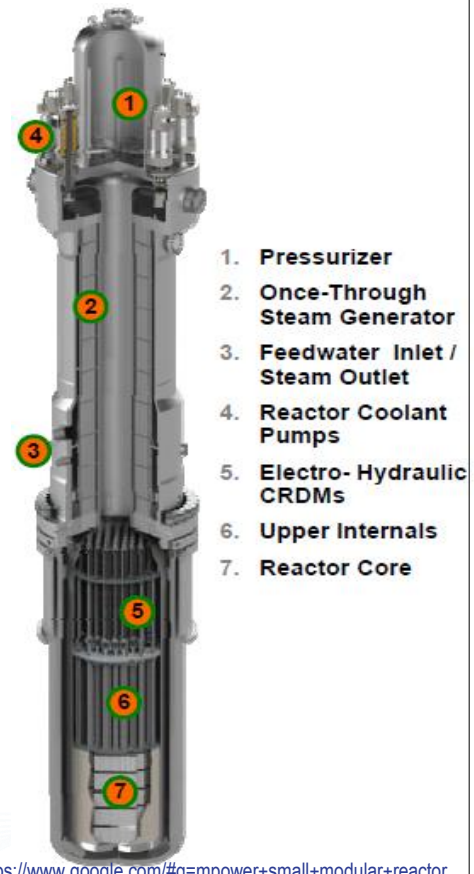
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

Introduction

- The objective of this study involved using VERA tools to perform a core cycle design for a typical iPWR SMR



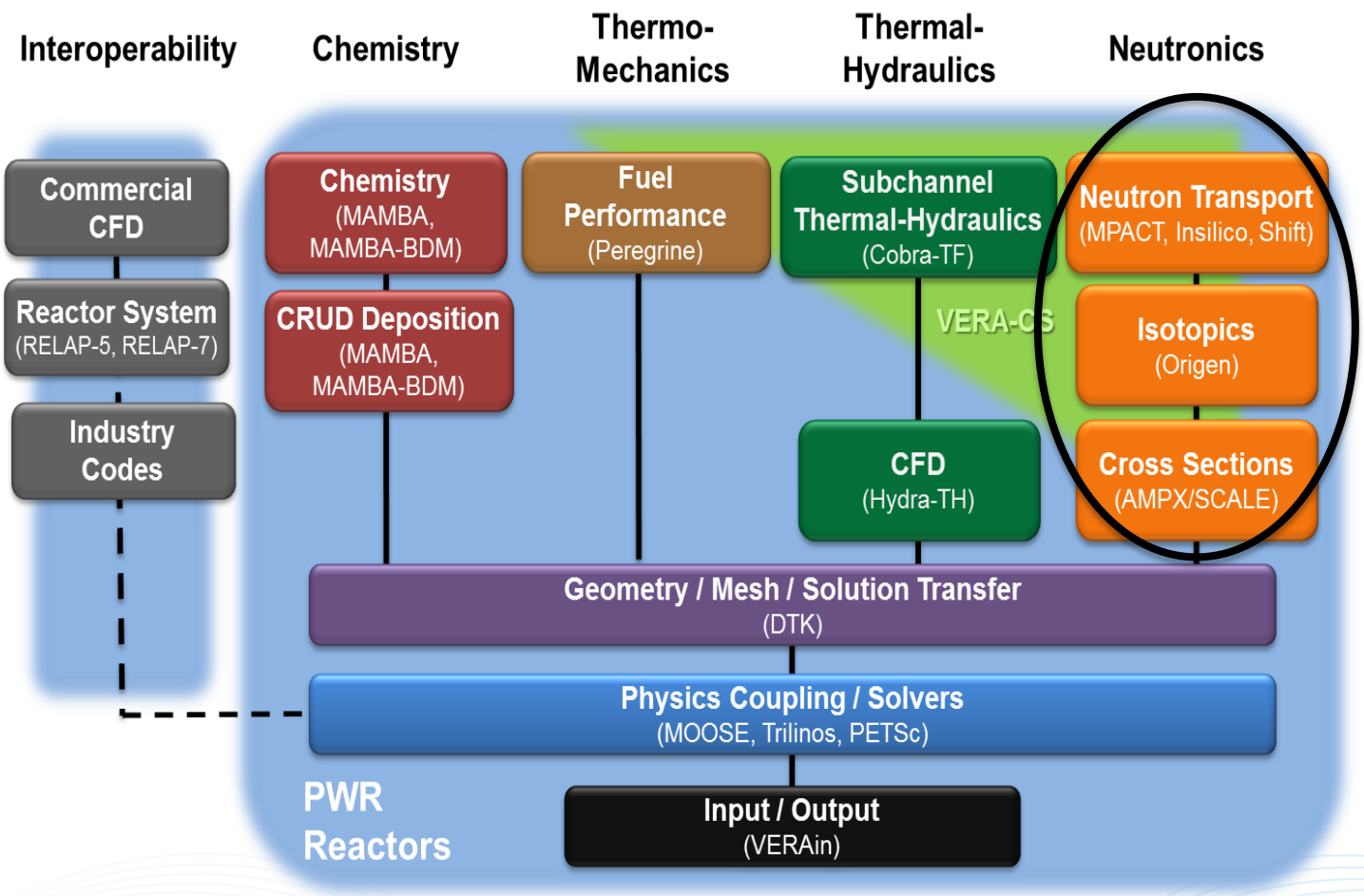
https://www.google.com/#q=mpower+small+modular+reactor+pressurizer+once-through+steam

- 69 17x17 fuel assemblies
- No soluble boron
- Active fuel height of 241.3 cm
- Core power of 530 MWt and 180 MWe
- ~4 kW/ft average linear power density
- 4.95% standard fuel enrichment
- Fixed BPRs and gad rods

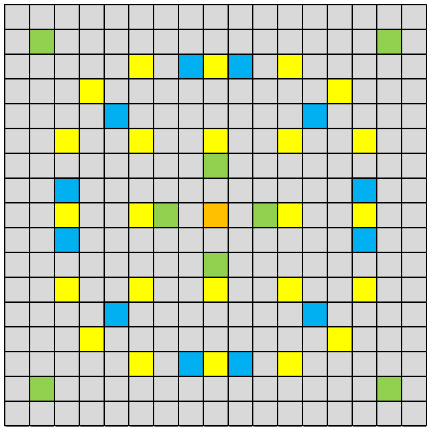
Introduction

- No soluble boron is used for reactivity control of the SMR
- Each fuel assembly type has varying number of BPRs of B_4C-Al_2O_3
- BPR pins do not include fuel, and are in fixed locations in each assembly (not inserts in guide tubes)
- Additionally, some assembly types include fuel rods of UO_2 mixed with gadolinia

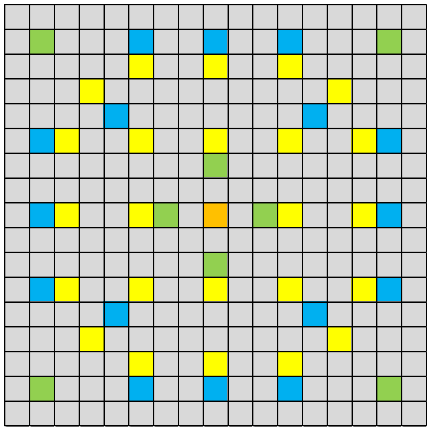
CASL Tools Used in This Study



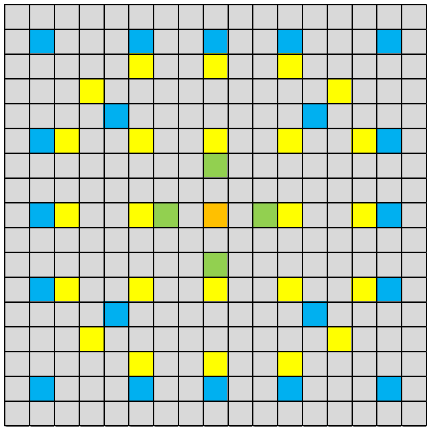
2D Single Assembly Lattice Models (1 of 2)



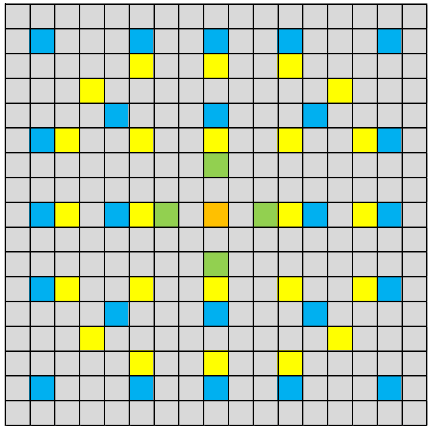
Type A: 12-BPR



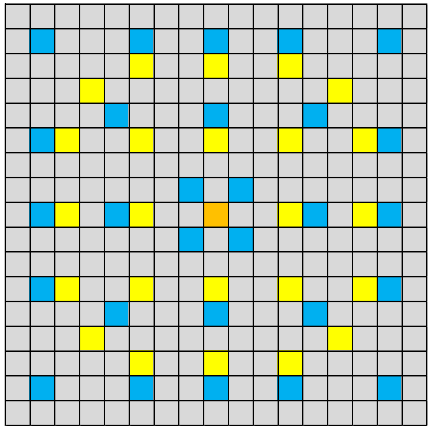
Type B: 16-BPR



Type C: 20-BPR



Type D: 24-BPR

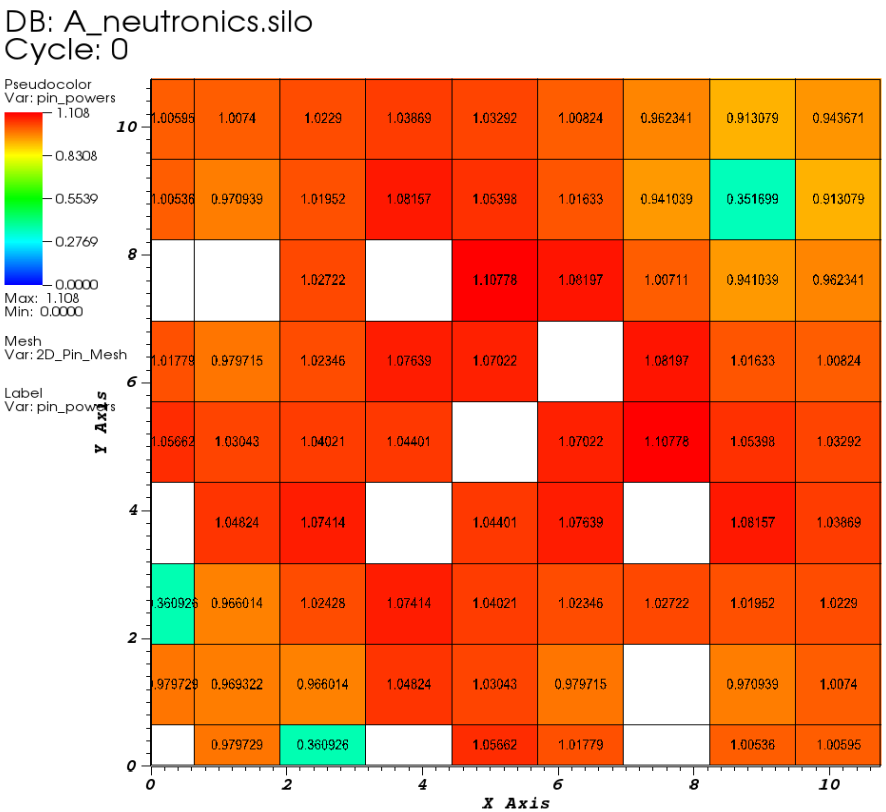


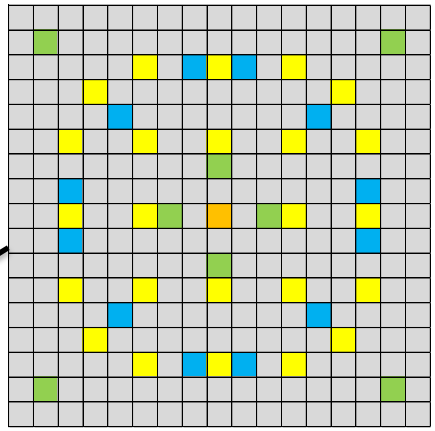
Type E: 28-BPR

	Standard Fuel Pin
	Control Rod
	Gd Fuel Pin
	BPR
	Instrument Tube

- Several lattices were evaluated for eigenvalue and peak pin power
- The initial core loading plan was selected based on the results from this 2D study

Example 2D Lattice Calculation





Example of a type A assembly (12-BPR) relative pin power distribution across the top right quadrant of the lattice.

Assembly	Peak Relative Pin Power	Minimum Relative Pin Power	k-inf
Type A	1.1078	0.3517	1.2152
Type B	1.1120	0.3545	1.1739
Type C	1.1010	0.3699	1.1686
Type D	1.1281	0.3686	1.0823
Type E	1.1241	0.9239	1.0717

Final Core Loading Plan

		A	B	A	B	A		
	D	B	D	B	D	B	D	
A	B	C	C	C	C	C	B	A
B	D	C	D	D	D	C	D	B
A	B	C	D	E	D	C	B	A
B	D	C	D	D	D	C	D	B
A	B	C	C	C	C	C	B	A
	D	B	D	B	D	B	D	
		A	B	A	B	A		

- Several configurations were tested
- The final configuration was selected based on power peaking
- The reference limit used for this study was for a typical PWR
  - Average relative assembly power of ~1.45

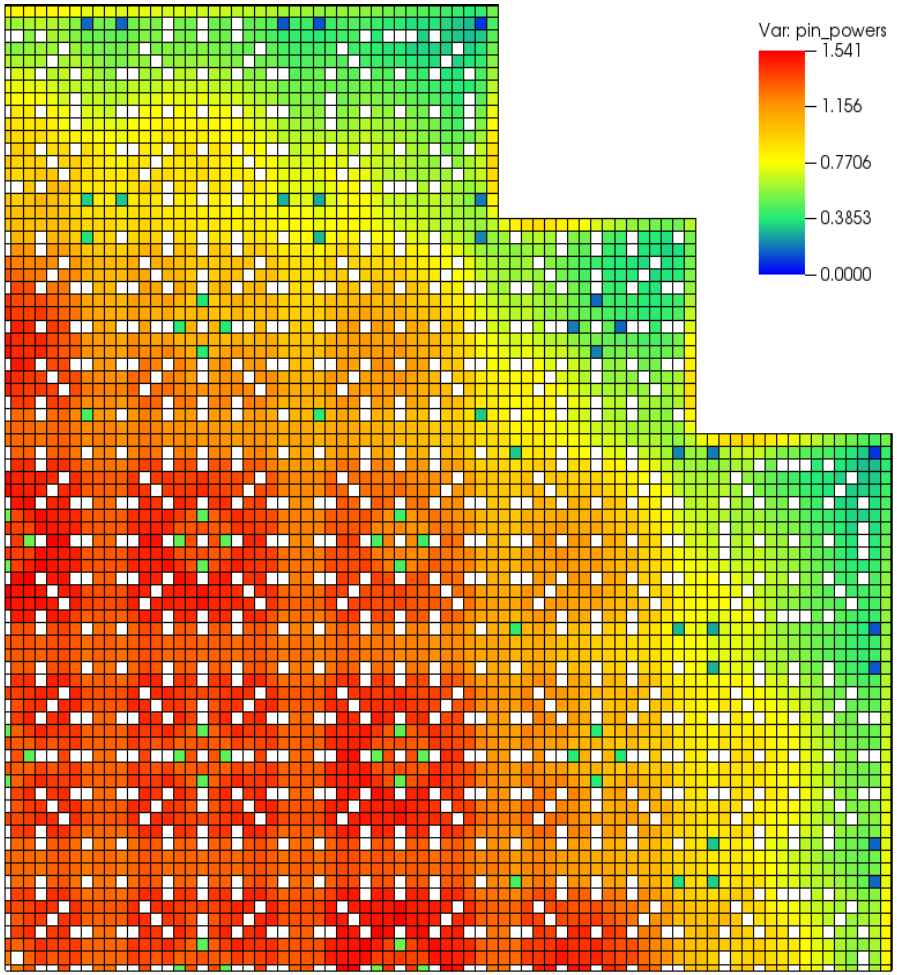
[Ref. *Sequoyah HTP Fuel Transition*. Attachment 8, Rev 2. AREVA NP Inc. June 2011. Print.]

1.352 1.447	1.379 1.480	1.424 1.566	1.274 1.520	0.791 1.077
1.379 1.480	1.334 1.469	1.325 1.522	1.055 1.318	0.697 0.957
1.424 1.566	1.325 1.522	1.194 1.402	0.935 1.185	0.553 0.803
1.274 1.520	1.055 1.318	0.935 1.185	0.593 0.862	
0.791 1.077	0.697 0.957	0.553 0.803		

Avg Pwr
FΔH

Assembly Type	# Standard Fuel Pins	Standard Fuel Pin Enrichment	# Gd Fuel Pins	Wt% Gd	Enrichment of Gd Pins	# BPR Pins
A	248	4.95	4	3	3.95	12
B	244	4.95	4	3	3.95	16
C	240	4.95	4	3	3.95	20
D	236	4.95	4	3	3.95	24
E	236	4.95	0	3	3.95	28

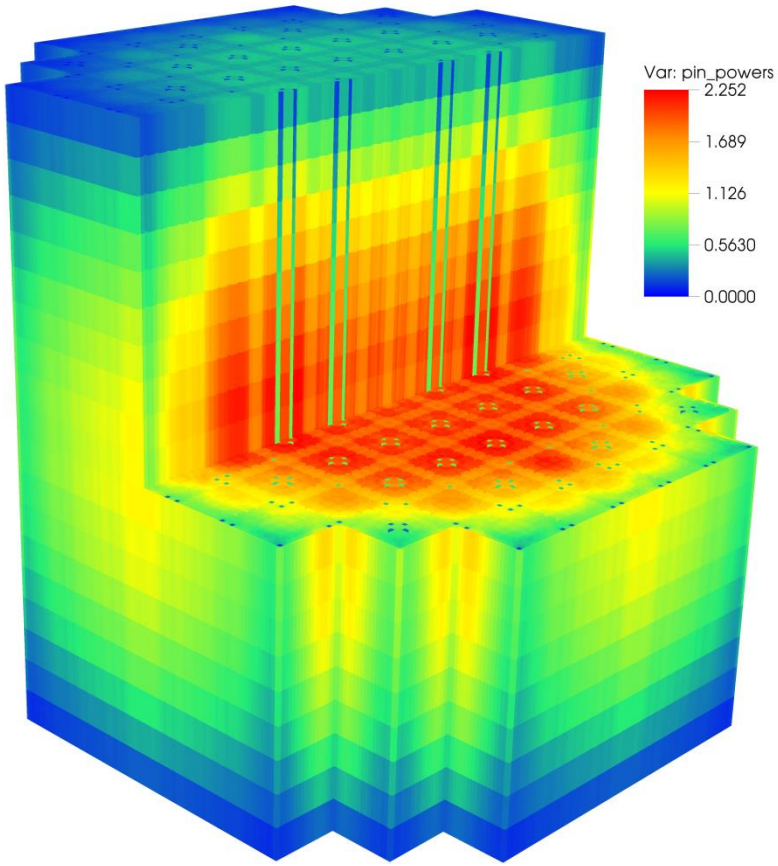
Final Core Loading Plan, Hot Full Power, Beginning of Cycle

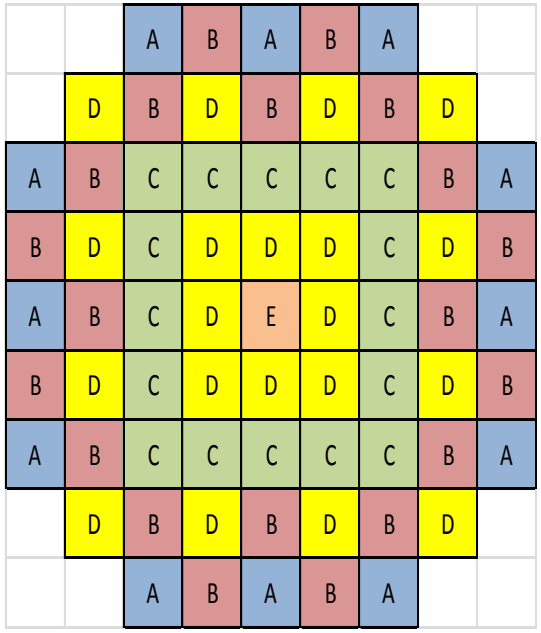


- Eigenvalue: 1.1287
- Max Relative Pin Power: 1.541
- Runtime: ~2.5 minutes for up to 49 cores on the Fissile-4 machines with Insilico
  - SP_5 angular approximation
  - PN order of 3
  - 252-group cross sections
  - 2-by-2 pin mesh

Reference Limit: FΔH < 1.55 for a typical PWR
[Ref. *Watts Bar Nuclear Reactor FSAR.* Tennessee Valley Authority. Print.]

3D Study with Insilico, HFP, BOL



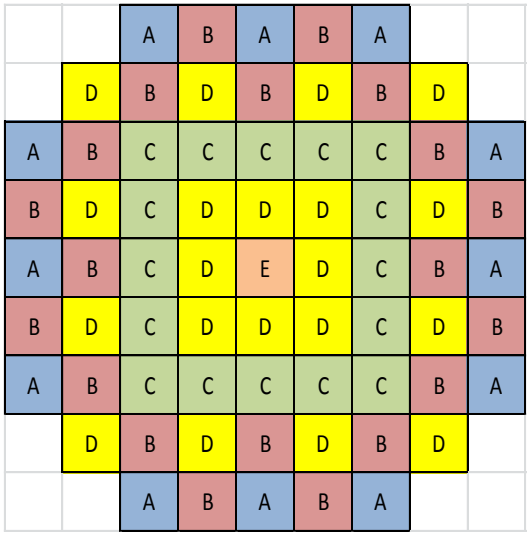


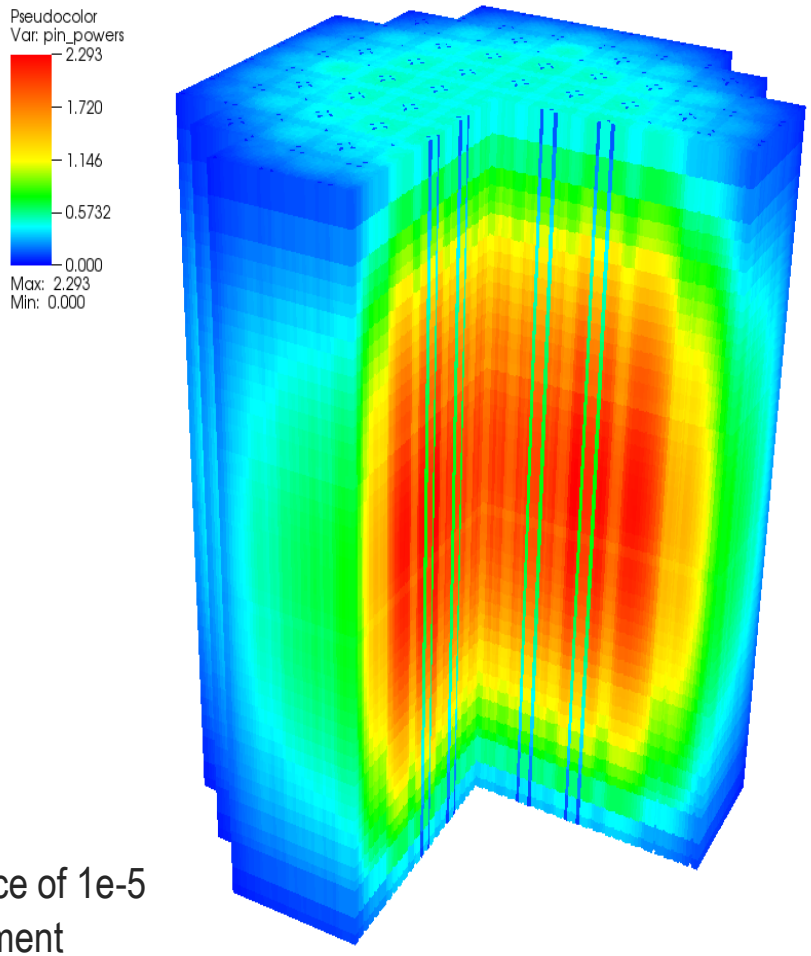
Number of Cores	400
Runtime	~20 minutes
Eigenvalue	1.1049
Peak relative pin power	2.252

Reference Limit: FQ < 2.4

[Ref. *Watts Bar Nuclear Reactor FSAR.* Tennessee Valley Authority. Print.]

3D Modeling with MPACT (no depletion)





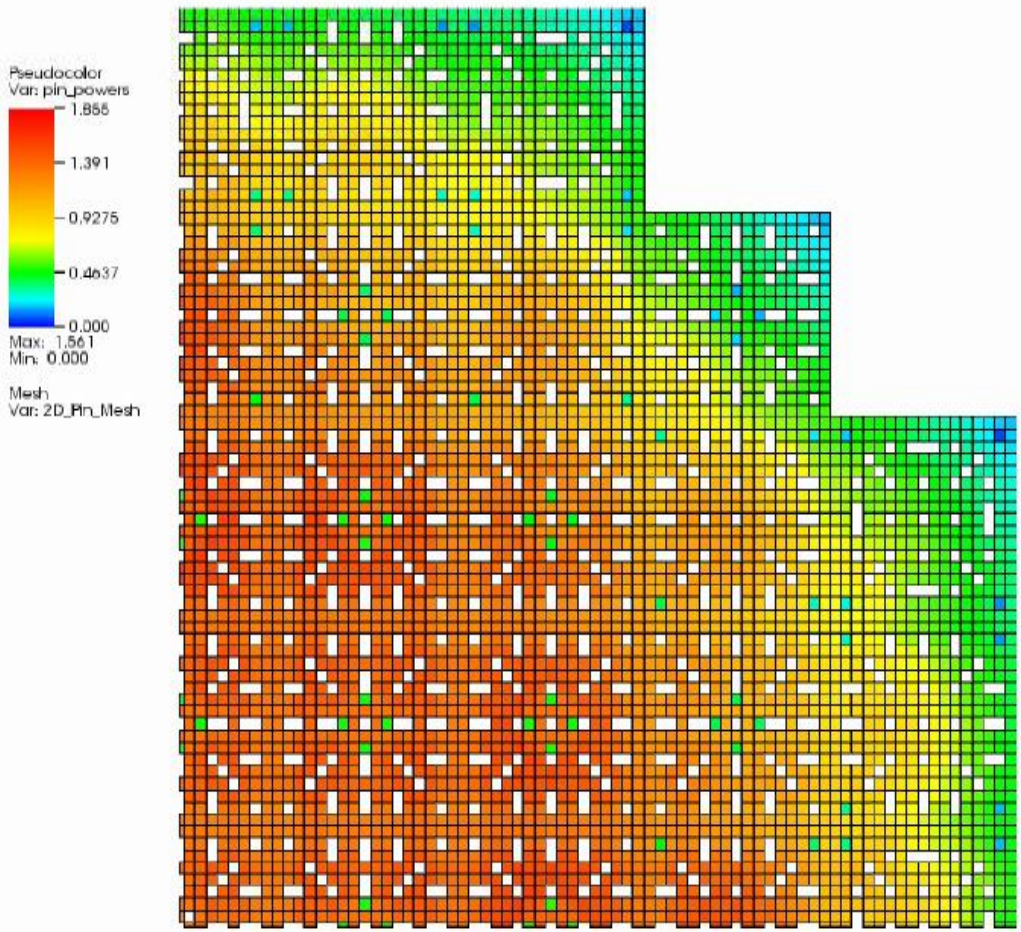
Number of Cores	1155
Runtime	~1 hour
Eigenvalue	1.1184
Peak relative pin power	2.293

- 0.1 cm ray spacing
- 8 azimuthal angles/octant
- 2 polar angles/octant
- Chebyshev-Yamamoto quadrature set
- Flux tolerance of 1e-4
- Eigenvalue tolerance of 1e-5
- P2 scattering treatment
- CMFD solver
- NEM nodal method
- 56 group cross section library

Determination of a Target Eigenvalue

- The desired cycle length for this iPWR is 1400 EFPD. Unfortunately, 3D depletion is not yet available, so the depletion study was performed in 2D using MPACT.
- Because the 2D configuration does not account for all leakage, a target eigenvalue for the 2D study was calculated based on undepleted 2D and 3D MPACT models.
  - Using MPACT, the initial core design was modeled in 2D and 3D to determine the target eigenvalue for the end of cycle in 2D depletion.
  - The eigenvalue in 2D was subtracted by the eigenvalue in 3D, and the difference was added to 1.0 to give the target eigenvalue.
    - 1.1392 - 1.1184 = 0.028 + 1 = 1.028

MPACT Depletion of the 2D Core



		A	B	A	B	A		
	D	B	D	B	D	B	D	
A	B	C	C	C	C	C	B	A
B	D	C	D	D	D	C	D	B
A	B	C	D	E	D	C	B	A
B	D	C	D	D	D	C	D	B
A	B	C	C	C	C	C	B	A
	D	B	D	B	D	B	D	
		A	B	A	B	A		

- This core produces the rated power for 1210 EFPD.
- Video shows depletion of the 2D core in EFPD time steps to 1300 EFPD.
  - Consistent scale for relative pin power throughout depletion, with a max relative pin power of 1.855

Cycle Length Not Achieved with the Selected Core Loading Plan

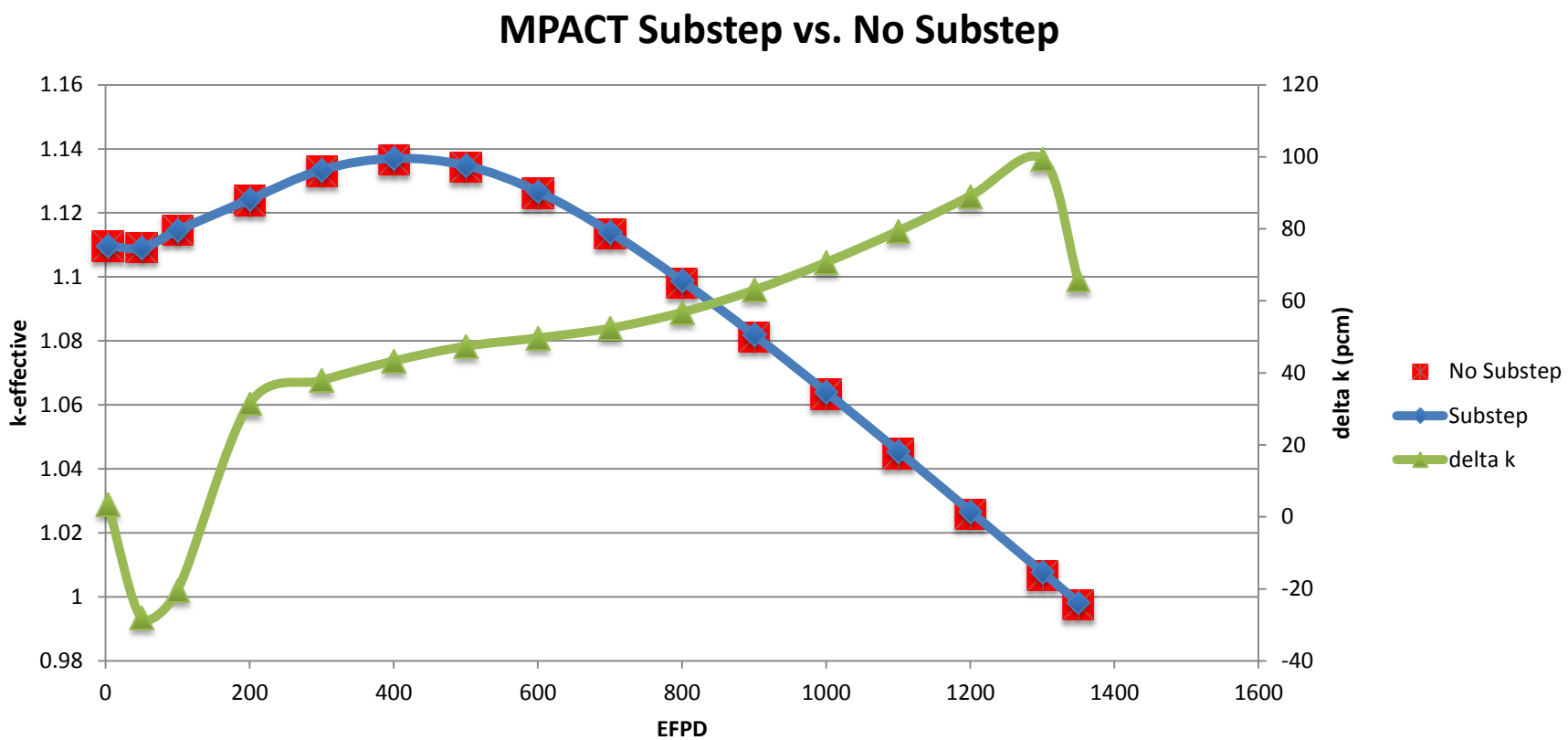
- This core did not reach 1400 EFPD (the goal lifespan of the core) and went subcritical between 1300 and 1400 EFPD.

MWD/kgHM	EFPD	k-effective
0.0797	3	1.1103
1.3287	50	1.1099
2.6574	100	1.1152
3.9861	150	1.1207
5.3148	200	1.1266
6.6435	250	1.1318
7.9722	300	1.1352
9.3009	350	1.1370
10.6296	400	1.1378
11.9583	450	1.1372
13.287	500	1.1352
15.9444	600	1.1264
18.6018	700	1.1137
21.2592	800	1.0983
23.9166	900	1.0814
26.574	1000	1.0635
29.2313	1100	1.0449
31.8887	1200	1.0260
34.5461	1300	1.0069
35.8748	1350	0.9977

- A 2D study using MPACT was performed to try to find a core design that would allow the reactor to remain critical to 1400 EFPD.
  - Only in extreme cases did the iPWR core reach 1400 EFPD.
- This study did not include control rod management
  - iPWRs are expected to operate their control components similar to a BWR, and this is expected to increase the cycle length.

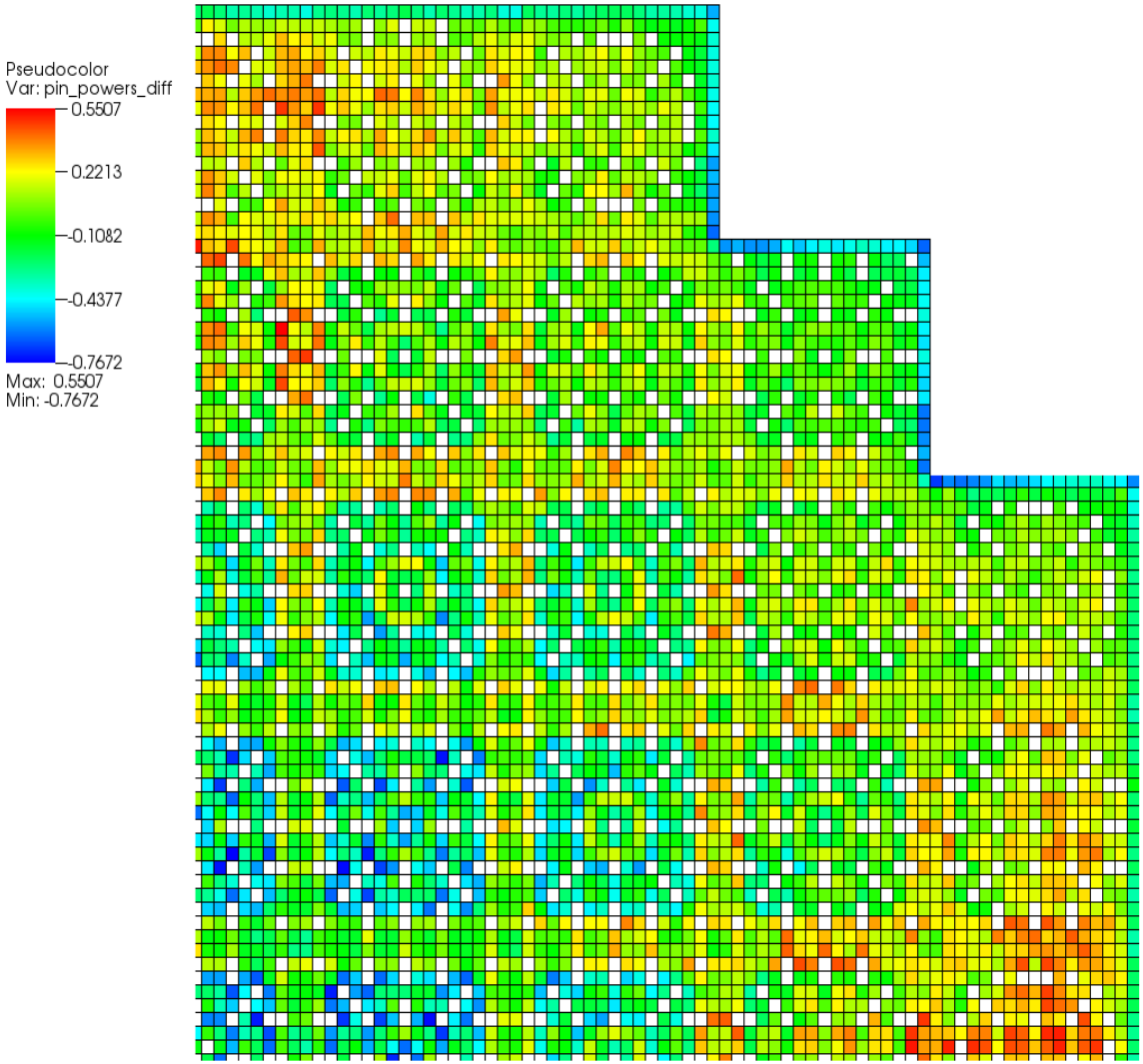
Below target eigenvalue of 1.028

Using Substepping in MPACT



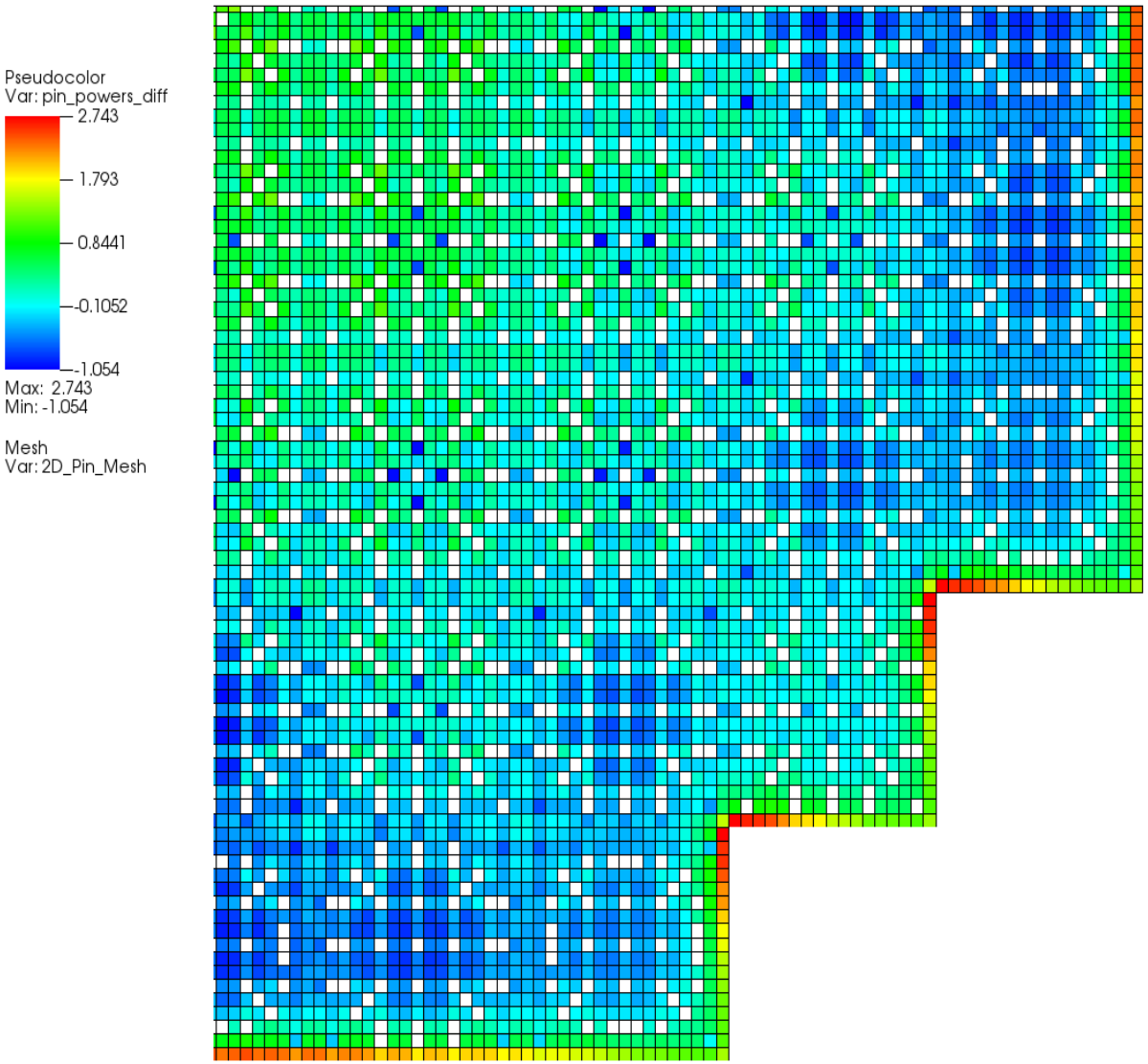
- The graph above shows a comparison between using the substepping option in MPACT
  - Substepping is advertised as a more accurate solution without increasing calculations of flux
- Runtime of ~30 minutes (coarse settings, few time steps) to ~1.5 hours (finer settings, many time steps).

2D Calculations with Shift for Comparison with MOC Results



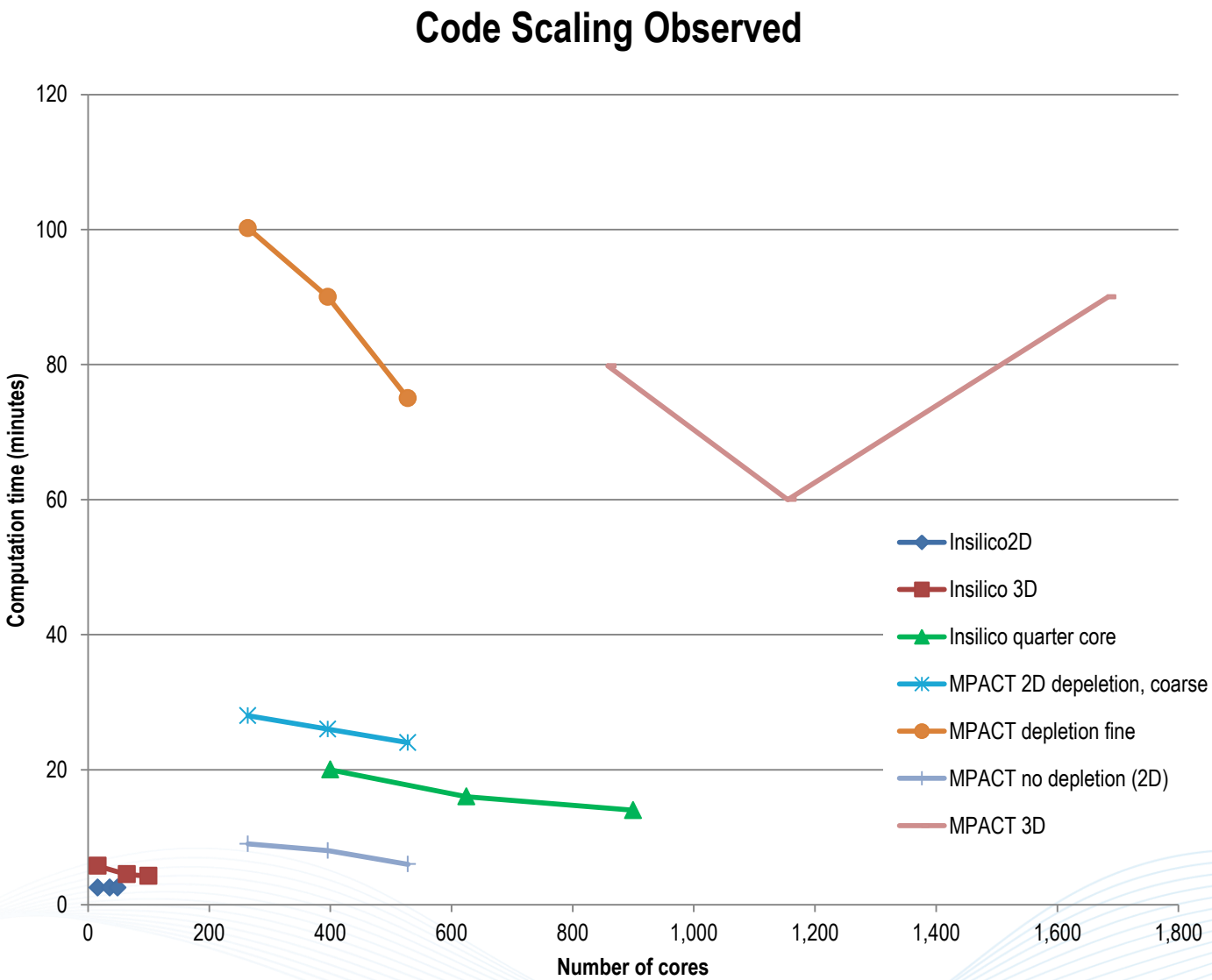
- An average -327 pcm difference exists between the k-effective for the 2D Shift case and the 2D MPACT case.

2D Calculations with Shift for Comparison with SP_N Results

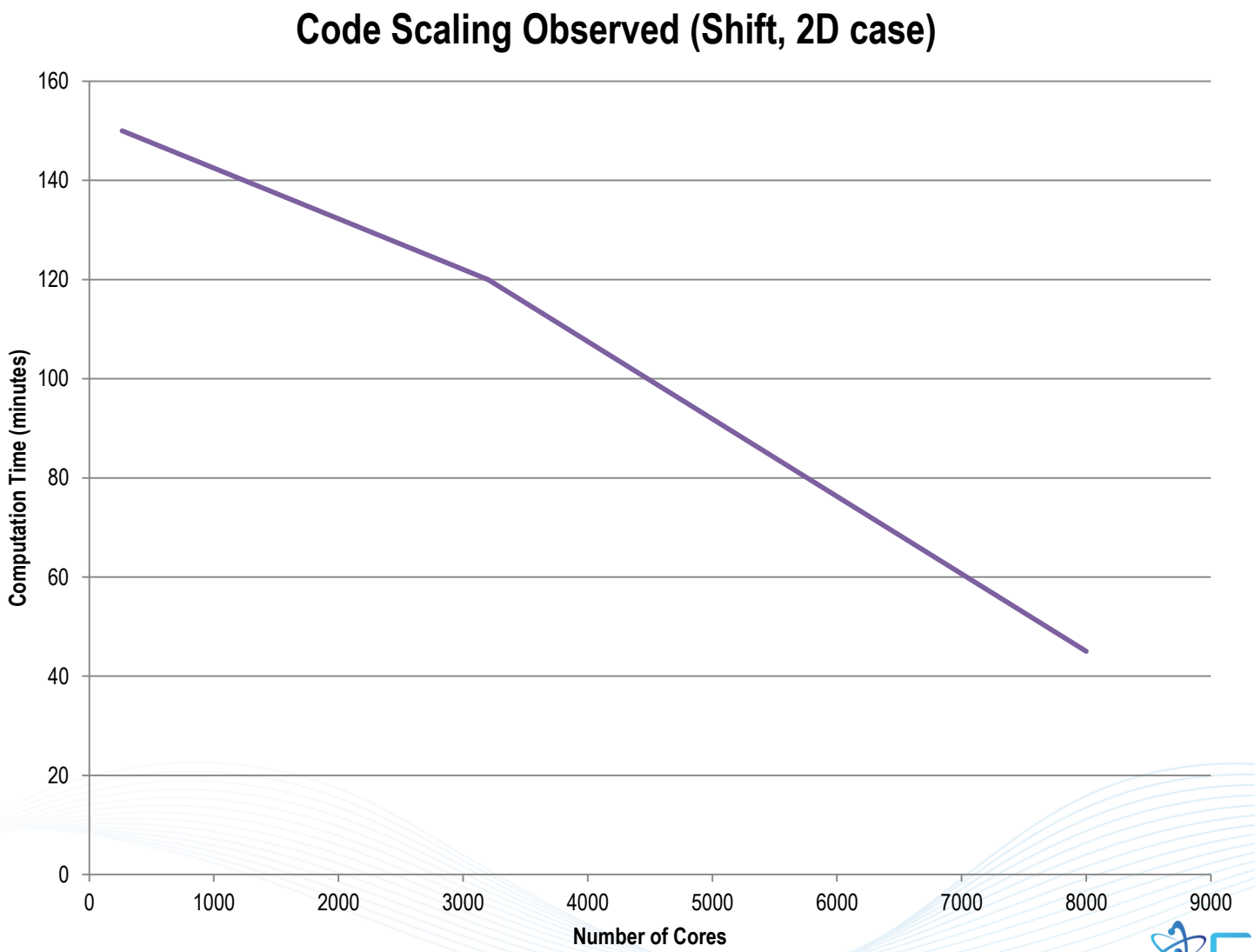


- An average -163 pcm difference exists between the k-effective for the 2D Shift case and the 2D Insilico case.

Experience Using CASL Tools (1 of 2)



Experience Using CASL Tools (2 of 2)



Challenges

- VERA is not intended for core design optimization as codes have slower runtimes
  - Core design selected was optimum design that could be created in the available time
- 3D depletion capability is not yet available
  - Target eigenvalue assumption had to be made
  - Control rod management could not be studied
- Identified Insilico limitations for core cycle analysis
  - Could not handle the larger baffle size

Conclusions

- VERA successfully modeled the iPWR SMR
- MPACT pin power and Insilico eigenvalue results agree well with Shift; MPACT and Shift eigenvalue difference is higher than expected
- Scalability appears to be good for all three neutronics codes
  - Coupled T/H was not studied
  - Longest runtime for 3D cases was ~1.5 hours using MPACT on 1683 cores
  - Longest runtime for 2D cases was ~2.5 hours using Shift on 264 cores
- Insilico did not have the capability to handle a larger baffle size
- MPACT substepping did not appear to have a significant affect on the solution
- There was difficulty reaching the goal cycle length of 1400 EFPD
  - Only extreme cases had the capability of reaching the goal cycle length. Therefore, the original core design was used to complete the study, reaching a goal cycle length of 1210 EFPD.

Acknowledgements

Many thanks and much gratitude to:

- Rose Montgomery, Dan Stout, Gary Adkins, TVA, and CASL
- Dr. Maldonado, Andrew Godfrey, Andy Worrall, Mark Baird, Jess Gehin, AJ Ierulli, Cole Gentry, Ben Collins and the MPACT developers
- This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

- Questions?

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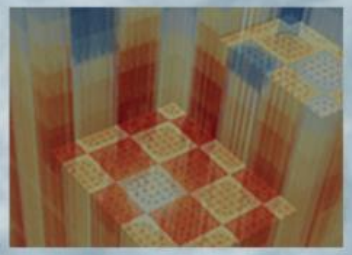
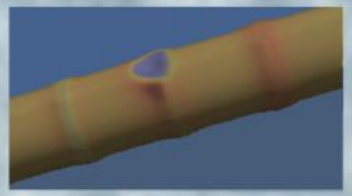
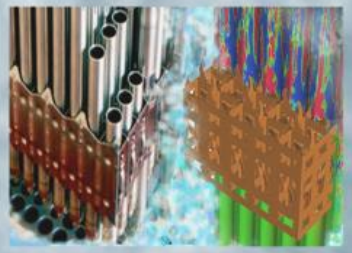
Phase 2 Industry Council Planning

Dennis Hussey (EPRI)

CASL Industry Council Meeting
Oak Ridge National Laboratories
September 9-10, 2014







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Overview

- Role of IC in Phase 2
- Expanded IC/CASL interaction
- Review of CASL Website
- Industry Council Chairman

Role of IC in Phase 2

- The Industry Council will be the executive connection to industry
  - All potential stakeholders of VERA in one committee
  - Members vary from project initiation and execution to results review

- CASL may request IC subcommittees
  - Many VERA applications are possible
  - Different skillsets and data needed for different challenges
  - 'Used and useful' will need focus from stakeholder needs

Industry Council will help drive Phase 2 direction

Expanded IC/CASL Interaction

- IC meetings are useful for information and feedback
- VERA is coupling is nearly ready for practical industrial application
  - Opportunities exist for IC to apply to VERA to actual problems
- Several venues for interaction
  - VERA Working Group-Rose Montgomery
  - Test Stands—Steve Hess
  - Special cases/applications
- CASL needs from IC
  - Validation data will always be needed
  - Help define margins of interest
  - Outreach to potential users

CASL Website

- CASL website will be a significant outreach tool
- www.casl.gov

IC Chairperson

- Phase 2 Proposal requires an IC Chairperson
  - Similar to EPRI model for industry committees
  - Provides a person closer to industry leading the group
- Process is outlined in Phase 2 Renewal Proposal
  - The Industry Council members nominate and select a Chairperson using the process stated above.
  - Chairperson is required to represent the nuclear industry (e.g. owner/operators or NSSS vendors).
  - Term of the Chairperson is one year with no term limit.

Target having IC Chairperson when Phase 2 commences

Summary

- CASL will need Industry Council involvement in more areas
  - CASL tools are developed for broad applications
  - IC can help shape the near and long term use of CASL codes
- CASL will request increased IC involvement
  - Working group
  - Test stands
  - Special problems

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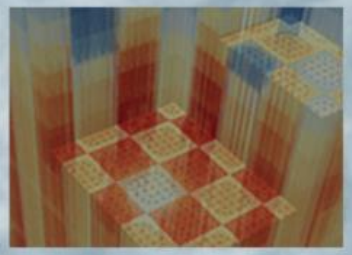
Developing a VERA Working Group

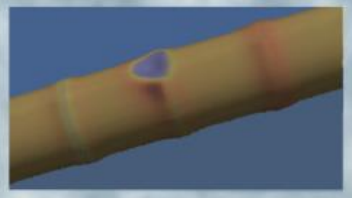
Rose Montgomery, TDO

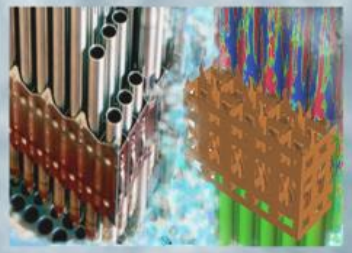
Industry Council Meeting

Oak Ridge National Laboratory

September 10, 2014







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VERA Working Group

- The VERA Working group (WG) will be stood up early in Phase 2 and will provide open forums focused on CASL technology.

- The goals of the WG are to:
  - **SUSTAIN** VERA User interest and connections post-CASL;
  - **CONNECT** users of the VERA tools;
  - **SHARE** training, experience, best practices, simulation and validation data, and successes;
  - **COLLABORATE** on the future development of the VERA.

Sustain

- Initial structure suggested:
  - Co-chaired by a CASL team member (Executive Director) and a WG-elected member (Chairperson).
  - Post-Phase 2, executive direction will be provided by the WG.
- General membership expected from:
  - Nuclear vendors
  - Nuclear utilities
  - Independent software vendors
  - National Labs
  - Universities
- Membership is open to all organizations / individuals eligible to license VERA.
- Phase 2 expects minimal (possibly zero) dues to start

Sustain

- The WG will enable users to:
  - Receive product information / updates
  - Receive software support for VERA
  - Participate and support VERA's Verification and Validation testing program
- The WG will work with TDO and CASL to investigate and develop a post-CASL entity.
  - The post-CASL entity is expected to administer the WG
- To establish the WG, TDO will leverage existing VERA subcomponent User Groups
- CASL Industry Council is encouraged to join

Sustain

- Phase 2 expects minimal (possibly zero) dues to start
  - CASL funds are budgeted for early support
- Post-Phase 2, User fees or VERA fees are expected to sustain the WG (likely through the post-CASL entity)
- The WG may develop a fee structure that is based on a market analysis
  - Examples of existing working groups have been identified, and initial studies have been completed
  - Further studies to be completed in year 1
- The WG is a candidate model for the post-CASL entity
- Source of WG operating budget could be either user-funded and/or funded collaborative projects, or something else
  - Pending study results

The WG is intended to be self-sustaining

Connect

- The combined WG will meet regularly to provide forums for User discussion, User Support, Training, and Alpha/Beta Testing.
- The WG will be empowered to establish subcommittees.
  - For example, a Training Subcommittee could be formed to help organize user training workshops and online materials.
  - Note that during Phase 2, the WG will likely work closely with TDO and CASL in support of outreach and education initiatives.

Share

- The WG, through meetings and webcasts, will facilitate the sharing of:
  - User experiences
  - Perceived best practices
  - Data
  - Successes
- The WG will further facilitate sharing through exploration of potential affiliations with other organizations such as ANS, ASME, AIAA, SIAM, EPRI, and utility owner's groups by coordinating delegates to meetings, sponsorship of cross-organization task teams, establishing new technical areas for discussion at meetings and conferences as deemed necessary or desirable.

Collaborate

- In Phase 2, the WG will collaborate with TDO, the post-CASL entity and CASL code development teams on:
  - VERA requirements and specifications
  - Testing and V&V
  - Source code development
  - Maintenance and usability
  - Funding opportunities as dictated by the interests and funding of the WG members
- The WG will explore potential collaborations across the nuclear industry to continue to develop the VERA functionality post-CASL

Other CASL Outreach Goals

- Nuclear community engagement is necessary for sustainability
- TDO will work with CASL staff to more fully develop communication vehicles
  - Website - Fact Sheets
  - TechNotes - Journal Articles / Conference Papers
- TDO plans to continue / expand engagements with selected groups
  - PWROG/BWROG
  - INPO Driving to Zero
  - EPRI Fuel Reliability Program
  - NRC (led by Jess Gehin, PHI)

Find Users; Manage Expectations

Other CASL Outreach Goals

- Demonstrations and Workshops will offer potential users the opportunity to work with VERA.
  - CASL Industry and Science Councils
  - Selected industry conferences
  - Support for CASL Education Program
- Initial Demonstration will be held at 'Advances in Nuclear Fuel Management' Conference in Hilton Head March 29-April 1, 2015.
- Training opportunities will be developed and coordinated with VMA and the Education Program.
  - Materials developed will leverage already existing CASL-edu materials
  - Summer school a possibility
  - Delivery vehicles to be investigated

The Timing

Year	Category	Level 2 TDO Milestones
1	Business operations	Establish a business case, identify and evaluate options for the post-CASL entity, determine mode of recruitment, and make recommendation for post-CASL entity
2	Business operations	Select the post-CASL entity
	Working Group	Establish the VERA Working group
	Training	VERA Training Pilot
5	Business operations	Finalize transition of CASL-supported functions to post-CASL entity

Lots of work in Y2 to 5 to fully develop the WG and the post-CASL entity, and to establish a large, trained VERA user pool before handing over the keys.

QUESTIONS?

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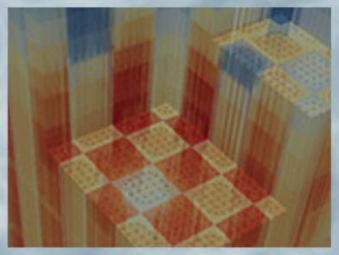
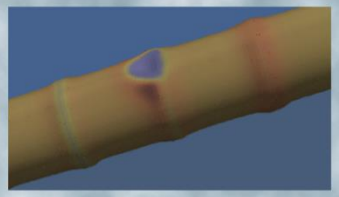
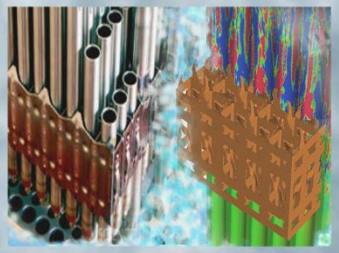
Thoughts on Phase 2

Doug Kothe
Director







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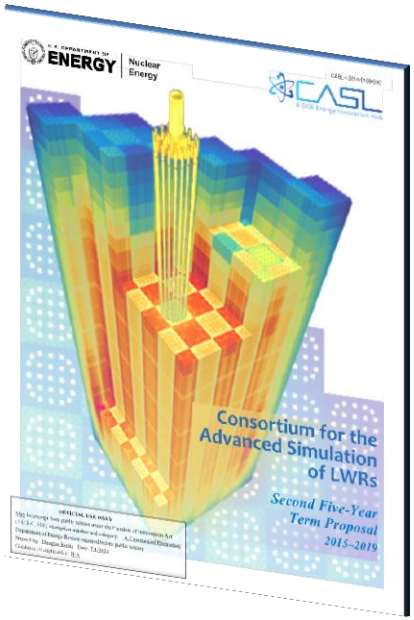

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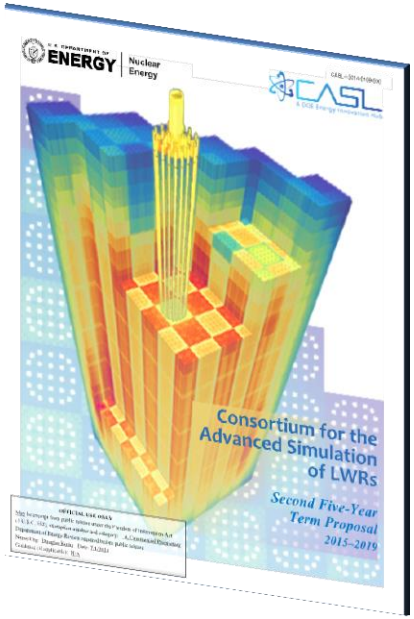

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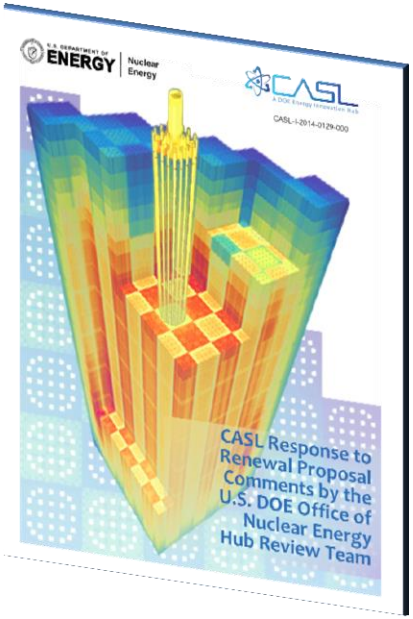
We appreciate the detailed and helpful comments received by the Review Team. Our responses in some cases reflect assumptions and best estimates by the CASL leadership at the present time, which may change as further knowledge and experience is gained



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Phase 1
Milestone Completion

- Relative to its proposed Phase 1 plan of 17 L1 and 126 L2/L3 milestones, CASL has delivered over 12 L1 and 529 L1/L2 milestones to date in support of its CP objectives, with that number expected to increase ~20% by the end of Phase 1.
- Milestones have been delivered in support of each CP, with some CPs (e.g., GTRF, FAD, LE) de-scoped relative to the proposed Phase 1 plan.
- VERA is progressing aggressively as planned and directed by CP objectives and now embodies a core simulator that represents a technology step change for industry.
- The executed milestone plan has differed slightly from the proposed plan, as it was not specific enough to meet the objectives and expected deliverables. The development path evolved as the CASL technology matured, with new avenues of research opening as the team discovered novel solutions and overcame roadblocks. The executed milestones provided more focused direction that resulted in better requirements-based outcomes.
- Further information is provided in Appendix A.1, A.3, A.4, and A.5.

Phase 1

Completion of Annual Reviews

- Each of the three annual reviews identified findings in technical and programmatic areas for improvement, which CASL has responded to and found invaluable in guiding continuous improvement (Table 5, Appendix A.6).

Phase 1

Publications and Innovations

- Over 1300 publications and related records through the first four years have been generated (~20 per month), including approximately 650 milestone reports and 450 journal articles, conference proceedings, and technical reports (Table 6, Appendix A.3.1-2).
- 90 undergraduate/graduate students and 15 postdoctoral associates have contributed directly to CASL R&D activities, and over 100 have participated in annual CASL summer workshops. A CASL School with an associated certificate is scheduled in FY15.
- Beside an active Industry Council, CASL is having an impact on M&S communities in the nuclear enterprise (VERA Test Stands, EPRI Advisory Committees, Owners Groups, NRC), professional societies, and the DOE (NE/NEAMS, SC/ASCR, NNSA/ASCR).
- Numerous innovations and discoveries have resulted from each CASL FA's focus technical work (Table 7, Table A-3).

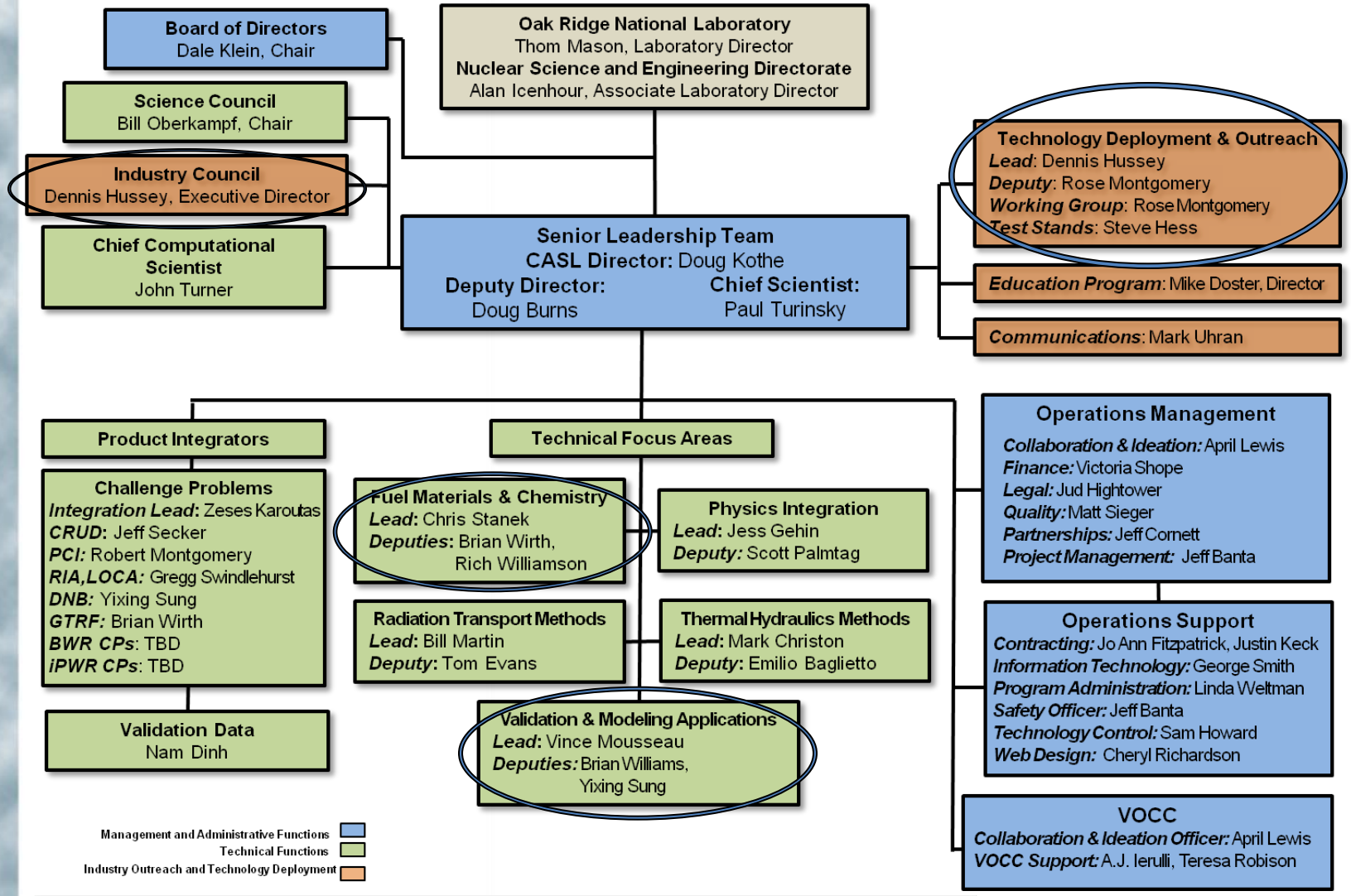
Phase 1

Technology Deployment

- Formal VERA releases have occurred annually, with the first limited release outside of CASL (thru RSICC) in late 2013 (Table 4). Broader release is planned for late FY14 and beyond.
- Government Use and Test and Evaluation (Appendix A.2.1) Licenses have been executed, with draft language in process for Non-Commercial and Commercial (Appendix B.4.3) Licenses.
- Signed IPMP is in place with another revision (Appendix B.4.1) currently under review.
- Three VERA Test Stands executed, with another 1-2 per year planned in Phase 2 based on significant interest expressed by IC members.
- An Advanced M&S User Group being chartered for implementation based on IC member interest.
- VERA components not subject to export control are being made available via open source release.

CASL Organization

Extended leadership team



Capability-based structure appropriate for CASL's mission of technology and product development. Basic structure remains intact from Phase 1. Could change as products mature and evolve into deployment and more heavy usage.

EF 1,2

CASL Organization

Extended leadership team

- Senior Leadership Team
  - Director, Deputy Director, Chief Scientist
- Board and Councils
  - Board Chair, Science Council Chair, Industry Council Executive Director
- Chief Computational Scientist
- Challenge Problem Product Integrators
- Technology Deployment and Outreach
  - Lead and Deputy Lead, Test Stands, Education Program, Communications
- Focus Area Leads and Deputy Leads
- Operations Management
  - Collaboration and Ideation, Project Management, Legal, Finance, Partnerships, Quality
- Operations Support
  - Technology Control

- Position responsibilities require from 10% to fulltime focus
- Most leadership positions are “player coaches” - doing technical work while leading

EF 1

Phase 2 Team Capabilities

Industry participation: partner, affiliate

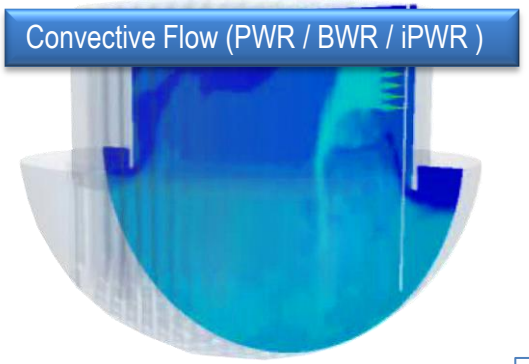
- R&D organizations and consultants
  - EPRI (Founding), Core Physics, GS Nuclear, Battelle, Bettis, Rolls Royce
- Nuclear vendors (fuel, designs)
  - WEC (Founding), AREVA, GNF, B&W mPower, NuScale
- Utilities (owner/operators)
  - TVA (Founding), Dominion, Duke, Exelon, EDF
- Independent Software Vendors (ISVs)
  - CD-adapco, ANATECH, GSE Systems, ANSYS, Studsvik Scandpower
- HPC and IT
  - Vidyo, NVIDIA, Cray, IBM
- Expand industry partnership beyond current (as VERA matures)
  - Seek **more nuclear vendor/utility partners** with help of IC and TDO element

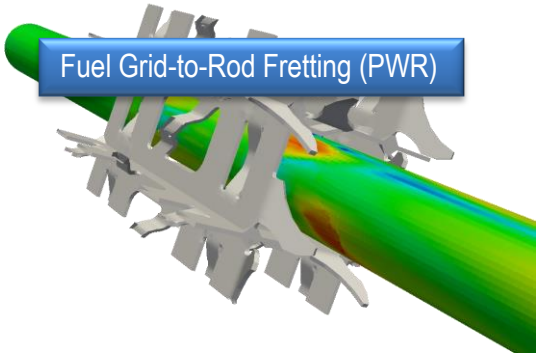
Industry letters of commitment (Renewal Proposal Appendix E):

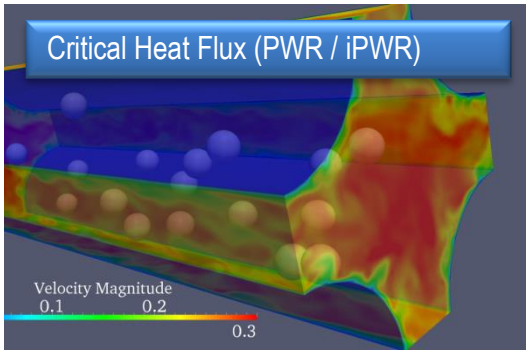
- Vendors: WEC, AREVA, GNF, B&W mPower, NuScale
- Utilities: TVA, Dominion, Duke, Exelon
- Others: EPRI, GSE Systems, Vidyo

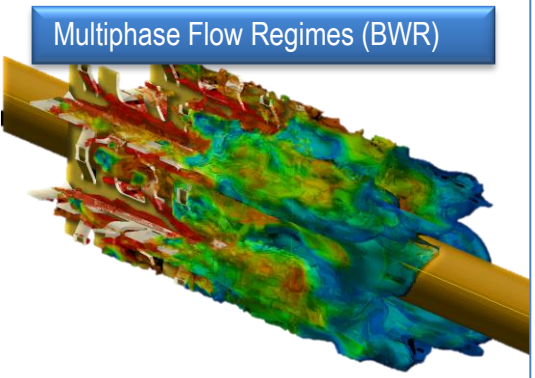
EF 1,2

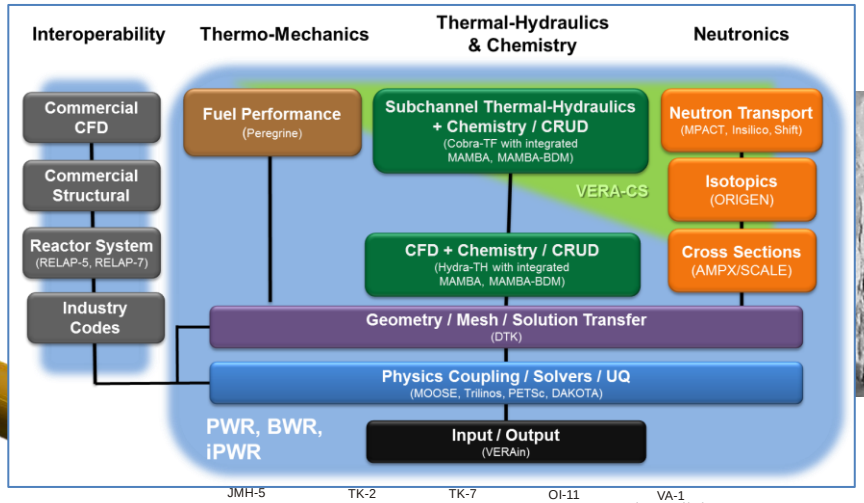
CASL Proposed Phase 2 Scope: 2015 – 2019

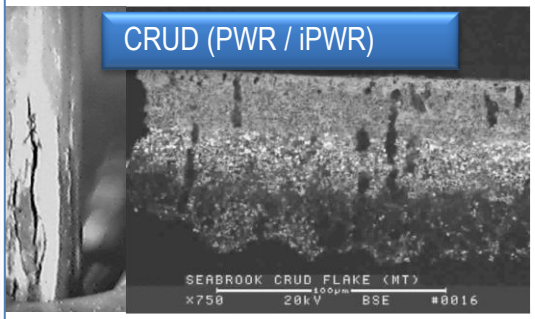


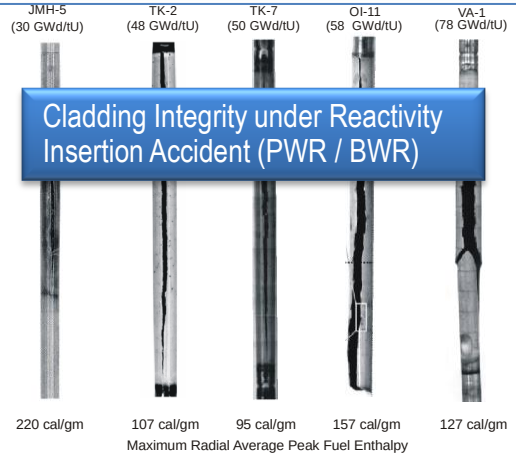


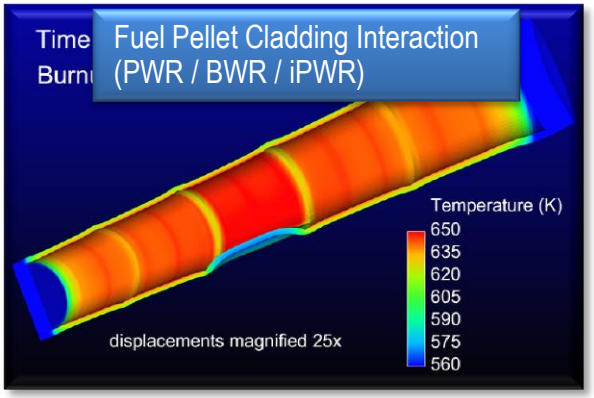










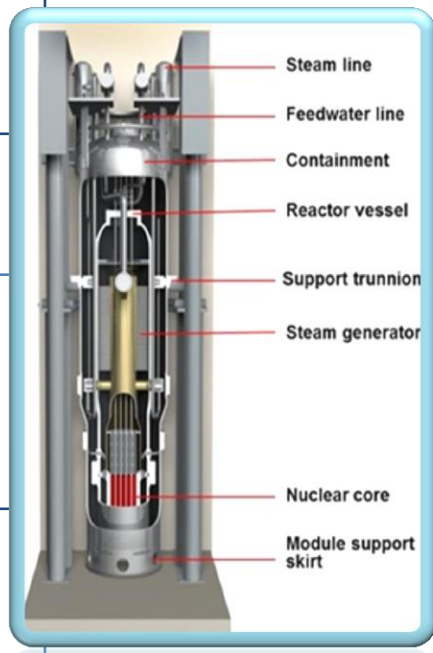


Selected Phase 2 Challenge Problems

BWRs

Category	Phase 2 New Challenge Problems	Phase 1 CPs targeted for Phase 2 Deepening
Thermal-Hydraulics	Convective Flow (thermal and solutal) iPWR CHF (DNB) BWR Flow Regimes	CHF (DNB)
Cladding Performance	BWR PCI iPWR PCI BWR RIA BWR LOCA	PCI RIA LOCA
Coolant / Corrosion Chemistry	iPWR CRUD (CIPS & CILC)	CRUD (CIPS & CILC)
VERA Core Simulator	Supporting: All BWR and iPWR CPs	Supporting: CRUD (CIPS & CILC) PCI DNB RIA
Interoperability	Supporting: GTRF, FAD LOCA, RIA	

iPWRs



A DOE Energy Innovation Hub

Roadmap for Phase 2

- Level 1 milestones provide a roadmap of the major objectives.
- Supporting Level 2 milestones are developed by focus areas

ear	Category	CP	No.	Milestone Description
1	Coolant / Corrosion Chemistry	CIPS / CILC	1	Qualify core-wide PWR CIPS capability with corrosion product treatment: Add corrosion product source term and mass balance to MAMBA, and utilize in VERA-CS to simulate multi-cycles of a PWR that experienced CIPS.
	Core Physics	PWR CPs	2	Qualify multi-cycle PWR core simulator capability: Using VERA-CS simulate first and reload cycles of the Watts Bar Unit 1, with predictions compared to plant measurements with regard to in-core, ex-core and selected startup physics test measurements.
	Core Physics	PCI / RIA / LOCA	3	Demonstrate iPWR core simulator capability: Utilizing VERA-CS, establish an iPWR core model and simulate cycle depletion.
	Thermal-Hydraulics	CHF (DNB) Convective flow	4	Qualify multiphase CFD capability for bubbly flow regime: Hydra-TH will be used to simulate out-of-core fluid experiments targeted at providing validation data for the bubble flow regime, with predictions contrasted to measurements.
2	Cladding Performance	PCI / RIA / LOCA	5	Demonstrate core subregion & core-wide PWR PCI capability: Utilizing VERA-CS with Peregrine-2D, complete PWR multi-cycle core depletion for core maneuver to identify PCI limiting fuel rods; utilizing Peregrine-3D complete PCI analysis for limiting fuel rods.
	Coolant / Corrosion Chemistry	CIPS / CILC	6	Quality CFD-based PWR CILC capability for a subregion: Using the results of the Year 1 CIPS L1 milestone to identify CILC limiting fuel rods and associated powers, CILC analysis will be completed using Hydra-TH with embedded MAMBA coupled to Peregrine.
	Deployment	N/A	7	Create Working Group for CASL software: To support the release to external users, a Working Group will be formed, members recruited, charter written, and first meeting held in conjunction with training on selected usages of VERA.
3	Cladding Performance	GTRF	8	Demonstrate GTRF analysis methodology components: Using the fuel rod mechanical/material modeling of Peregrine, finalized rod wear model, Hydra-TH predicted turbulent pressure forces, and assumed gap opening, demonstrates interoperability capability of VERA with a structural mechanics code. Stretch goal: extend Peregrine to treat the change in spacer grid straps geometry and material properties to capture cladding-grip strap gap formation and impact on wear.
	Cladding Performance	LOCA	9	Demonstrate PWR LOCA fuel performance capability: Use Peregrine to predict the extent of clad ballooning and oxidation, as a function of initial fuel rod state (e.g. hydrogen pickup) using LOCA system transient code generated boundary conditions.
	Core Physics	All BWR	10	Establish BWR core simulator capability for core subregion: Use VERA-CS to simulate a subregion (i.e. one or more fuel assemblies) of a BWR core. Stretch goal: simulate full core.
	Thermal-Hydraulics	DNB	11	Qualify prediction of onset of DNB using M-CFD: Hydra-TH will be used to simulate out-of-core fluid experiments targeted at providing validation data for the onset of DNB, for a range of powers and coolant inlet enthalpy, flow and pressure.
	Thermal-Hydraulics	Convective flow	12	Qualify thermal/solutal convective fluid flow CFD capability: Hydra-TH will be modified via incorporation of appropriate turbulence model and boron solution/dissolution chemistry model and used to predict first thermal convective fluid flow and subsequently thermal/solutal convective fluid flow, with predictions contrasted to validation data where available.
4	Cladding Performance	RIA	13	Demonstrate core-wide PWR RIA capability to simulate ejected rod accident: VERA-CS with neutron kinetics and Peregrine-2D will be used to simulate a PWR ejected rod accident to identify RIA limiting fuel rods; utilizing Peregrine-3D complete RIA analysis for limiting fuel rod(s).
	Cladding Performance	PCI / RIA / LOCA	14	Demonstrate BWR PCI capabilities: Utilizing VERA-CS with Peregrine-2D coupled, complete BWR core subregion depletion from which a maneuver will be completed to identify PCI limiting fuel rods; utilizing Peregrine-3D complete PCI analysis for limiting fuel rod(s).
	Thermal-Hydraulics	BWR Flow Regimes	15	Demonstrate capability to simulate using M-CFD the flow regimes that exist during normal operations of a BWR. Hydra-TH will need to be modified to incorporate the appropriate closure relationships associated with each flow regime and recognize the flow topology in order to utilize the appropriate closure models, including addressing flow regime transitions.
5	Cladding Performance	RIA	16	Demonstrate BWR RIA capabilities: Utilizing Peregrine-3D complete RIA analysis for assumed limiting fuel rod(s).
	Cladding Performance	LOCA	17	Demonstrate BWR LOCA fuel performance capability: Use Peregrine to predict the extent of clad ballooning and oxidation, as a function of initial fuel rod state (e.g. hydrogen pickup) using LOCA system transient code generated boundary conditions.
	Thermal-Hydraulics	CHF (DNB)	18	Demonstrate prediction of onset of DNB using M-CFD for low flow conditions indicative of iPWRs and PWRs during post-trip loss of offsite power event.
	Deployment	N/A	19	Finalize transition of CASL-supported functions to post-CASL entity: Establish post-CASL entity and assist it to manage software release, distribution, training, and the bug fix and enhancement processes.

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Top Risks in Phase 2

Category	Risk Description	Risk Mitigation
Resource	Insufficient availability of experimental and operational reactor data for validation and insufficient effort available for validation activities.	Influence other programs, institutions, and vendors/utilities to fill data gaps; define and resource-load validation data needs and priorities; quantify M&S uncertainties resulting from data gaps with early PCMM analyses. Recognize that industry must complete validation task; clearly communicate this need.
Technical	Multiphase CFD closure relationships beyond bubbly flow require more effort than planned. Extensions to Gen-I/Gen-II closure models and BWR-like flow regimes lead to excessively complex models and numerical algorithm challenges.	Establish evolution and maturity of Hydra-TH effort as the singular focus of THM with highest priority for resources as early as possible. Seek and extend existing Gen-1/Gen-II closure models and numerical algorithms. Reduce scope on depth of closure modeling if necessary. Communicate this is an immature and active area of research to temper expectations.
Technical	Transient neutronics capability is too compute intensive.	Have trigger to implement interoperability with existing industry transient neutronics capability to minimize delay of dependent work; engage computer science expertise if necessary in scrutinizing and implement compute efficiency opportunities.
Technical	COBRA-TF subchannel T-H model for BWRs is not sufficiently validated for predicting void distribution and unable to model BWR features such as water rods and bypass flow are insufficient. Also not able to yield acceptable steady-state full-core BWR solutions.	Address physical models and computational algorithms in COBRA-TF to correct issues by drawing in part on existing BWR work as guided by validation results. If not feasible, develop new steady-state subchannel T-H capability.
Technical	Unable to devise compute-efficient, accurate, and robust multi-physics coupling models, algorithms and software implementations, especially for the BWR core simulator.	Perform research on advanced coupling methods as a backup to standard Picard iteration to provide an alternative approach with improved convergence properties.
Programmatic	Inability to expand industry interest and engagement through the effective deployment of CASL-developed technologies.	Implement software license agreements for VERA and its components; formulate and enforce a useful and actionable IP Management Plan; work proactively with BOD; understand and quantify industry requirements; and ensure adequate resources are available for TDO and VMA activities to support software users.
Programmatic	Post-CASL entity not ready or not capable of accepting ownership of CASL processes.	Establish TDO area; diversify post-CASL candidates; coordinate early with active post-CASL entities; perform benchmarking; perform pre-transition demonstrations during Phase 2.
Programmatic	Overall scope outpaces constrained budget and schedule for the BWR core simulator, where development proves more difficult than planned and results in delays in delivery of capability.	Implement multiple technical paths where possible, proactively engage BWR fuel vendors, IC and SC for requirements definition and review/consultation, and insert decision point milestones for go/no-go or de-scoping. Utilize predictions from industry-based core simulator in interim until CASL capabilities are available.
Programmatic	IPMP is unable to accommodate potentially conflicting requirements and priorities of DOE and consortium partners.	Proactively review and revise IPMP on a quarterly basis to ensure pace is keep with deployment goals. Seek DOE policy guidance where necessary to resolve conflicting partner needs and interests.
Technical	Run times for MPACT full-core, multi-cycle depletion with TH-feedback are too high for industry class clusters.	Several efforts are underway to improve MPACT run times, with expected gains of 5-10. If these fail, Moore's Law continues to make computing cheaper and may allow re-definition of "industry class cluster".
Programmatic	Fuel/clad materials phenomena undertaken to model too complex given scope, schedule, and funding constraints.	Coordinate actively with other DOE programs (e.g. Office of Science, NEAMS, etc.) to ensure optimized scope definition and maintain flexibility in resource allocation should certain multi-scale approaches pursued for specific materials issues prove unsuccessful. Revert to phenomenological models if physics based models prove unrealizable.

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
- VUQ: Capabilities integration

Phase 2

Expected Accomplishments

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

AREVA

CASL Project

A Vendor's Perspective

Chris Lewis
AREVA Sr. Project Manager

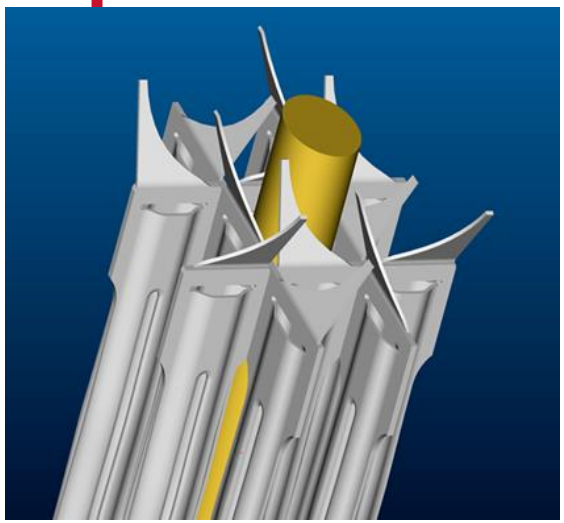
AREVA

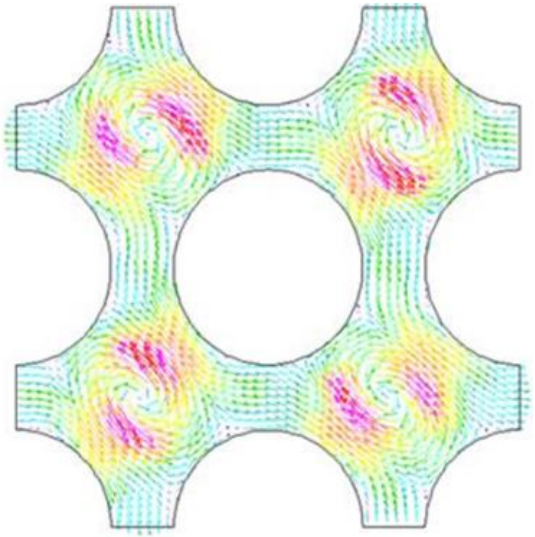
Outline

- Potential Areas for Use
  - Product Development
  - Evaluation of Operational Issues
  - Licensing Applications
- Potential Issues
- Conclusions

Product Development

- **Potential Benefits**
  - **Product optimization outside of expensive testing**
  - **Performance evaluations under conditions that cannot be tested**
  - **No NRC approval required**
- **Requirements for code:**
  - **Reasonable computation time**
  - **Adequately benchmarked against relevant phenomena**
  - **Must be accurate enough to:**
    - Predict actual or relative change between designs
  - **Must be versatile for different designs**
    - Minimal tuning between designs
    - Ability to incorporate proprietary models





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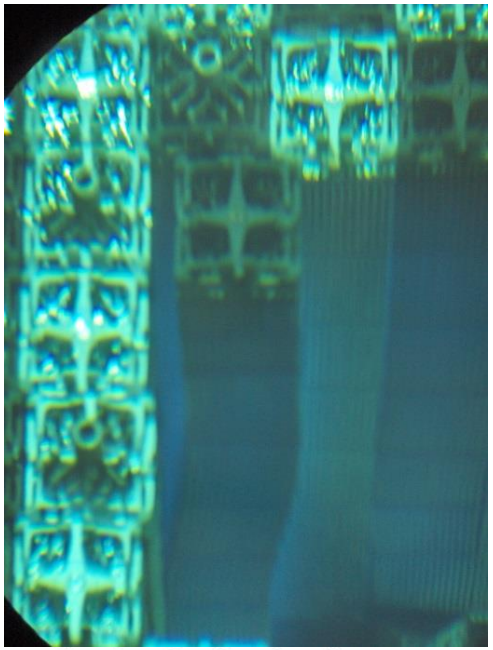
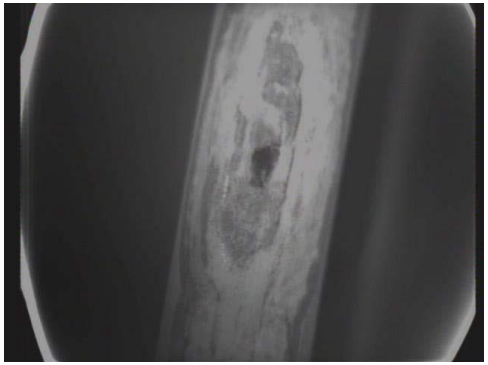
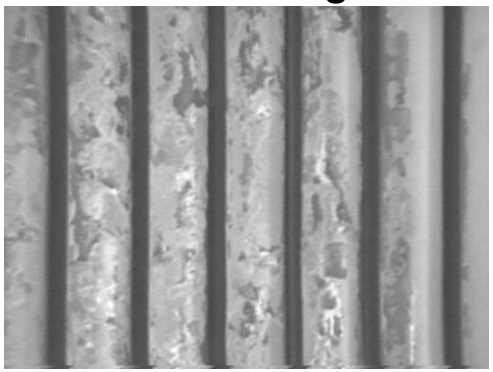
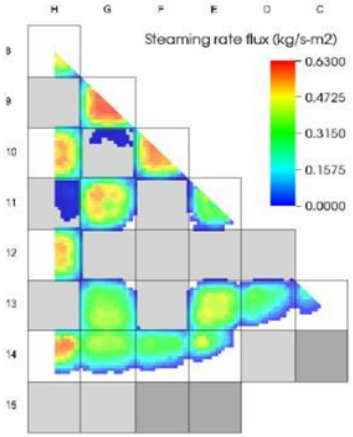
Evaluation of Operational Issues

- **Potential Benefits**
  - **Solve issues impacting plant operating operations**
  - **Avoid plant downtime or costly mitigation**
  - **Does not require NRC approval**
- **Requirements for code:**
  - **Rapid analysis turnaround time**
  - **Benchmarked against operational data**
  - **Accurate enough to predict relative change**
    - Would like to understand absolute margins where possible
  - **Versatile across different reactors/FA design**









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Licensing Applications

- **Potential Benefits**
  - **Provide additional licensing margin**
  - **Allow better understanding of transient progression**
  - **Use to qualify less sophisticated codes**

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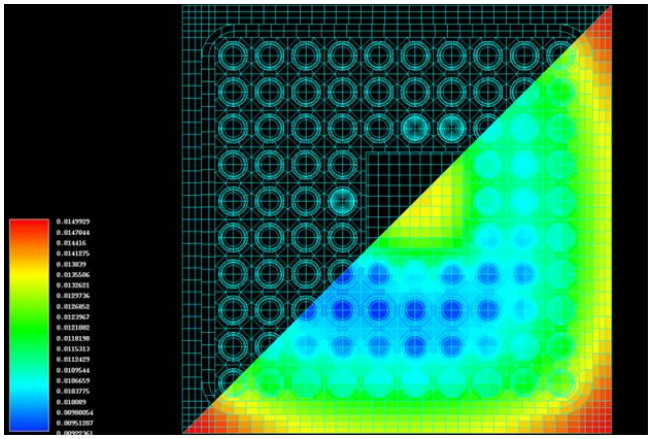
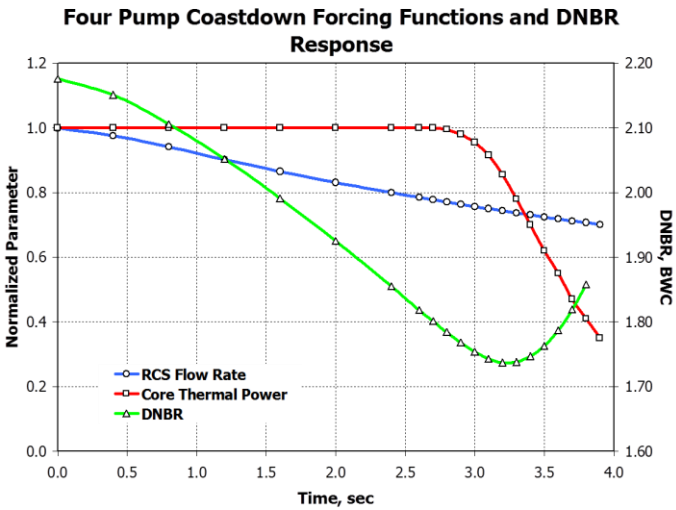


- **Requirements for code:**
  - **Requires relatively fast analysis turnaround**
  - **Must be benchmarked against measured data/phenomena**
  - **Must quantify uncertainty in analysis**
  - **Must be versatile across different reactor/FA designs**
  - **Requires NRC approval**



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Potential Barriers

- **Improvement over existing technology?**
  - **Limit to how low you can drive calculation uncertainties**
- **Speed of analysis in context of typical reload or outage time frames?**
  - **Will benefits warrant cost of 1000+ core machines**
- **Confidence of industry that the code can perform as advertised?**
- **If code is submitted to NRC later for approval:**
  - **Qualification of coupling methodology (impact on accuracy and stability) will likely need to be addressed**

>> Requires benchmarking to actual data

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Conclusions

- **Several areas for industry application of VERA**
  - **Product development (vendors) and evaluation of operational issues (vendors/utilities) have the fewest hurdles for immediate entry**
    - Does not require NRC approval for use
  - **Speed of analyses will dictate most appropriate uses**
  - **Significant improvement in predictions (and/or costs) over current methods will be required to justify costs to adopt**
- **Work to validate the code is not insignificant**
  - **What areas warrant most attention?**
    - Gen 2 plants are nearing end-of-life, Gen 3, Gen 4, SMR
    - Benchmarking is critical to establishing confidence

>> Need to demonstrate solution of current problem

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CASL/NRC Meeting Summary

February 25, 2014
NRC Headquarters
One White Flint North, CR 4-B6
Rockville, MD

Meeting Objective: Provide update to NRC staff on CASL R&D activities, validation data needs, planning for phase 2 proposal, and areas of mutual interest and collaboration for CASL and the NRC.

Summary

This meeting represented the next in a series of status update and discussion meetings held with NRC staff since the beginning of CASL. The meeting provided an opportunity to provide a briefing of on-going activities and to identify areas for further discussion. The agenda and participants are included below. Note that because of inclement weather, a number of the participants had to participate via phone. Despite the weather there was good participation by NRC staff from the Office of Regulatory Research (RES) and the Office of Nuclear Reactor Regulation (NRR). All presentations are attached. The discussions with the NRC are to inform them of the ongoing research and seek areas of interest for future discussions and information exchanges. The following text is the CASL summary of the meeting.

The CASL Director, Doug Kothe, provide a status update of CASL providing a background of CASL given a number of NRC participants that had not attended past meetings. This was followed by an overview of the status and development activities for VERA given by the Physics Integration Focus Area Lead, Jess Gehin. The NRC staff expressed interest in the developments to improve COBRA-TF including the ability to represent all of the fuel rod channels in the core (not just a single channel per assembly). There was additional interest in the use of the VERA core simulator to understand approximations made with current design and analysis tools. However, they expressed concern over the large computational requirements and felt that would be a barrier for the use of these tools at the NRC.

Zeses Karoutas, the CASL Challenge Problem Integrator, provided a summary of the progress on modeling and simulation of the CASL Challenge Problems. This presentation included a status of the current status of work, the definition of success for CASL on the challenge problems, and implementation plans for performing the work.

A discussion of CASL's work on thermal-hydraulics modeling was provided by the Thermal-Hydraulics Deputy FA Lead, Emilio Baglietto focusing on computational fluid dynamics (CFD) development. The presentation included details on the development of Hydra-TH, comparisons with measured data, experiments that are being undertaken by THM. There was considerable discussion on the use of CFD for licensing activities with the NRC staff stating that it appears that the industry is reluctant to use CFD to support licensing submissions. The current licensing basis for most thermal-hydraulics is based on subchannel methods and there is a need and driver to develop an approach for using CFD in licensing submissions.

Paul Turinsky, the CASL chief scientist, provided the Validation and Uncertainty Quantification presentation on behalf of Vince Mousseau. The presentation covered the strategy being used by VUQ including the Predictive Capability Maturity Model (PCMM). It was recommended that further follow-up with information on PCMM be provided to the NRC.

Because of time constraints, the discussion of validation data availability and needs was limited. A new effort involving the DOE, NRC and OECD Nuclear Energy Agency to establish a validation center was briefly discussed and given this broader engagement, it was felt that a follow-on meeting including people engaged in this activity be held.

The final presentation topic presented focused on the plans for CASL's Phase II (second five years). Paul Turinsky presented the candidate problems for Challenge Problems for Phase II including deepening PWR scope and broadened to SMRs and BWRs. There were several suggestions including RIA fuel dispersal consequences, full core high-fidelity modeling to support current methods to understand approximations, simplifications, as well as detailed capabilities to look at individual models to understand sensitivities in current codes that may contribute significantly to margins). For BWRs, while the focus of understanding fibrous debris has been with PWRs, it may be of interest for BWRs as well and overall improved tools could be helpful. For SMRs topics related to severe accidents, containment modeling, criticality safety, and natural circulation were discussed.

At the close out of the meeting CASL agreed to send additional information related to specific challenge problem charters and that Jess Gehin would work with Steven Bajorek to schedule the next meeting in the Fall 2014 time frame.

Agenda

Time	Agenda Item	Participants
1:00 pm	CASL Update	Doug Kothe
1:30 pm	VERA Status/Development	Jess Gehin
1:50 pm	Challenge Problems Status	Zeses Karoutas
2:10 pm	TH Status/Development	Emilio Baglietto
2:30 pm	Validation and Uncertainty Quantification	Vince Mousseau
3:00 pm	Break	
3:15 pm	Validation Data Availability and Needs	Nam Dinh
3:45 pm	CASL Phase 2 proposal planning	Paul Turinsky
4:00 pm	Discussion	
5:00 pm	Adjourn	

Participants

Name	Organization
Stephen Bajorek	NRC/RES
Dan Collins	NRC/R-I
Istvan Frankl	NRC/RES
Jennifer Gall	NRC/NRR
Kathy Gibson (Phone)	NRC/RES
Chris Hoxie	NRC/RES
Christoher Jackson	NRC/NRR
Josha Kaizer	NRC/NRR
Timothy McGinty	NRC/NRR
Stuart Richards	NRC/RES
Harold Scott	NRC/RES
Peter Yarsky (Phone)	NRC/RES
Doug Kothe	CASL (ORNL)
Paul Turinsky (Phone)	CASL (NCSU)
Emilio Baglietto	CASL (MIT)
Nam Dinh (Phone)	CASL (NCSU)
Jess Gehin	CASL (ORNL)
Zeses Karoutas (Phone)	CASL (Westinghouse)
Vince Mousseau (Phone)	CASL (SNL)
Alex Larzelere	DOE Office of Nuclear Energy