CASL Industry Council Meeting
March 11-12, 2014 Charlotte, NC
Minutes

The eighth meeting of the Industry Council (IC) for the Consortium for Advanced Simulation of Light Water Reactors (CASL) was held on March 11-12, 2014; at EPRI in Charlotte, NC. The meeting was chaired by Heather Feldman. The meeting presentations are available on the CASL website.

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. Fifteen members of the Industry Council attended representing 15 organizations. Members of the CASL project team participated in the meeting including the program director, program deputy 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 during both days. The BOD ex-officio attended the second day.

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

Heather Feldman began the meeting with a warm welcome. She provided an overview of the Industry Council, the current membership, reviewed action items, and discussed the agenda. Heather noted that CASL is actively updating the website (www.casl.gov) with invited presentations, reports, and publications.

Doug Kothe, CASL Director, provided an overview of the CASL project including: the milestones that are formally reportable to DOE in fiscal year 2014, the status of VERA, a summary of the Data Transfer Kit (DTK), an update on the DNB Challenge Problem, Hydra development, the solid model and mesh available for Watts Bar 1 in-vessel, an update from RTM on depletion capability, and an VUQ update. Doug provided the highlights from the CASL-NRC meeting that was held on February 25, 2014.

Scott Palmtag, PHI Deputy, provided an update on the core simulator (VERA-CS). Scott summarized the ten core simulator progression problems that are used to test out capabilities of VERA-CS, provided an update on code coupling, results for the progression problems that were completed since the last Industry Council meeting, and the status of the progression problem currently in-progress.

Brian Wirth, MPO Deputy, provided an overview of the MPO area, a summary of the validation and benchmarking of Peregrine (fuel performance code), a comparison of Mamba (coolant chemistry code) results of a CIPS/CILC with plant data, and a summary of the approach to GTRF. The validation and benchmarking of Peregrine showed that the thermal, mechanical, and irradiation behavior of UO2/Zr-alloy fuel rods is similar to results from Peregrine for the thirty test rods that were assessed. The key result from the CIPS/CILC analysis is that both axial and azimuthal thermal hydraulic effects dramatically affect CRUD deposition patterns; however,

azimuthal power variations have very little impact on CRUD deposition patterns. Brian noted that the staged model approach that is being used to develop the engineering scale wear model for GTRF is a significant enhancement.

Matt Sieger, QA/Release Manager, provided an update on VERA releases and software licensing. A VERA test and evaluation release will be available as soon as the Test and Evaluation License agreement is finalized. The release will be available from RSICC (ORNL Radiation Shielding Information Computational Center). The released components are limited and include: COBRA-TF, Insilico, MPACT, Core Simulator (Coupled COBRA-TF + Insilico), and Dakota. This release lays the groundwork for future releases. The next release is being planned for November 2014. The release is expected to include: full core modeling of multiple PWR cycles (including depletion), fuels modeling, and computational fluid dynamics. CASL anticipates using four type of licensing agreements:

- Open Source: some of the components are available as open source (currently computational infrastructure components)
- Government Use: use must fall within scope of an existing government project (in place)
- Test & Evaluation: use for a limited period (under core partner review)
- Non-Commercial: restricted to R&D/educational/nonprofit purposes (in progress)
- Commercial: use as part of a profit-based business plan (in progress)

During the working lunch, Alex Larzelere, DOE-NE, shared an overview of the DOE Advanced Computing Tech Team. The mission includes promoting and facilitating the improved use of advanced computing technologies. Doug Kothe briefly talked about CORAL which is a Collaboration of Oak Ridge, Argonne, and Lawrence Livermore Labs to acquire three leadership class computer systems for delivery in 2017. Heather Feldman wrapped up the working lunch with an overview of EPRI's initiative of high performance computing and Phoebe (EPRI's industry class cluster). Phoebe was acquired by EPRI to support the CASL Test Stand at EPRI.

Doug Burns, CASL Deputy Director, described the status of the Test Stands. Deployment of the initial Test Stands was to the CASL core partners:

- WEC: Deployment during June 2013; focus on VERA simulation of AP1000 first core startup
- EPRI: Deployment during December 2013; new EPRI computing capabilities will be utilized to test VERA fuel (Peregrine) performance applications
- TVA: Deployment planned for Q2 2014; lower plenum flow anomaly

The first External Test Stand deployment target is September 2014. Over five external organizations have expressed interest in deploying a Test Stand.

Brenden Mervin, EPRI Test Stand Project Engineer, summarized the status of the EPRI Test Stand. Phoebe, the EPRI cluster with 496 cores, became operational in late 2013 to support deployment of the EPRI Test Stand. The EPRI Test Stand is focused on fuel performance using Peregrine, the fuel performance code. To date, the EPRI team has installed Peregrine on Phoebe, attended a training session, and has started the initial simulations.

Rose Montgomery, TVA Test Stand Manager, provided a status update on the TVA Test Stand. TVA has selected lower plenum flow anomaly for the problem to address for the Test Stand. A memo was submitted to CASL in late December and TVA is waiting for a response from CASL. TVA has assembled a collaboration for the Test Stand which includes: Exelon as an independent reviewer, UT-C will be assisting with mesh generation, and Westinghouse has contributed a geometry file. TVA has evaluated several options for a computing resource and the current plan is to apply for an allocation on Titan.

Fausto Franceschini, Westinghouse, provided a comprehensive presentation on the Westinghouse Test Stand which was used to simulate zero power physics tests for the AP1000® PWR. The Test Stand was deployed in June of 2013 and the final report was completed in January 2014. The simulations were run on an in-house Westinghouse cluster with 576 cores. Results VERA with SP_N 3D flux solver were compared with the reference solution from KENO-VI Monte-Carlo. This was considered an advanced application for VERA since the AP1000® core has some unique features. The features of the core are described in the presentation. The simulations were built up from a 2D simulation to a 3D assembly and finally to a 3D core. Overall, VERA compared favorably with the reference solution. Details of the results are in the presentation. Computational resources are summarized and demonstrate time duration of the VERA simulations is reasonable and much less than for the reference solution. Westinghouse noted some desired capabilities as well as the need to improve the documentation and decrease computational resources.

A summary of the outcome of the value proposition subcommittee was provided by Heather Feldman, EPRI. Dan Wells (CIPS/CILC), Rob Daum (PCI and GTRF), and Steve Hess (DNB, RIA, LOCA), EPRI, provided the information that was used to develop the overall value proposition. The effort of the entire subcommittee is acknowledged and appreciated. A subcommittee of the Industry Council was formed last year. The subcommittee met eleven times to develop and refine the process as well as to assess data to use in the value proposition. The value in CASL can be realized through many ways including: providing operational understanding (challenge problems and margin improvement), research and development (using the code for applications beyond the challenge problems), and core modeling (the codes). Value can be defined in other ways and in other areas as well. The subcommittee focused on the value of the challenge problems and acknowledges that there is value beyond just the challenge problems. Each of the six challenge problems were assessed for the cost impact to industry (to bracket the cost of a future unknown unknown and the saving opportunity if CASL tools can change or eliminate a mitigation strategy. The return of investment (ROI) when only looking at the challenge problems was estimated. It was noted that the CASL tools are not quite at the maturity level to address the challenge problems, but upon execution of CASL's plan it is anticipated the CASL tools will reach the necessary level of maturity to impact the industry.

Paul Turinsky, Chief Scientist, provided an overview of potential scope for phase 2. He noted the guiding principles that are being used for the selection process. He provided an overview and the Industry Council agreed to resume a discussion the following day. In addition, the planned discussion on the Deployment Area and the evolution of the Industry Council was moved to the following day.

The meeting was adjourned for the day.

The next morning was started with a presentation on Interoperability given by Jess Gehin, PHI Lead. Eric Volpenhein, CD-adapco, then provided an update on their project for interoperability of STAR-CCM+ with NEAMS and CASL. Jess indicated that interoperability is the process of CASL software working with software external to the CASL program. There are three primary scenarios for interaction with external codes / components (CASL is currently working on the first two):

- Share data through data files (input, output, restart or other data formats)
- Software coupling and data transfer with external (potentially proprietary) components
- Use VERA components (or applications) in another environment

CASL is planning for VERA to be interoperable with ANC, RELAP5 , REPLAP7, STAR-CCM+, and others. CASL has initiated planning and discussions with ANSYS for interoperability with Fluent and is considering the need for interoperability with a structural mechanics code. Eric indicated that internal discussion on interoperability with STAR-CCM+ began in March of 2013. The concept worked its way through their internal process including a proposal to and review by their Innovation Forum. The concept was accepted in early 2014 and CD-adapco has put together functional requirements and a conceptual design. It is under review by the Product Development Team Steering Committee. CD-adapco plans to develop a API for MOAB / DTK which is anticipated to be available in the 9.06 release in September 2014. Eric also noted that STAR-CCM+ is interoperable with RELAP5 and ABAQUS.

Didier Banner, EDF, provided an overview of modeling and simulation activities at EDF. EDF is using modeling and simulation for addressing issues in terms of safety, performance, integrity and fuel. EDF (and in conjunction with partners) has developed a suite of codes which are listed in the presentation. The codes are built on the Salome environment for interoperability purposes. EDF made the decision to develop codes in-house when commercial codes were not adequate for its own use. Most of the EDF codes have an open source license. Didier also gave example applications that included simulation of pressurized thermal shock in the context of safety, simulation of thermal fatigue at a tee junction in a piping system, simulation of thermal and irradiation degradation of bolts, fuel assembly vibration and distortion, and deposition of iron oxide in the secondary system. He noted that EDF has three neutronics projects at various stages in their life cycle.

Paul Turinksy, Chief Scientist, lead a discussion about technical scope for a potential Phase 2. He reviewed five possible option (there are many others). The scope of the various options includes various combinations of deepening Phase 1 Challenge Problems and broadening scope to include structural, SMRs, BWRs and accident tolerant fuel. The Industry Council drove home the point that the value needs to be demonstrated and that is done by industry adoption. CASL asked the Industry Council to provide input using the scope assessment matrix that is being used by the partner organizations. Heather Feldman, Industry Council Chair, suggested changes to the Industry Council charter to enable more engagement and to provide CASL with actionable feedback. The three significant suggestions are:

- Expanding the purpose to include "provide guidance/direction and functional requirements to CASL on the application of VERA to a problem that is relevant to industry (from initiation to completion)."
- Adding a Chairman from the Industry Council
- Forming subcommittees

The Industry Council generally agreed with these changes, but further discussion is needed. Heather will be leading phone discussions on this topic with the goal to implement the agreed upon changes at the September 2014 Industry Council meeting.

The Round Robin allowed each IC member to summarize significant suggestions, concerns, or comments about the meeting agenda items. Comments are captured by the list below. Since the discussion was quite robust and free-form, it was not possible to attribute each comment to a specific IC member:

- Deliberate emphasis on deployment is needed to make CASL tools used and useful by the industry especially when CASL is no longer a hub
    - Deployment needs focus, resources, and Industry Council engagement.
    - Formation of subcommittee is important.
    - Validation (VUQ) work is critical
    - Challenge Problems are use cases (examples) of how VERA can be used. It is important that the tools that CASL develops and leaves behind can be picked up and used by the industry. The tools must have documentation and VUQ. Interoperability is also important for this purpose.
- Phase 2 Scope
    - Need to extend into new areas
    - SMRs are a small extension to the existing capabilities. This should be pursued.
    - Higher enrichment and fuel burn up extension have significant value to some owner/operators.
- Test Stands
    - Important to have Test Stands to get technology out to end users
    - Useful update on Test Stands.
    - Impressed with the Westinghouse Test Stand.
- Value
    - Value of CASL tools is directly related to cost savings of plant operation. For example, the value is in using the CASL tools to address issues that allow a plant to lower the number of fuel assemblies loaded, increase enrichment (above current limits, for instance), improve thermal margin capability (either the limits or the fuel's ability to perform) or extend the burnup (that is, lowering the number of fuel assemblies loaded).
    - Demonstrate the impact of VERA by solving an industry issue. The codes for that specific issue need VUQ first.
- Topics for the Next Webcast or Meeting
    - Information on how the codes scale and computing resourced needs for codes
    - Test Stands, Releases and Licensing

- Meeting Improvements
    - Provide meeting presentation ahead (1 week) of the meeting

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

1. Turinsky/Feldman: Provide IC with list of Phase 1 Challenge Problem Charters and Implementation Plans. Due: April 15, 2014
2. Gehin/Feldman: Gehin send NRC Meeting Minutes and Attendee List to Feldman. Feldman distribute to IC. Due: April 15, 2014
3. Feldman: Update IC on relevant reports as they are posted on website. Due: On-going
4. IC: Provide CASL with your feedback on the Value Proposition. Feldman to request input via email. Due: April 15, 2014.
5. IC: Phase 2 Technical Scope – what's missing, complete matrix by March 14th. Action Complete
6. Turinsky: Provide IC with list of Phase 2 Mini-Charters. Due: April 15, 2014
7. Feldman: Discussions with IC on IC evolution. Due: September 12, 2014
8. Feldman: Provide updates to IC on Phase 2. Due: on-going
9. Kothe/Turinsky: Work with SMR vendors to identify specific scope. Due: April 15, 2014
10. Feldman: Work with Kurt Flaig – CASL presentation to PWROG Analysis Subcommittee. Due: April 30, 2014
11. Banta/Feldman: Banta send Feldman QA plan. Feldman send QA plan to IC. Due: April 15, 2014.
12. Banta/Feldman: Evaluate the existing CASL metrics and determine if CASL should develop metrics based on user base (number of published reports, number of users, etc) Due: September 12, 2014.

The next in-person meeting of the Industry Council will be a joint meeting with the Science Council and will be held on Tuesday-Wednesday, September 9-10, 2014 at Oak Ridge National Laboratory in Oak Ridge, TN. A webcast is planned for early Summer.

The meeting was adjourned at approximately 12:30 pm on March 12, 2014. Following lunch, a subset of the Industry Council joined Jess Gehin, Scott Palmtag, and Andrew Godfrey for a deep dive into the VERA Core Simulation and Progression Problems.

Prepared: March 20, 2014
Distributed to Industry Council for Review: March 20, 2014
Finalized: March 31, 2014

By Heather Feldman, Industry Council Chair

CASL Presentations and Reports

CASL presentations and reports are available on the CASL website. Go to www.casl.gov then R&D – Publications:

Presentation

- Turinsky, Paul, Modeling & Simulation Goals and Accomplishments, SNA and MC 2013 Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo, October 27-31, 2013, Paris, France, 2013.

Technical Reports

To find a report go to the Technical Report section of the website and "find" the report number (i.e. CASL-U-2014-0012-001)

- **Westinghouse Test Stand Report**
  F. Franceschini, A. Godfrey, et al., Westinghouse VERA Test Stand: Zero Power Physics Test Simulations for the AP1000® PWR; L3.AMA.VDT.P8.01 Milestone Report CASL-U-2014-0012-001; March 2014 (Revision 1)
- **CASL Progression Problems Benchmark Specifications:**
  Godfrey, A., *VERA Core Physics Benchmark Progression Problem Specifications*, CASL Technical Report: CASL-U-2012-0131-002, March 2013.
- **CASL Progression Problems - Problem 5 Results:**
  Gehin, J., A. Godfrey, F. Franceschini, T. Evans, B. Collins, S. Hamilton, *Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Test*, CASL Technical Report: CASL-U-2013-0105-001, June 2013.
- **CASL Progression Problems - Problem 6 Results:**
  Palmtag, S., *Coupled Single Assembly Solution with VERA (Problems 6)*, CASL Technical Report: CASL-U-2012-0150-000, July 2013.
- **CASL Progression Problems - Problem 7 Results:**
  Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using VERA, CASL Technical Report: CASL-U-2013-0196-000, December 2013.
- **THM Milestone Report**
  Demonstration & Assessment of Advanced Modeling Capabilities to Multiphase Flow with Sub-Cooled Boiling, CASL Technical Report: CASL-U-2013-0181-001, August 2013
- **MPO Milestone Report**
  Kendrick, B., V. Petrov, D. Walter, A. Manera, CILC Studies with Comparative Analysis to Existing Plants, CASL Technical Report: CASL-U-2013-0224-000, September 2013.
- **Validation Needs Survey**
  Dinh, N., Validation Data Needs Survey, CASL Technical Report: CASL-U-2013-0194-001, September 2013.

Attendance

	Name	Institution	March 11	March 12 (AM)	March 12 (PM)
1.	Walt Schwarz	ANSYS	Y	Y	N
2.	Chris Lewis	AREVA	Y	Y	Y
3.	Bob Wall	Bechtel Marine Propulsion Corporation / Naval Nuclear Propulsion Program	Y	Y	Y
4.	Eric Volpenhein	CD-adapco	Y	Y	Y
5.	Scott Palmtag	Core Physics	Y	Y	Y
6.	Mahesh Lailasam	Dassault Systems SIMULIA Corporation	N	N	N
7.	Ian Stevenson	Dassault Systems SIMULIA Corporation	Y	Y	Y
8.	Alex Larzelere	DOE	Y	Y	N
9.	John Harrell	Dominion	Y	Y	N
10.	Scott Thomas	Duke	Y	Y	Y
11.	Didier Banner	EDF	Y	Y	N
12.	Heather Feldman	EPRI	Y	Y	N
13.	Steve Hess	EPRI	Y	Y	N
14.	Brenden Mervin	EPRI	Y	Y	Y
15.	Rob Daum	EPRI	Y part	N	N
16.	Dan Wells	EPRI	Y part	N	N
17.	Tyrone Stevens	Exelon	Y	Y	N
18.	Russell Stachowski	Global Nuclear Fuels	Y	Y	Y
19.	Zen Wang	GSE Systems	Y	Y	N
20.	Doug Burns	INL	Y	Y	N
21.	Bill Arnold	mPower	Y	Y	Y
22.	Paul Turinsky	NCSU	Y	Y	N

23.	Dan Ingersoll	NuScale	Y	Y	N
24.	Jeff Banta	ORNL	Y	Y	N
25.	Jess Gehin	ORNL	Y	Y	Y
26.	Doug Kothe	ORNL	Y	Y	N
27.	Matt Sieger	ORNL	Y	Y	N
28.	John Turner	ORNL	N	N	N
29.	Andrew Godfrey	ORNL	Y	Y	Y
30.	Alan Copestake	Rolls Royce	Y	Y	Y part
31.	David Brown	TVA	Y	Y	N
32.	Rose Montgomery	TVA	Y	Y	N
33.	Brian Wirth	UTK	Y	Y	N
34.	Zeses Karoutas	WEC	N	N	N
35.	Bob Oelrich	WEC	Y	Y	N
36.	Sumit Ray	WEC	Y	Y	N
37.	Fausto Franceschini	WEC	Y	Y	N

CASL Industry Council Meeting

Agenda

March 11-12, 2014

Location: EPRI Office Bldg 3 Rm 741 B, C & F Charlotte, NC

Tuesday, March 11

8:00	Gather and Coffee	
8:30	Welcome and Introductions	Heather Feldman
8:45	CASL Results • Look back – since last (September 2013) meeting • Look ahead – to next (September 2014) meeting	Doug Kothe / Paul Turinsky
9:15	VERA Core Simulator Updates	Scott Palmtag
10:15	Break	
10:45	Update on Fuel Performance Modeling Efforts within MPO: CRUD, PCI and GTRF	Brian Wirth
11:45	VERA Releases and Licensing	Matt Sieger
12:00	Lunch	
1:00	Test Stand Update	Doug Burns Brenden Mervin Rose Montgomery
1:30	Zero Power Physics Test Simulations for the AP1000® PWR (Westinghouse Test Stand)	Fausto Franceschini
2:15	Break	
2:30	Value Proposition	Heather Feldman
3:15	Phase 2 (Technical Scope and Deployment)	Doug Kothe Paul Turinsky Heather Feldman
5:00	Adjourn	

Wednesday, March 12

8:00	Gather and Coffee	
8:30	Review of Day 1	Heather Feldman
8:45	Interoperability	Jess Gehin Eric Volpenhein
9:15	EDF Activities in Modeling and Simulation	Didier Banner
9:45	Break	
10:15	Evolution of the Industry Council	Heather Feldman
11:00	Round Robin	All
11:30	Wrap Up – Action Items, Next Meeting	Heather Feldman
12:00	Adjourn	

Optional Meeting – March 12 1:00 pm

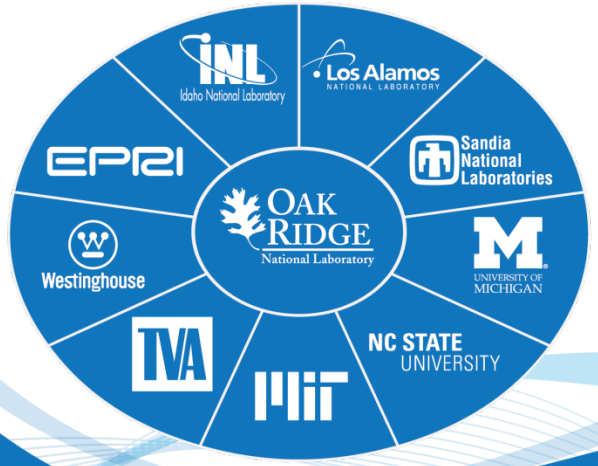
Deep Dive into the Core Simulator and Progression Problems

CASL is interested in getting feedback on the Core Simulator and Progression Problems. This meeting is being set up to enable Industry Council members to take a deeper dive into these activities to provide feedback to CASL.

Welcome to the Eighth Industry Council Meeting!

Industry Council Chairman: Heather Feldman (EPRI)

CASL Industry Council
Charlotte, NC
March 11-12, 2014



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CASL
Consortium for Advanced Simulation of LWRs

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			

Actions from September Industry Council Meeting

- Determine process to obtain IC input on current list of Phase II Challenge Problems. Heather Feldman to work with Doug Kothe. Due December 23, 2013. Process established.
- Heather Feldman to provide IC members with the HUB lessons learned document "what went right" once it is received from Alex Lazelere (DOE-NE). Emailed on Jan 15, 2014
- Industry Council members to contact Heather Feldman to join the Value Proposition subcommittee. Complete
- Industry Council members to contact Heather Feldman if you want to give a perspective presentation and to provide any topics that you would like to hear about at the March 2014 Industry Council meeting. Complete
- Industry Council to provide Heather Feldman with comments on Progression Problem 5 report on "Watts Bar 1 Cycle 1 Zero Power Physics Tests". (http://www.casl.gov/ – R&D – Publications – Technical Reports). Complete
- Heather Feldman will provide the Industry Council with the following documents:
  - CASL Program Plan – will not be distributed at this time
  - Industry Workflows and Use Cases document – will not be distributed at this time
  - Document on Validation Data effort - document and presentation are in review for posting on CASL website
  - VERA Common Input document – available upon request, but not on the CASL website

Technology Transfer Vehicle

Industry Council Website - http://www.casl.gov/IndustryCouncil.shtml

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Industry Council

Chairman: Heather Feldman, EPRI

The mission of the Industry Council (IC) is to ensure that CASL solutions are "used and useful", and that CASL provides effective leadership advancing the Modeling and Simulation state-of-the art in the nuclear industry.

LINK TO RESOURCES

Industry Council Resources

LINK TO UPDATES

Upcoming Webcast and Meeting

Specific objectives of the Industry Council are:

- 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

The CASL Project benefits from advice on expected virtual reactor (VERA) capabilities, validation and test plans, quality assurance plans, priorities and schedules, rollout and commercialization strategies, and computer requirements.

IC members benefit by influencing the VERA product and its development process to be compatible with expected applications. They can also prepare their business and technical processes to make use of VERA products.

Finally, both CASL and end-users can identify opportunities for validation, pilot studies, early applications, and other beneficial collaborations.

A CASL team member chairs the Industry Council. Membership is drawn from prospective technology-providers and end-users of CASL products. Members represent fuel vendors, design engineering companies, engineering service providers, computer technology companies, and owner/operators of nuclear plants. DOE and the CASL Board of Directors (BOD) have ex-officio members. A list of current members and other contacts are included in the Industry Council Resources on this website.

- Organization
- Senior Leadership
- Technical Leadership
- Outreach
- Board of Directors
- Industry Council
- Science Council
- One-Roof Culture

Documents Recently Added to CASL Website

CASL Website (www.casl.gov)

Overview Presentation in R&D – Invited Presentations

- Turinsky, Paul, *Modeling & Simulation Goals and Accomplishments*, SNA and MC 2013 Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo, October 27-31, 2013, Paris, France, 2013.

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

- THM
  - Demonstration & Assessment of Advanced Modeling Capabilities to Multiphase Flow with Sub-Cooled Boiling, CASL Technical Report: CASL-U-2013-0181-001, August 2013
- Westinghouse Test Stand report
  - Franceschini, F., A. Godfrey, J. Gehin, S. Palmtag, W. Martin, T. Evans, Westinghouse VERA Test Stand - Zero Power Physics Test Simulations for the AP1000 PWR, CASL Technical Report: CASL-U-2014-0012-000, January 2014.

Agenda – Day 1

- CASL Results
- VERA Core Simulator
- CRUD, PCI, GTRF
- VERA Releases and Licensing

→ CASL Update

- LUNCH!

- Test Stand Updates
- Zero Physics Test Simulations for the AP1000®
- Value Proposition
- Phase 2

→ Test Stands, Value, Phase 2

- DINNER – Ciro's at 6:30 pm

Agenda – Day 2

- Interoperability
- EDF Activities in Modeling and Simulation
- Evolution of the Industry Council
- Round Robin
- Wrap Up

→ IC Member Engagement and Looking Forward

- Optional at 1 pm
  - Deep Dive into Core Simulator and Progression Problems

September 2014 Meeting

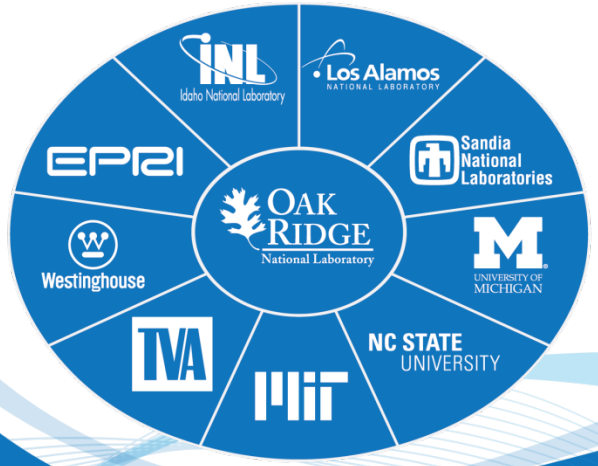
- Save the Date
  - Tuesday-Wednesday, September 9-10, 2014
  - ORNL in Oak Ridge, TN
- Potential Topics?

CASL Results

Industry Council Meeting

Charlotte, NC

Mar 11-12, 2014



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CASL Status and Looking Forward

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

Scientific Output thru Year 3

- Virtual Reactor M&S technology integrated, under active development and assessment, and deployed for beta testing
- 81+ journal articles
- 328 conference papers
- 28 technical reports
- 51+ invited talks
- 382 milestone reports
- 216 programmatic reports

CASL FY14 Plan (Oct 2013 – Sep 2014)

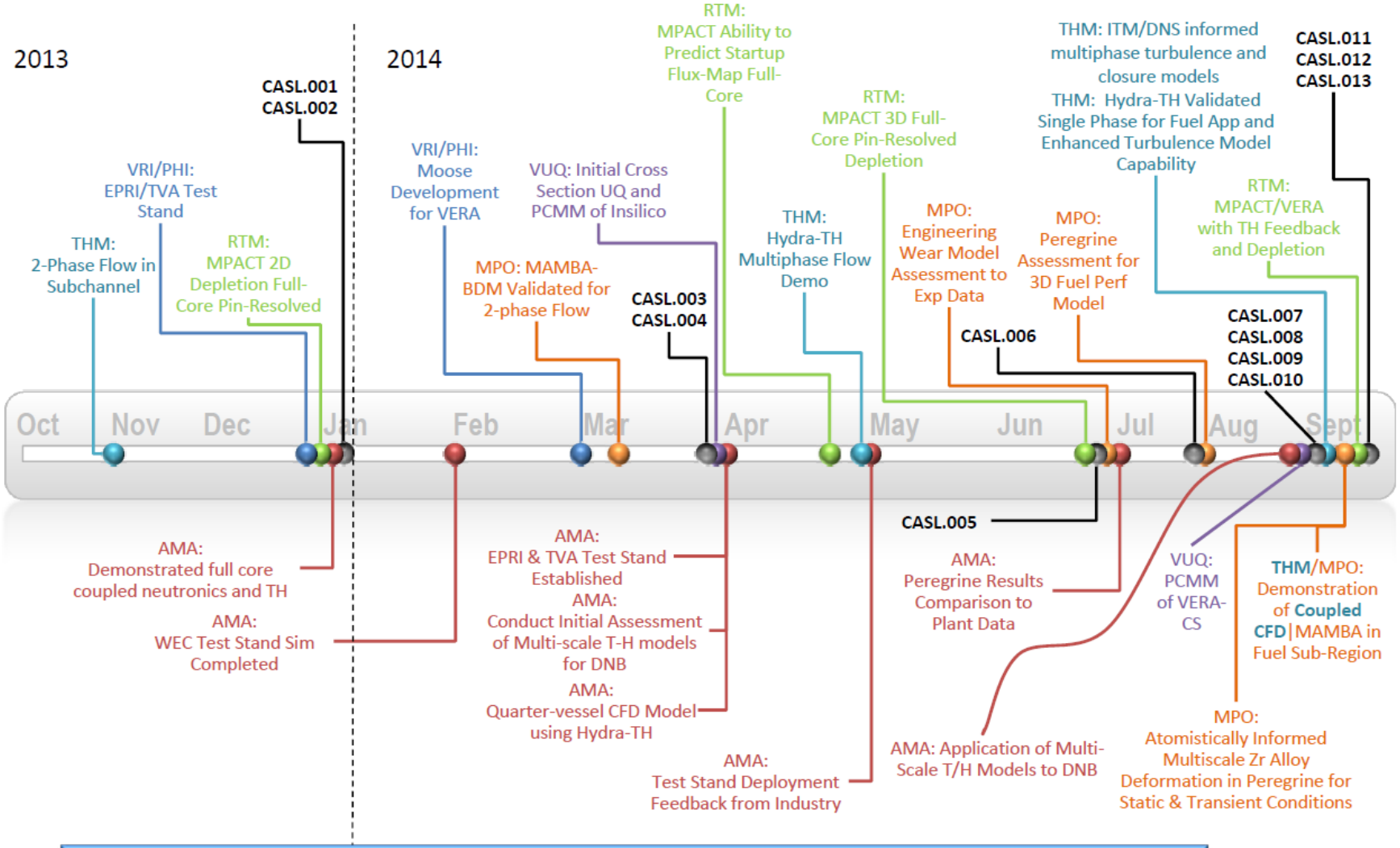
DOE reportable milestones

Reportable #	Milestone ID	Milestone Description	Finish Date	Owner	Status
FY14.CASL.001	L2:PHI.P8.01	VERA Deployment for EPRI Test Stand on PCI	Dec 2013	Jess Gehin	Complete
FY14.CASL.002	L2:RTM.P8.01	PWR Full Core 2D Depletion Capability with Pin Resolved Transport	Dec 2013	Bill Martin	Complete
FY13.CASL.011	L2:AMA.P7.02	Demonstration of neutronics coupled to thermal-hydraulics for a full-core scenario using VERA.	Dec 2013	Scott Palmtag	Complete
FY14.CASL.003	L3:VUQ.V&V.P8.01	User Guidelines and Best Practices for CASL UQ Analysis using DAKOTA	Mar 2014	Brian Williams	On Track
FY14.CASL.004	L2:AMA.P9.01	Experience with use of VERA in Industry Test Stands	Mar 2014	Steve Hess	On Track
FY14.CASL.005	L2.MPO.P9.01	Assessment of CASL Engineering Wear Model Against Experimental Fretting Measurements	Jun 2014	Chris Stanek	On Track
FY14.CASL.006	L1:CASL.P9.01	Assess Peregrine as a 3D Fuel Performance Model for the PCI Challenge Problem	Jul 2014	Rob Montgomery	On Track
FY14.CASL.007	L1:CASL.P9.02	Application of Multi-Scale Thermal Hydraulic Models to DNB Analysis	Aug 2014	Yixing Sung	On Track
FY14.CASL.008	L1:CASL.P9.03	Demonstrate integrated VERA-CS for the PCI Challenge Problem	Aug 2014	Scott Palmtag	On Track
FY14.CASL.009	L2:VUQ.P9.01	Demonstration of Integrated DA/UQ for VERA-CS on a Core Physics Progression Problem	Aug 2014	Vince Mousseau	On Track
FY14.CASL.010	L2:THM.P9.01	Single Phase Validation of Hydra-TH for Fuel Applications	Aug 2014	Emilio Baglietto	On Track
FY14.CASL.011	L1:CASL.P9.04	Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback	Sep 2014	Bill Martin	On Track
FY14.CASL.012	L2:MPO.P9.02	Demonstration of Coupled CFD and Crud/Corrosion Chemistry for a Fuel Sub-region	Sep 2014	Jeff Secker	On Track
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	Chris Stanek	On Track

Currently on track

CASL FY14 Plan (Oct 2013 – Sep 2014)

Timeline of key milestones



Period 8 and 9 Baseline Plan of Record (PoR-8/9) for FY14

- 4 L1, 15 L2, and 98 L3 technical milestones
- 14 milestones formally "reportable" to DOE

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 **			
Reactor internals integrity **			

* Delayed
** LWRS

Significant Progress

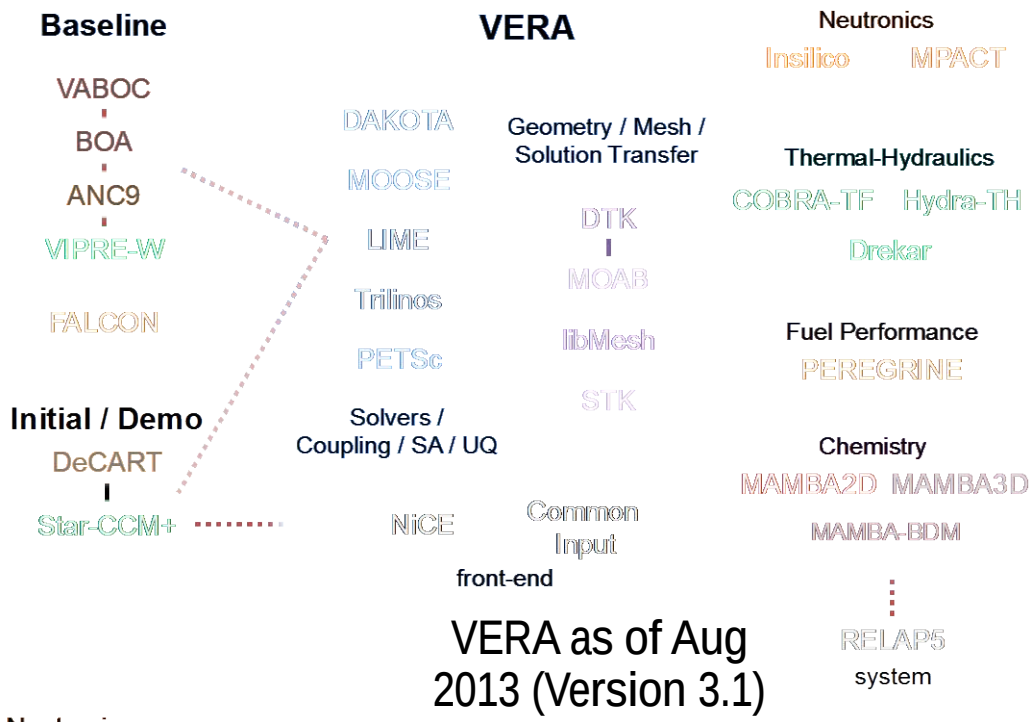
Planning & Scoping

Good Progress

Not Started

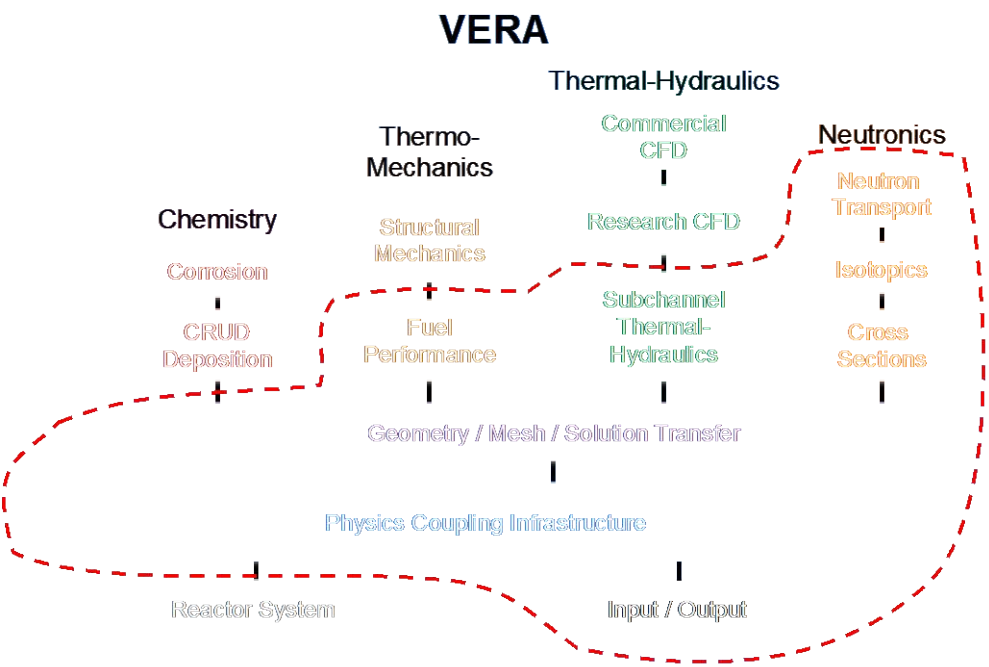
VERA: Virtual Environment for Reactor Applications

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



VERA as of Aug 2013 (Version 3.1)

Required functional capabilities



CASL has 3 M&S technology products

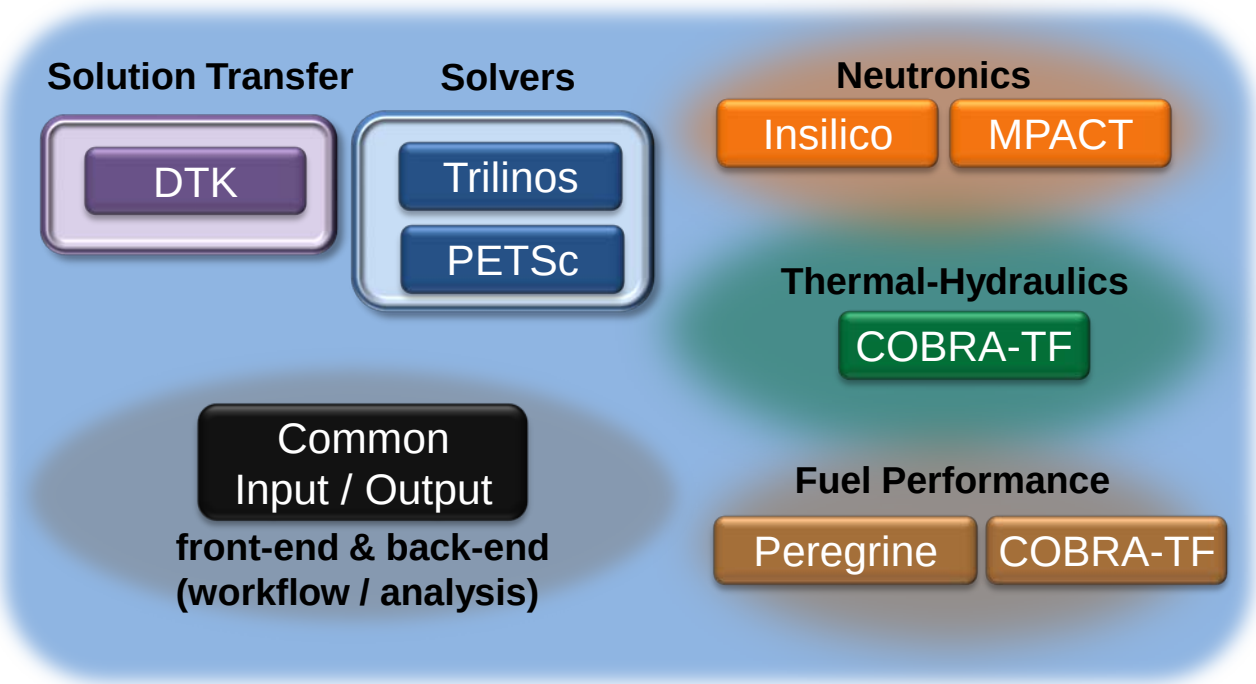
1. VERA-CS as the fast running core simulator, which has value both standalone and for providing power histories, etc for more detailed codes
2. Engineering suite of standalone codes with ability to couple 2 or more within VERA or in other environments
3. Leadership suite of high fidelity codes used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

VERA supports a range of PWR core physics and spatial scales

- Neutron transport/Cross Sections
  - Spatial scale: fuel pellet to fuel rod to fuel assembly to full core
  - Components: Insilico, Shift (ORNL), MPACT (UMich)
- Single-phase and multi-phase thermal hydraulics
  - Subchannel spatial scale: fuel assembly to full core
  - CFD Spatial scale: fuel sub-assembly (3x3 rods) to fuel assembly (17x17 rods)
  - Components: COBRA-TF (PSU), Hydra-TH (LANL)
- Nuclear fuel behavior and performance
  - 2D R-Z Spatial scale: fuel rods to full core
  - Unstructured-mesh 3D spatial scale: fuel pellet to fuel sub-assy (3x3 rods)
  - Component: PEREGRINE (INL)
- Coolant chemistry and CRUD deposition/buildup
  - Spatial scale: fuel pellet to fuel rods to fuel sub-assembly
  - Components: MAMBA (LANL), MAMBA-BDM (MIT)

VERA Core Simulator (VERA-CS)

- Simulate steady-state reactor operation during depletion
- Contains only neutronics (transport, cross sections, depletion), thermal-hydraulics and fuel rod temperature components

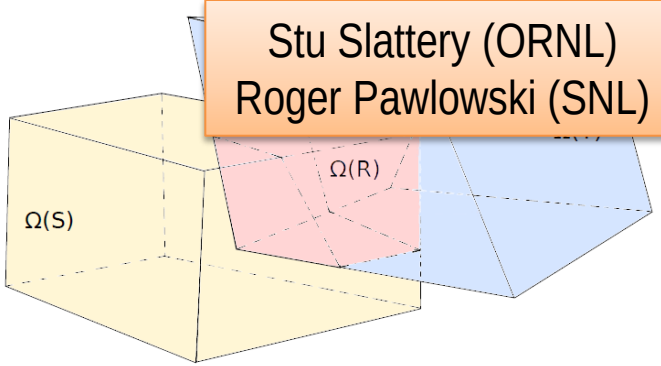


VERA Usage for Challenge Problems

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	MPACT- COBRA - MAMBA (light)
Crud-CILC	Y	Few pin-wide	MPACT/Insilico – Hydra – Peregrine – MAMBA
GTRF	Y + 50 Hz	Few pin-wide	MPACT - Hydra – Peregrine –STK or TPLs
PCI	Y + M to H	Few pin-wide	MPACT/Insilico - Hydra - Peregrine
DNB	Y + S to M	System to assembly-wide	MPACT – COBRA/Hydra – Peregrine - RELAP
LOCA	Y + S to M	Pin-wide	Peregrine (B.C. from WEC)
RIA	Y + S	Few pin-wide	MPACT – Hydra – Peregrine

Data Transfer Kit (DTK) (Slattery, Wilson, Pawlowski)

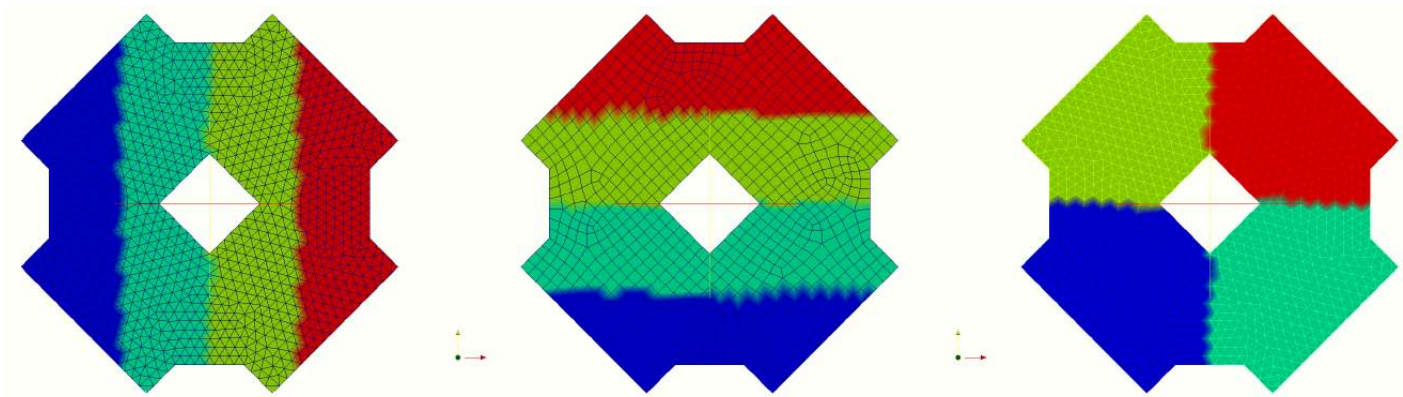
Stu Slattery (ORNL)
Roger Pawlowski (SNL)



$$\mathbf{M} : \mathbb{R}^D \rightarrow \mathbb{R}^D, \forall r \in \Omega_R$$

$$\mathbf{G}(t) \leftarrow \mathbf{M}(\mathbf{F}(s))$$

- Collection of geometry-based data mapping algorithms for shared domain problems
  - Rendezvous Algorithm, Initially developed by the Sandia SIERRA team in mid-2000's for parallel mesh-based data transfer
- Data maps allow for efficient movement of data in parallel
  - e.g. between meshes of a different parallel decomposition
- Ideally maps are generated in desirable time complexity (logarithmic)
- Does not provide general interface for all physics codes to couple to all other physics codes
- Does not provide discretization services (e.g. basis functions)
- Open-source BSD 3-clause license - https://github.com/CNERG/DataTransferKit



Ω_source Ω_target Ω_rendezvous

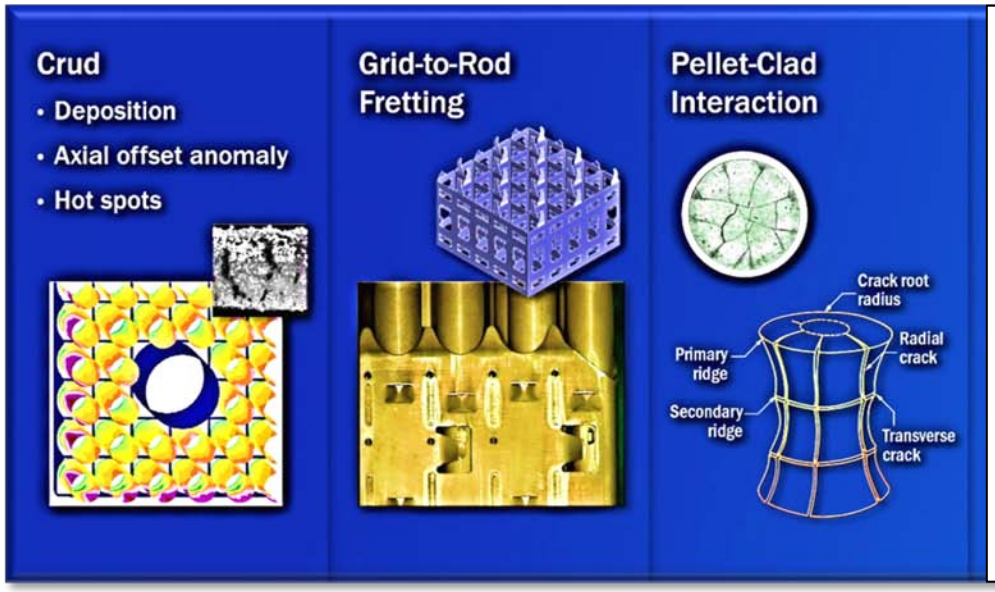
CASL Challenge Problems

Key safety-relevant reactor phenomena that limit performance

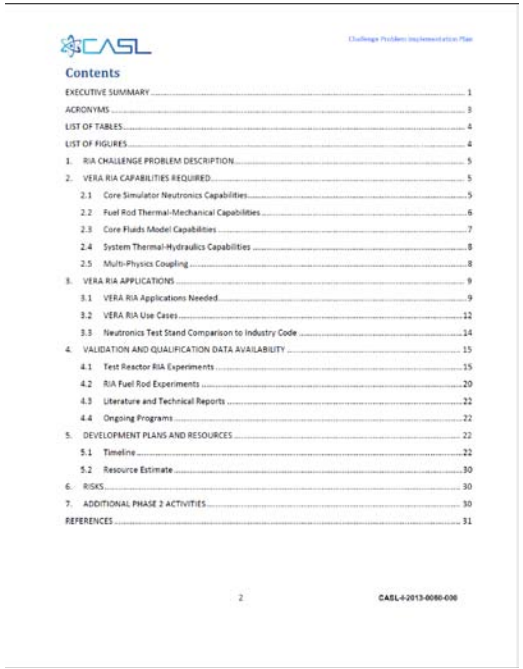
Safety Related Challenge Problems

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



Operational Challenge Problems



CASL

Challenge Problem Implementation Plan

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2 CASL-I-2013-0060-000

Fuel temperature

Subchannel flow, pressure, temperature, void fraction

RELAP5-3D
(FOM system pressure)

MPACT or Insilico

Peregrine
(FOM cal/gm; incipient melting)

COBRA-TF
(FOM % fuel rods that fail DNBR)

Core inlet flow, pressure, temperature

Direct moderator heating

3D fuel rod power

Cladding heat flux

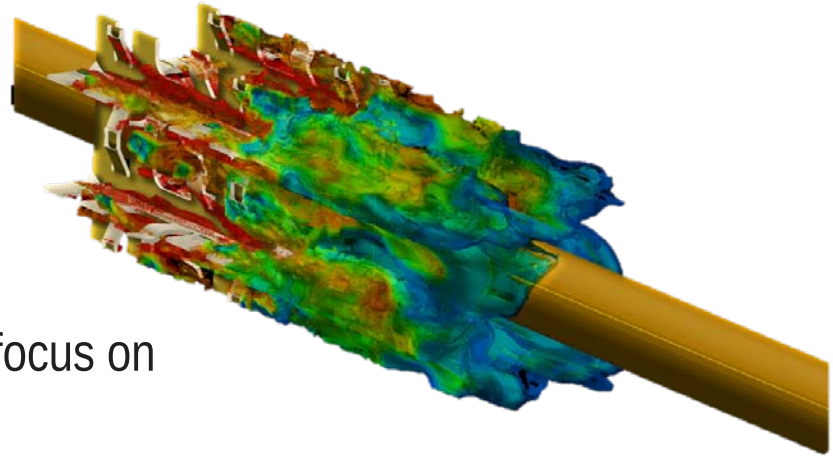
DNB Challenge Problem [PHI, RTM, THM, MPO, VUQ, AMA]

- Simulations by COBRA-TF and VIPRE-W of voiding for the PSBT transient tests
- Simulation of 5x5 rod DNB tests using STAR-CCM+ in preparation for later comparisons with Hydra-TH
- Implementation of Hydra-TH within WEC
- DNB Challenge Problem Implementation Plan completed

Supporting Activities

- Identification of validation data needs
- Assessment of COBRA-TF for prediction of subcooled boiling conditions
- *Most of the supporting activities listed under CRUD Challenge Problem apply to CHF Challenge Problem*

MCFD: Hydra-TH Code



- Attributes
  - Builds upon existing LANL Hydra code
  - Multiphase/multi-field equations solved with focus on bubble flow
  - Higher-order temporal and spatial treatments
  - State-of-art nonlinear solver routines
  - CFL condition can be violated
  - Utilizes capabilities of evolving HPC architectures
- Current activities
  - Closure relationships (e.g. bubble drag, lift and wall effect, nucleate boiling energy partition, bubble departure and coalescence) being evaluated via contrasting experimental data & simulations, supported by DNS
  - Implicit, nonlinear solver being added for multiphase/multi-field equations
  - Validation experiments on bubble creation/departure and turbulent flow continuing

Hydra-TH Development Path

Mark Christon (LANL)
Emilio Baglietto (MIT)

FY2011 - 2012

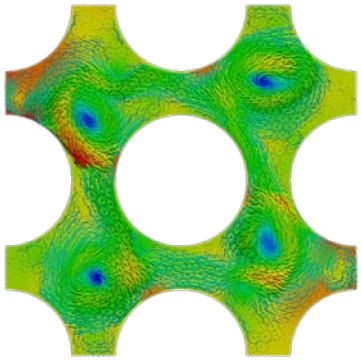
- Hybrid Parallel Meshing of V5H. 3x3 and 5x5 V5H meshes up to 192M cells
- Development of a priori mesh assessment based on y+
- Runtime turbulence statistics
- Parallel Visualization (ParaView)
- L1 Milestone: Determine sensitivity of structural response to GTRF RMS forces
- Investigate sensitivity 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 ~ 50 licensed users

FY2014

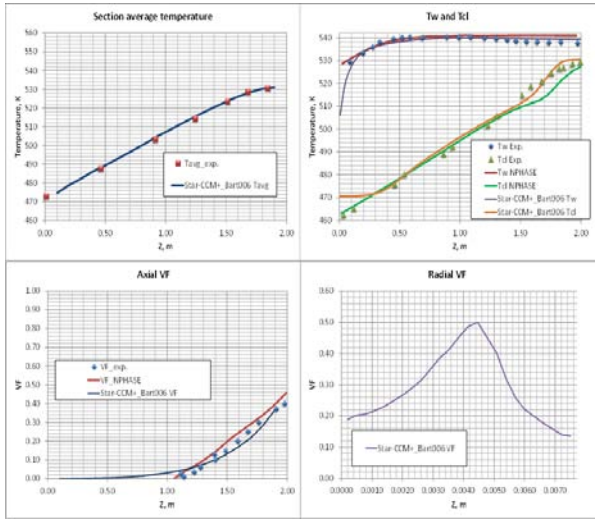
- Expose Native CHT Capabilities
- Release porous drag for simplified meshing
- Single-phase validation for fuel applications
- Improved parallel linear algebra
- Enhanced turbulence single/multiphase turbulence models
- Fully-implicit multiphase
- Boiling closure models
- Single/multiphase V&V
- Hydra-Mamba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



Deliverables

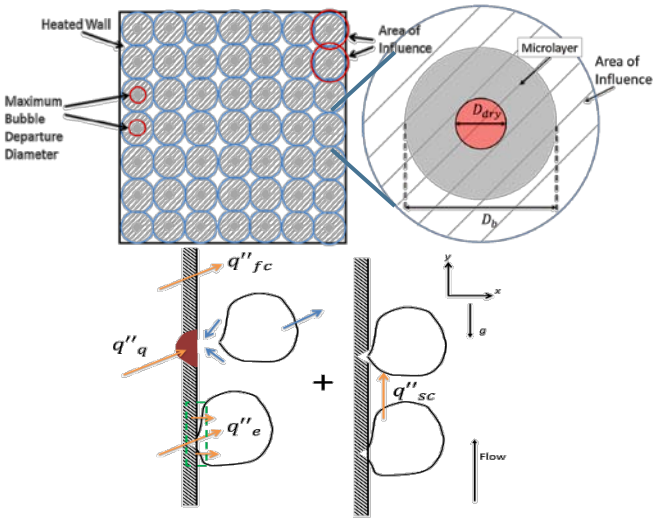
Mark Christon (LANL)
Emilio Baglietto (MIT)

Robust Baseline Closure



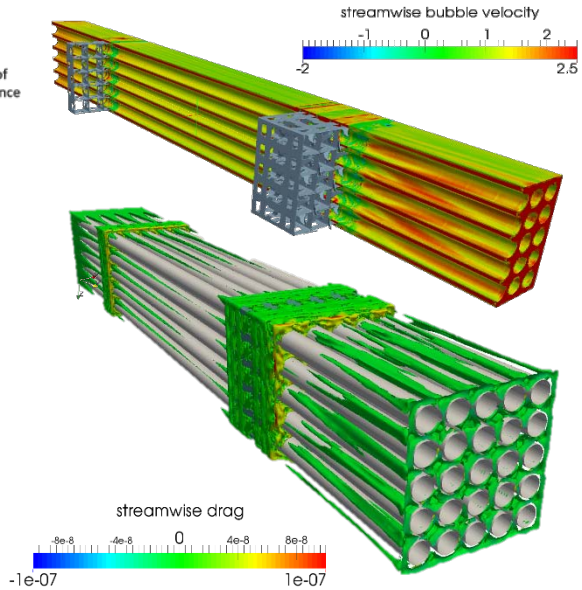
- First Generation Closure in Hydra-TH should leverage existing experience
- Implementation of baseline closure in STAR-CCM+ allows direct comparison to CD-adapco baseline closure results (platform independent)
- Sensitivity of model parameters should confirm PoR-3 studies

Innovative GEN-II Closure

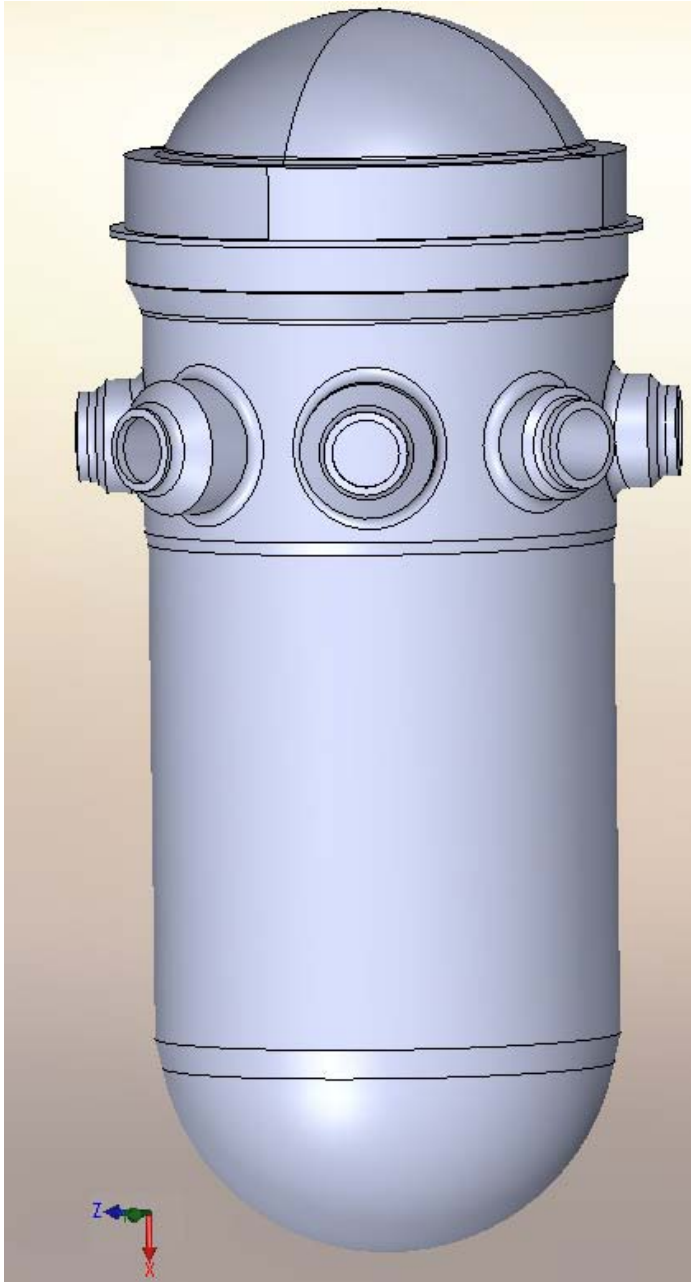


- Second Generation Closure should incorporate new physical understanding
- Increased synergy with experimental "micro" measurements
- Extended applicability (lower/ higher vapor generation)
- Include modeling toward limiting behavior (CHF)

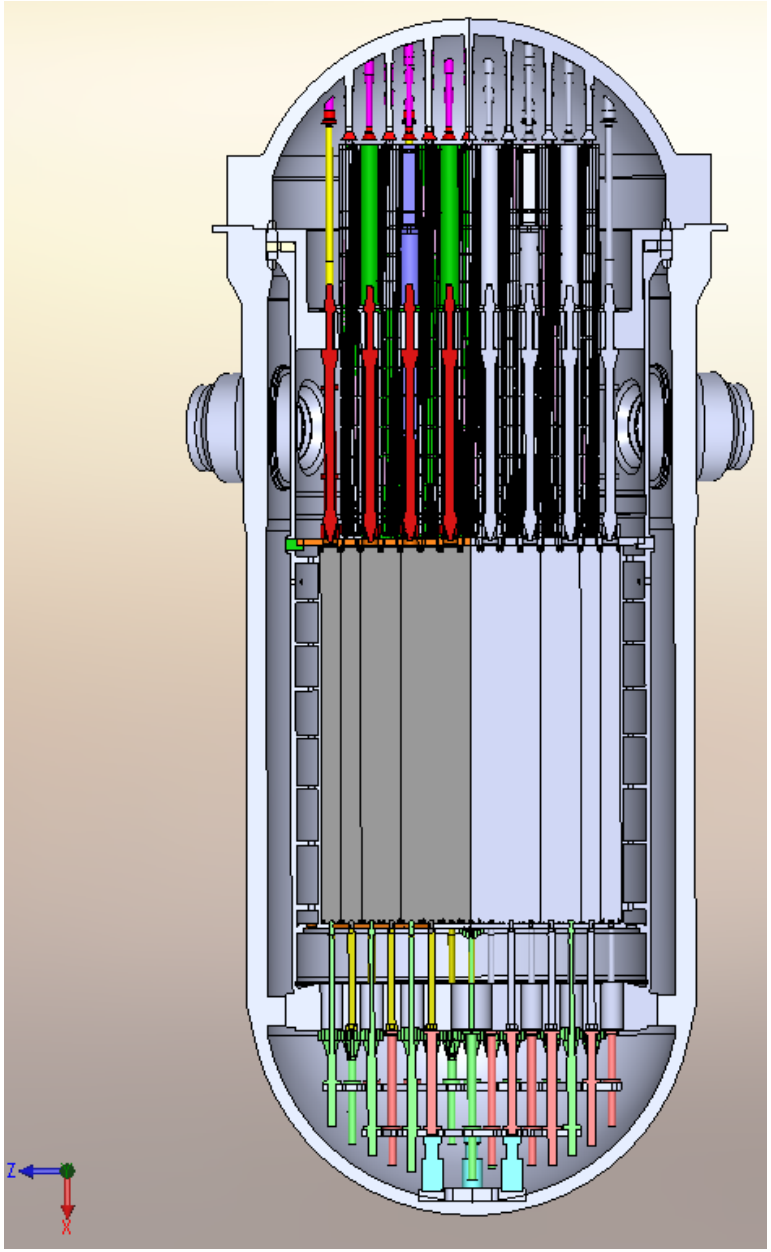
New M-CFD Platform



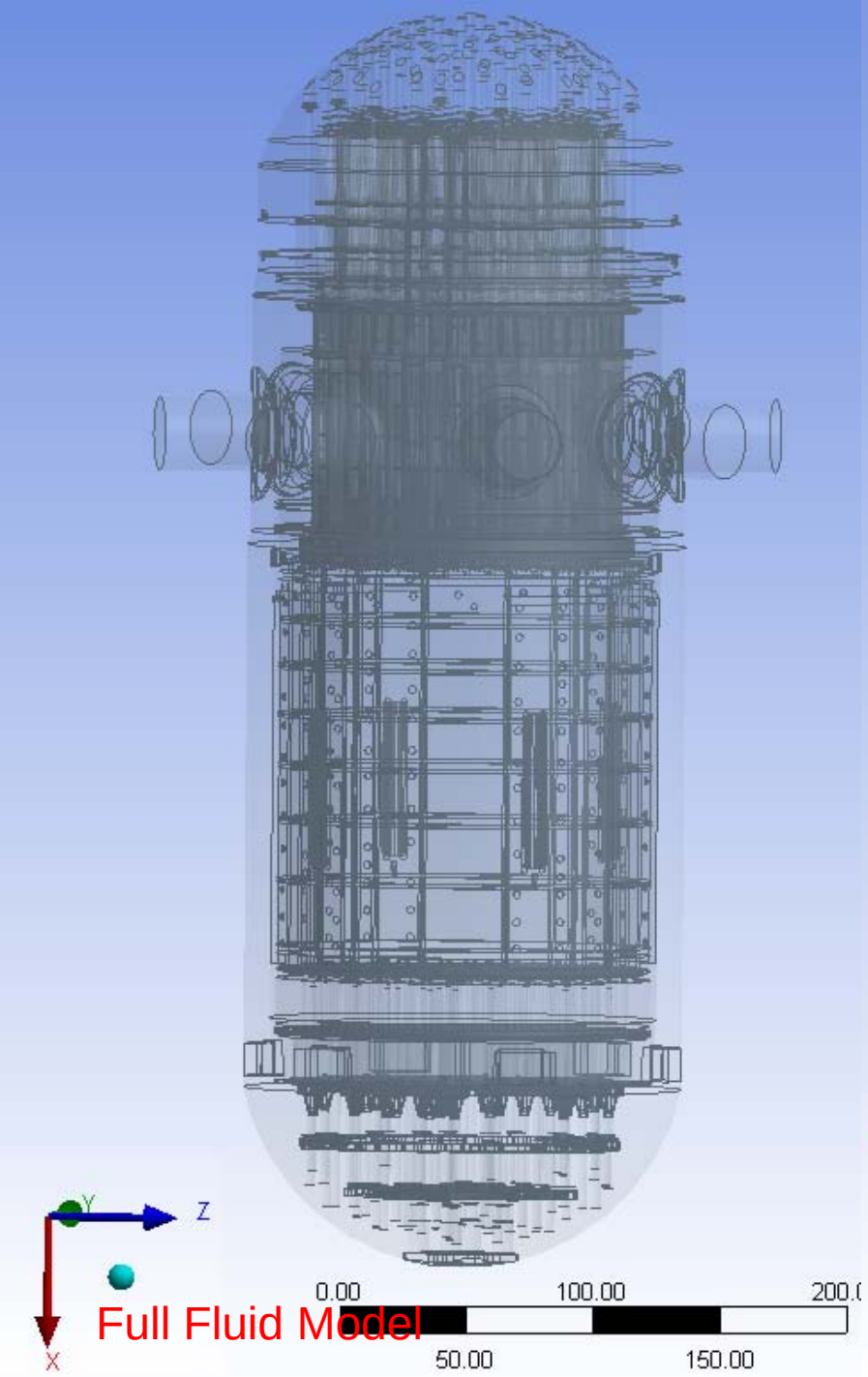
- Hydra-TH baseline multiphase capabilities first shakedown
- Hydra-TH Mupltiphase implementation should target enhanced applicability towards transient simulations (including fast transients)



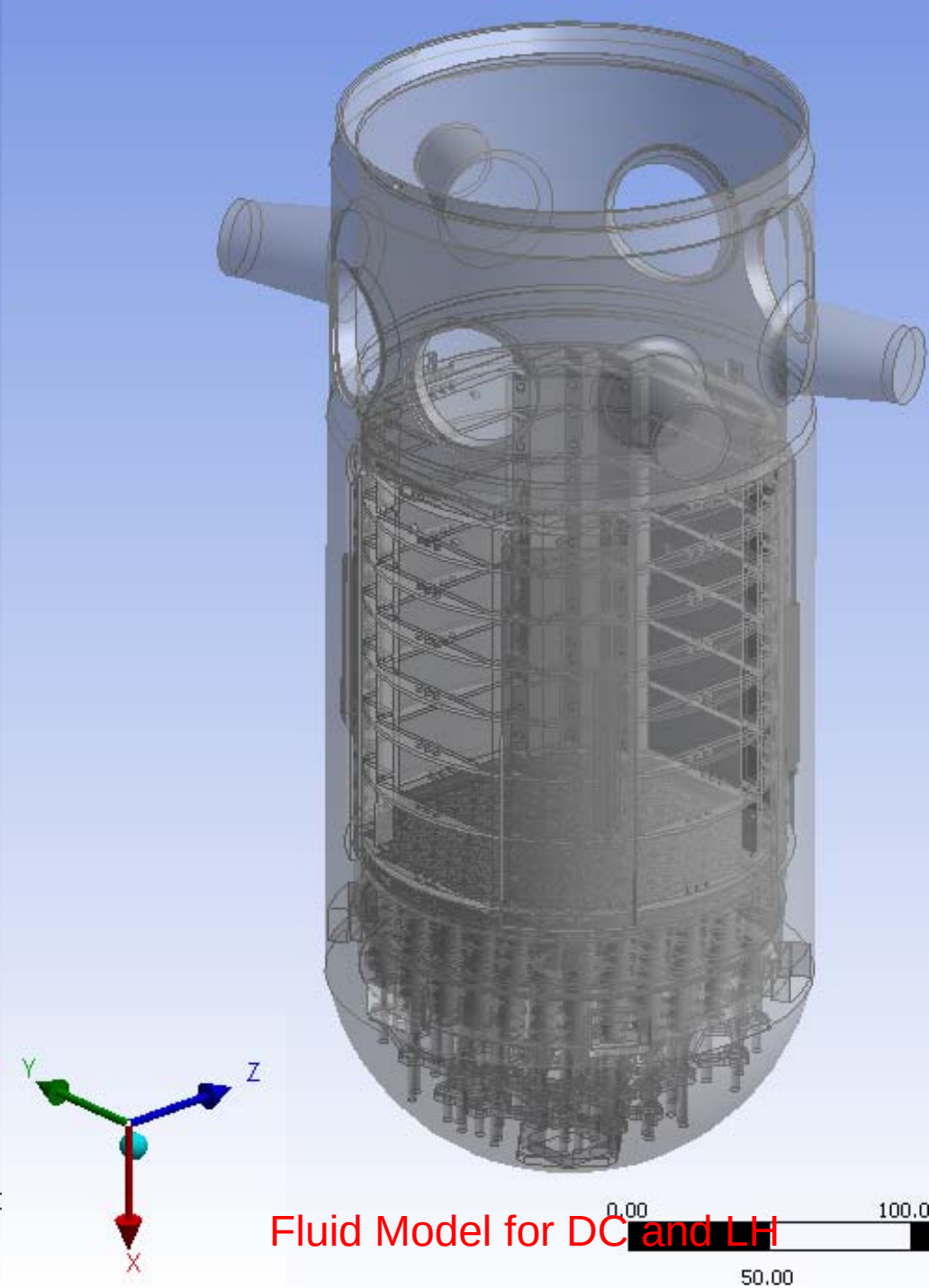
Reactor Solid Model



Reactor Solid Model (Cut Plane View)

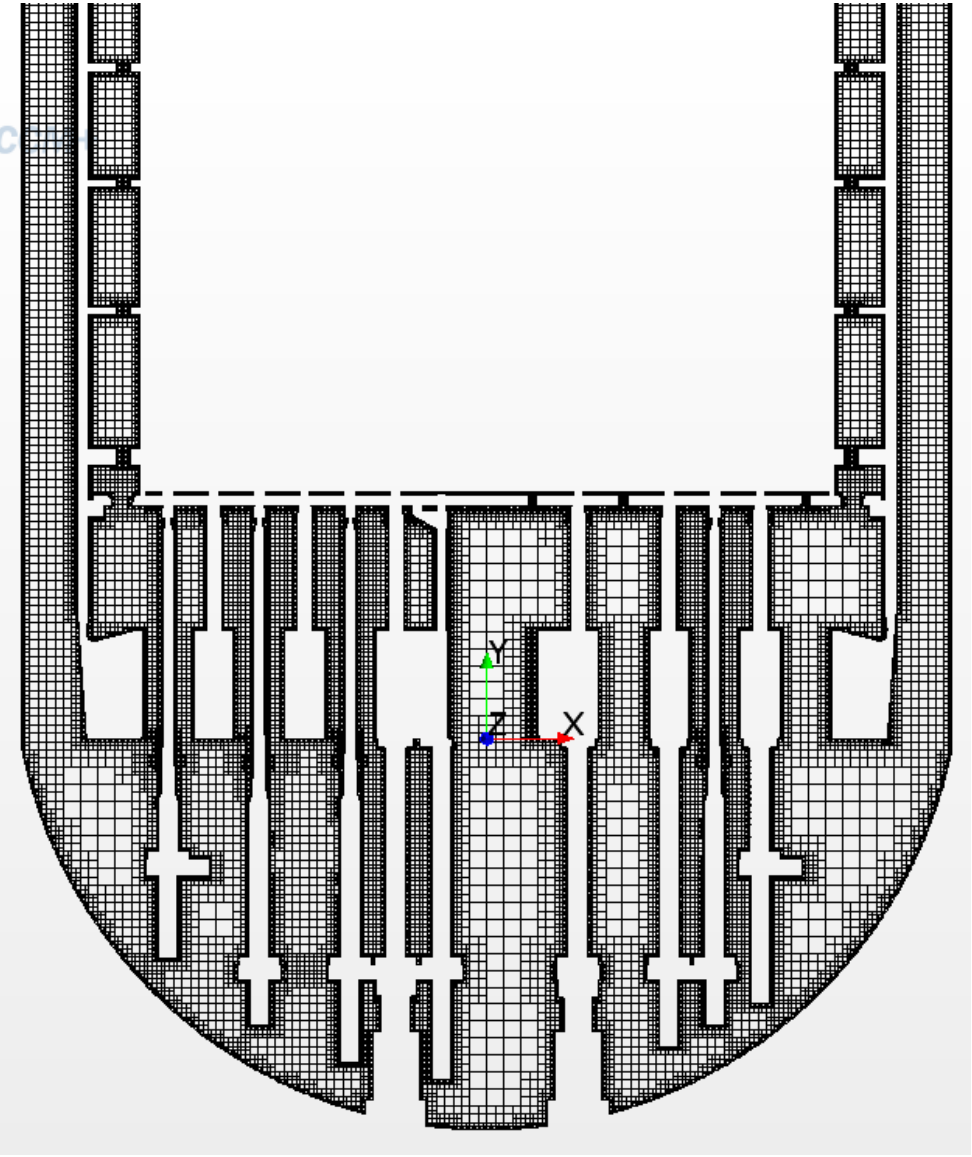


Full Fluid Model

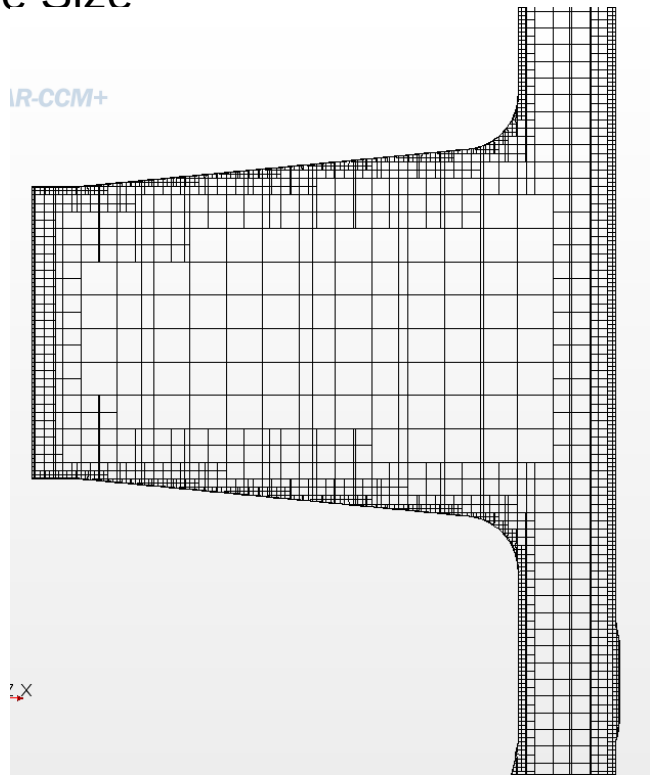


Fluid Model for DC and LH

Typical Meshes



Total No. of Cells: 72 million
Mesh Settings:
Base Size=10 mm
Prism Layers: 2
Stretching: 1.5
Prism Layer Thickness: 10% of Base Size



Radiation Transport: Adding microscopic depletion capability

- Capability added to MPACT (2D MOC/1D Diffusion) code for radial plane utilizing OREGIN type formulation.

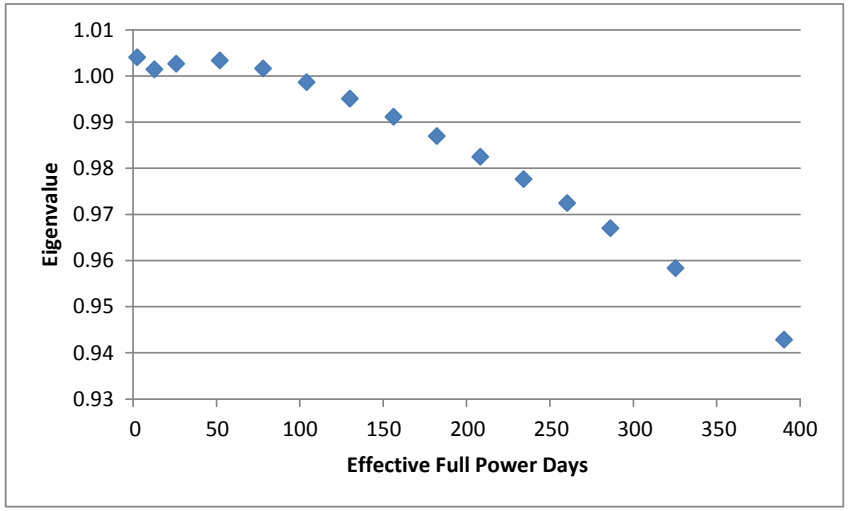
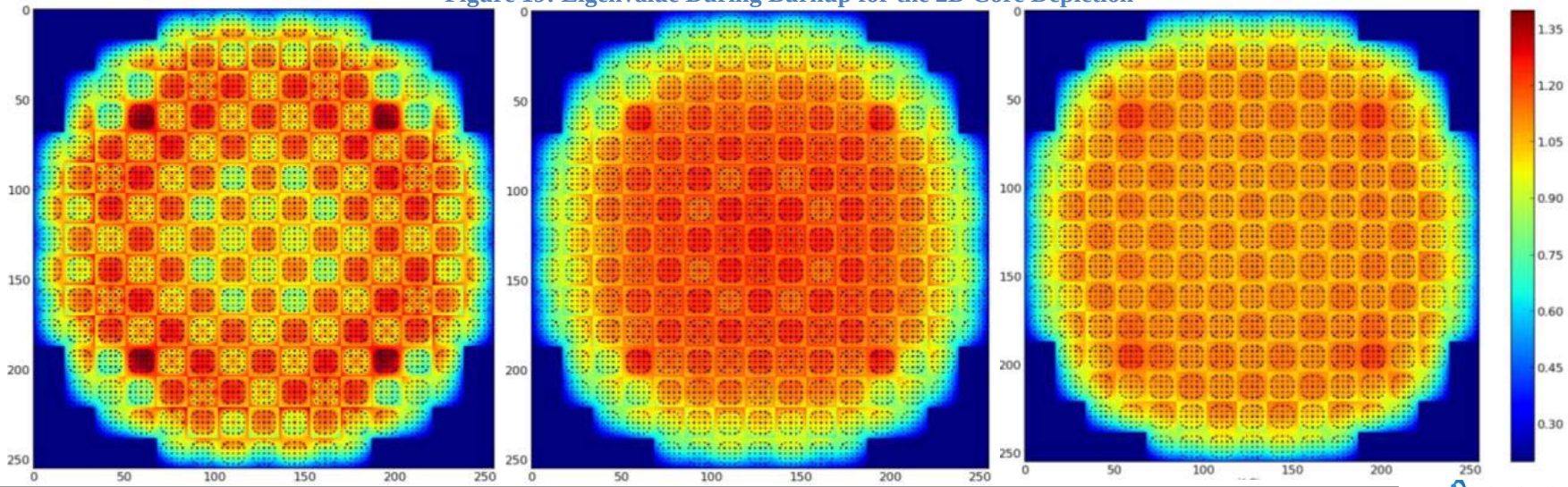


Figure 19: Eigenvalue During Burnup for the 2D Core Depletion

Later in year will incorporate OREGIN

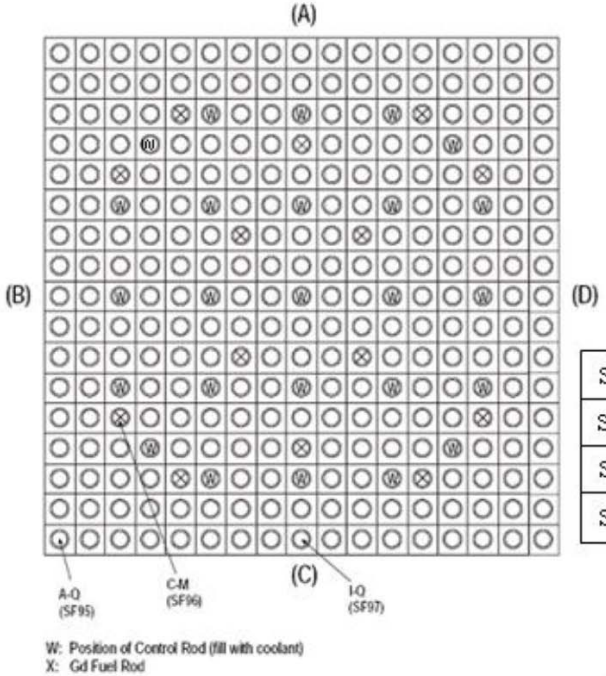


2D Core Power Distribution at Beginning (left), Middle (center), and End (right) of Cycle

MPACT Depletion Validation

Table 1: Takahama-3 Initial Fuel Composition (wt%)

Isotope Ratio	Fuel Rods	Burnable Absorber Rods
$^{234}U/U$	0.04	0.02
$^{235}U/U$	4.11	2.63
$^{238}U/U$	95.85	97.25
Gd_2O_3/Fuel	0.00	6.00



Sample ID	Location	Assembly
SF95	A-Q	NT3G23
SF96	C-M	NT3G23
SF97	I-Q	NT3G24

Figure 11: Takahama-3 Assembly Measurement Locations

Table 3: SF97 Comparisons

	MPACT (HELIOS Lib)		MPACT (ORNL Lib)		DeCART [7] (HELIOS Lib)		SAS2H [6]		HELIOS [6]	
	C/E	St Dev	C/E	St Dev	C/E	St Dev	C/E	St Dev	C/E	St Dev
234U	1.09	1.26%	1.11	0.92%	1.09	1.28%	1.08	1.53%	0.95	2.49%
235U	1.01	0.64%	1.01	0.67%	1.00	0.62%	0.97	1.38%	1.02	0.29%
236U	0.99	0.27%	0.99	0.24%	1.00	0.28%	0.99	0.20%	0.96	0.86%
238U	1.00	0.03%	1.00	0.03%	1.00	0.03%	1.00	0.04%	1.00	0.19%
237Np	0.94	1.80%	0.95	1.79%	0.93	1.76%	1.01	2.09%	0.87	4.72%
238Pu	0.86	1.36%	0.89	1.70%	0.87	1.41%	0.90	2.04%	0.80	3.88%
239Pu	1.01	1.13%	1.01	1.13%	0.99	1.14%	1.00	1.69%	1.03	2.30%
240Pu	1.02	0.43%	1.04	0.48%	1.01	0.45%	1.04	1.00%	1.01	2.13%
241Pu	0.97	1.29%	0.97	1.27%	0.95	1.24%	0.96	1.56%	1.02	1.84%
242Pu	0.88	0.36%	0.95	0.37%	0.88	0.38%	1.01	0.83%	0.98	2.69%
241Am	1.16	7.95%	1.17	7.99%	1.19	8.71%	1.18	9.72%	1.23	11.61%
242mAm	1.12	7.16%	1.19	7.41%	0.93	6.77%	1.10	9.65%	1.02	6.49%
243Am	0.95	1.54%	0.99	1.52%	0.94	1.58%	1.13	1.91%	0.89	5.09%
242Cm	1.04	8.11%	1.04	7.99%	1.15	8.83%	1.04	6.76%	1.09	11.75%
243Cm	0.61	1.77%	0.67	2.30%	0.69	1.95%	0.79	1.36%	0.69	12.77%
244Cm	0.82	1.99%	0.88	2.00%	0.81	2.03%	0.93	2.45%	0.77	5.90%
245Cm	0.77	2.70%	1.00	3.46%	0.74	2.65%	0.57	3.40%	0.51	6.17%
246Cm	0.67	1.85%	0.87	2.37%	0.66	1.80%	0.81	4.38%	0.58	12.94%
143Nd	0.99	0.36%	0.99	0.36%	0.99	0.33%	1.00	0.51%	0.99	0.73%
144Nd	0.97	2.20%	0.97	2.16%	0.98	2.25%	0.99	1.96%	0.97	1.18%
145Nd	1.01	0.17%	0.99	0.37%	1.01	0.17%	1.01	0.18%	1.02	0.62%
146Nd	1.00	0.16%	1.01	0.09%	1.00	0.14%	1.01	0.20%	0.97	0.85%
148Nd	1.00	0.07%	1.00	0.06%	1.00	0.07%	1.00	0.29%	--	--
150Nd	1.00	0.21%	1.00	0.21%	1.00	0.22%	1.01	0.27%	1.00	0.69%
137Cs	0.99	0.44%	0.99	0.45%	0.97	0.38%	1.00	0.43%	0.97	1.20%
134Cs	0.84	3.55%	0.90	2.93%	0.82	3.60%	0.84	2.46%	0.75	3.63%
154Eu	1.06	2.39%	1.06	1.60%	1.04	2.29%	1.00	2.61%	0.89	2.70%
144Ce	0.99	7.46%	0.99	7.49%	0.94	7.01%	0.99	7.41%	0.99	7.99%
125Sb	1.62	30.02%	1.58	29.20%	1.56	29.11%	1.54	28.79%	1.82	18.40%
106Ru	1.12	38.68%	1.13	38.76%	1.08	37.25%	1.13	38.64%	1.11	32.01%

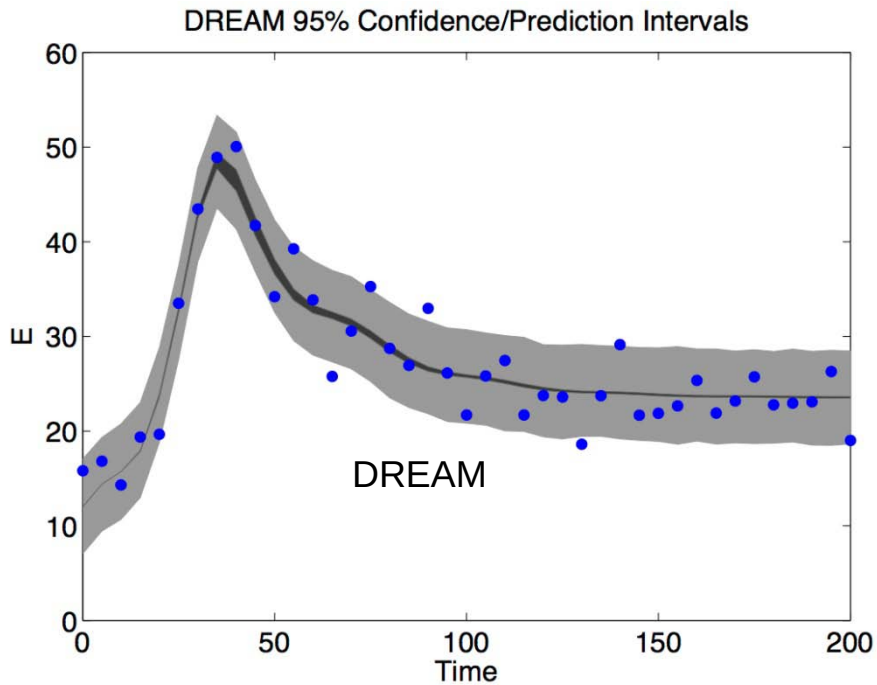
143Nd	0.99	0.36%	0.99	0.36%	0.99	0.33%	1.00	0.51%	0.99	0.73%
144Nd	0.97	2.20%	0.97	2.16%	0.98	2.25%	0.99	1.96%	0.97	1.18%
145Nd	1.01	0.17%	0.99	0.37%	1.01	0.17%	1.01	0.18%	1.02	0.62%
146Nd	1.00	0.16%	1.01	0.09%	1.00	0.14%	1.01	0.20%	0.97	0.85%
148Nd	1.00	0.07%	1.00	0.06%	1.00	0.07%	1.00	0.29%	--	--
150Nd	1.00	0.21%	1.00	0.21%	1.00	0.22%	1.01	0.27%	1.00	0.69%
137Cs	0.99	0.44%	0.99	0.45%	0.97	0.38%	1.00	0.43%	0.97	1.20%
134Cs	0.84	3.55%	0.90	2.93%	0.82	3.60%	0.84	2.46%	0.75	3.63%
154Eu	1.06	2.39%	1.06	1.60%	1.04	2.29%	1.00	2.61%	0.89	2.70%
144Ce	0.99	7.46%	0.99	7.49%	0.94	7.01%	0.99	7.41%	0.99	7.99%
125Sb	1.62	30.02%	1.58	29.20%	1.56	29.11%	1.54	28.79%	1.82	18.40%
106Ru	1.12	38.68%	1.13	38.76%	1.08	37.25%	1.13	38.64%	1.11	32.01%

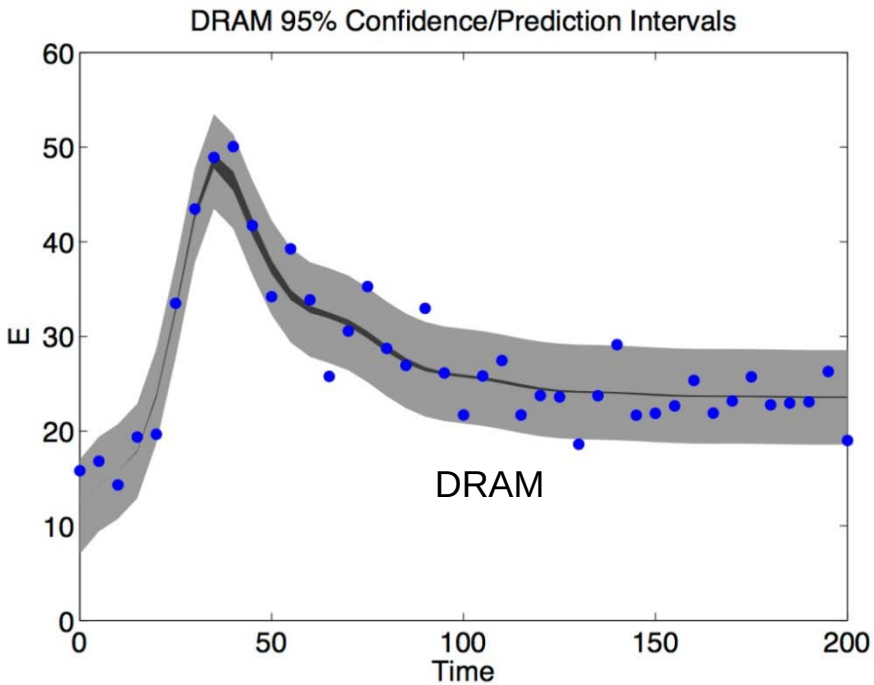
Data Assimilation & Uncertainty Quantification: Dakota Code

- Attributes
  - Builds upon existing SNL Dakota code
  - Nonintrusive approach (after exposing parameters) with many algorithmic options
  - Added capabilities particularly in the areas of surrogate model development & data assimilation
- Current Activities
  - Testing of capabilities for single physics applications
  - VERA specific users guide for Dakota usage
  - Integration into Dakota of capabilities that have been developed
  - Extension of capabilities to support PCMM

Data Assimilation & UQ: Prediction intervals for DREAM versus DRAM data assimilation algorithms

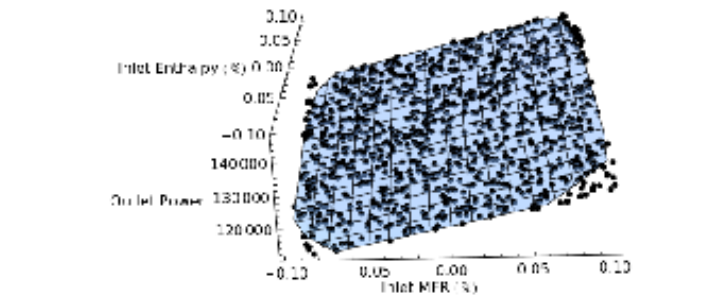
Test case with 16 parameters





Application to the Cobra-TF code

First generate surrogate model (GP model)

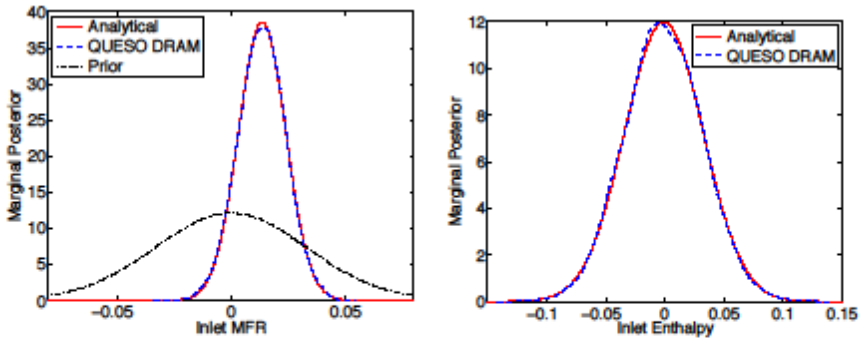


(a) Front View

(b) Side View

Figure 9: Comparison of true response to surrogate.

Next use surrogate model to determine posteriori parameter distributions by MCMC



(a) (b)

Figure 11: QUESO DRAM and analytic marginal posterior densities for the (a) Inlet MFR with prior density and (b) Inlet Enthalpy.

Exercise of capabilities developed

Validation Experiments: Summary of CASL's Highest Priorities Needs

Challenge Problem	# Proposed Key Exp.	Types of Test	Total Cost	Execution Difficulty
CIPS	7	6 SET, 1 IET	$4 M	Medium
CILC	2	1 SET, 1 IET	$1.2M	Medium
GTRF	5	3 SET, 2 IET	$3M	Medium
PCI	4	2 SET, 2 IET	$15+M	High
DNB	4	3 SET, 1 IET	$5M	Medium
RIA	3	1 SET, 2 IET	$12M	High
LOCA	4	2 SET, 2 IET	$4M	Medium

Needs reflected in appendix of NEUP RFP

Productive CASL/NRC Meeting Results in Topics for Potential Future Engagement

CASL

- Well attended by NRC staff from key offices
  - 12 NRC attendees representing staff, branch chiefs, and division directors.
  - Office of Regulatory Research
  - Office of Nuclear Reactor Regulation
- Supports objective to keep NRC informed on CASL activities
  - Inform NRC on research to support eventual use of CASL tools in licensing activities by industry
  - Seek area for potential collaboration
  - Discuss potential Phase 2 scope of interest to NRC
- Topics identified for potential engagement
  - Advances/improvements in subchannel T/H modeling
  - Creating an industry "push" for CFD in license applications
  - Interoperability of VERA with NRC TRACE reactor systems code
  - CASL core simulator to assess impact of approximations in current approaches
  - Computing resource requirements and availability

CASL/NRC Meeting
February 25, 2014
Rockville, MD

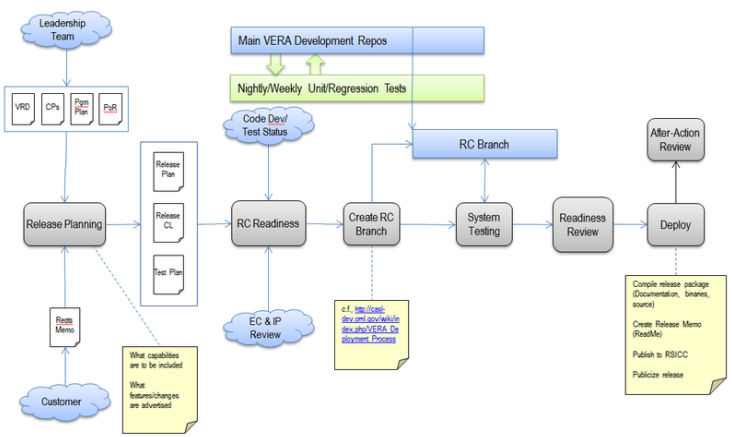
Time	Agenda Item	Presenter
1:00 pm	CASL Update	Doug Kothe
1:30 pm	Challenge Problems Status	Zeses Karoutas
1:50 pm	VERA Status/Development	Jess Gehin
2:10 pm	TH Status/Development	Emilio Baglietto
2:30 pm	Validation and Uncertainty Quantification	Vince Mousseau
3:00 pm	Break	
3:15 pm	Validation Data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

CASL Consortium for Advanced Simulation of LWRs

U.S.NRC

First RSICC Release of VERA Delivered

- Release candidates for selected VERA components finalized in Dec 2013
  - What is the capability? VERA-CS? What can it simulate?
- Licensing terms
  - Test & Evaluation license completed
  - Completed review of component code licenses
- Final documentation delivered as part of release
  - Revised installation guide
  - README files for components
  - Theory & User Manuals
- Export control determination completed
- Process for approving distribution under test & evaluation terms drafted
- Final software tested & delivered to RSICC



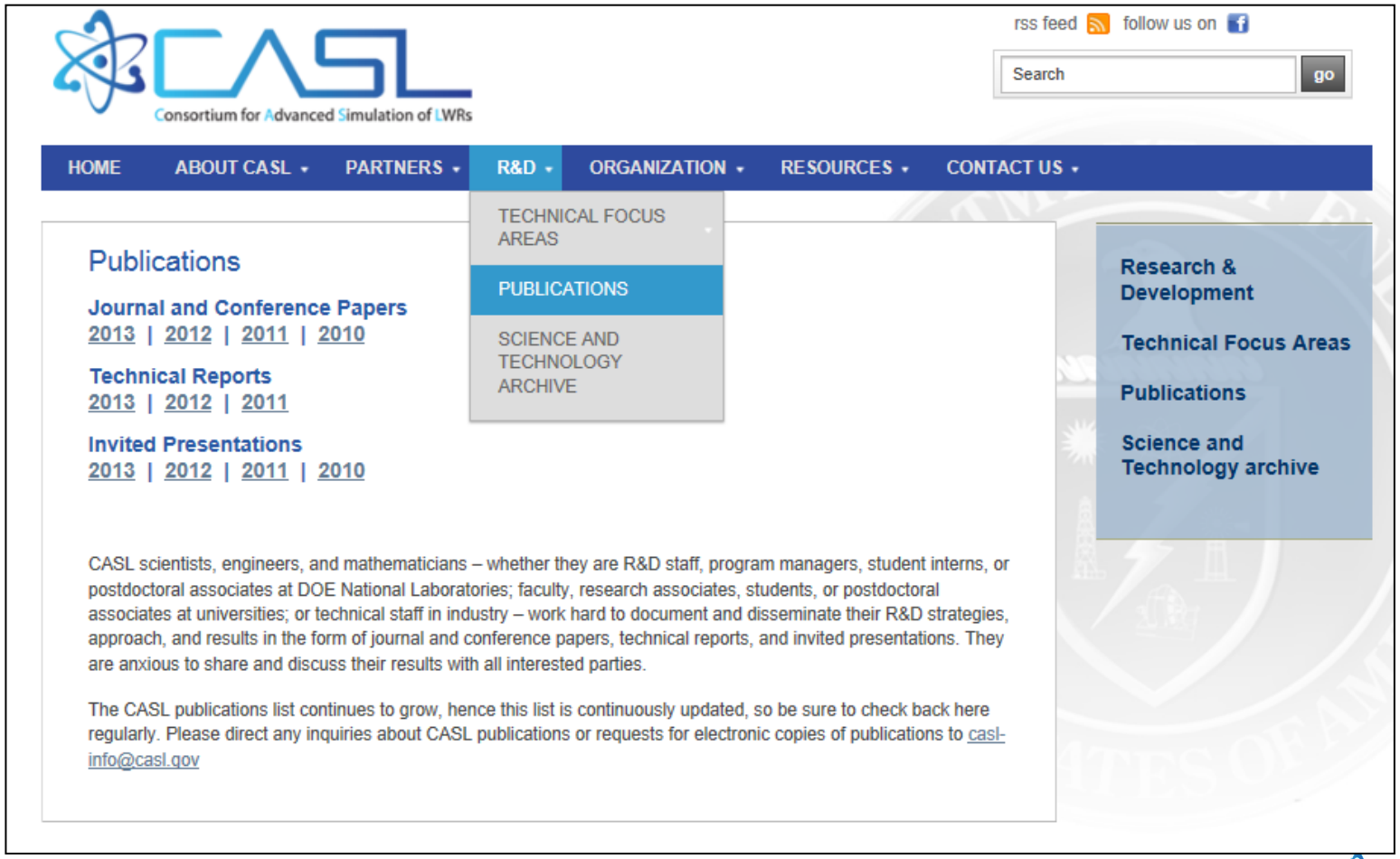
SOFTWARE TEST AND EVALUATION LICENSE AGREEMENT

[SOFTWARE NAME & VERSION]

UT-BATTELLE, LLC, hereinafter referred to as, a _____ company having its principal place of business at _____, hereinafter referred to as the "LICENSOR," and **[COMPANY]**, a **[STATE]** company, having its principle place of business at [ADDRESS], hereinafter referred to as "EVALUATOR" agree as follows, with both hereinafter referred to collectively as the Parties:

We are Making a Concerted Effort to Publish our Results Online

- http://www.casl.gov/
- Significantly more reports are available



Questions?

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

Demonstration of Neutronics Coupled to Thermal-Hydraulics for a PWR Core using VERA-CS

Scott Palmtag

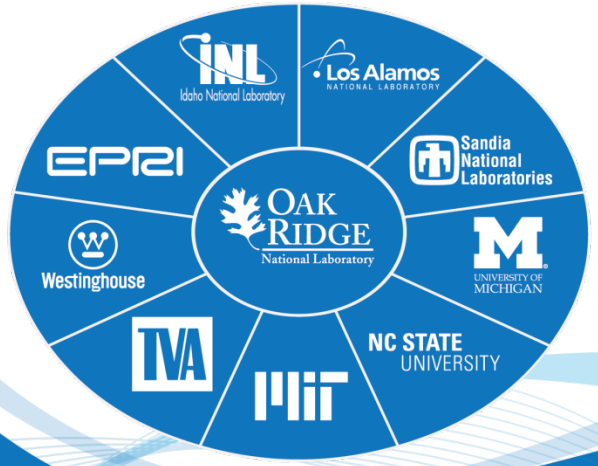
CASL, Physics Integration

Industry Council Meeting

Electric Power Research Institute

Charlotte, NC

March 11-12, 2014



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

Overview

- Background – Progression Benchmark Problems
- Codes being coupled
- Problem Description
- Results
- Future Work

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 ✓

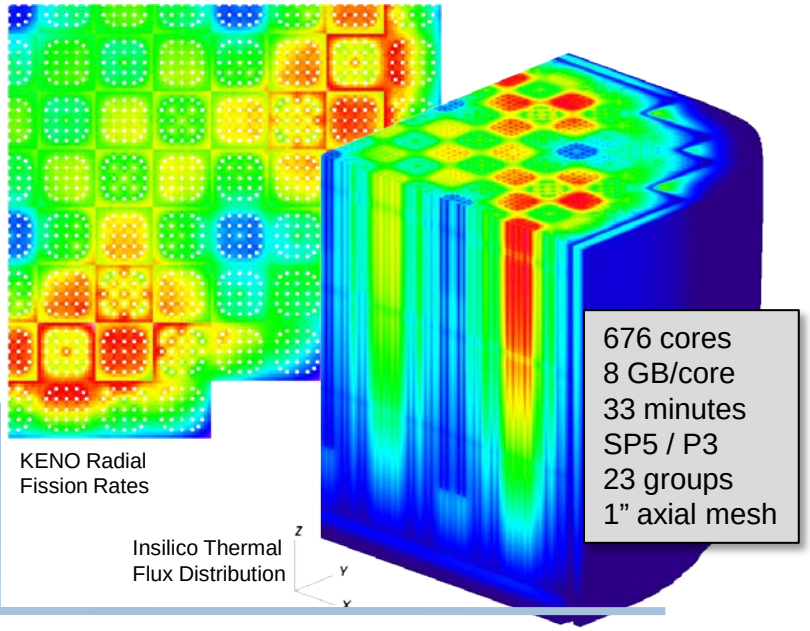
FY14

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

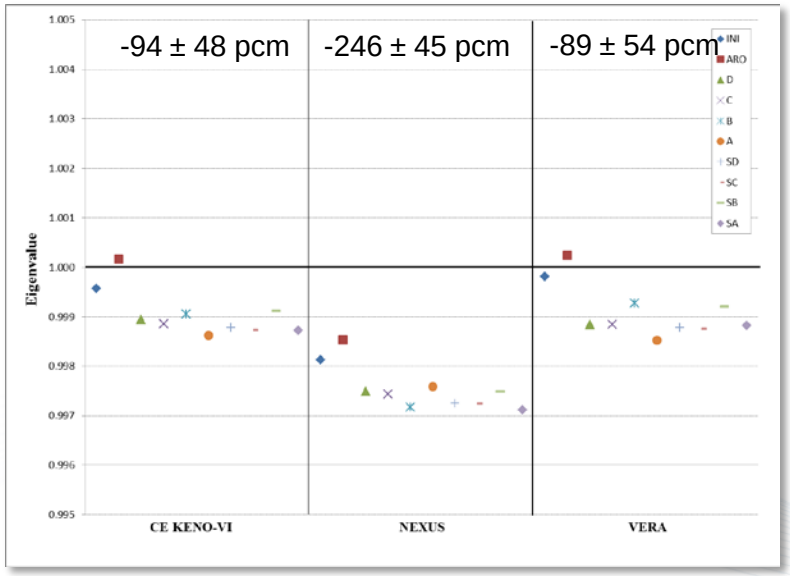
*** Bold text signifies ability to compare to measured plant data**

Problem 5 – Operational Reactor at HZP (June 2013)

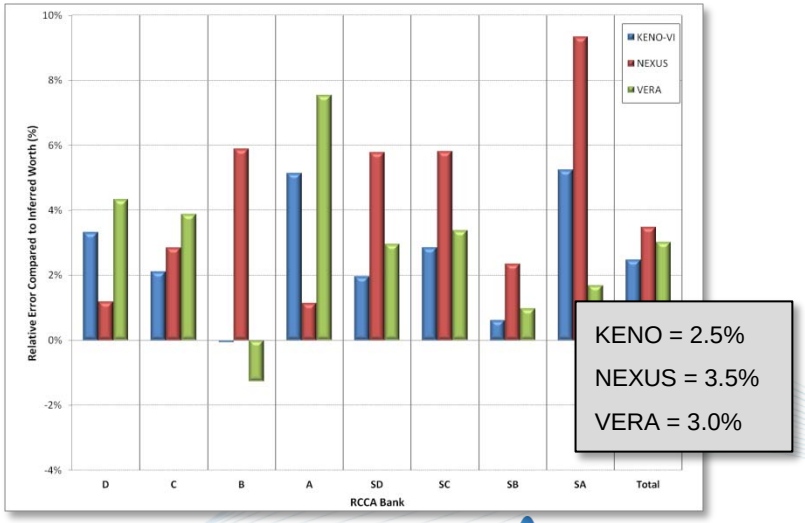
- Comparisons to startup physics tests results for Watts Bar Nuclear Unit 1 Cycle 1 (HZP)
- Analyses include:
  - VERA (*Insilico*) – 3D pin homogenized transport using SP_N methods
  - KENO-VI – 3D continuous energy Monte Carlo from SCALE 6.2
  - NEXUS – Westinghouse NRC-licensed 2D lattice physics + 3D nodal diffusion methodology
- Excellent reactivity results - except for ITC
- No power distribution comparisons performed



Ten Critical Conditions (initial, ARO, and rod swaps)

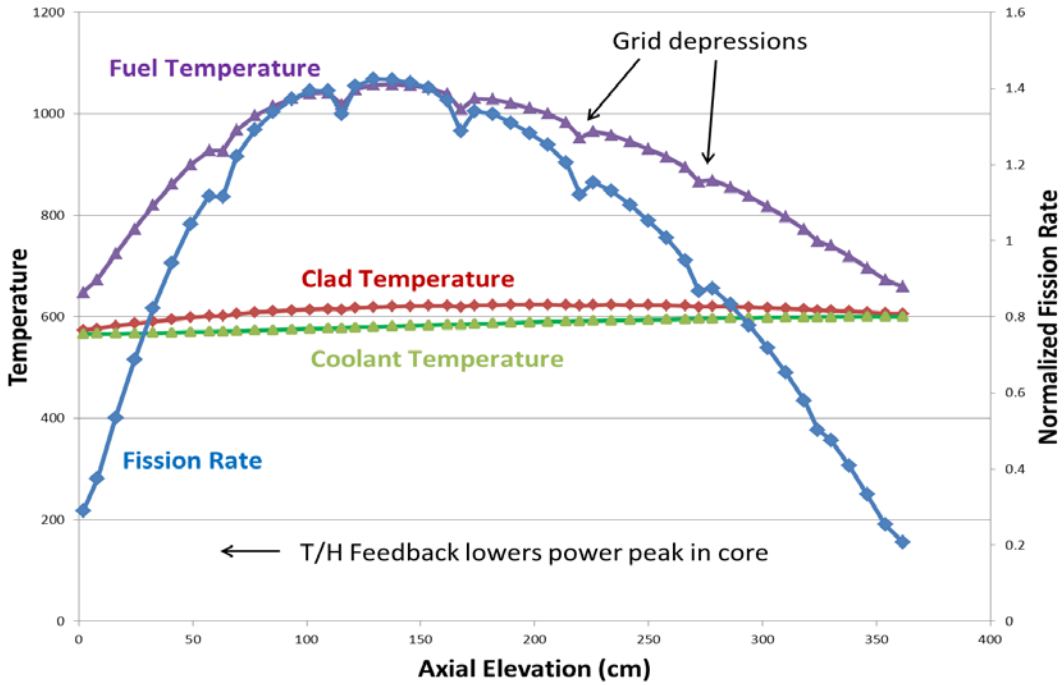


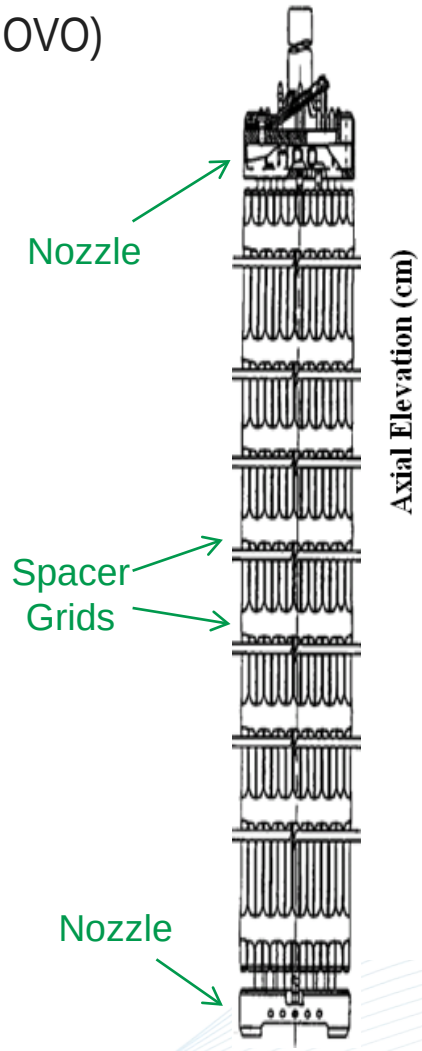
Eight Control Rod Bank Worths

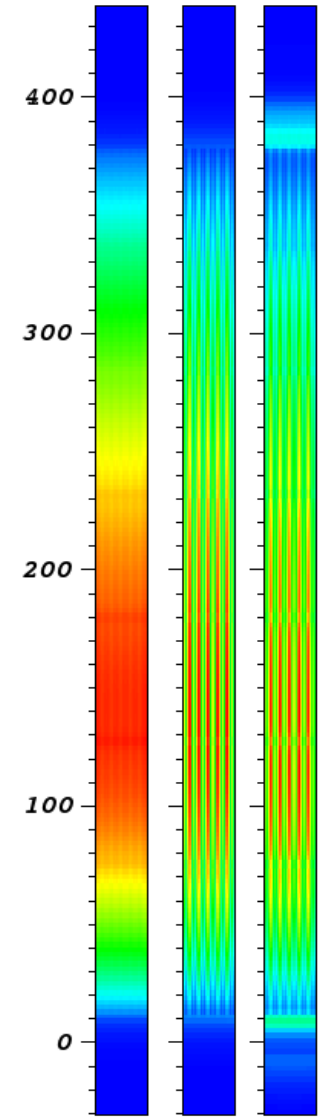


Problem 6 – Coupled Single-Assembly (July 2013)

- Coupled Multiphysics Model of PWR Fuel Assembly
  - Neutron transport to calculate power distribution (DENOVO)
  - Thermal-Hydraulics in coolant (COBRA-TF)
  - Heat conduction in fuel rods (COBRA-TF)
  - Neutron cross sections as function of temperature and density (SCALE)







Fast, Epithermal, and Thermal Flux Profiles

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

- 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

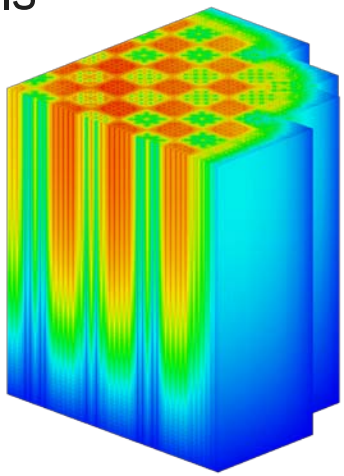
- No reference results available due to feedback
  Future Problems will include flux maps and depletion

Development Activities

1. Scale unique cross sections from single-assembly to full-core
   - Coupled problems require each geometry region to have “unique” cross sections (fuel/clad/coolant temperatures, coolant density is unique)
   - Optimized mesh construction for homogenized pins
   - More than 1,000,000 cross section sets for qtr-core problem
2. Develop parallel CTF to reduce run time
   - Full-core CTF runtime reduced from ~20 hours to ~10 minutes
   - Domain decomposition parallelism with one assembly per core
3. Add boron search capability
4. Add restart capability
   - Run-times exceed maximum job-time on Titan
   - Need to split runs into multiple jobs

Neutronics – INSILICO

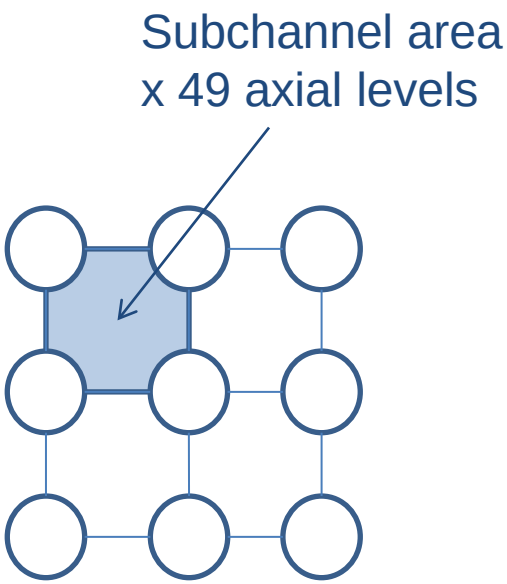
- Input directly from common input (VERAIn)
- Built in cross section processing with XSPROC
  - 56-group pincell calculations for every rod on 49 axial levels
- SP_N neutron transport solver (pin homogenized)
  - SP_3 transport / P_1 scattering
  - 2x2 radial mesh in each rod
  - 7.64 cm (3 inch) maximum axial mesh
  - 11-group 3D transport
- Accuracy of SP_N demonstrated in Problem 5 report



Efficient Scaling to Large 3D Problems

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)

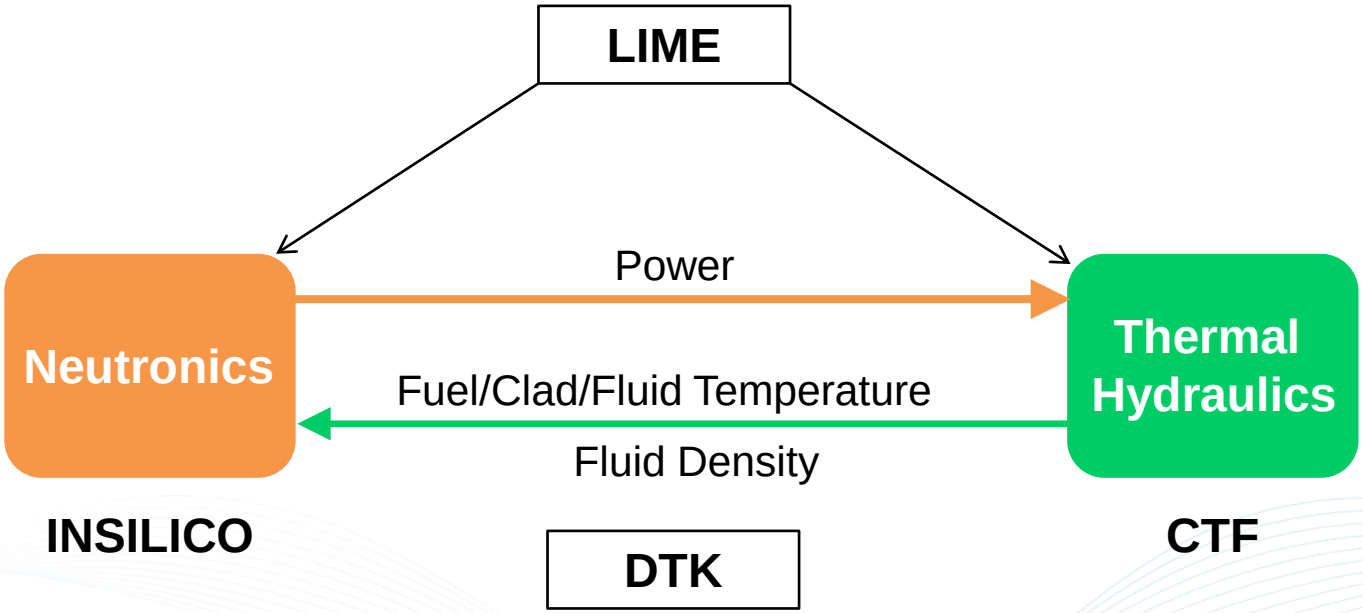


Parallel CTF Developed for Problem 7

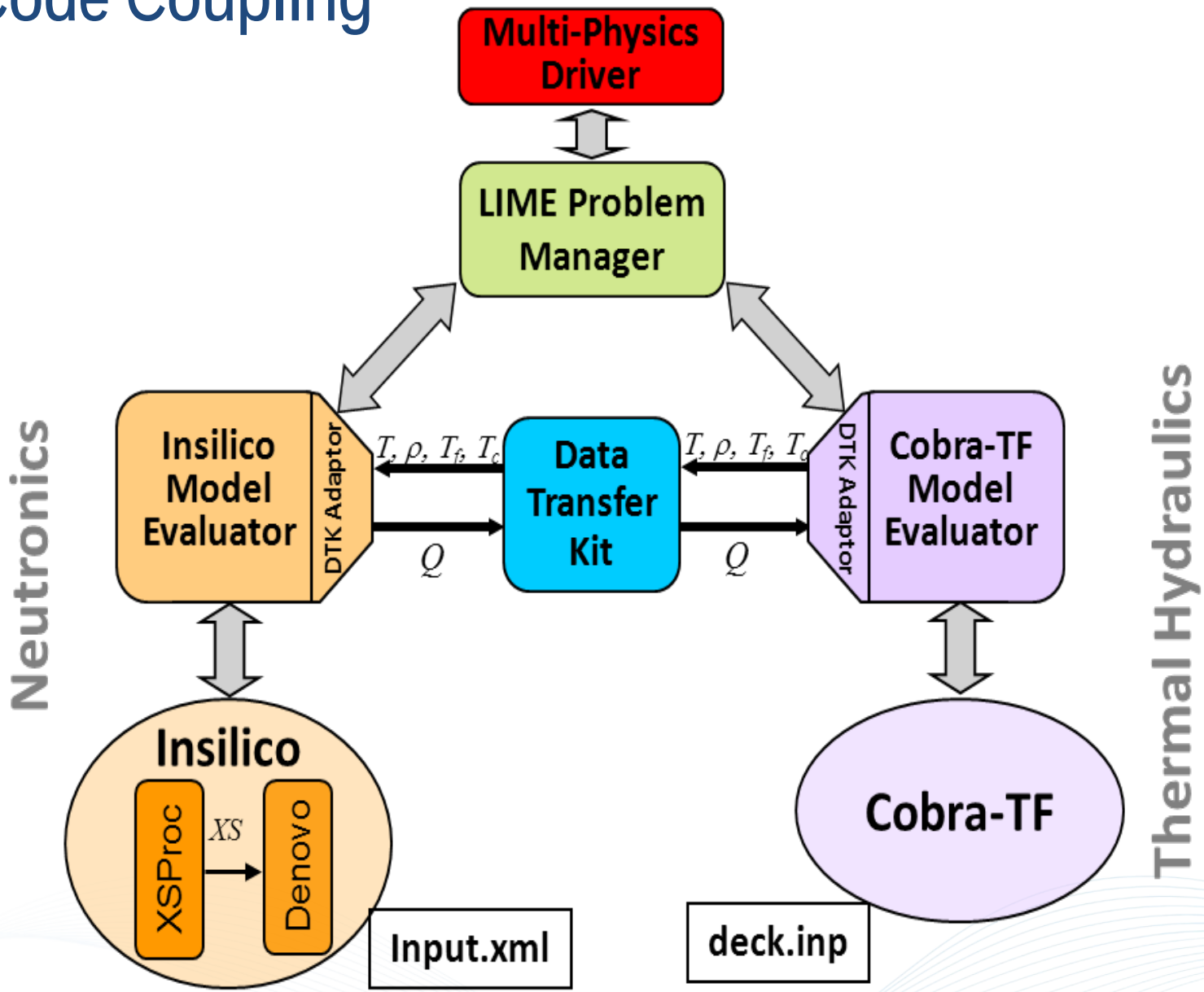
Code Coupling

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

(both are open source toolkits)



Two Code Coupling



Coupling Mesh

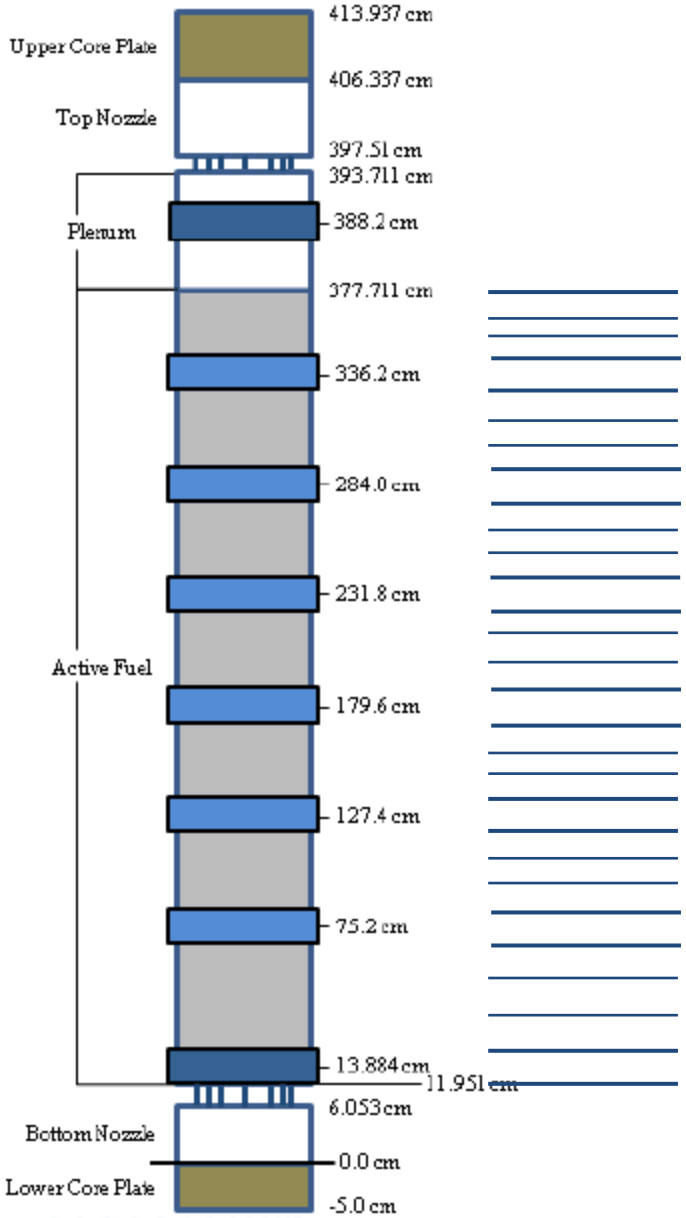
Insilico model spans from below lower core plate to above upper core plate

(Typically 1” intervals)

CTF model spans active fuel region

(49 levels)

recently extended to cover entire rod



Coupling is performed on CTF mesh

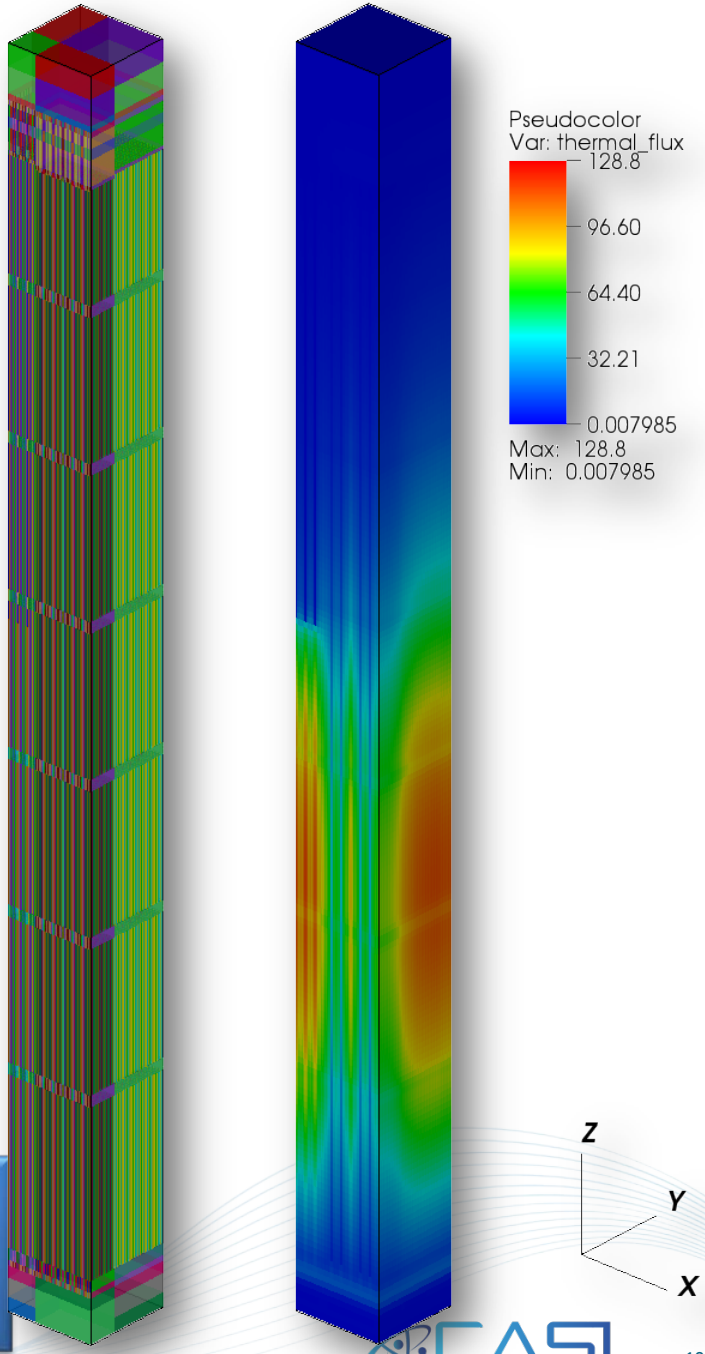
(49 axial levels)

Grids are resolved + equal spacing between grids

Drawing not to scale

VERA Common Output

- Fine-mesh results written to **SILO** files for visualization in tools such as Visit / Paraview
- Pin-by-pin distributions (from multiple codes) written to a common **HDF5** format that can be post-processed to create user edits
  - 2D/3D pin distributions
  - 2D/3D assembly distributions
  - peaking factors
  - Compare distributions (e.g. Keno vs. VERA)
- Recognition that industrial users need **both** visualization and "real numbers"



DENOVO fission rate for full assembly, generated with SILO file and VISIT

Problem Description and Results

Watts Bar Unit 1 Cycle 1

Problem Description

Core Features:

- 193 Fuel Assemblies
- 17x17 Rods/assembly
- 3 Enrichment Zones
- Pyrex Burnable Absorber Rods
- Guide Tubes
- Soluble Boron
- Spacer Grids
- Top and Bottom Nozzles
- Core Plates
- Core Baffle

	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1	3.1 16	3.1	3.1		
15	3.1 12	3.1	3.1 8	3.1				

Enrichment
Number of Pyrex Rods

Each pincell has a *unique* fuel temperature, coolant temperature, and coolant density

193 assemblies x 289 rods/assembly x 49 axial levels

= **2.7M** unique regions in full-core (not including baffle, reflectors, etc.)

Common Input – VERAIN (Core)

```
[CORE]
  size 15                  ! assemblies across core
  rated 3411 131.68        ! MW, Mlbs/hr
  apitch 21.5              ! Assembly pitch
  height 406.337

  core_shape
    0 0 0 0 1 1 1 1 1 1 1 0 0 0 0
    0 0 1 1 1 1 1 1 1 1 1 1 1 0 0
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
    0 0 1 1 1 1 1 1 1 1 1 1 1 0 0
    0 0 0 0 1 1 1 1 1 1 1 0 0 0 0

  assm_map
    1
    2 1
    1 2 1
    2 1 2 1
    1 2 1 2 2
    2 1 2 1 2 3
    1 3 1 3 3 3
    3 3 3 3
```

	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1	3.1 16	3.1	3.1		
15	3.1 12	3.1	3.1 8	3.1				

Enrichment
Number of Pyrex Rods

```
insert_map
     -
    20  -
     - 24  -
    20  - 20  -
     - 20  - 20  -
    20  - 16  - 24 12
     - 24  - 16  -  -
    12  -  8  -

baffle ss 0.19 2.85
vessel mod 219.71 cs 241.70

lower_plate ss  5.0 0.5   ! mat, thickness, vol frac
upper_plate ss  7.6 0.5   ! mat, thickness, vol frac

xlabel  R P N M L K J H G  F  E  D  C  B  A
ylabel  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
```

Common Input – VERAIN (Assembly)

```
[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260

  fuel U31 10.257 95.0 / 3.1

  cell 1    0.4096 0.418 0.475 / U31 he zirc
  cell 10          0.561 0.602 / mod    zirc       ! guide tube
  cell 20          0.561 0.602 / mod    zirc       ! instrument tube
  cell 7           0.418 0.475 / mod    mod        ! empty location
  cell 8           0.418 0.475 /     he zirc       ! plenum
  cell 9                 0.475 /        zirc       ! pincap

  lattice FUEL1
     20
      1 1
      1 1 1
     10 1 1 10
      1 1 1  1 1
      1 1 1  1 1 10
     10 1 1 10 1  1 1
      1 1 1  1 1  1 1 1
      1 1 1  1 1  1 1 1 1

 lattice PLEN1
     20
      8 8
      8 8 8
     10 8 8 10
      8 8 8  8 8
      8 8 8  8 8 10
     10 8 8 10 8  8 8
      8 8 8  8 8  8 8 8
      8 8 8  8 8  8 8 8 8
```

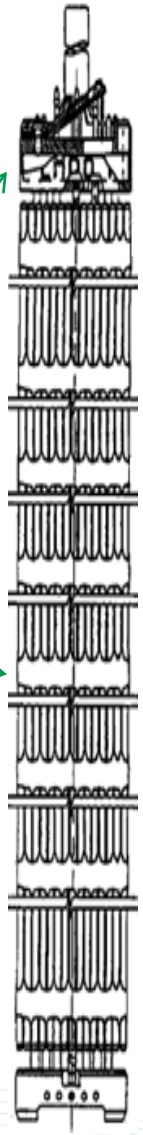
```
 axial A1    6.050
     LGAP1  10.281
     PCAP1  11.951
     FUEL1 377.711
     PLEN1 393.711
     PCAP1 395.381
     LGAP1 397.501

 grid END inc  1017 3.866  ! grid mass, height (cm)
 grid MID zirc 875  3.810  ! grid mass, height (cm)

 grid_axial
     END  13.884
     MID  75.2
     MID 127.4
     MID 179.6
     MID 231.8
     MID 284.0
     MID 336.2
     END 388.2

 lower_nozzle  ss 6.05  6250.0  ! mat, height, mass
 upper_nozzle  ss 8.827 6250.0  ! mat, height, mass
```

Information shown originates from FSAR document (ref 4 from L1:CASL.P7.01)



Coupled Iterations

Calculation took longer than maximum run-time on Titan, so it was split into two jobs with a **restart**

	its	xkeff	keff_dif	powr_dif	cool	clad	fuel	cool delta	clad delta	fuel delta
1	1247	0.986477	-1352.3	1.000000	622.00	693.70	1525.00	64.62	95.07	127.20
2	1042	0.984064	-241.3	0.065975	634.42	723.89	2399.87	12.47	30.16	875.10
3	908	0.983410	-65.4	0.012352	638.80	735.91	2649.67	4.38	12.02	249.80
4	351	0.983204	-20.6	0.002382	639.75	738.99	2717.49	0.95	3.08	67.82
5	569	0.983137	-6.7	0.001741	640.00	739.73	2738.42	0.25	0.74	20.93
6	502	0.983113	-2.4	0.000622	640.18	740.06	2744.71	0.18	0.33	6.29
7	152	0.983103	-1.0	0.000081	640.26	740.19	2746.94	0.08	0.12	2.23

Start date: Thu Dec 19 23:29:56 EST 2013
End date: (job stopped after 12:00 hours)

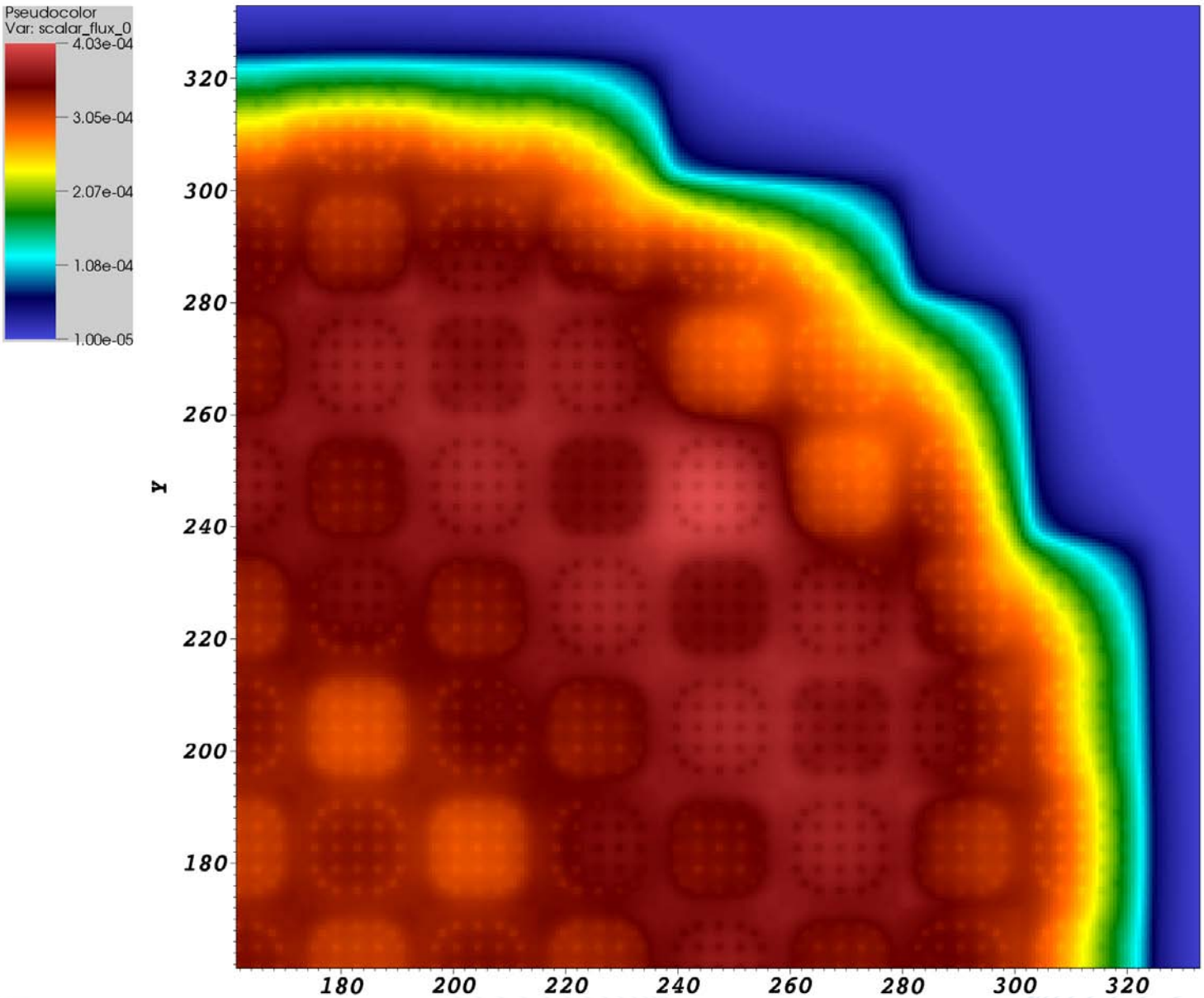
Converged after 7 iterations?

	its	xkeff	keff_dif	powr_dif	cool	clad	fuel	delta	delta	delta
1	1443	0.983100	-1690.0	0.000668	640.90	740.40	2748.00	83.62	141.70	1350.00
2	241	0.983101	0.1	0.000419	640.97	740.35	2747.97	0.01	0.01	-0.51
3	10	**0.983100**	-0.1	0.000002	640.97	740.35	2748.07	0.00	-0.00	0.10

Start date: Fri Dec 20 18:08:37 EST 2013
End date: Fri Dec 20 23:40:50 EST 2013
elapsed time 5:32:13 332.22 min

18,769 cores (137x137)
~ 12 - 17.5 hours on Titan

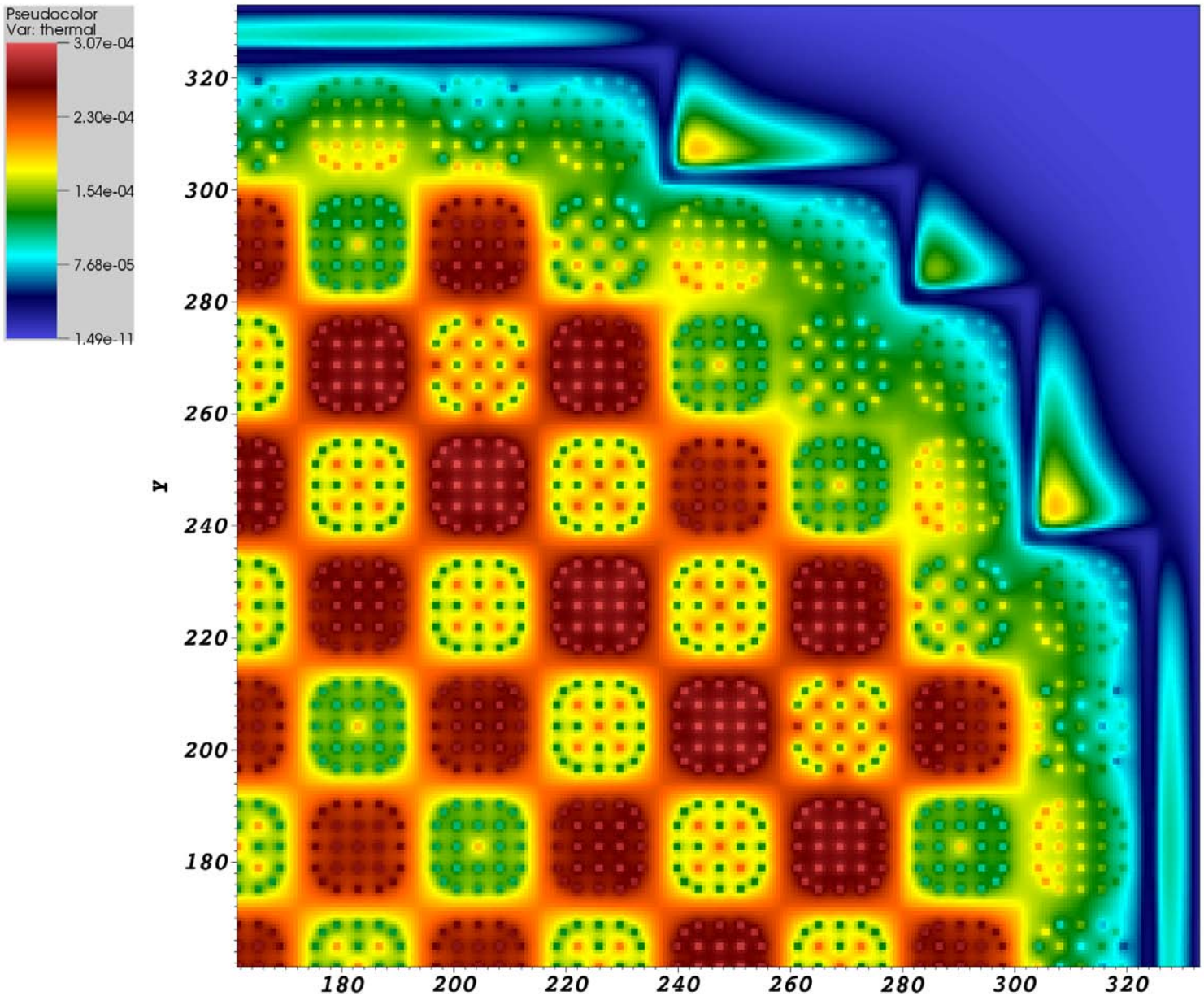
Fast Flux Results



Fast Flux at mid-plane
(Group 1 of 11)

Highest energy neutrons, Longer mean-free-paths

Thermal Flux Results



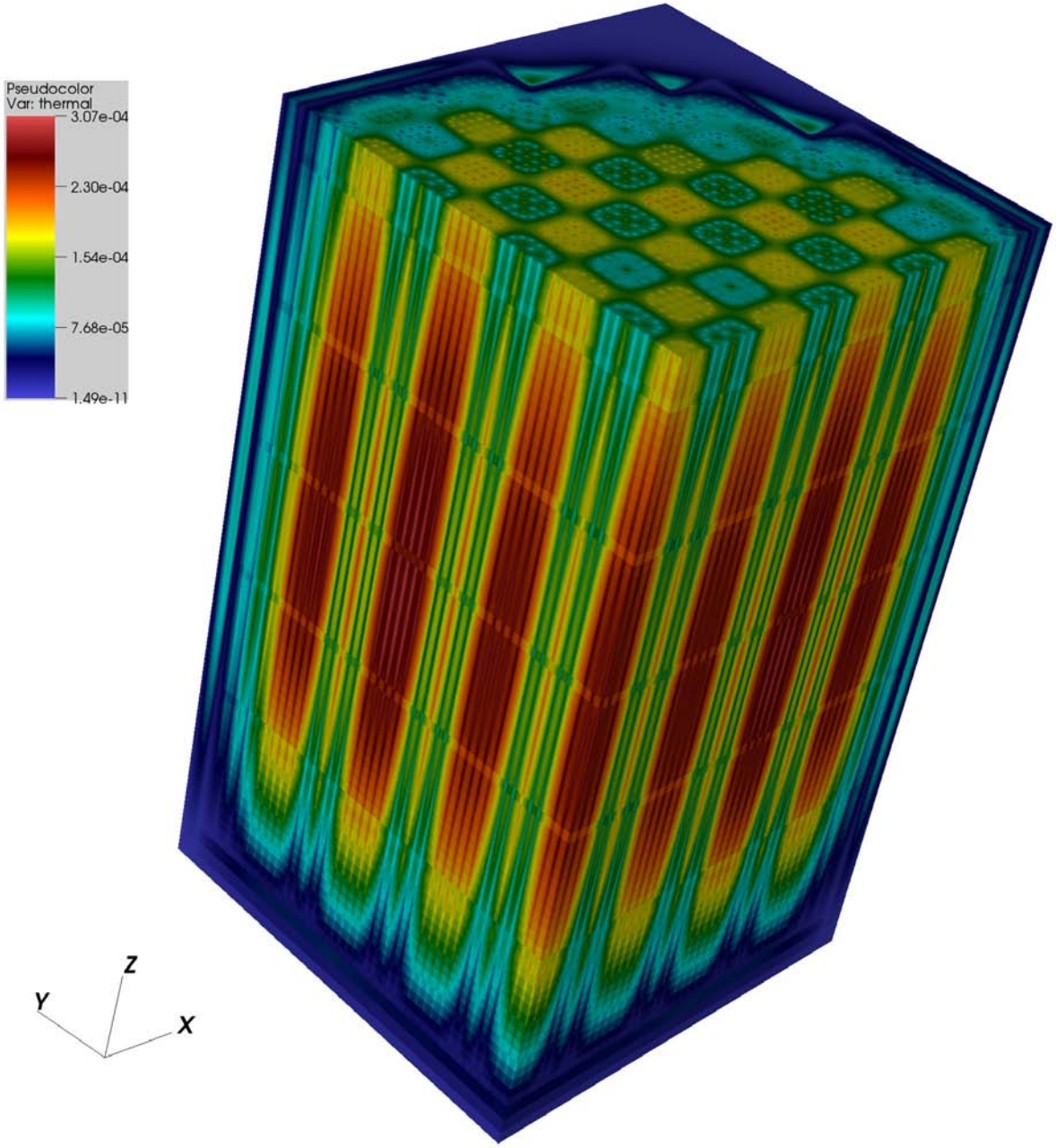
Thermal Flux
0.625 eV
at midplane
(Groups 8-11 of 11)

Low energy neutrons, Short mean-free-paths

Peaks formed in reflector from downscatter source

Low flux in baffle

Thermal Flux Results

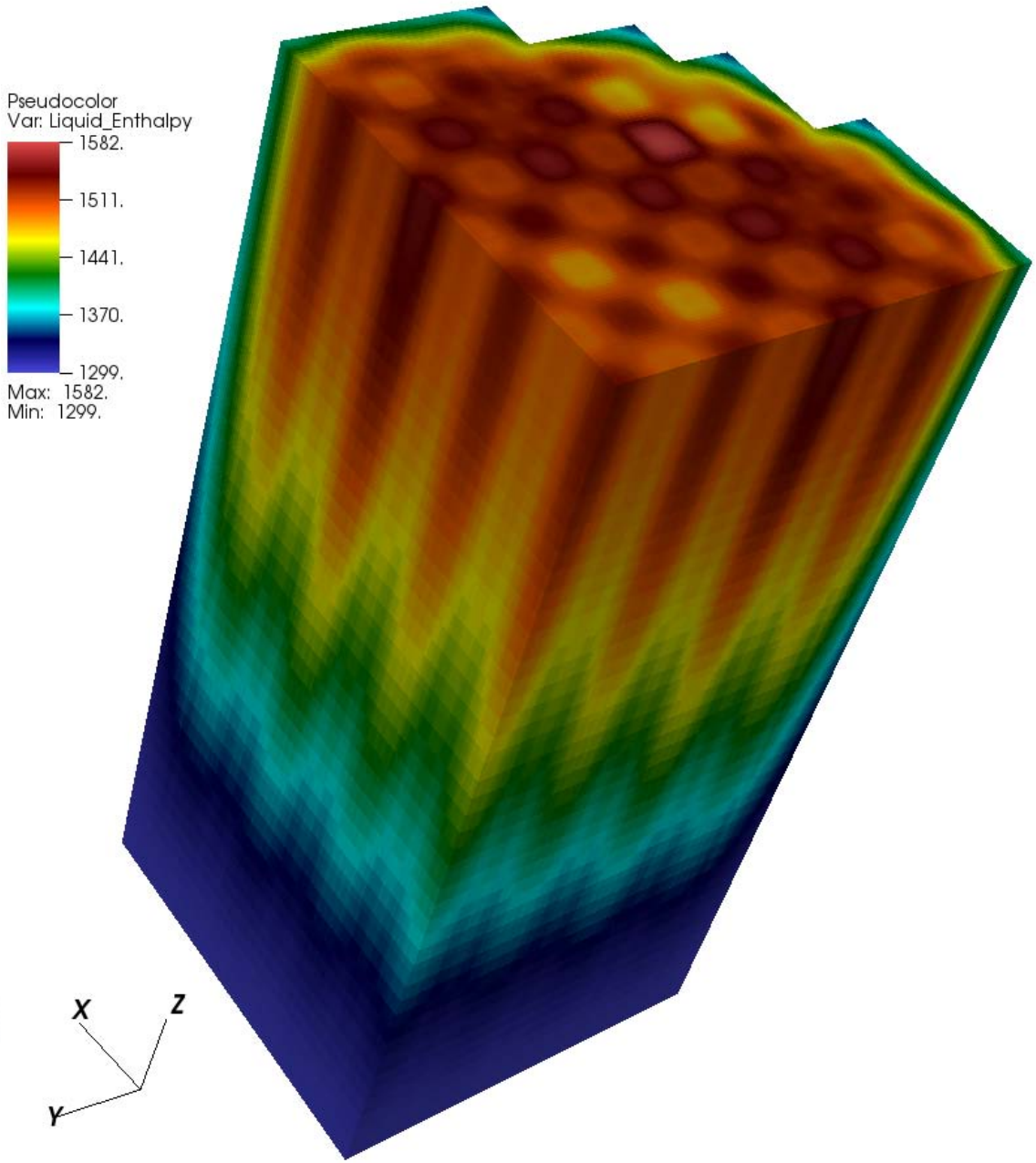


Thermal Flux
0.625 eV
at core midplane
(Groups 8-11 of 11)

Flux depressed in assemblies with Pyrex absorbers

Can make out baffle, nozzles, and spacer grids

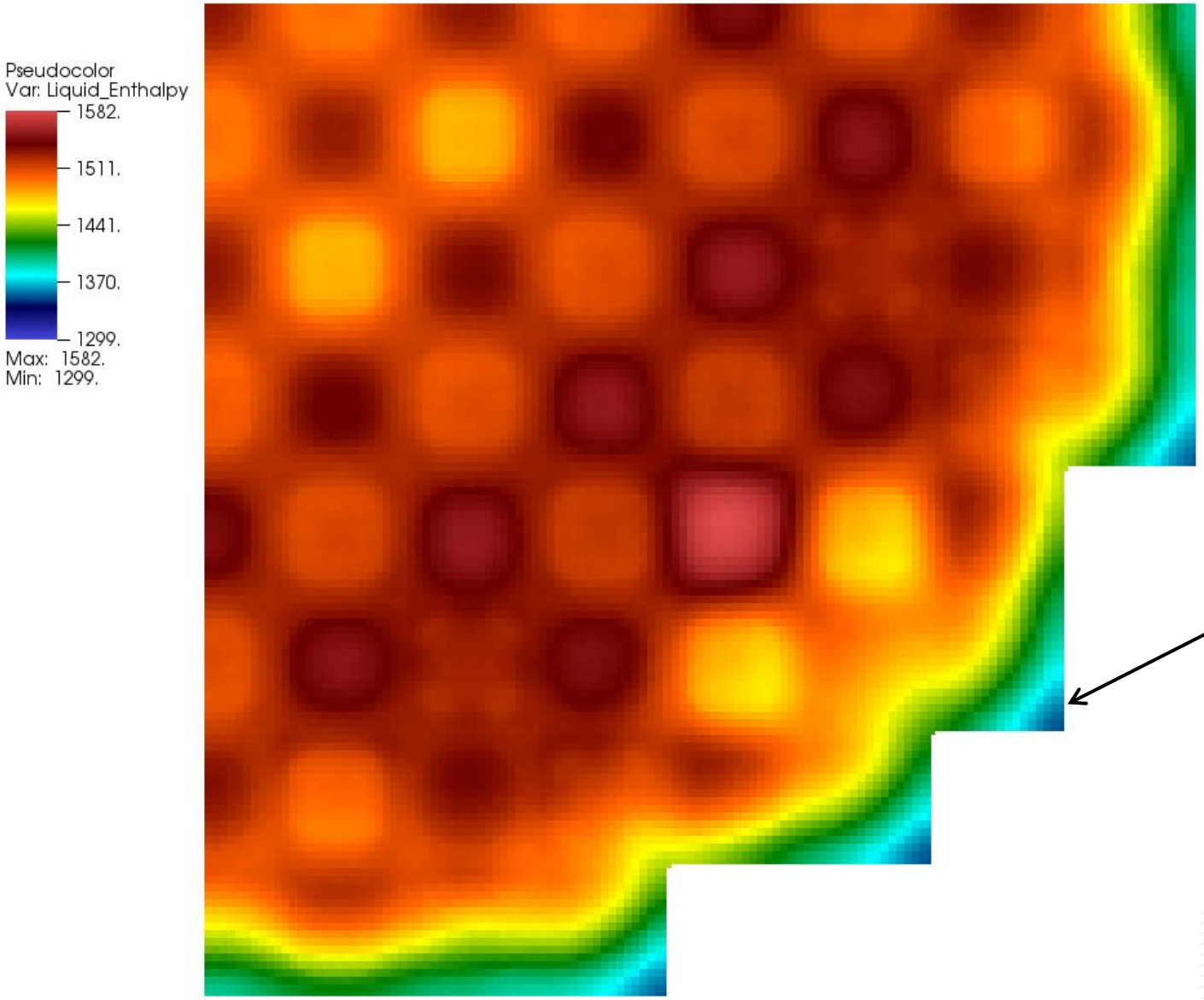
3D Coolant Enthalpy



VTK file created by CTF

Note the lower enthalpy in assemblies with Pyrex absorbers

Exit Coolant Enthalpy



2D plot of coolant enthalpy at core exit

Large gradients at outer corners next to baffle

Common Output - Post Processing

Assembly Power (averaged over all rods axially)

	H	G	F	E	D	C	B	A
8	1.0619	0.9815	1.0605	1.0222	1.1330	1.0491	1.0550	0.7740
9	0.9815	1.0500	0.9428	1.1053	1.0612	1.1452	1.0334	0.8806
10	1.0605	0.9428	1.0856	1.0489	1.1641	1.1257	1.0682	0.7859
11	1.0222	1.1053	1.0489	1.1592	1.0830	1.1298	1.0218	0.6516
12	1.1330	1.0612	1.1641	1.0830	1.2758	0.8979	0.9334	
13	1.0491	1.1452	1.1257	1.1298	0.8979	0.9134	0.6337	
14	1.0550	1.0334	1.0682	1.0218	0.9334	0.6337		
15	0.7740	0.8806	0.7859	0.6516				

2D and 3D Pin Powers

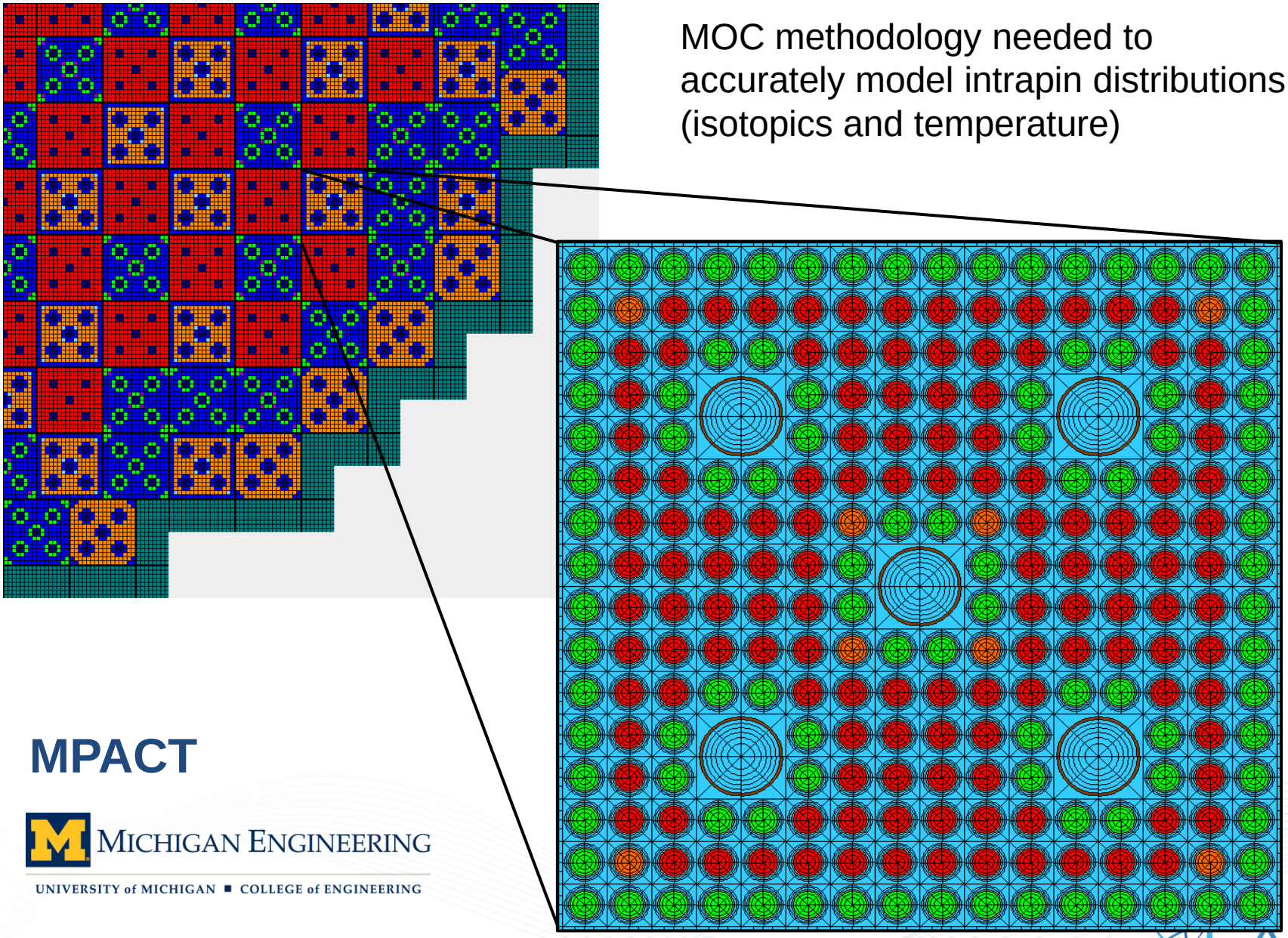
	Power	Pin Location	Level	Assembly
2D min rod	0.1544	(4,5)	--	C-14/B-13
2D max rod	1.3981	(17,17)	--	D-12
3D min	0.0246	(4,5)	1	C-14/B-13
3D max	1.9756	(17,17)	20	D-12

Pictures are nice, but we also need numbers!

Work in Progress

Problems 8-10 (Depletion with MOC)

Method of Characteristic (MOC) Transport in 2D



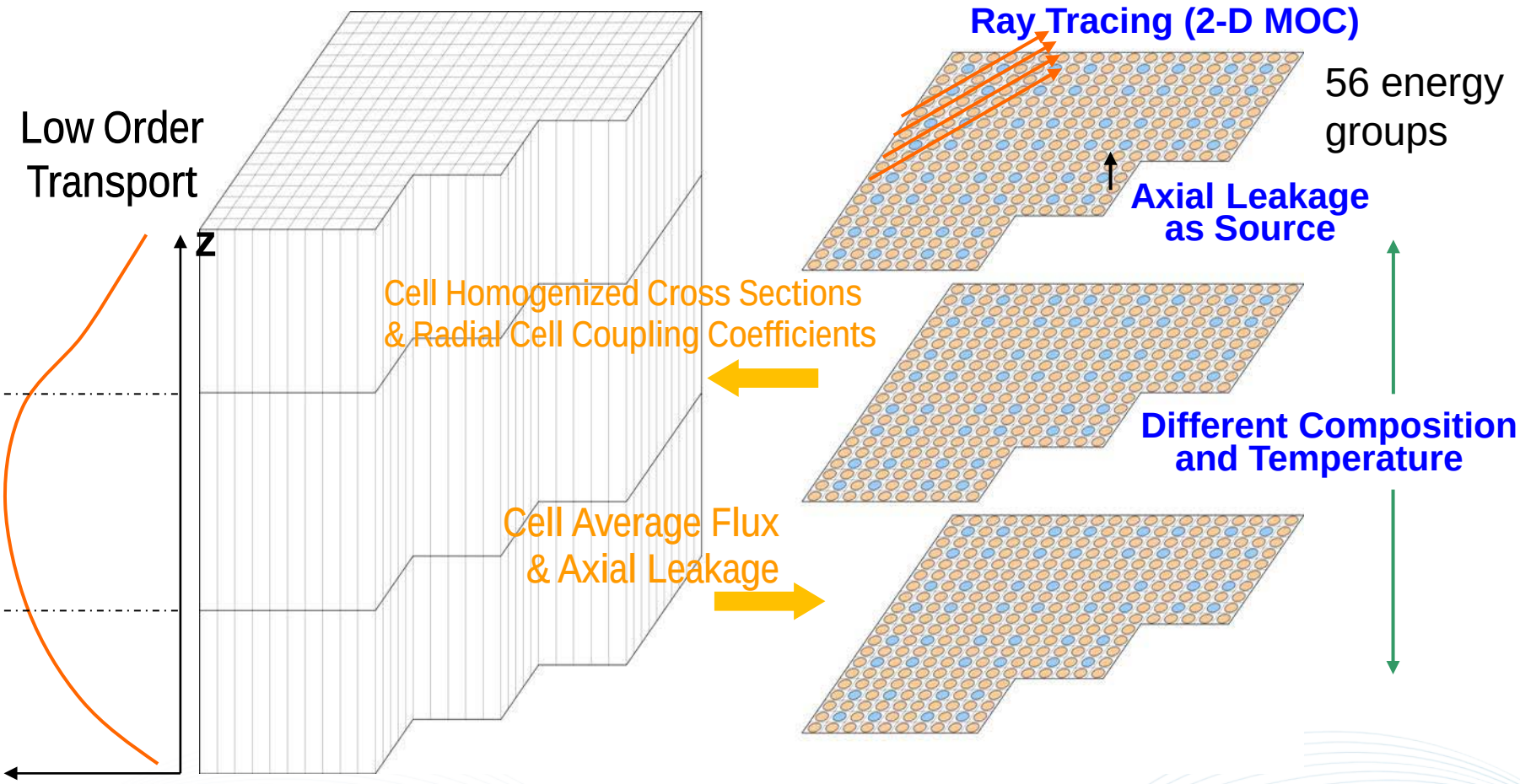
MOC methodology needed to accurately model intrapin distributions (isotopics and temperature)

MPACT

MICHIGAN ENGINEERING
UNIVERSITY of MICHIGAN ■ COLLEGE of ENGINEERING

Consortium for Advanced Simulation of LWRs

Coupled MOC Planes for 3D Transport (2D/1D)

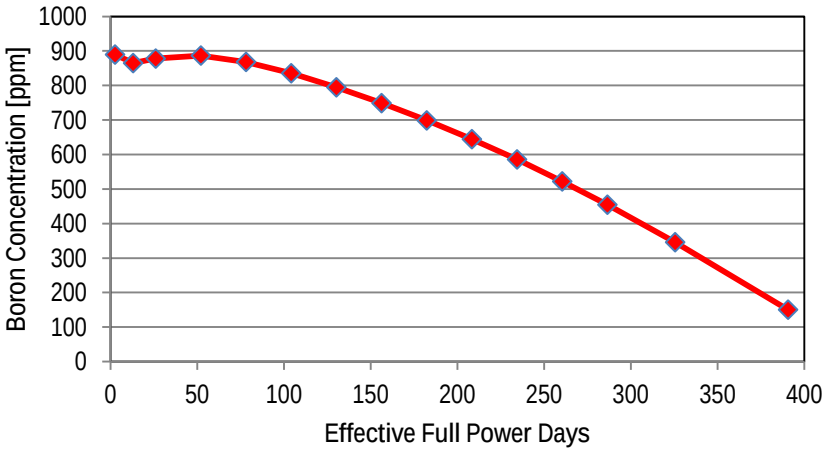


Global 3-D CMFD Problem

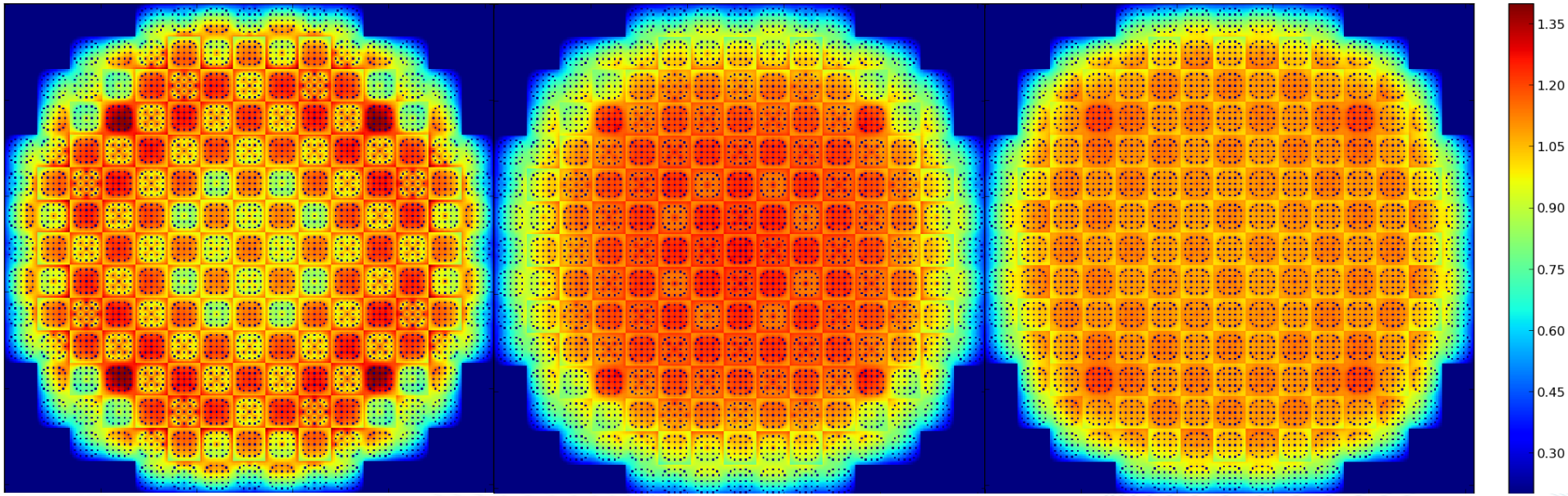
Local 2-D MOC Problems

Initial 2D Core Depletion Capability

- 2D slice of Watts Bar Core was used at core average temperature and density
- Boron search was used to make reactor critical



BOC **MOC** **EOC**



MOC Advantages

- Intrapin distributions for depletion, power, and temperature
  - Need radial and azimuthal distributions for Challenge Problems
- More efficient memory and run-times
  - Many factors go into this including cross section methodology, solvers, and iteration strategies

***Initial/Estimated* Problem 7 Results**

	Cores	Wall-Time	CPU-hour
Insilico-CTF	18,769	14:30	272,150
MPACT-CTF	2,880	16:00	46,080

Very preliminary results!

- Could expect another 50% reduction with further development

Lots of room for improvement!

“Deep Dive”

- Wednesday afternoon we will present more information on the MOC methods and future development tasks
- We are looking for feedback and suggestions for future direction!

Questions?

INL
Idaho National Laboratory
Los Alamos
NATIONAL LABORATORY
EPRI
Sandia
National
Laboratories
OAK
RIDGE
National Laboratory
Westinghouse
UNIVERSITY OF
MICHIGAN
TVA
NC STATE
UNIVERSITY
MIT

References

The following reports are available from the public CASL website www.casl.gov

CASL Progression Benchmark Specifications:

Godfrey, A., *VERA Core Physics Benchmark Progression Problem Specifications*, CASL Technical Report: CASL-U-2012-0131-002, March 2013.

Problem 5 Results:

Gehin, J., A. Godfrey, F. Franceschini, T. Evans, B. Collins, S. Hamilton, *Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Test*, CASL Technical Report: CASL-U-2013-0105-001, June 2013.

Problem 6 Results:

Palmtag, S., *Coupled Single Assembly Solution with VERA (Problems 6)*, CASL Technical Report: CASL-U-2012-0150-000, July 2013.

Problem 7 Results:

Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using VERA, CASL Technical Report: CASL-U-2012-0196-000, December 2013.

Westinghouse Test Stand Results:

Franceschini, F., A. Godfrey, J. Kulesza, R. Oelrich, Westinghouse VERA Test Stand - Zero Power Physics Test Simulations for the AP1000 PWR, CASL Technical Report: CASL-U-2014-0012-000, January 2014.

Update on Fuel Performance Modeling Efforts within MPO: CRUD, PCI and GTRF

Chris Stanek
Los Alamos National Laboratory

Brian Wirth
University of Tennessee
On behalf of the MPO team

CASL Industry Council Meeting
EPRI, Charlotte, NC
March 11, 2014

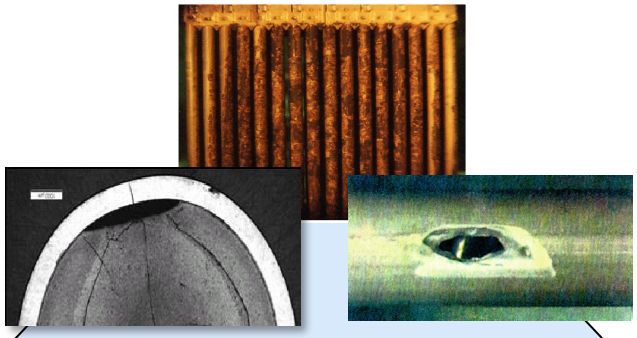
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

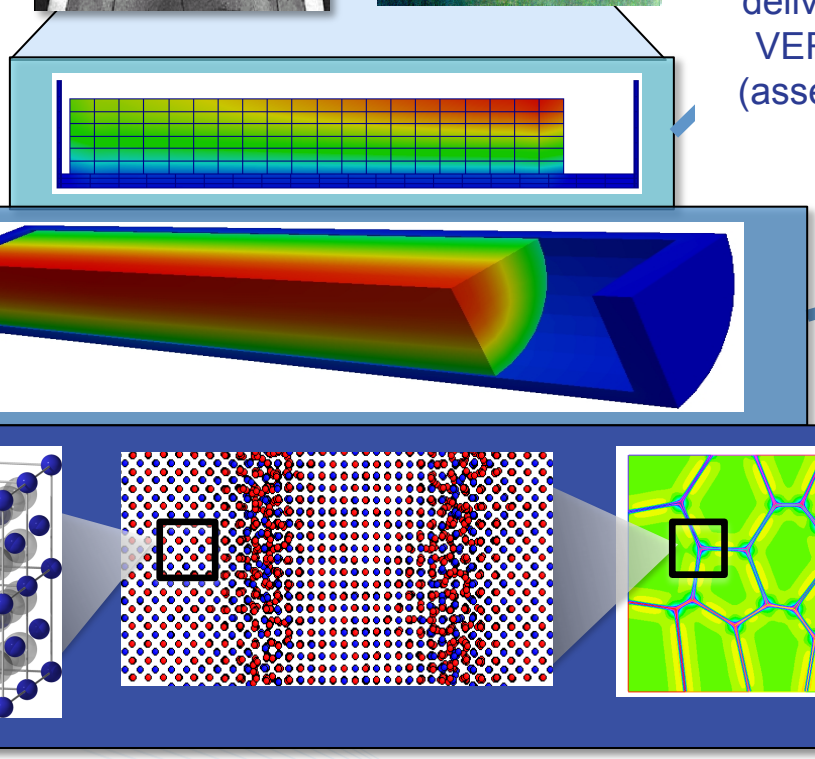
CASL
Consortium for Advanced Simulation of LWRs

Materials Performance Optimization (MPO)

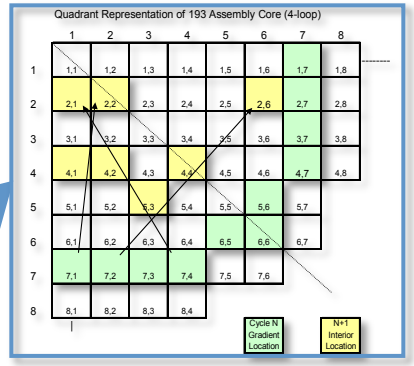
Enabling Improved Fuel Performance through Predictive Simulation

Deliver engineering-scale fuel performance models to VERA for CASL challenge problems

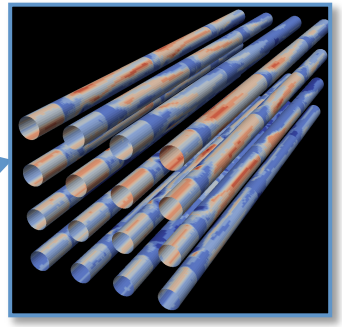




2D engineering scale models delivered to VERA-CS (assemblies)



3D engineering scale models delivered to VERA (few pins)



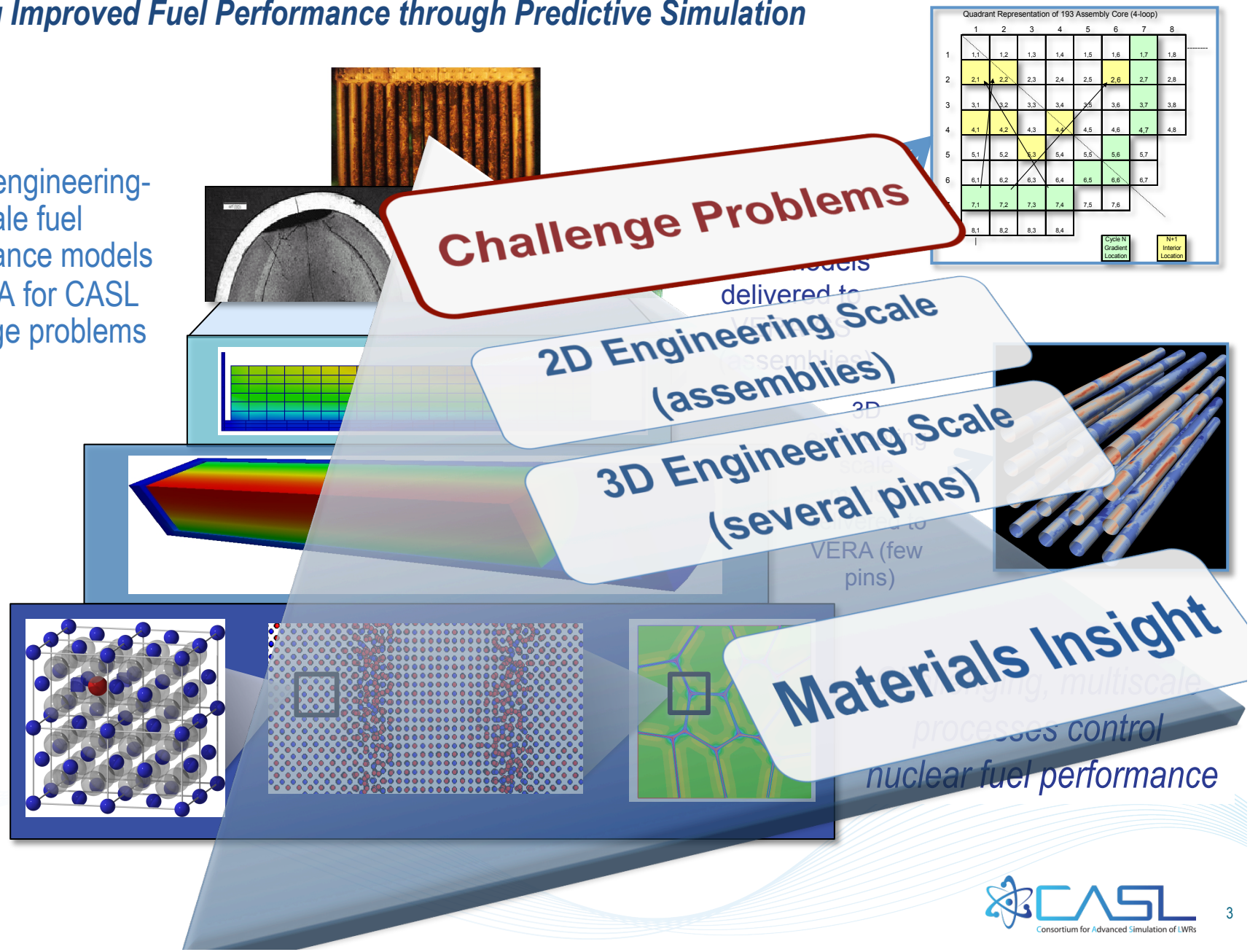
Improved physics and chemistry insight delivered via constitutive relations and behavioral models

Challenging, multiscale processes control nuclear fuel performance

Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

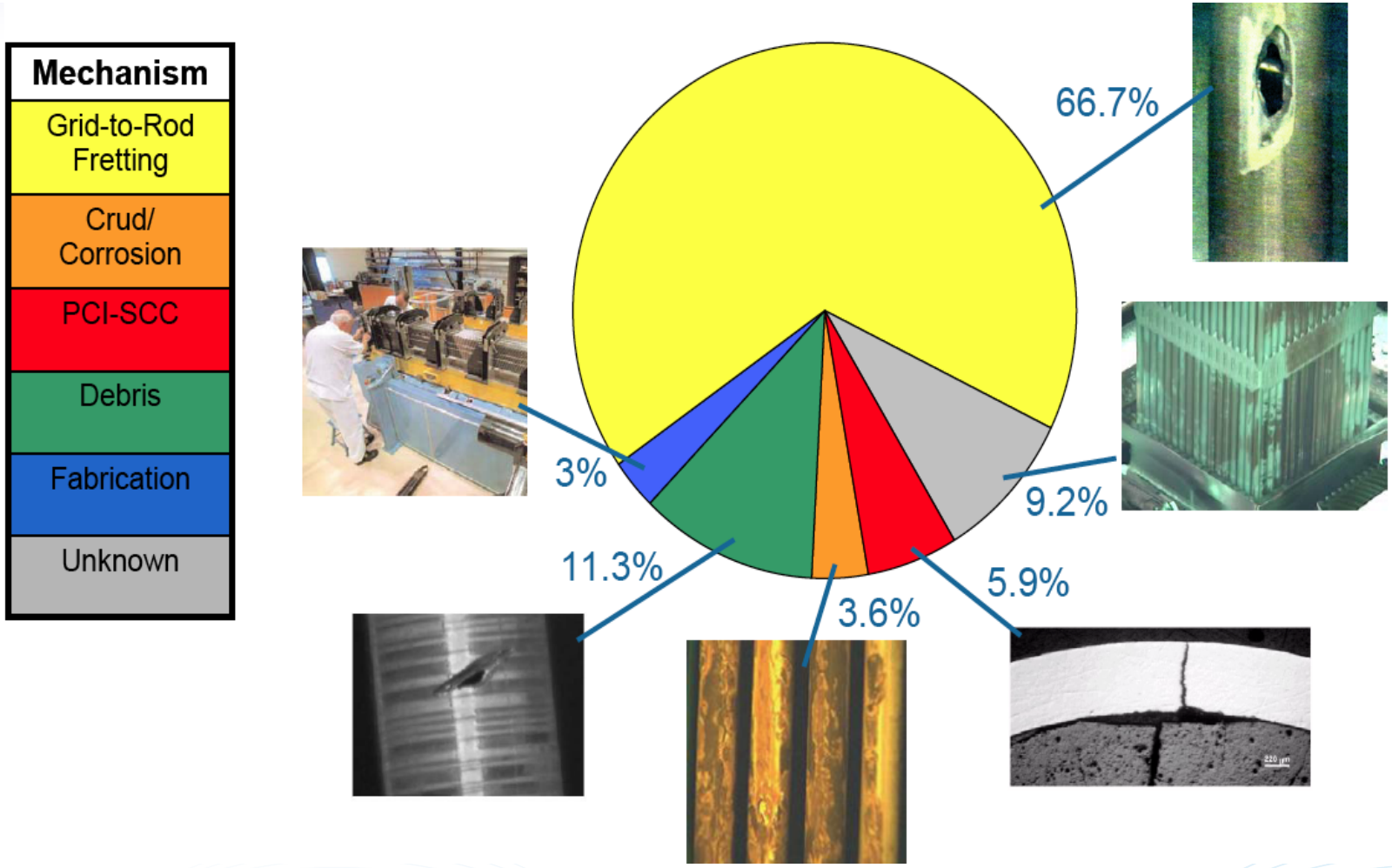
Deliver engineering-scale fuel performance models to VERA for CASL challenge problems



Improved physics and chemistry insight delivered via constitutive relations and behavioral models

CASL Challenge Problems

Summary of US fuel failure mechanisms (2000-2008)

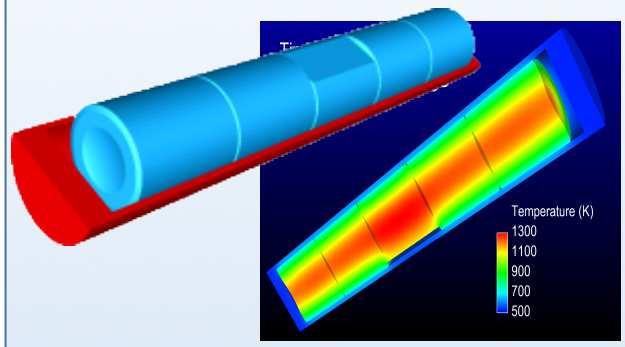


* Edsinger, Stanek, Wirth, JOM **63, no. 8** (2011)

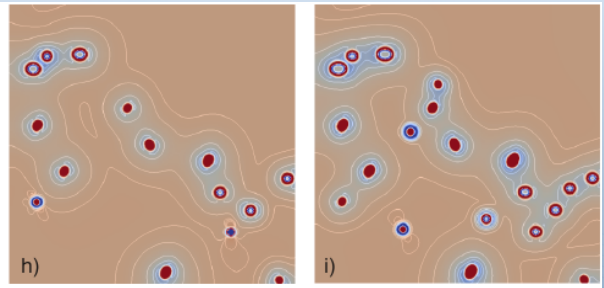
MPO delivers engineering scale fuel performance models and materials physics-based constitutive models for CASL challenge problems

For CRUD, GTRF and PCI - 3-D, high resolution coupled physics simulation capability demonstrated for interface with virtual reactor;

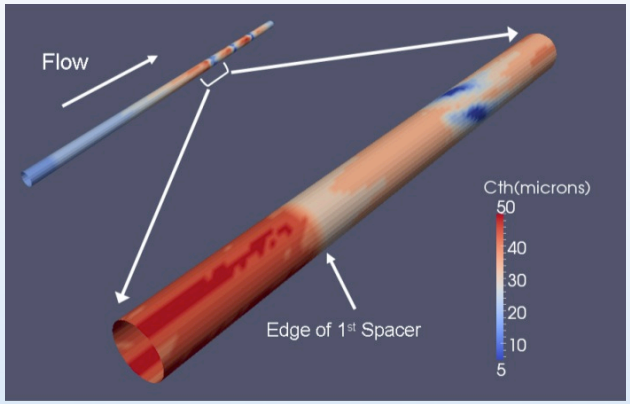
PCI



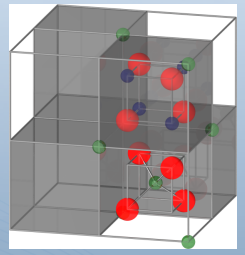
Peregrine
(Fuel Performance)

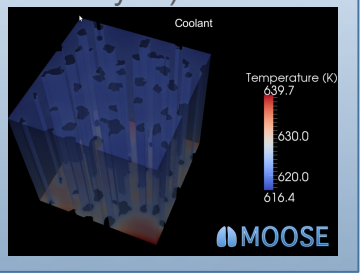


CRUD

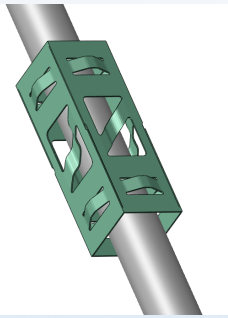


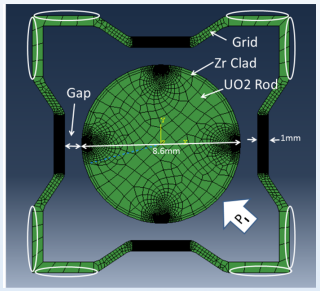
MAMBA
(MPO Advanced Model for Boron Analysis)



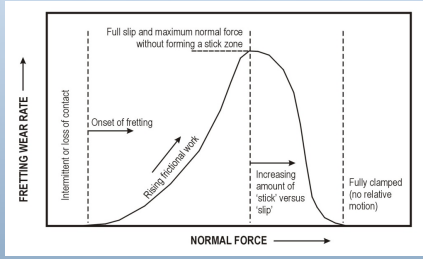


GTRF





Structural Mechanics & WEAR MODELS



Microscale activities underway to provide mechanistic/physical insight into complex degradation phenomena

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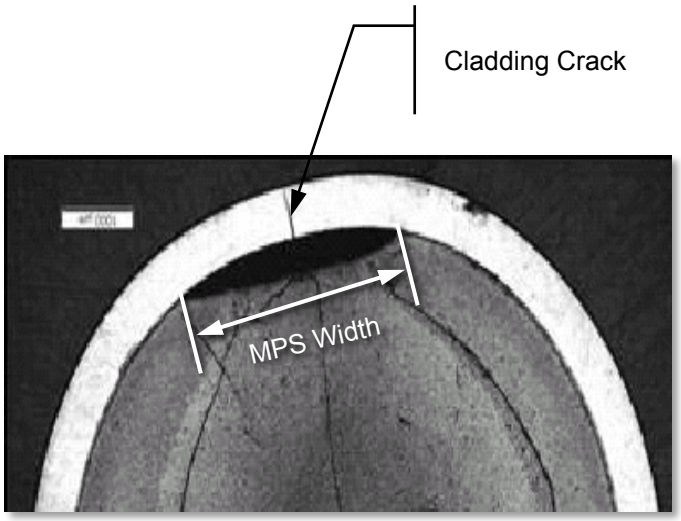
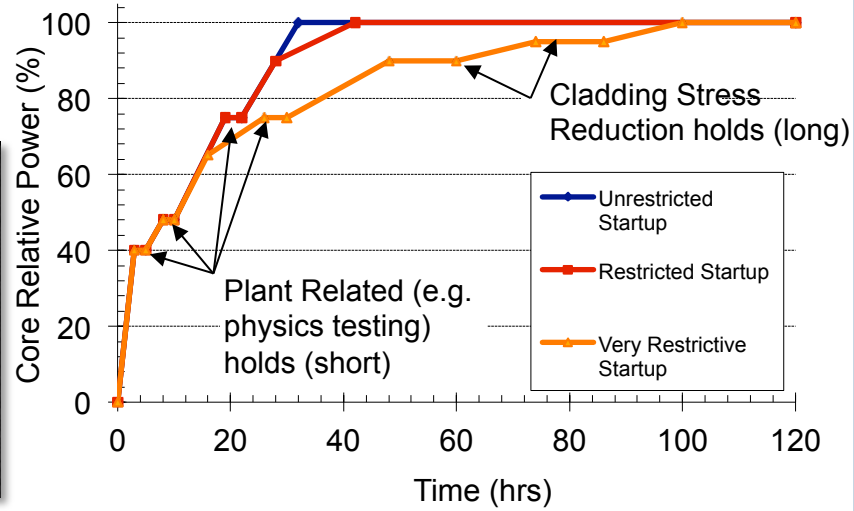
PCI Challenge Problem

Typical MPS Defect in PWR Fuel



Impact of MPS Defect on Power Operation



Question posed by industry:

"What specific benefits will be realized after CASL completes its PCI Challenge Problem?"

Answers:

1. 3D fuel performance, i.e. Peregrine
2. Improved materials/behavioral models
3. Coupled fuel performance, neutronics and thermal hydraulics

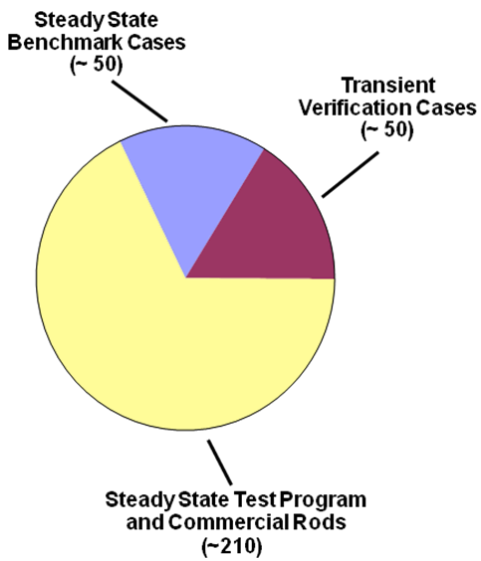
The above answers combine to reduce uncertainty

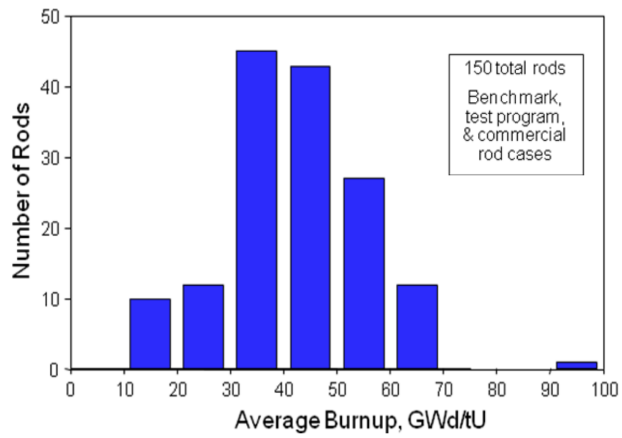
Validation and Benchmarking of Peregrine

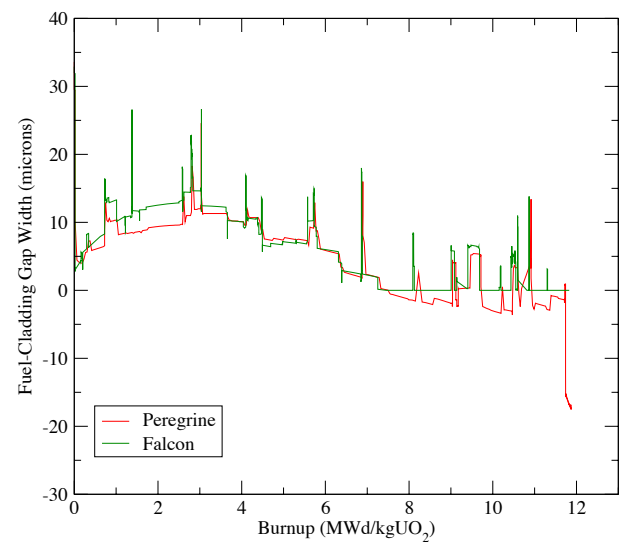
- Emulating rigorous and systematic benchmarking approach of Falcon
- Evaluate Peregrine to calculate the thermal, mechanical, and irradiation behavior of UO_2/Zr-alloy fuel rods
- 30 test rods (of 300+ in Falcon database) selected to evaluate key phenomena: First priority = temperature comparisons, second priority = cladding deformation, third priority = PCI ramp tests fail/no fail

TEAM:

Robert Montgomery
Wenfeng Liu
Dion Sunderland
Joe Rashid
Nathan Capps
Brian Wirth
Jason Hales
Chris Stanek







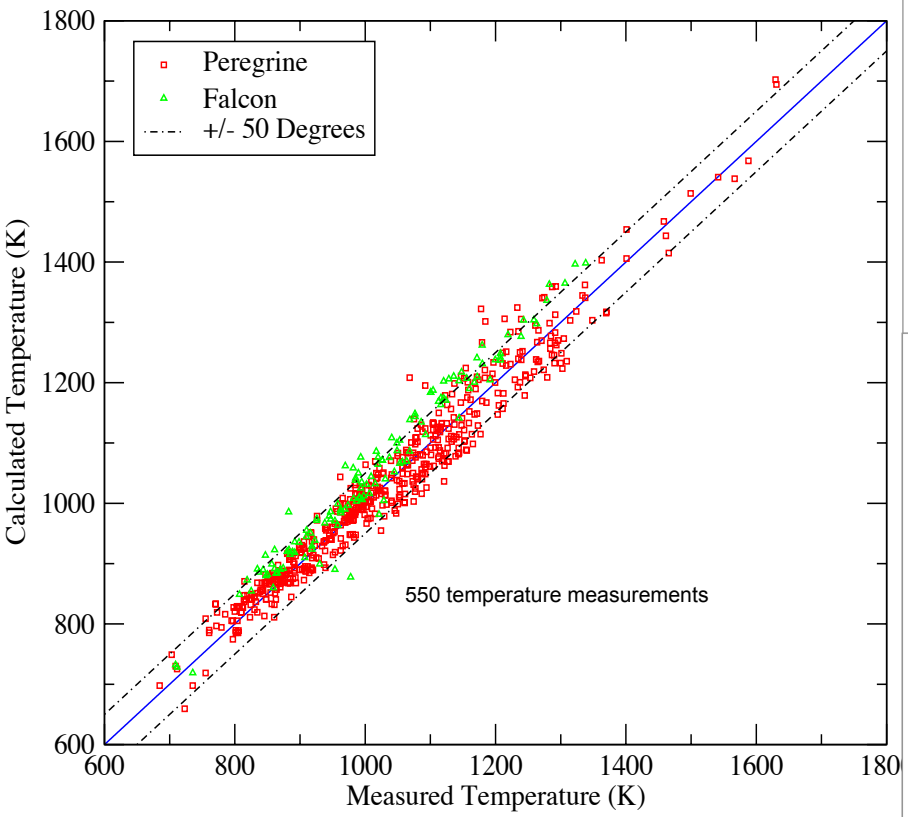
Peregrine is on par with industry standard codes (e.g. FALCON) up to 75 GWd/tU

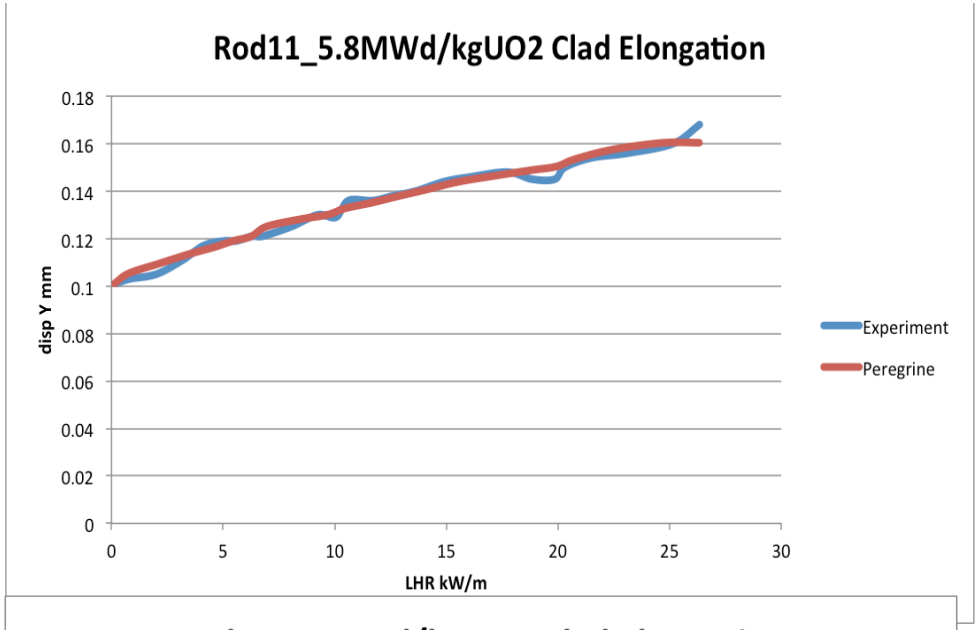
Path Forward:

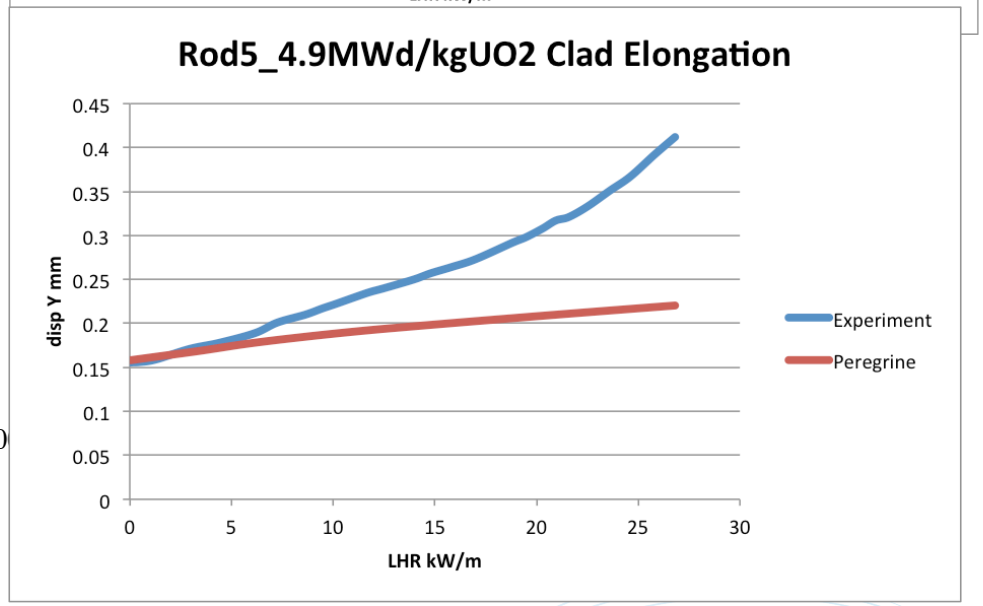
Expand to 3D and improve physics-based models

* CASL-I-2013-0122-000 and CASL-I-2013-0165-000

Peregrine: V&V Experience







Improved materials and behavioral models will provide for higher fidelity calculations of time dependent phenomena

Improved Mechanistic Models of Cladding Deformation

VPSC successfully integrated in to Peregrine and constitutive models include creep, growth and plastic deformation of Zr-4

Improved models for clad deformation required for PCI and safety assessments

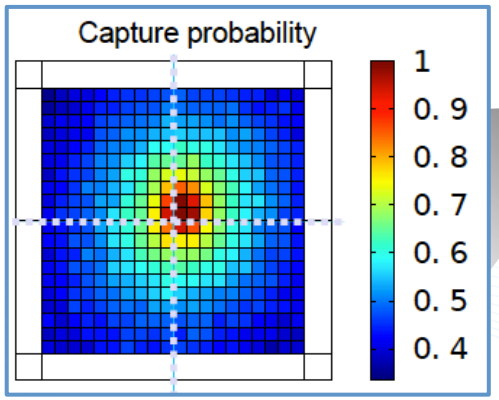
TEAM:

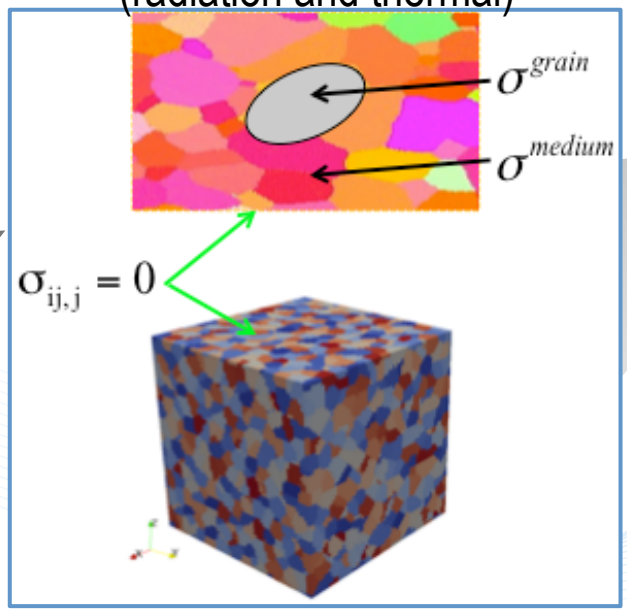
Carlos Tome
Alankar
Gopinath Subramanian
Stas Golubov
Sasha Barashev
Roger Stoller
Jason Hales

Los Alamos NATIONAL LABORATORY EST. 1943
OAK RIDGE National Laboratory
INL Idaho National Laboratory

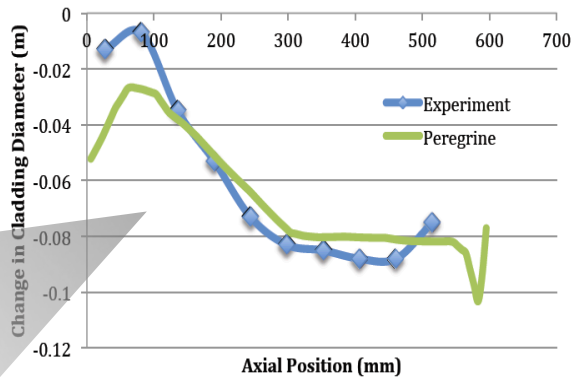
Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)

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





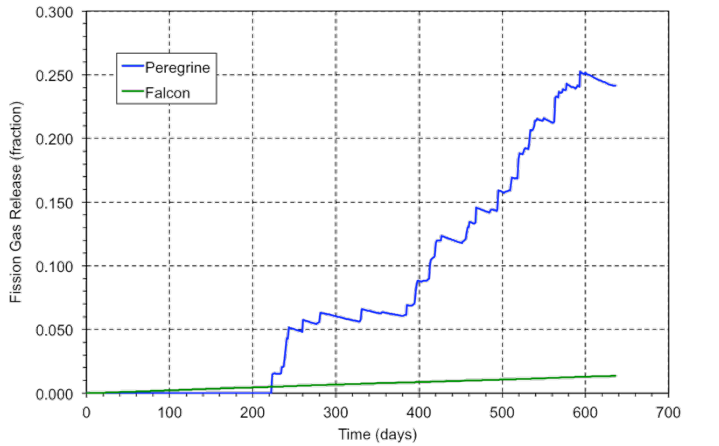
Peregrine engineering scale fuel performance

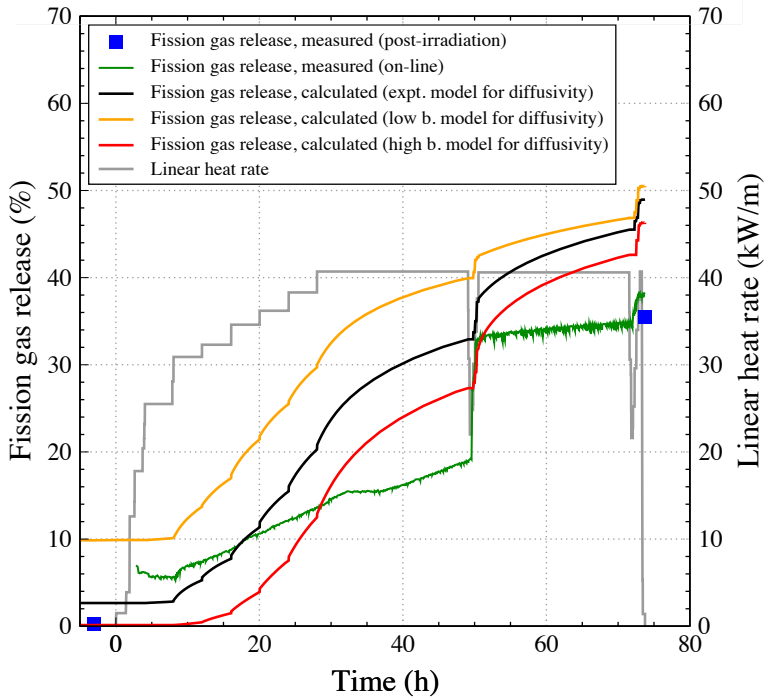


* Alankar and Tome, LA-UR-13-25085

CASL Consortium for Advanced Simulation of LWRs

Positive Interaction with NEAMS-Fuels

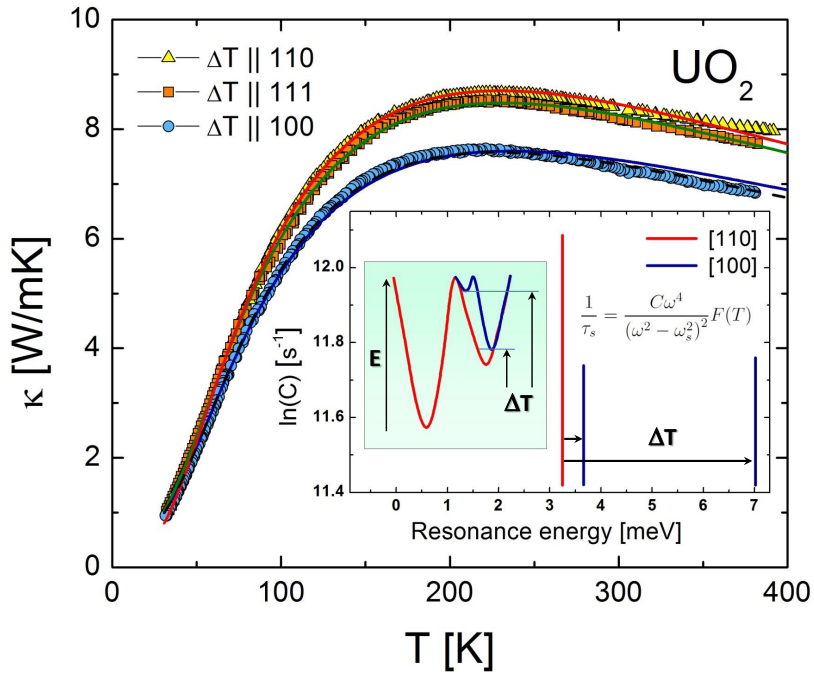




Fission Gas Release

CASL and NEAMS share fuel performance modeling framework.

Additionally, opportunities exist to improve the fidelity of fuel performance models for mutual benefit.

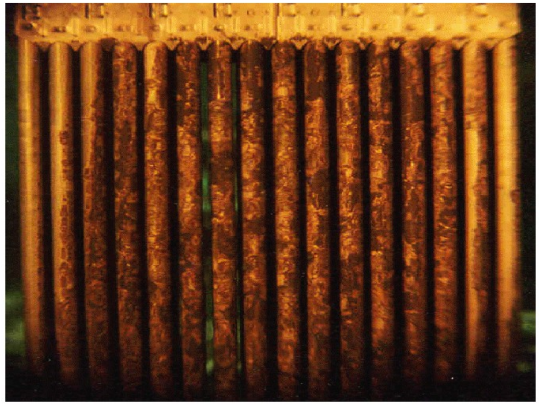


Thermal Conductivity

CRUD Challenge Problem:

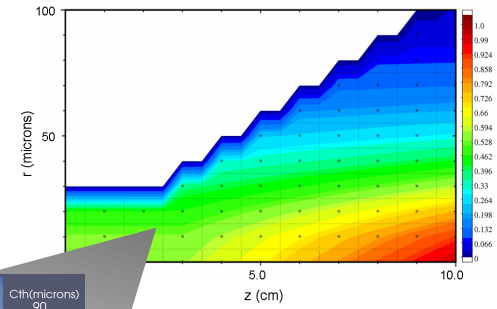
Motivation and Key Issues

- Chalk River Unidentified Deposit, is predominately a nickel-ferrite spinel corrosion product that deposits on hot fuel clad surfaces in nuclear reactors.
- For **performance** issues, CRUD incorporates lithium and boron impurities. Boron, in particular, is a strong neutron absorber – and thus leads to reactor power level variations known as axial offset anomaly
- For **reliability** issues, CRUD deposits are responsible for local temperature increases that can further accelerate CRUD formation rates, leading to localized corrosion induced failures.
- **Need** = accurate prediction of CRUD formation, including both the thickness, composition and the effects of CRUD on temperature(/corrosion rates) and reactor power level (which is complementary to existing industrial capabilities, e.g. BOA)



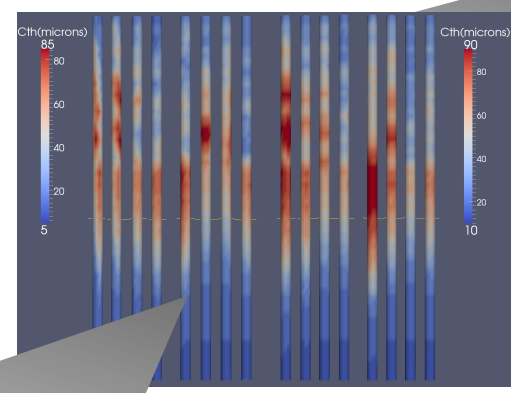
MPO Approach to CRUD

Pragmatic multiscale approach, complementary to BOA, to address the physics/chemistry of CRUD formation and growth, and subsequent impact on CIPS and CILC.



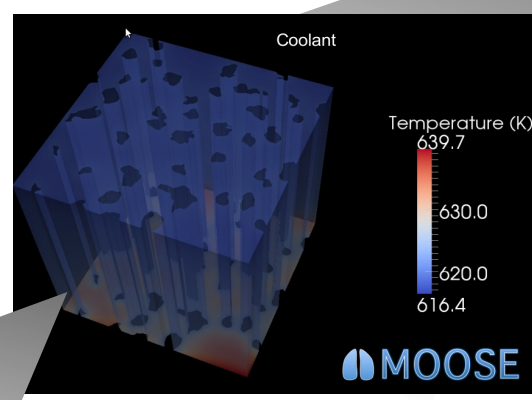
2D MAMBA

Pin-scale CRUD formation/ growth model, which can be used for VERA-CS CIPS-risk analysis (assemblies)



3D MAMBA

Pin-scale CRUD formation/growth model, which can be used for VERA CIPS-risk analysis (single to few pins)

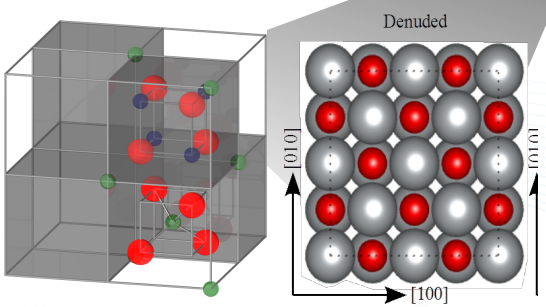


MAMBA-BDM

Microscale CRUD formation/growth model, which can be used for CILC-risk analysis

Thermodynamics

Mostly atomistic scale calculations that address CRUD phase stability, nonstoichiometry, solvation and potentially source term



Benefit to Industry:

1. 3D CRUD pin scale model
2. Improved materials models
3. Coupled CRUD, neutronics and thermal hydraulics model

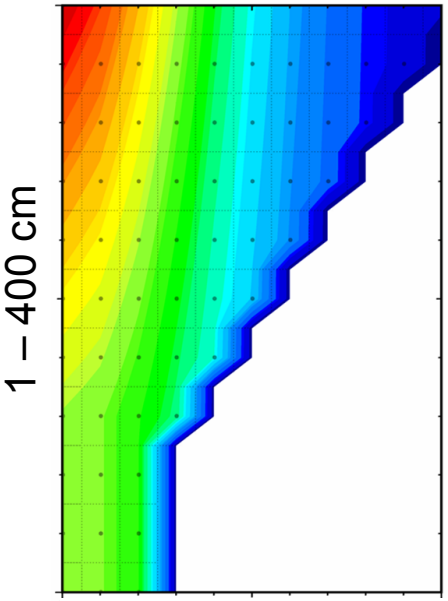
Thermodynamics of Boron Precipitation in PWR CRUD

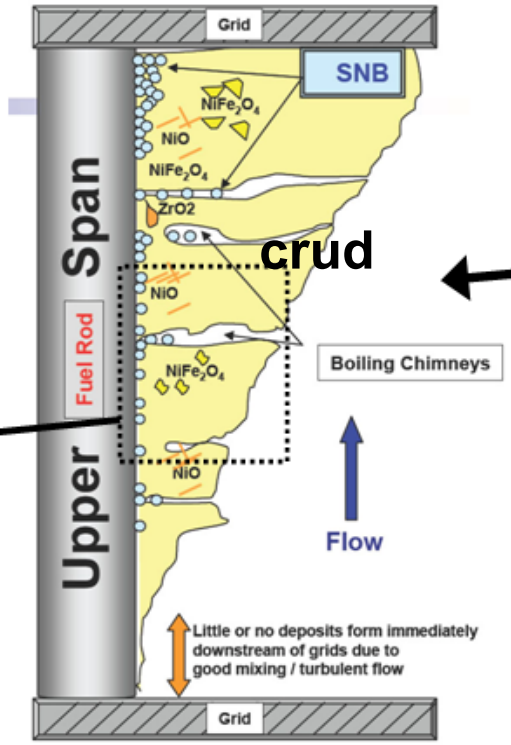
* BOA model has two boron precipitates
  - $LiBO_2$ (lithium metaborate)
  - $Li_2B_4O_7$ (lithium tetraborate)
* CASL-MPO thermodynamic studies have suggested the potential stability of other phases:
  - HBO_2 (metaborite)
  - B_2O_3 (boron trioxide)
  - Bonnacordite (Ni_2FeBO_5)
* During residual heat removal at a PWR, a boron "rock" comprised of metaborite was discovered.
* Implications for AOA mechanism
  - Multiple boron phases may be present in crud
  - Boric acid volatility is also maximized at high pressure

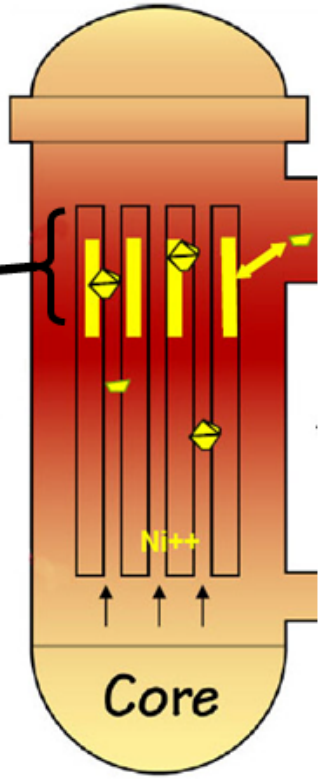
Photo courtesy of Dennis Hussey (EPRI)

MAMBA's 3D Computational Cell

2D profile view

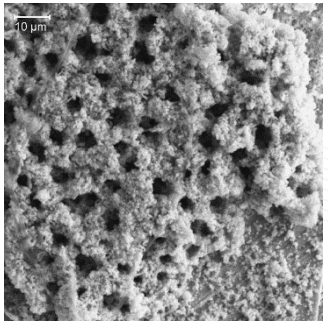


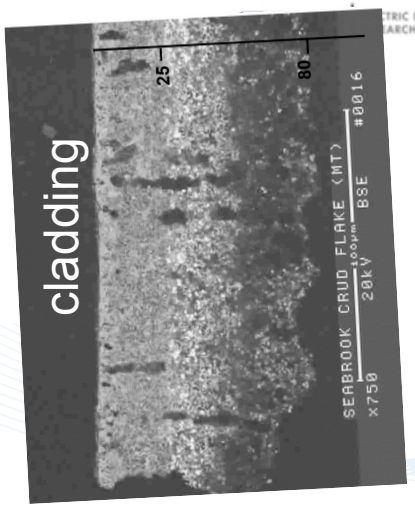




crud

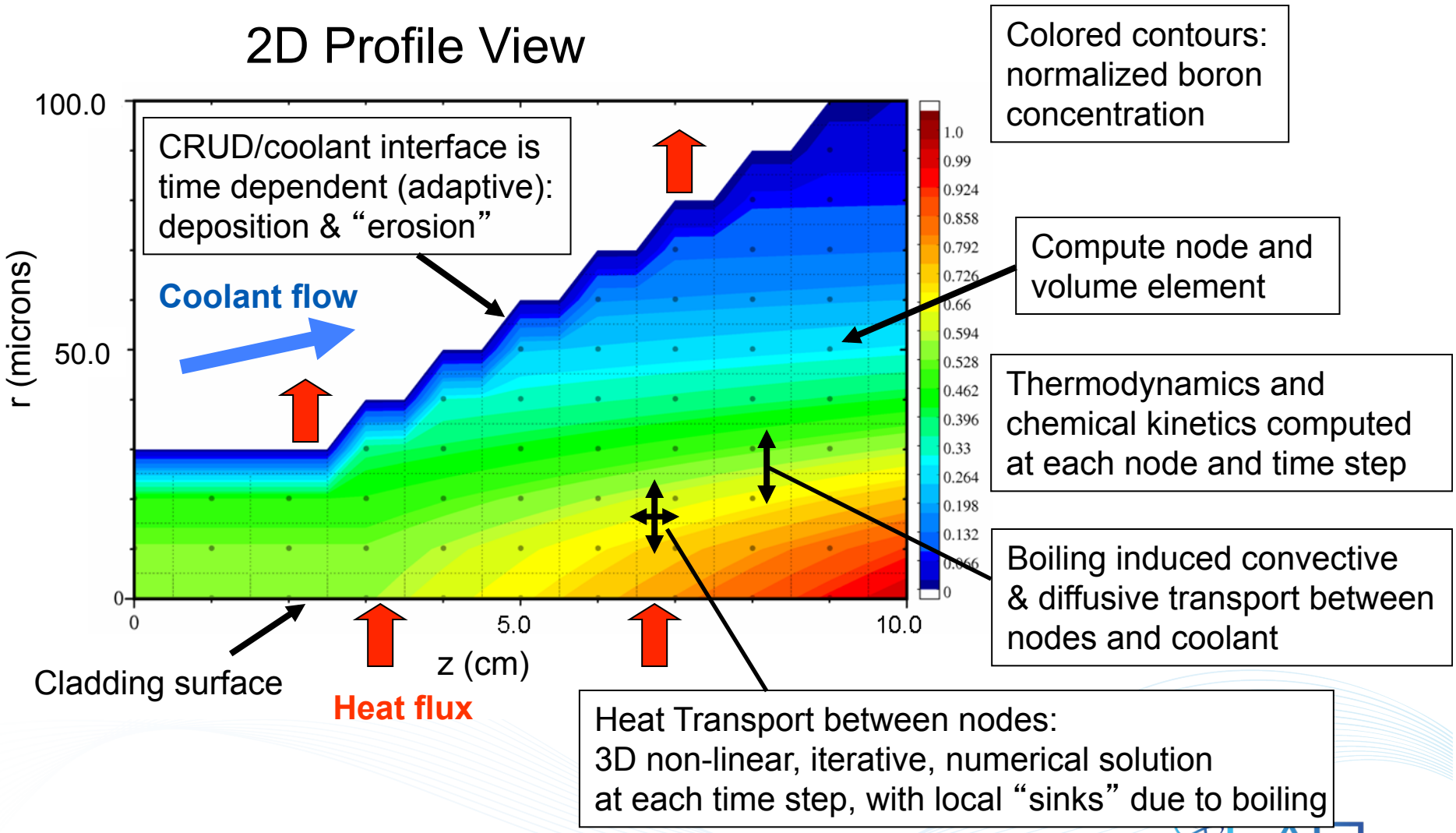
top view



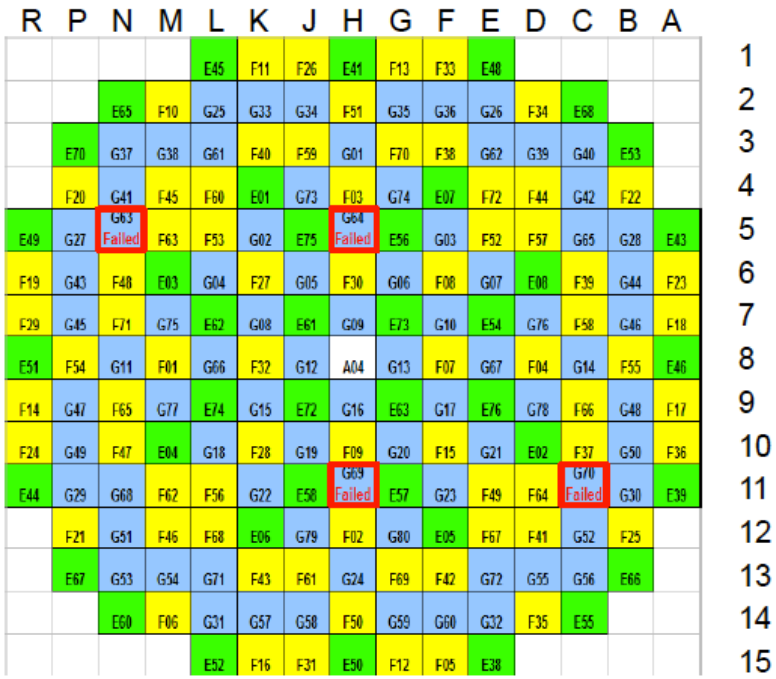


side view

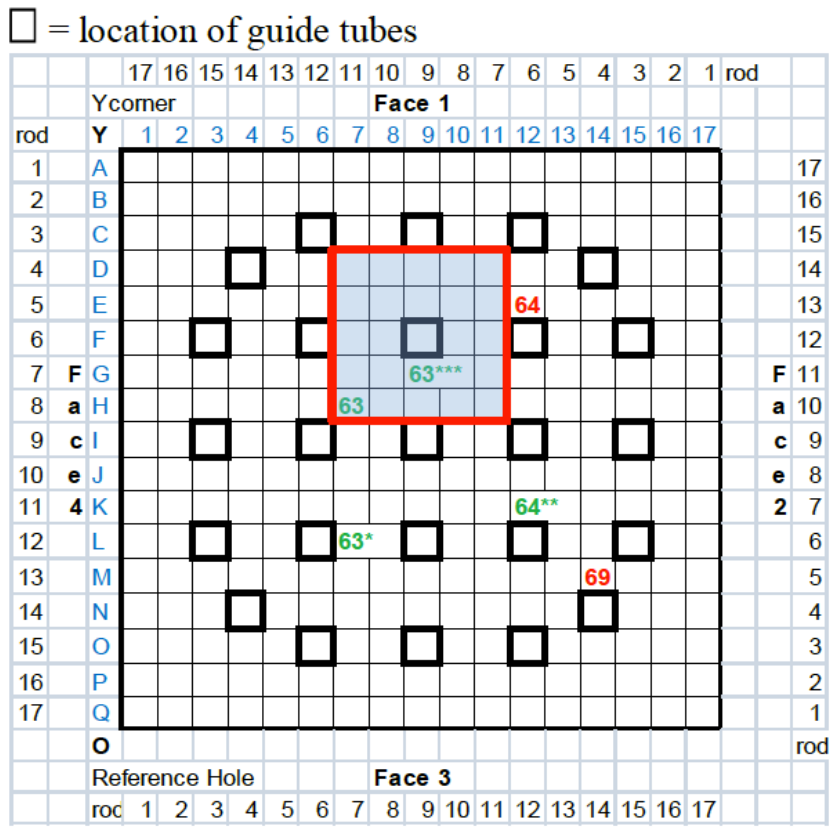
MAMBA example grid:



CIPS/CILC Analysis Compared to Existing Plant Data



Core configuration (assemblies with failed rods noted by red boxes)



Assembly map (where red box denotes 5x5 simulation cell)

TEAM:
Dennis Hussey
Jeff Secker
Zeses Karoutas
Brian Kendrick
John Barber
Annalisa Manera
Victor Petrov
Dan Walter
Tom Downar
Mike Short

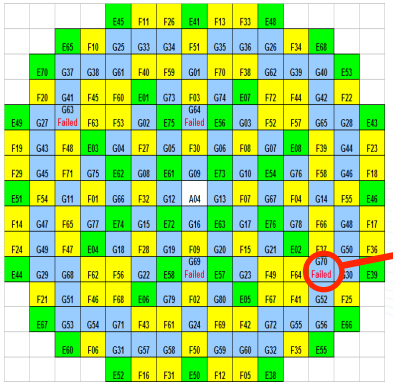
5x5 Sub-assemblies identified for Star-CCM+ - 3D MAMBA analysis for plant/cycle that experienced CRUD-related issues, and for which input and rod examination data (e.g. oxide thickness) exists.

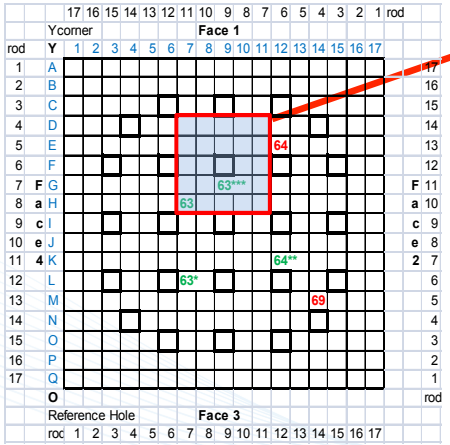
* CASL-U-2013-0224-000

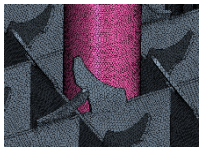
Simulation of Seabrook 1 Cycle 5 CRUD formation using coupled STAR-CCM+ and MAMBA3D

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

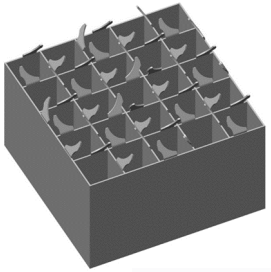
- 5-rod by 5-rod array for which qualitative and quantitative data is available was selected for analysis
- First high-fidelity, two-way coupled CFD/CRUD simulation of an industrial relevant plant cycle
- Input power provided by industry simulations
- Showed that <u>both</u> axial and azimuthal thermal hydraulic effects dramaticall 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

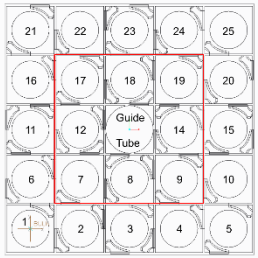






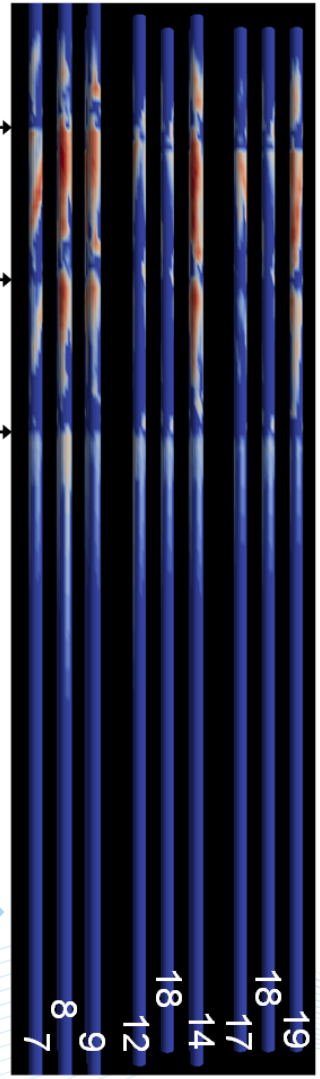
STAR-CCM+
5x5 spacer grid





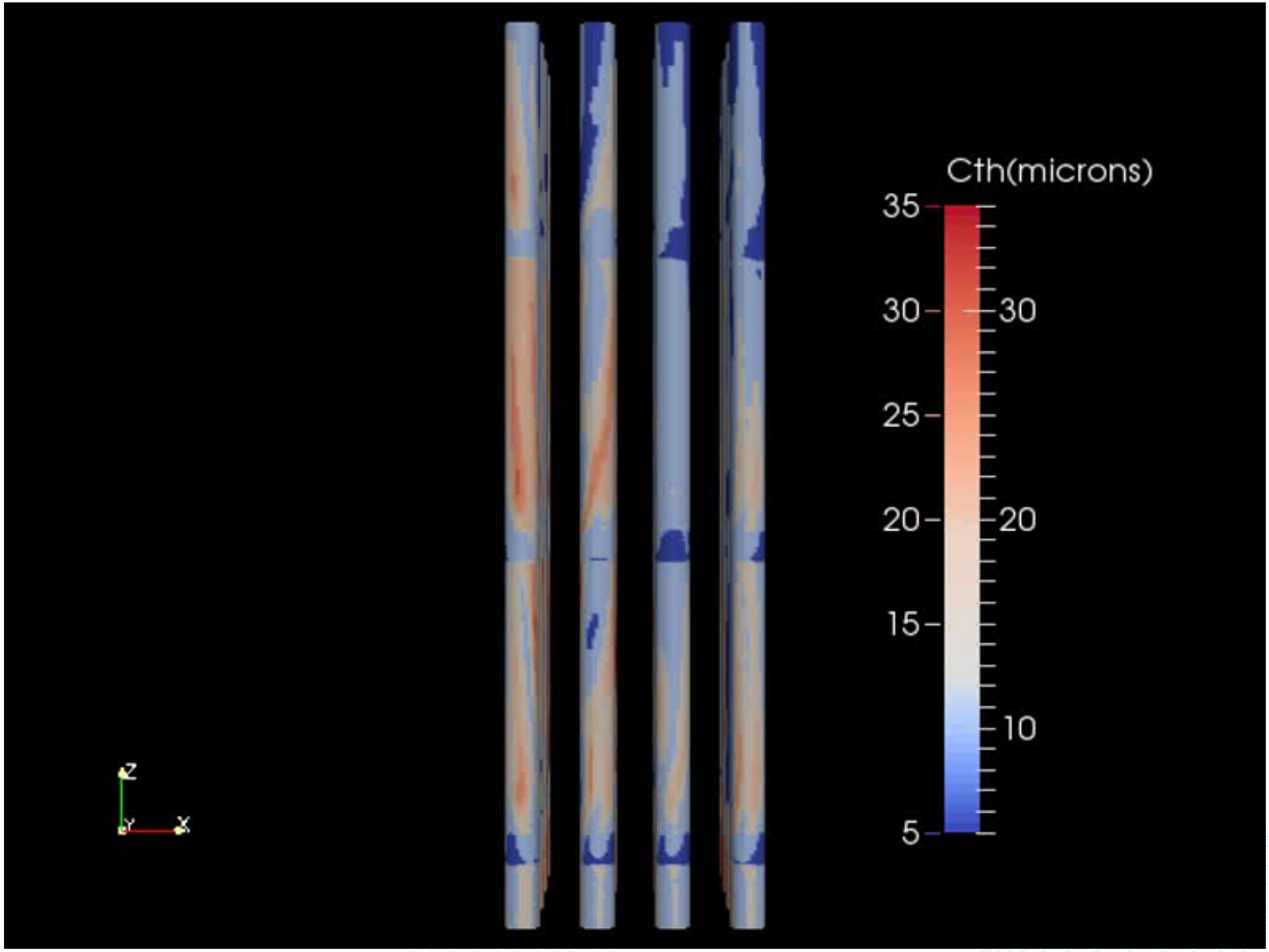
view

CRUD (red)

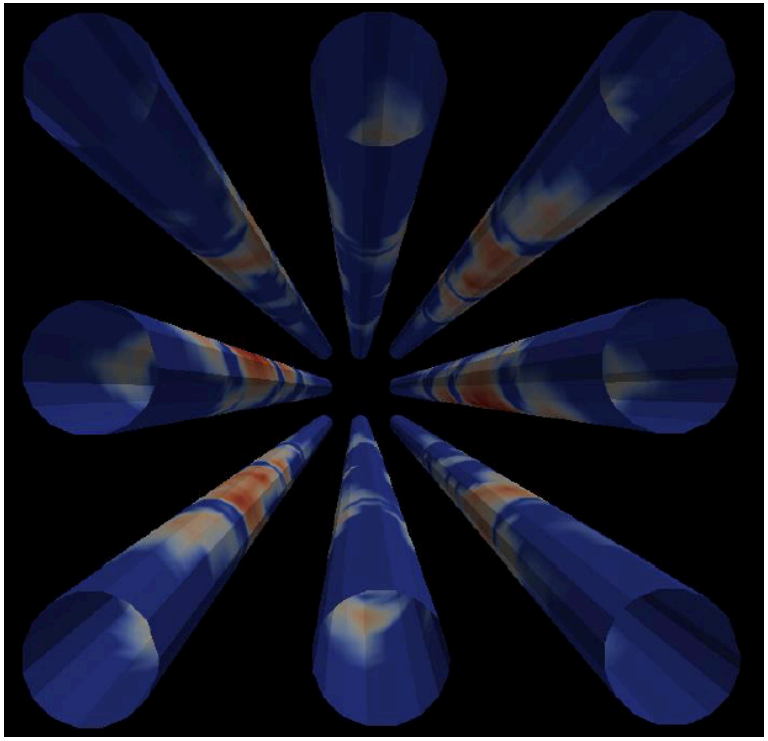


* CASL-U-2013-0224-000

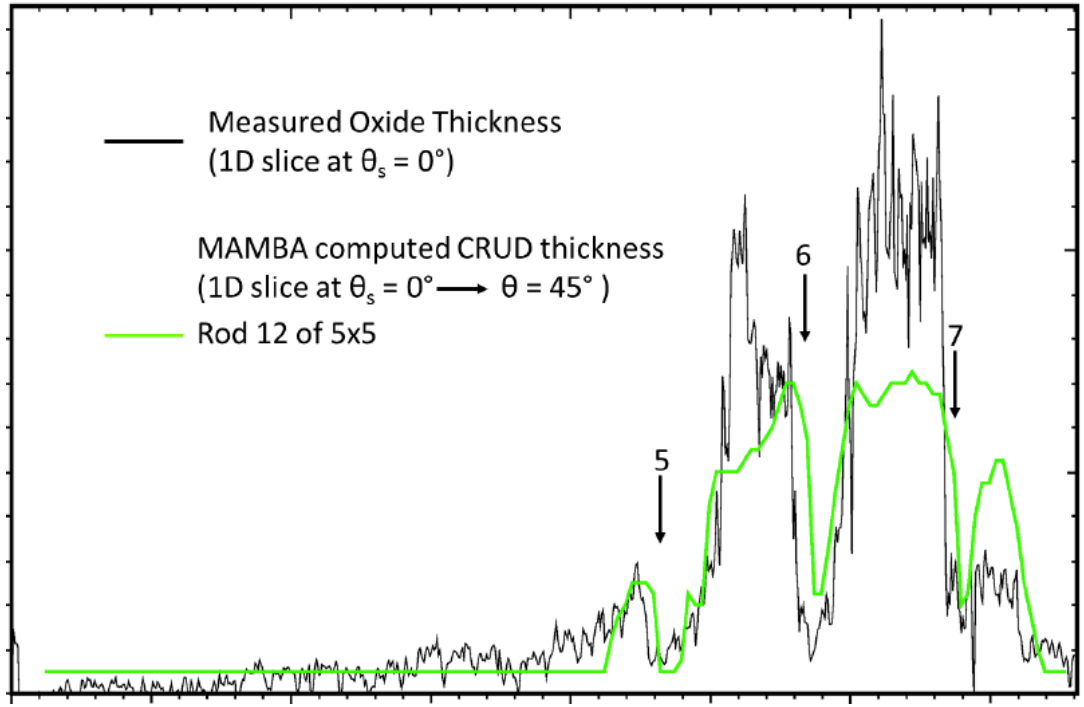
Preliminary 4x4 3D MAMBA Results



Coupled MAMBA-CFD Comparison to Plant Data



First high-fidelity, two-way coupled CFD/ CRUD simulation of an industrial relevant plant cycle



Both axial position and azimuthal thermal hydraulic flow dramatically affect CRUD deposition patterns

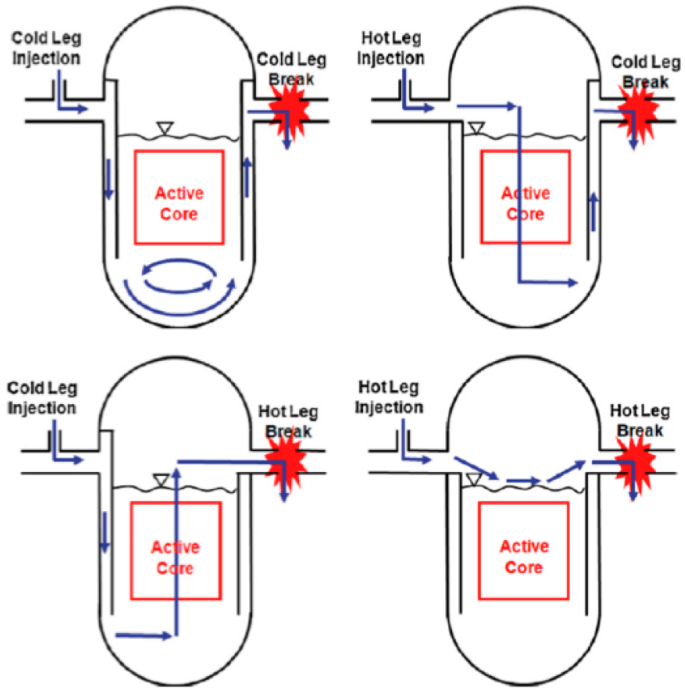
Initial comparison to plant oxide thickness data encouraging

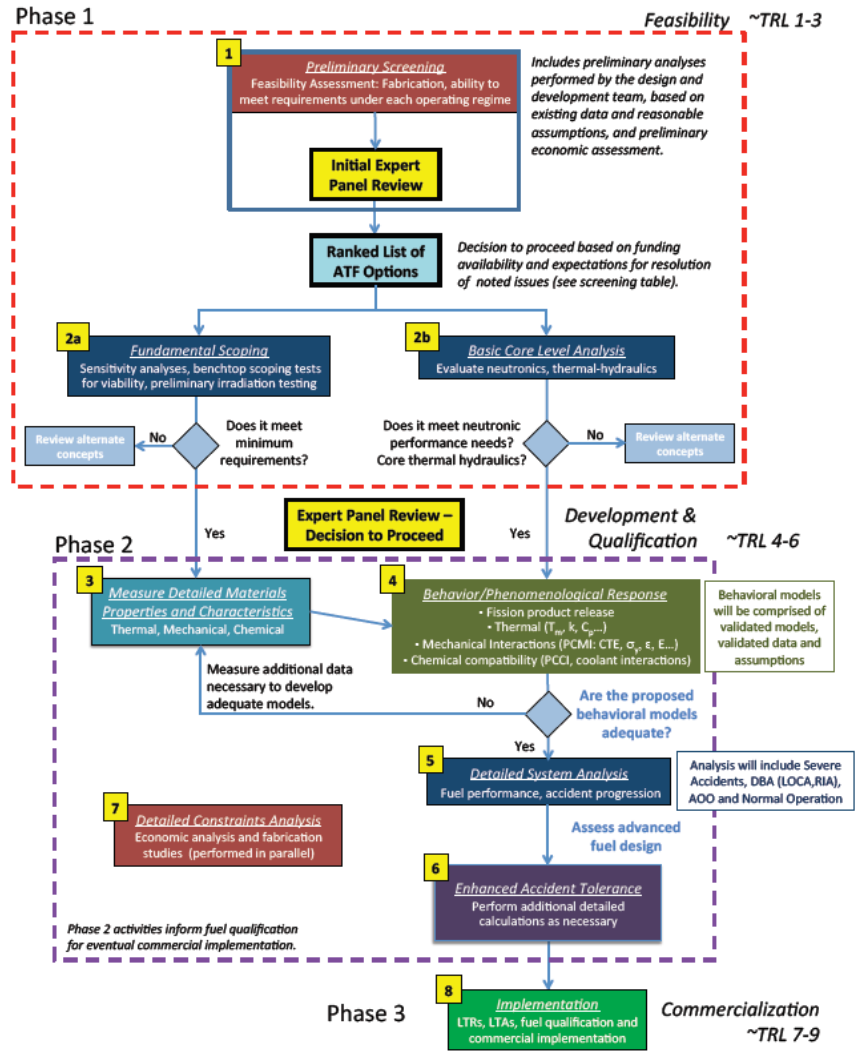
Improvements to BOA v3.1 are due to close coordination with the MAMBA team

MPO has established important foundational capability required for potential Phase 2 scope

Extension of fuel performance and chemistry capability to e.g. BWRs or iPWRs is evident

Other topics could leverage Phase 1 capability, e.g. Boron Acid Precipitation and Assessment of Accident Tolerant Fuels

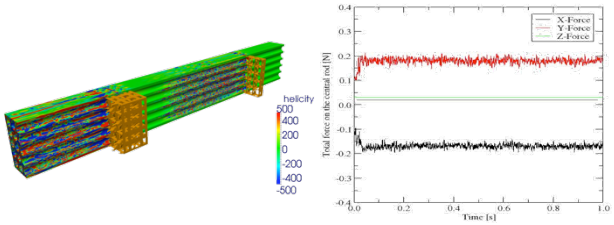




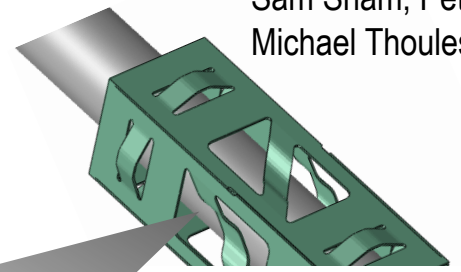
Opportunity and need for mechanistic/behavioral models to enable accurate predications of time dependent 3D fuel performance

CASL Approach to GTRF

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

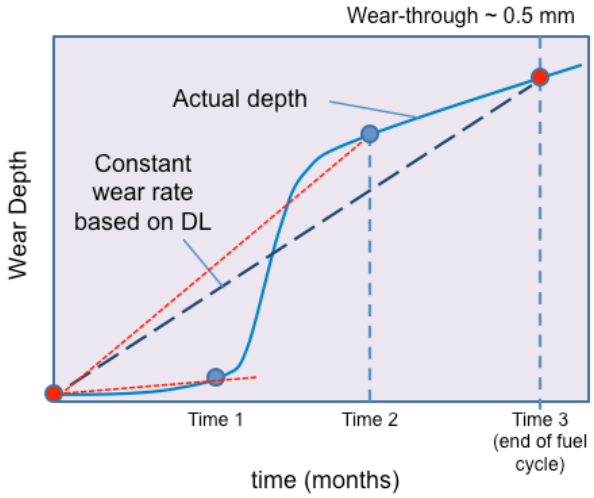


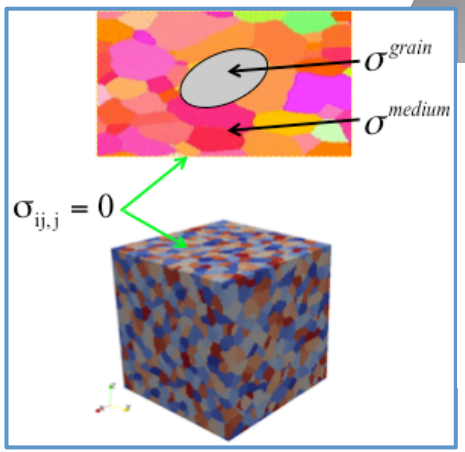
CFD Pressure Load History (Hydra-TH)

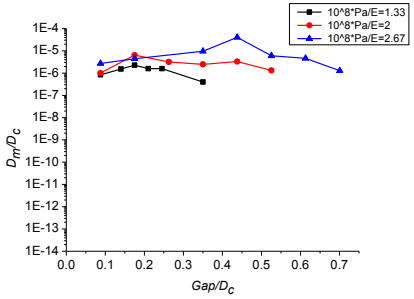


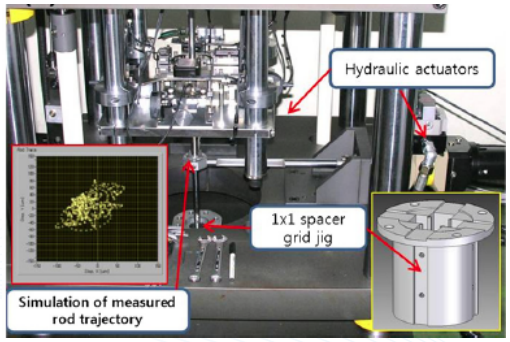
Structural mechanics

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







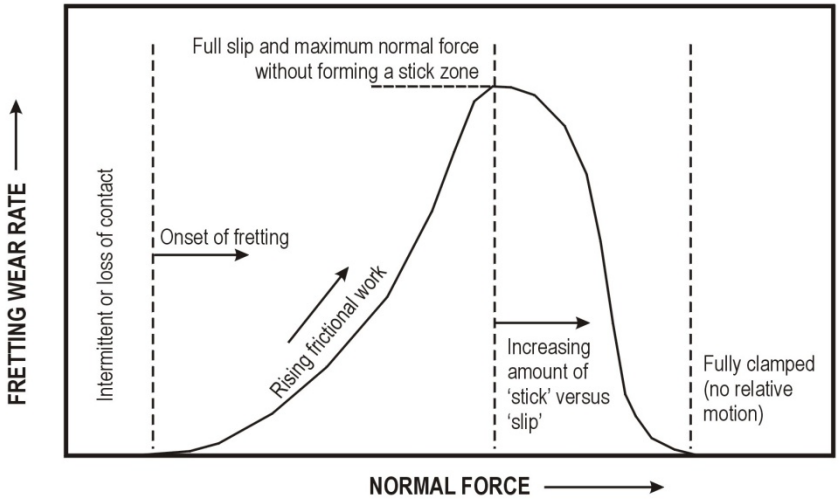


ORNL/KAERI controlled fretting wear measurements

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

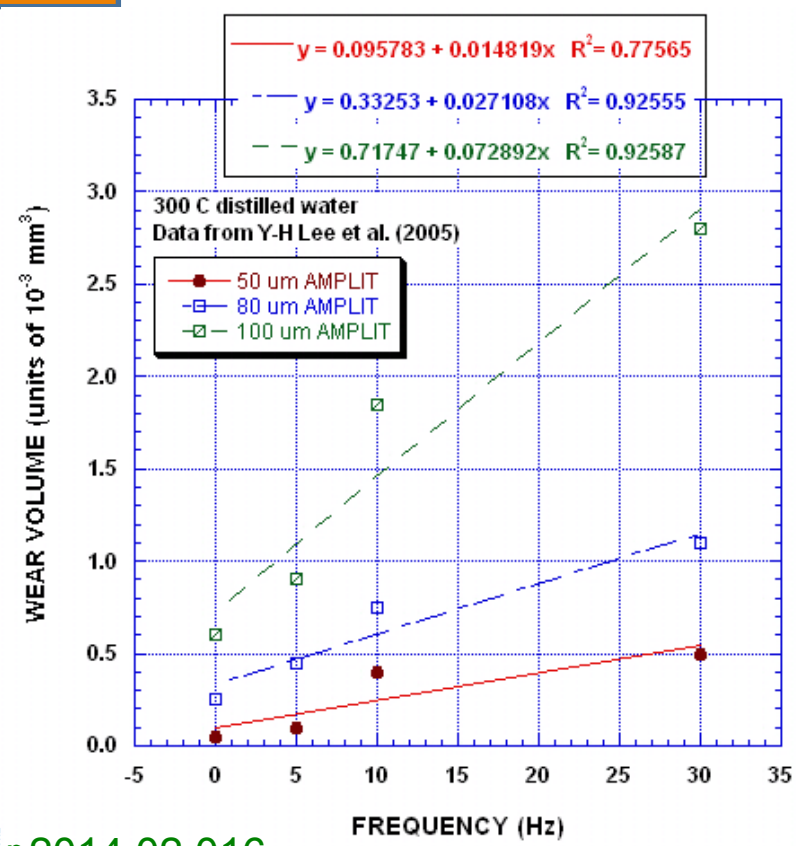
Engineering Wear Model development*

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



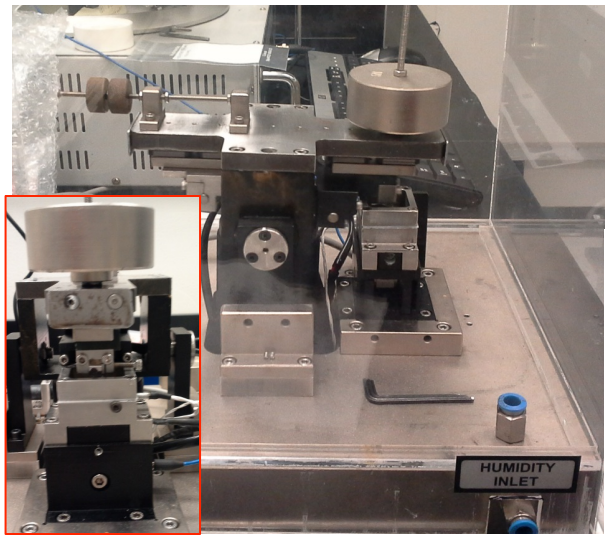
If normal force is either too high or two low, fretting is reduced or stopped.

High frequencies of impact and large oscillation amplitudes increase the wear rate.



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

Engineering Wear Model development

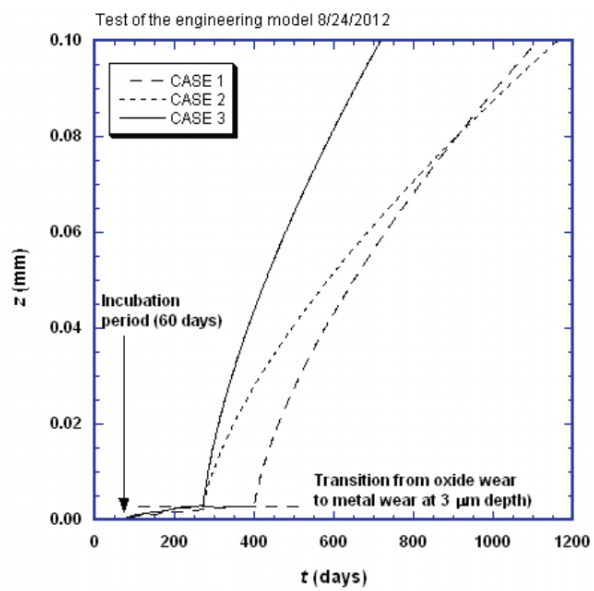


TR282 fretting wear testing at ORNL suitable for friction/wear testing under dry or lubricated conditions, ball on disk or tube or tube – provide laboratory data for engineering wear model validatic

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

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

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



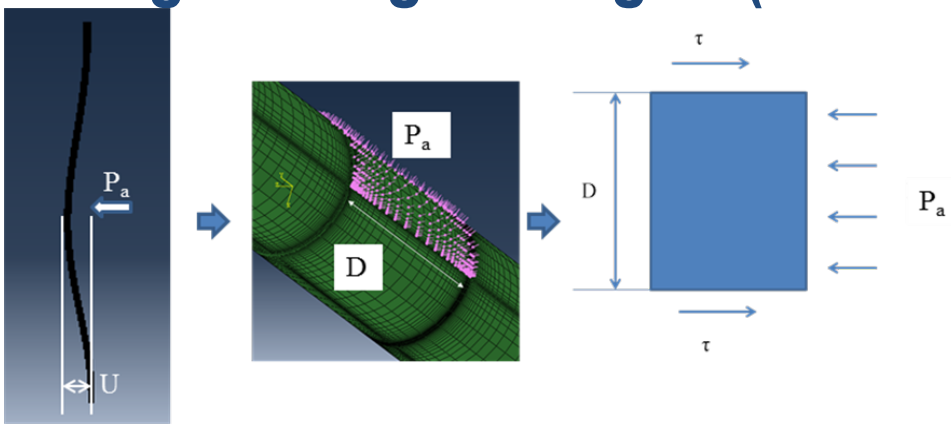
(μ) Friction coefficient

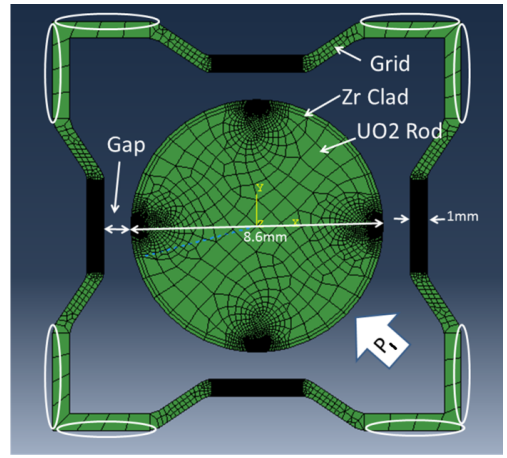
(P_{rec}) Normal force during time t

(X_{eff}) amplitude of oscillation

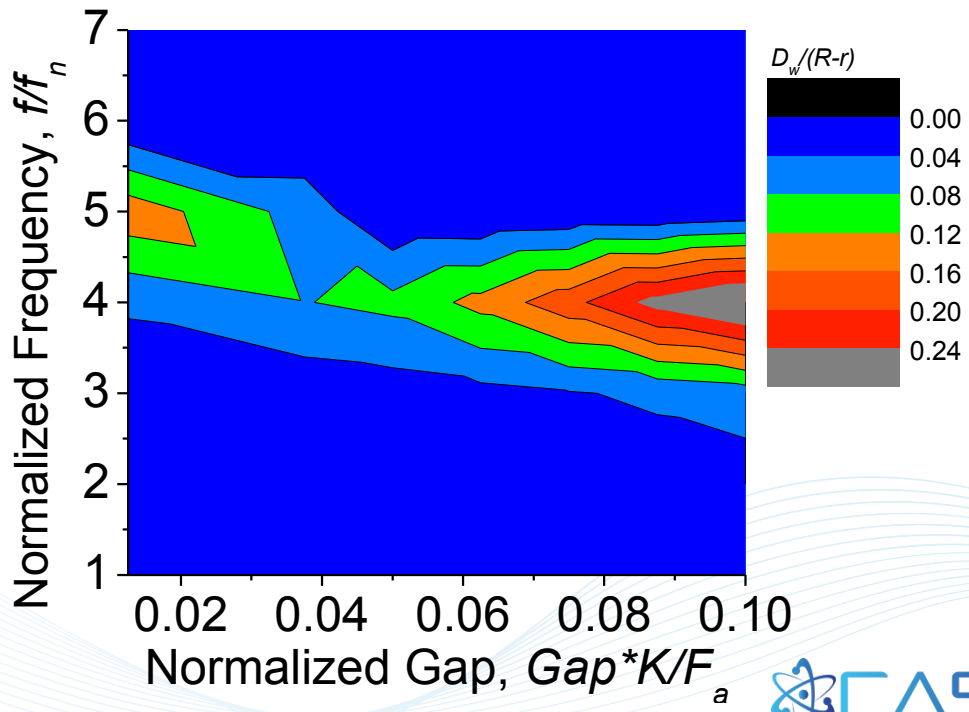
(f) oscillation frequency

Parametric variation of key assumptions within GTRF using 3D single cell grid (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' showing the overall dependence on grid-to-rod gap and load frequency



Mechanical Engineering

Consortium for Advanced Simulation of LWRs

Summary

- MPO benefits from: (1) strong working relationship between Industry, National Laboratories and Universities, and (2) challenge problem oriented focus

- Benchmarking of CRUD and PCI tools has demonstrated that MAMBA and Peregrine are on par with industry standard tools – Engineering Wear Model for GTRF under development.

- Much work still exists to improve materials and behavioral models resident within engineering scale capabilities, which will be benefited by effective coordination with other programs, e.g. NEAMS, EFRCs, etc.

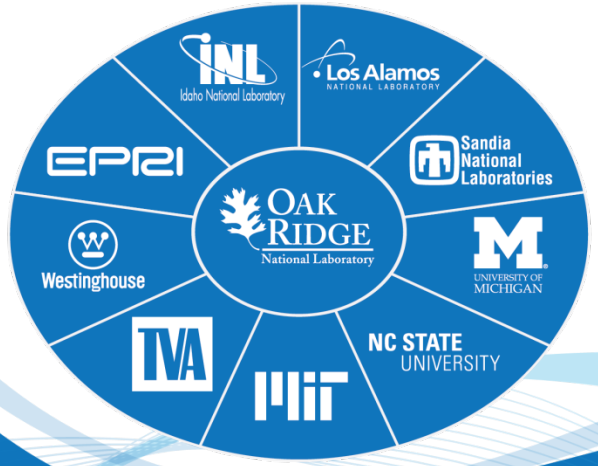
- Validation data remains a challenge, especially for the more fundamental activities.

- Path forward: Continue to merge fundamental models in to engineering scale capabilities and work across DOE programs to integrate complex multi-physics

A great deal of progress has been made, but "much work looms ahead to maintain momentum."

VERA Releases & Licensing

Matt Sieger
CASL QA/Release Manager



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

VERA 2013 Test & Evaluation Release

- First release of selected components to non-CASL participants
  - The ORNL Radiation Shielding Information Computational Center (RSICC) is coordinating the release
  - Distribution to users is subject to CASL approval
  - Available under a Test & Evaluation license agreement
  - Limited support
- Criteria for approval
  - Appropriate export control
  - Agree to Test & Evaluation license
  - The customer has a valid usage for VERA
  - Feedback from the customer is likely to inform future VERA development efforts
- Lays groundwork for future VERA releases
  - Exercise of the CASL release & support processes
  - Provide subset of VERA components for testing and evaluation by others

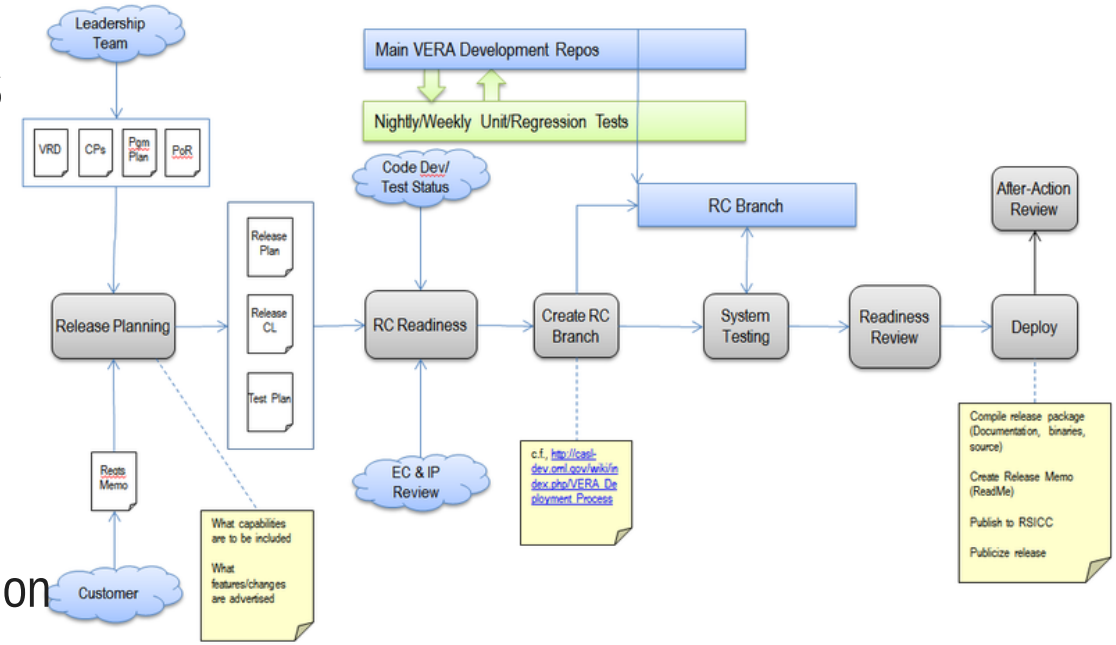
VERA 2013 Test & Evaluation Release Components

Component	Physics	Comments
COBRA-TF	Subchannel T/H	Standalone with VERAIn input.
Insilico	Neutronics	Sn/SPn with SCALE XSProc and VERAIn input.
MPACT	Neutronics	Lattice physics, no 3D.
Core Simulator (Coupled COBRA-TF + Insilico)	Coupled T/H + Neutronics	Single assembly.
Dakota	Uncertainty quantification	Standalone.

+ supporting infrastructure components

CASL Release Process

- A rigorous release process was developed for this release (and will be used going forward)
- Includes:
  - Software testing
  - Generation of release documentation
  - Readiness review
  - Creation of initial user support system
  - After-action review and lessons learned



VERA 2014 Release

- Planning has started for the 2014 VERA Release, targeting November 2014
- Capabilities based on FY14 developments
  - Expected to include full core modeling of multiple PWR cycles, including depletion
  - Fuels modeling
  - Computational Fluid Dynamics
- Plan to include a fuller set of components – updated 2013 release components plus:
  - Hydra-TH (CFD)
  - Peregrine/Bison (Fuel performance)
  - MAMBA (CRUD chemistry)
  - VERA-CS (depletion capability)

Software License Agreements

- What will CASL be prepared to license?
  - VERA in its entirety (including all core simulator and advanced components)
  - Selected VERA components (e.g., those necessary for a CIPS analysis)
- What types of license agreements will CASL execute?
  - ✓ *Open Source:* some of the components are available as open source (currently computational infrastructure components)
  - ✓ *Government Use*: use must fall within scope of an existing government project (in place)
  - ✓ *Test & Evaluation*: use for a limited period (under core partner review)
  - – *Non-Commercial*: restricted to R&D/educational/nonprofit purposes (in progress)
  - – *Commercial*: use as part of a profit-based business plan (in progress)
- Principles
  - Ability to license VERA with a single agreement
  - Consistent terms and conditions for each VERA component
  - Non-commercial and commercial may include minimal license fees

Advanced Computing Tech Team

Alex R. Larzelere

Chair, Advanced Computing Tech Team
Office of Nuclear Energy

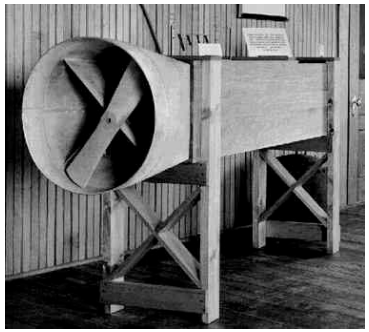
U.S. DEPARTMENT OF ENERGY

Advanced Computing Tech Team

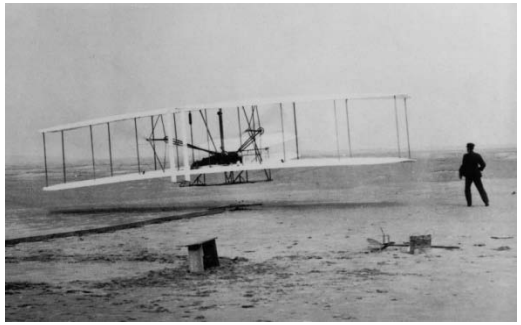
The Question Is . . .

Why did these guys fly?

1901 Wind Tunnel



These guys used this

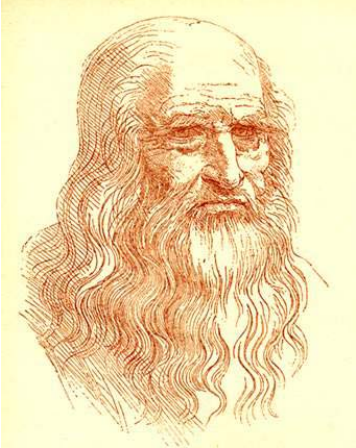


Before they did this in1903

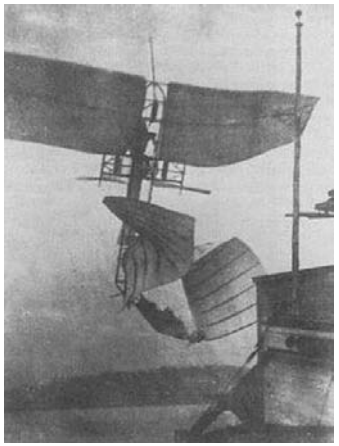
Modeling and Simulation is in the wind tunnel invention business.

When this guy could not?

This guy spent his time studying birds.



And his airplane looked like this.



But flew like this.

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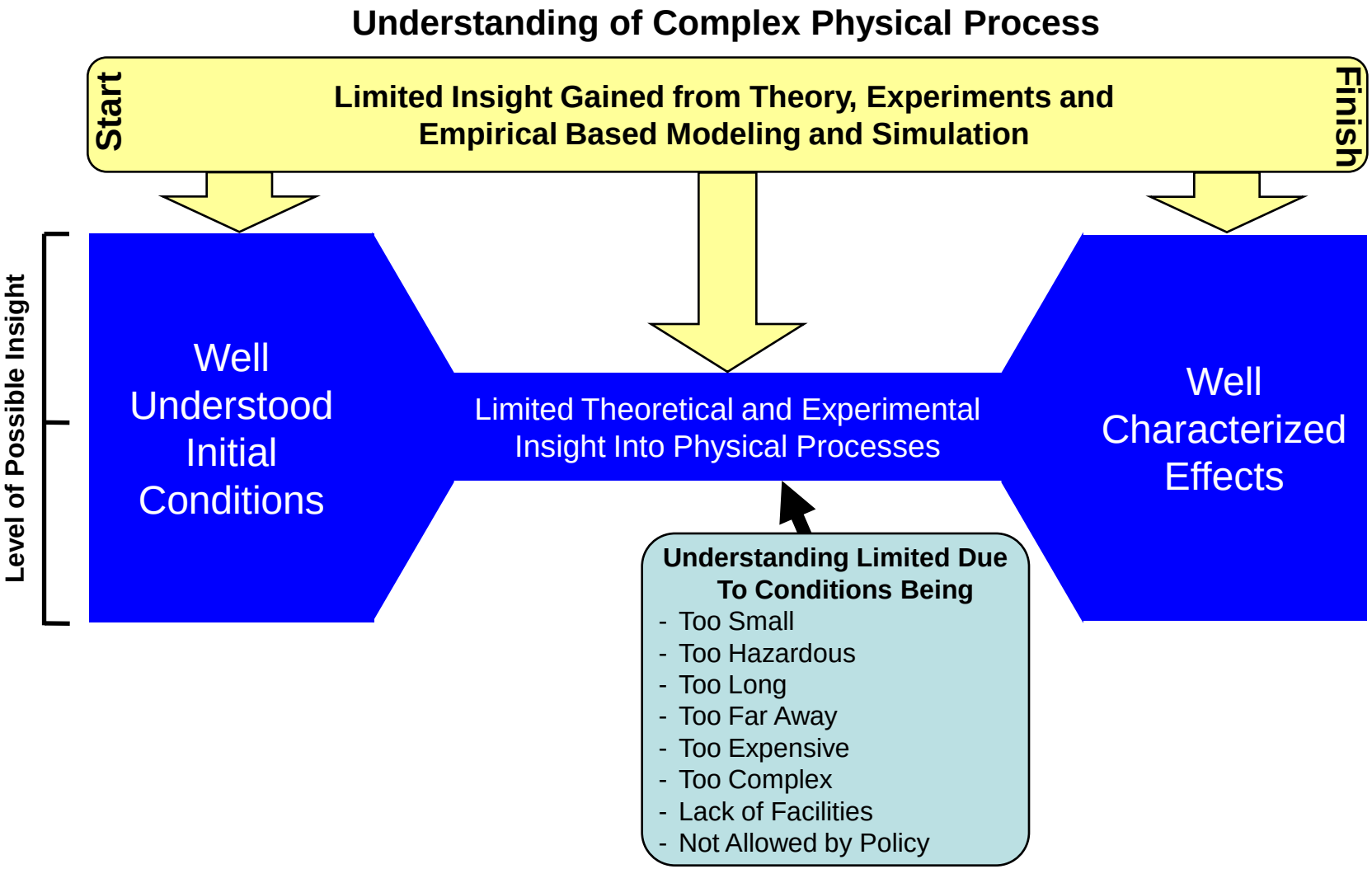
Advanced Computing Tech Team

Why Step Up to New Methods of Gaining Insight?



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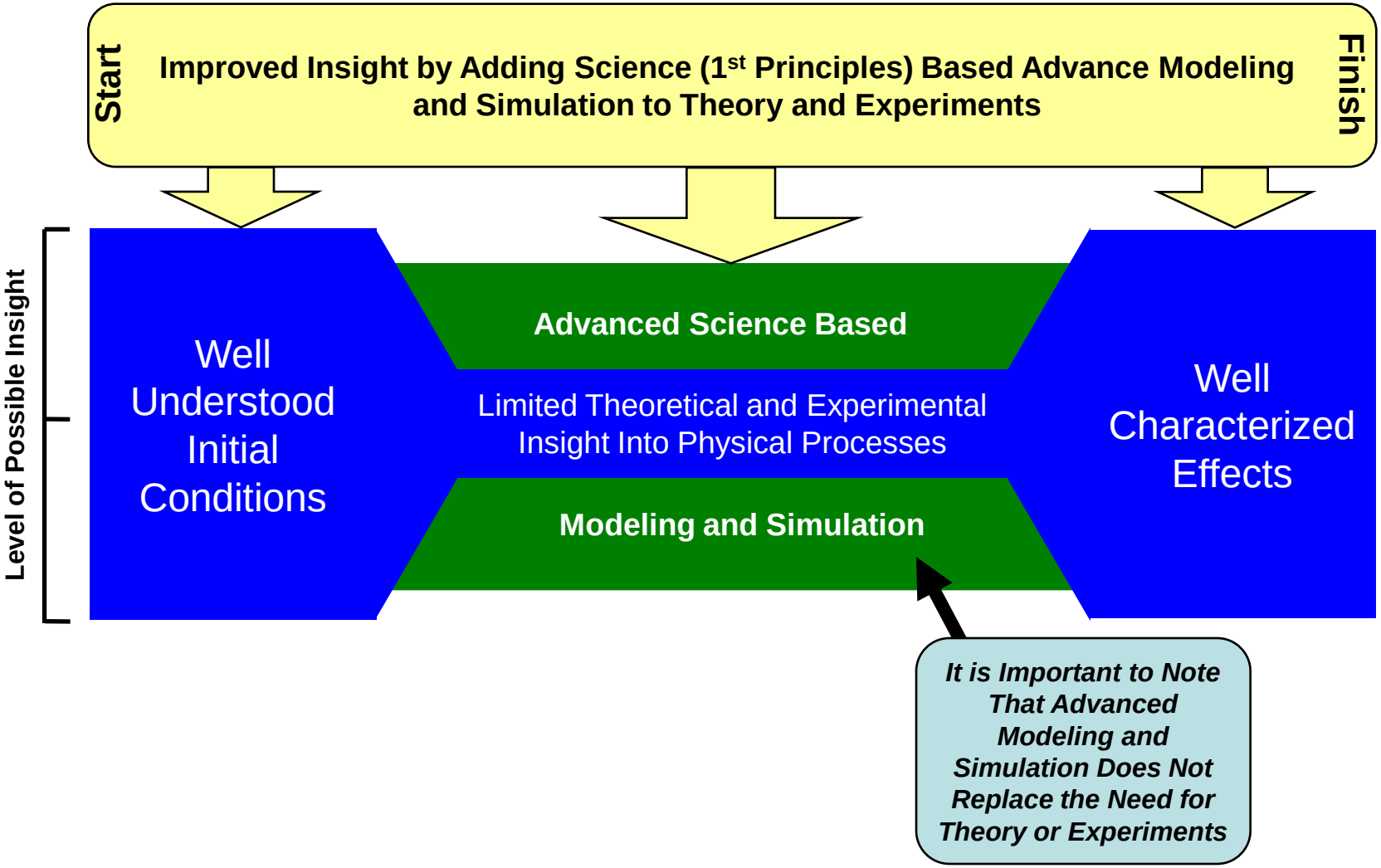
Advanced Modeling and Simulation Enables a New Approach for Gaining Insight

Understanding of Complex Physical Processes



It Started with a Question
Who else is doing this?

- **Broad Definition of Advanced Computing**
  - Advanced
    - Better than the current "state of industry usage"
  - Modeling and simulation
    - Improved dimensionality, resolution and fidelity
  - Data Analytics
    - Extracting knowledge out of large data
  - Enabled by High Performance Computing
    - Hardware, Middleware, Applications Software
    - Capabilities potentially deployable a full range of systems (laptops and up)

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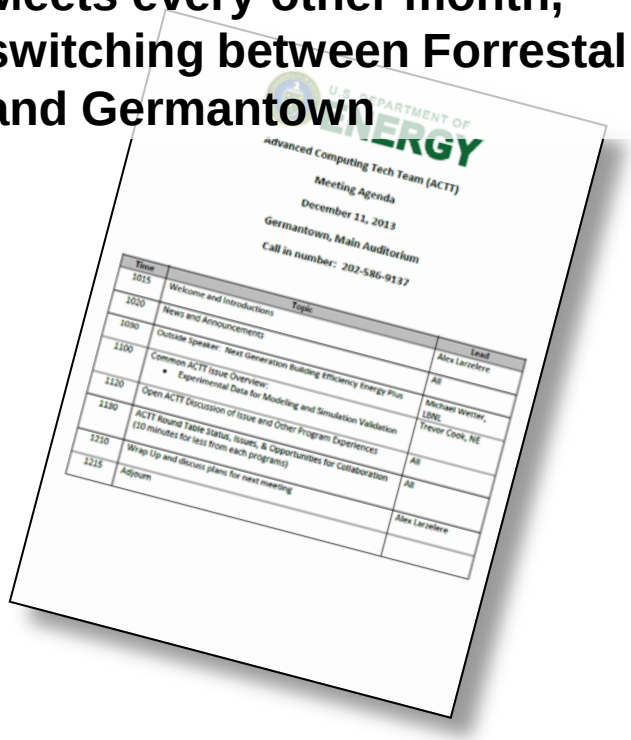
Advanced Computing Tech Team

The ACTT Today

- **Officially Designated a Tech Team by former Secretary Chu in June 2012**
- **Meets every other month, switching between Forrestal and Germantown**



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Advanced Computing Tech Team (ACTT)

Meeting Agenda

December 11, 2013

Germantown, Main Auditorium

Call in number: 202-586-9137

Time	Topic	Lead
1015	Welcome and Introductions	Alex Larzelere
1020	News and Announcements	All
1030	Outside Speaker: Next Generation Building Efficiency Energy Plus	Michael Wetter, LBNL
1100	Common ACTT Issue Overview: • Experimental Data for Modeling and Simulation Validation	Trevor Cook, NE
1120	Open ACTT Discussion of Issue and Other Program Experiences	All
1130	ACTT Round Table Status, Issues, & Opportunities for Collaboration (10 minutes for less from each program)	All
1210	Wrap Up and discuss plans for next meeting	Alex Larzelere
1215	Adjourn	

- **Current Membership:**
  - Electrical Delivery (OE)
    - Grid Modeling
  - Energy Efficiency and Renewable Energy (EERE)
    - Wind and Water, Fuel Cell, Vehicle Technologies, Solar
  - Environmental Management (EM)
    - ASCEM
  - Fossil Energy (FE)
    - Carbon Capture, NRAP
  - National Nuclear Security Administration (NNSA)
    - Defense Programs ASC, Nonproliferation DNN
  - Nuclear Energy (NE)
    - NEAMS, Energy Innovation Hub
  - Science (SC)
    - ASCR, Fusion Energy, Biological and Environmental Research

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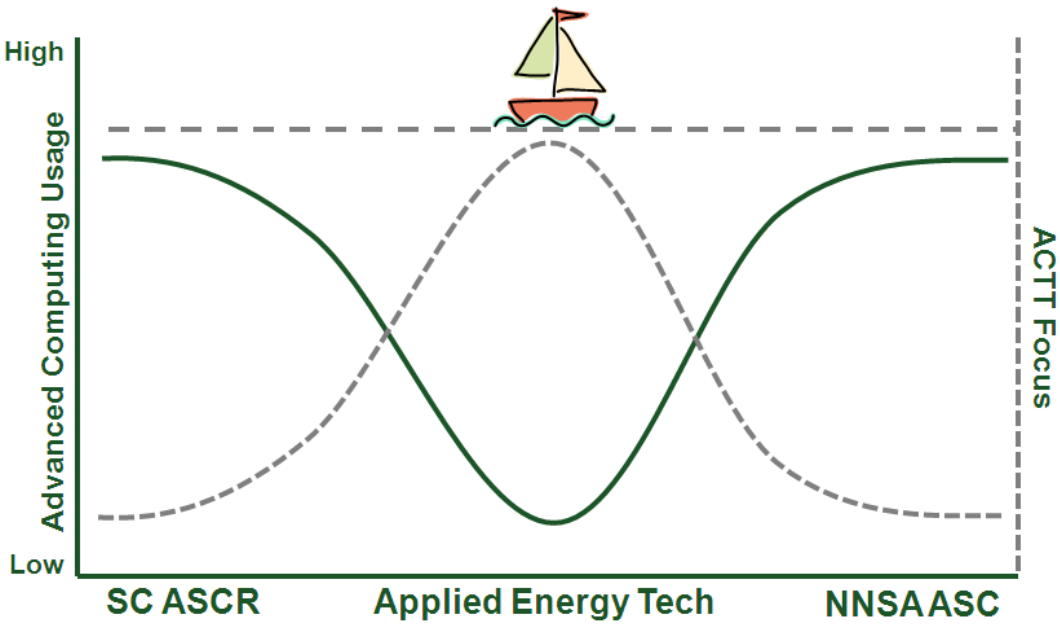
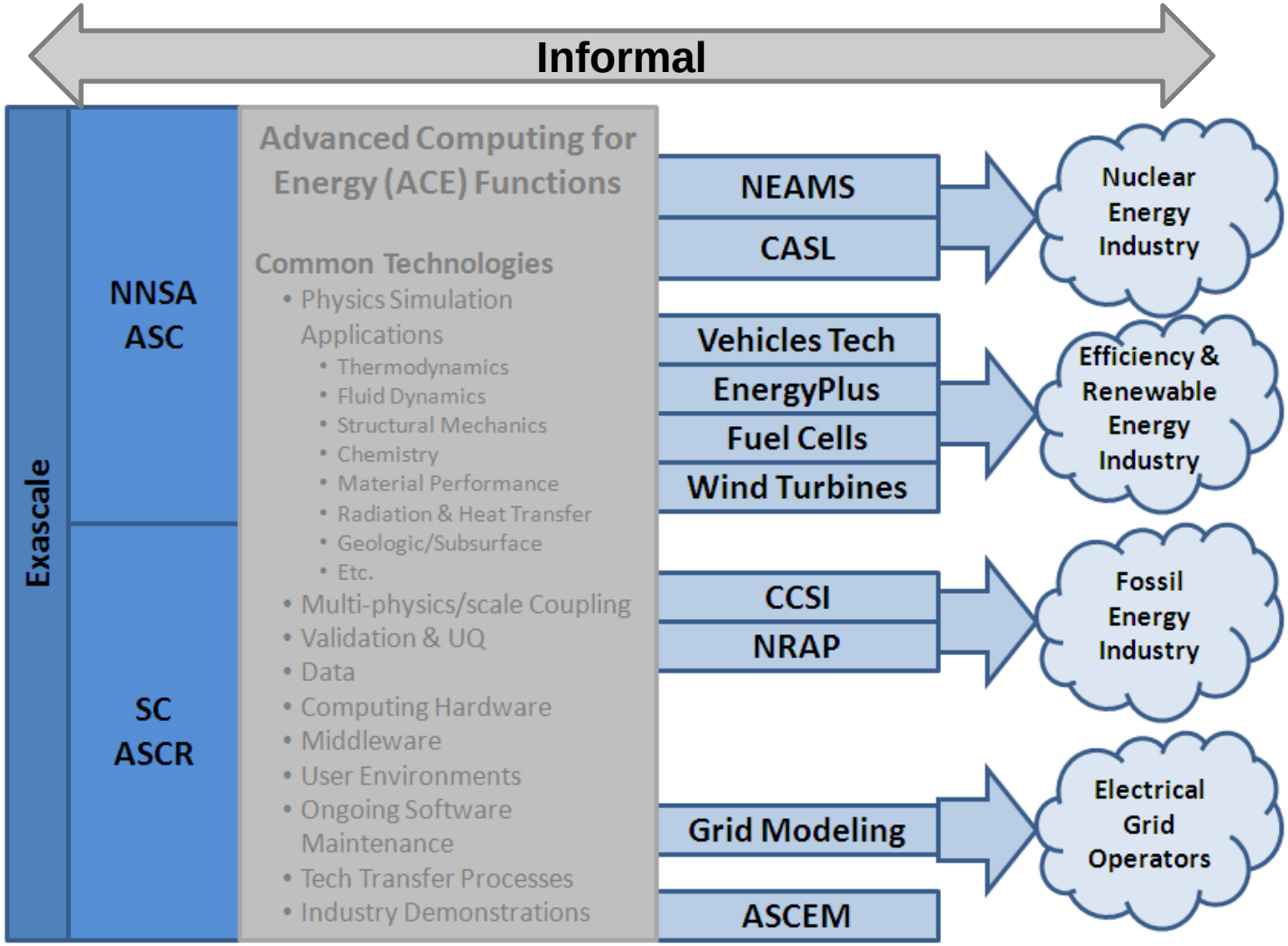
Advanced Computing Tech Team

ACTT Mission Statement

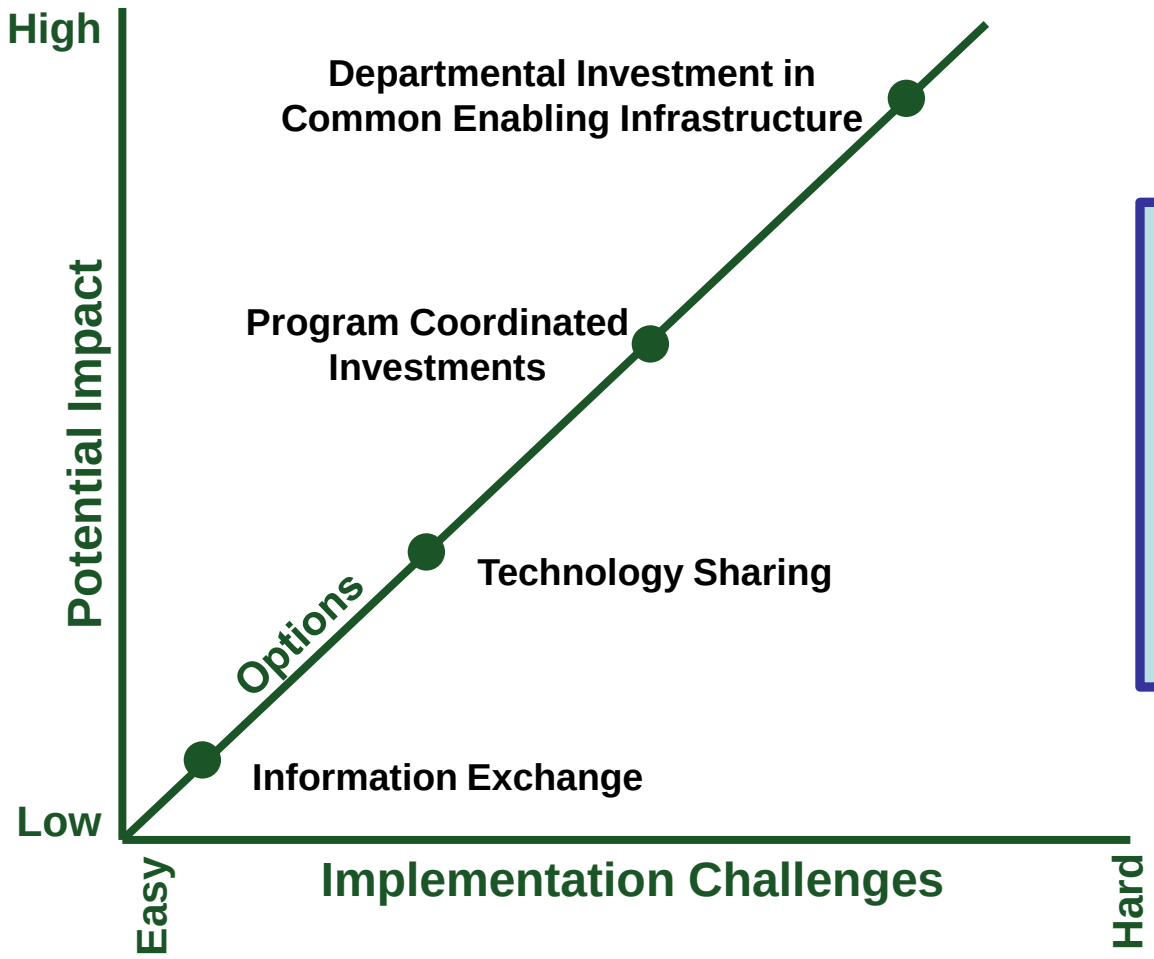
- Promote and facilitate the improved use of advanced computing technologies
- By scientists and energy innovators (in government, academia and industry)
- In support of the applied energy technology missions of the Department of Energy



Starting Point



Opportunities and Challenges



The ACTT will work to move DOE advanced computing activities "up and to the right" (as appropriate)

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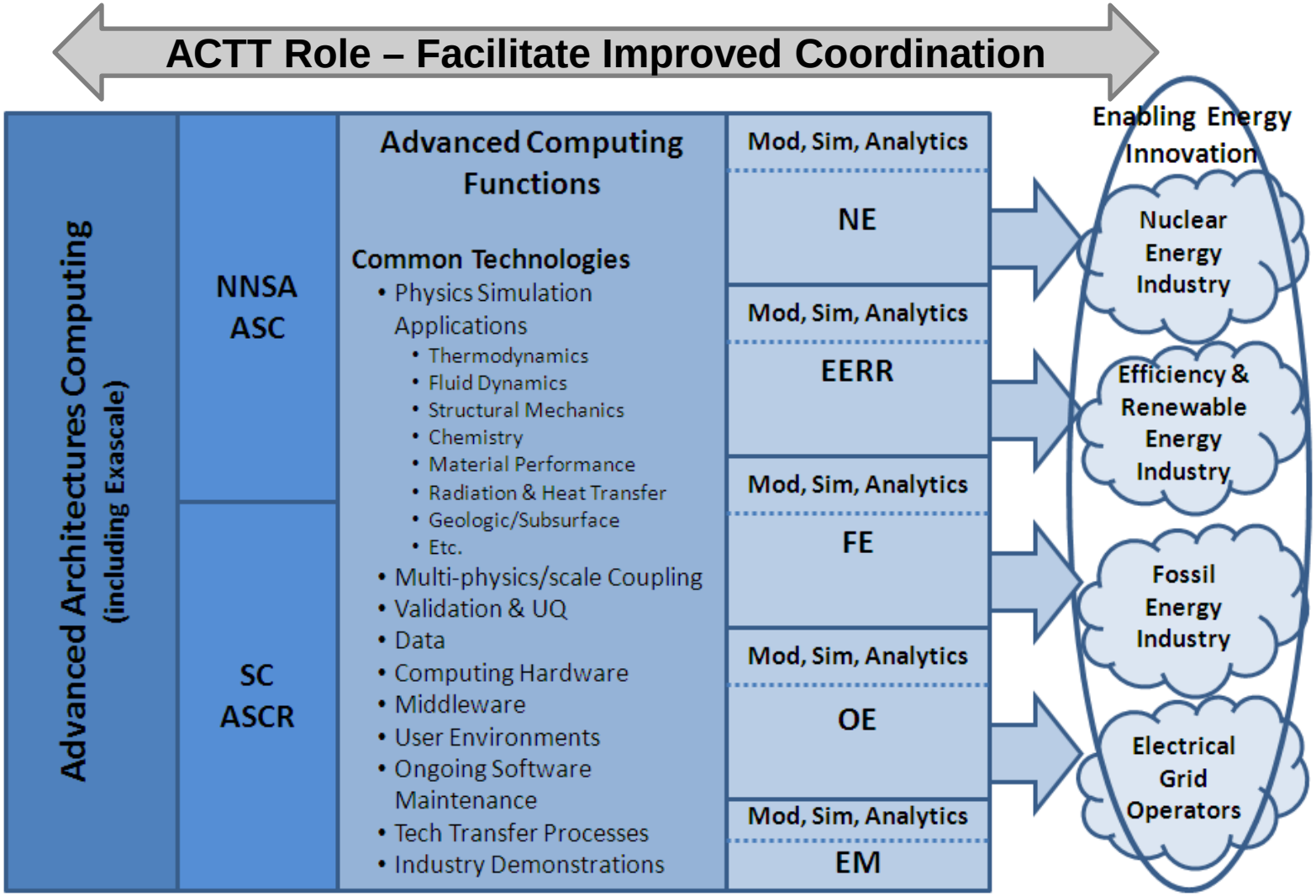
Advanced Computing Tech Team

Success



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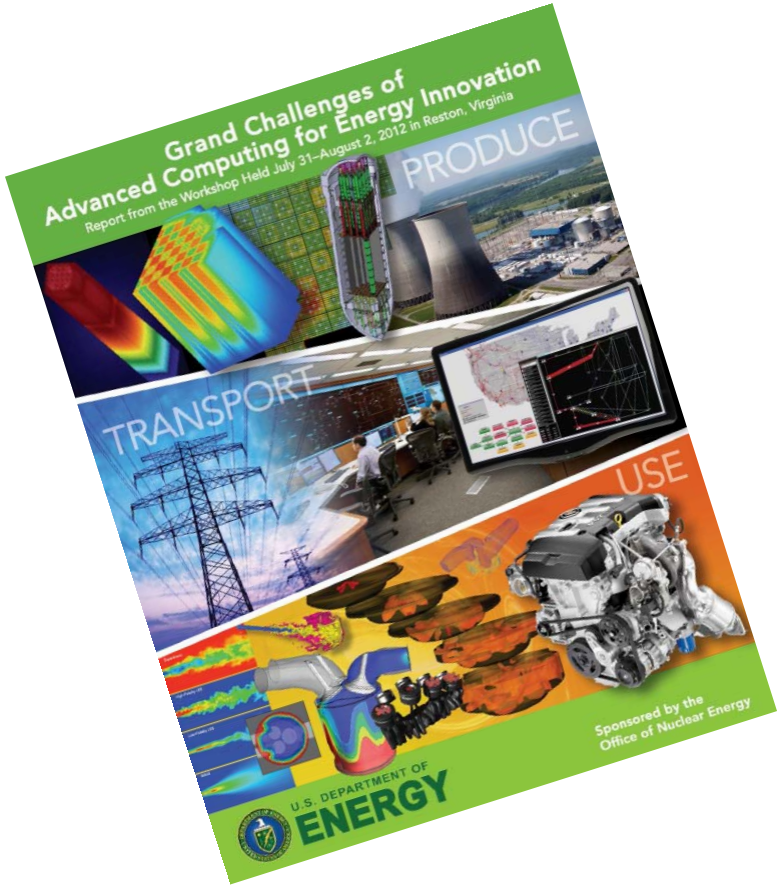
Build on the findings and recommendations of the July 2012 Workshop



- **Workshop Findings**
  - **Technical Challenges**
    - High level of expertise needed
    - Customize DOE developed tools to particular energy innovation needs
    - Transition of computing architecture programming models
  - **Structural Challenges**
    - Visibility into relevant activities
    - Opportunity to work with ISV
    - Tech Transfer
  - **Motivation Challenges**
    - Understanding ROI
    - Lack of “in-house” expertise
    - Improve understanding by the DOE and labs of the possible impact

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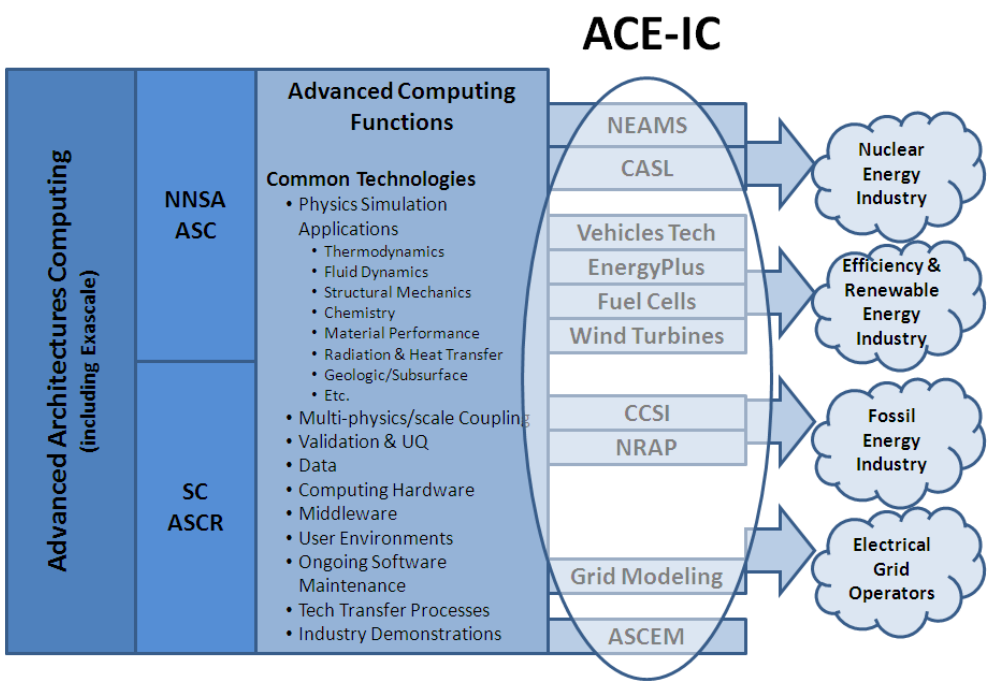
Advanced Computing Tech Team

ACTT Facilitated Innovation Centers to Overcome Grand Challenge

ACE Innovation Center Roles



- Build a confederation of existing advanced computing programs focused on
- Sharing methods to address Grand Challenges
  - Understand specific industry needs
  - Putting tools in form to be usable in industry settings
  - Technology transfer processes
  - Help industry understand investment requirements
  - Provide demonstrations opportunities to understand potential return

What is CORAL (Partnership for 2017 System)

- CORAL is a **C**ollaboration of **O**ak **R**idge, **A**rgonne, and **L**awrence Livermore Labs to acquire three systems for delivery in 2017.
- DOE's Office of Science (DOE/SC) and National Nuclear Security Administration (NNSA) signed an MOU agreeing to collaborate on HPC research and acquisitions
- Collaboration grouping of DOE labs was done based on common acquisition timings. Collaboration is a win-win for all parties.
  - It reduces the number of RFPs vendors have to respond to
  - It improves the number and quality of proposals
  - It allows pooling of R&D funds
  - It strengthens the alliance between SC/NNSA on road to exascale
  - It encourages sharing technical expertise between Labs

CORAL
COLLABORATION
OAK RIDGE ARGONNE LIVERMORE

CORAL Joint NNSA & SC Leadership Computing Acquisition Project

Current DOE Leadership Computers

Titan (ORNL)
2012 - 2017

Sequoia (LLNL)
2012 - 2017

Mira (ANL)
2012 - 2017

Objective - Procure 3 leadership computers to be sited at ANL, ORNL and LLNL in CY17

Leadership Computers run the most demanding DOE mission applications and advance HPC technologies to assure continued US/DOE leadership

Approach

Competitive process - one RFP (issued by LLNL) leading to 2 R&D contracts and 3 computer procurement contracts

For risk reduction and to meet a broad set of requirements,
2 architectural paths will be selected

Once Selected, Multi-year Lab-Awardee relationship to co-design computers

Both R&D contracts jointly managed by the 3 Labs

Each lab manages and negotiates its own computer procurement contract, and may exercise options to meet their specific needs

Understanding that long procurement lead-time may impact architectural characteristics and designs of procured computers

CORAL Management Structure

Top three levels of management and their responsibilities

CORAL Executives	
Rick Stevens, Associate Laboratory Director, Argonne **Jeff Nichols**, Associate Laboratory Director, ORNL **Mike McCoy**, ASC Program Director, LLNL	• Laboratory leadership oversight • Final decision authority

CORAL Directors	
Michael E. Papka, LCF Director, Argonne **Jim Hack**, LCF Director, ORNL **Terri Quinn**, LC Program Lead, LLNL	• Concur on system selection and ensures selected system meets DOE and facility (LC, ALCF, OLCF) mission needs • Coordination at facility level

CORAL Acquisition Leads	
Susan Coghlan, ALCF-3 Project Director, Argonne **Buddy Bland**, OLCF-4 Project Director, ORNL **Bronis de Supinski**, LC CTO, LLNL	• Responsible for the acquisition • Work with technical and procurement teams to gather requirements, develop RFP, prepare for and respond to IPRs, issue RFP, and recommend system selection

CORAL Procurement Model

Two Diverse Architecture Paths

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EPRI's High Performance Computing Initiative

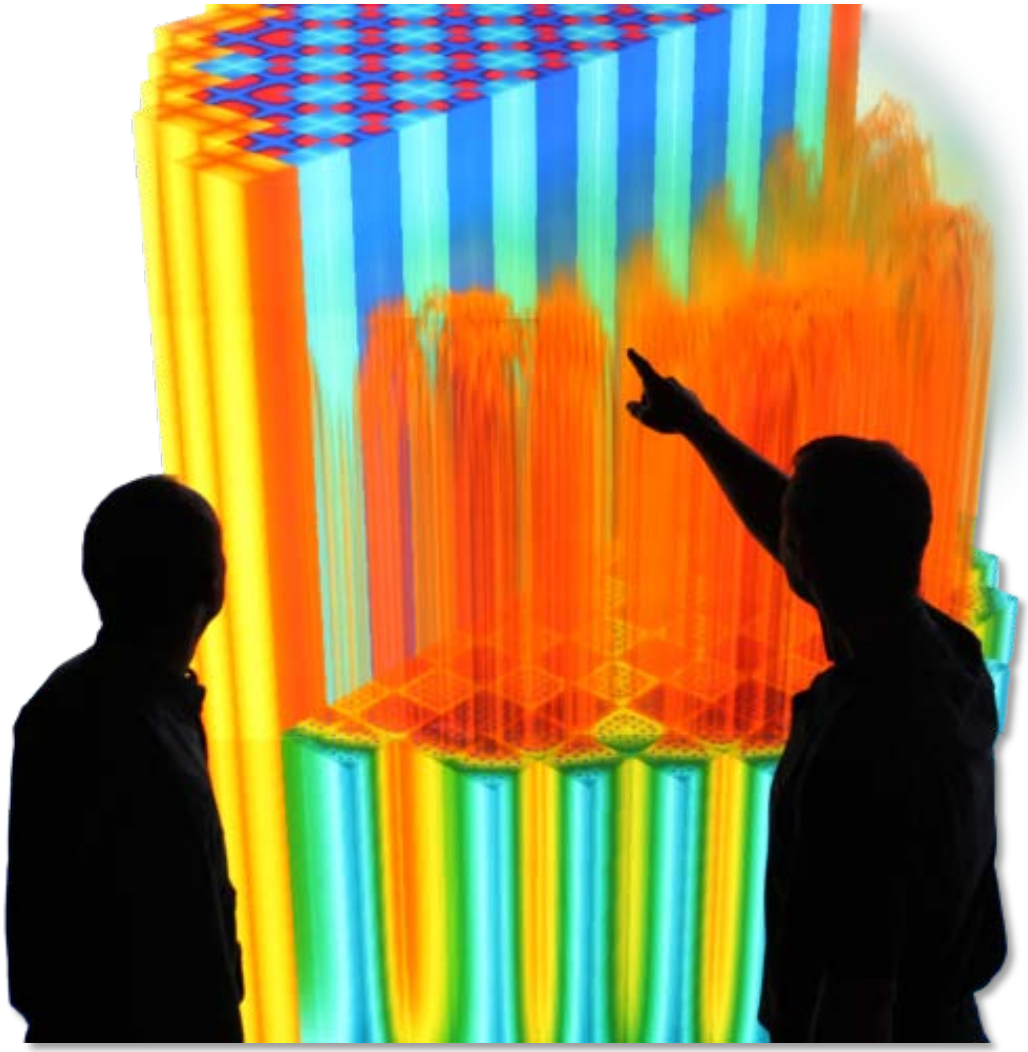
Heather M. Feldman

Manager, Thermal-Hydraulics

Lunch Talk CASL Industry Council

March 11, 2014

The Driver --- CASL



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Impacts of High Performance Computing

THEORY

EXPERIMENT

- SCENARIO EXPLORATION – MANY, MANY WHAT IFS
- VIRTUAL EXPERIMENTS – CAN'T BE DONE EXPERIMENTALLY
- HUMAN FACTOR – CHANGES WORKFLOW
- SECRET LIFE OF DATA – REVEAL TRENDS

HIGH END COMPUTING

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EPRI's High Performance Computing Initiative

- The mission of this EPRI-wide initiative is to bring high performance computing and modeling and simulation capability in-house at EPRI.

Where did the name Phoebe come from?

Phoebe is one of the Olympians from Greek mythology, and she is typically associated with intellect and prophecy. At EPRI, we believe Phoebe will demonstrate these same qualities, helping us uncover new knowledge and insights into the electric power industry.

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Compute Capabilities

Phoebe at EPRI

Industry-class, high-performance computer

~500 cores
8 Teraflops (10^{12})

Titan at Oak Ridge National Lab

Leadership-class, high-performance computer

~560,000 cores + GPUs
27 Petaflops (10^{15})

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Software List

- Linux
  - ABAQUS
  - Fluent
  - MAAP/Dakota
  - MAAP/Python
  - Matlab
  - VERA/Peregine
- Windows
  - Wave2000Plus, Wave300Plus

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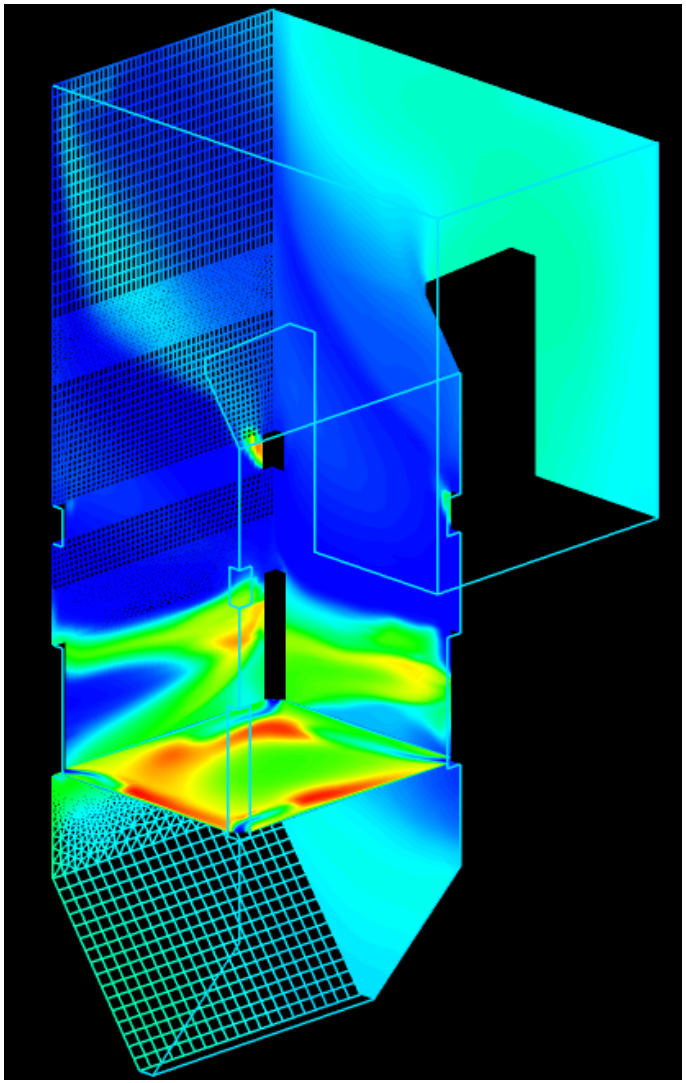
EPRI Example
Solve times decrease from 10 days to 1-2 days



Coal-Fired Boiler

- New burner design
  - Minimize nitrogen oxide (NO_X) release
  - But, they promote corrosion
- Combustion parameters and associated pathways that lead to corrosion

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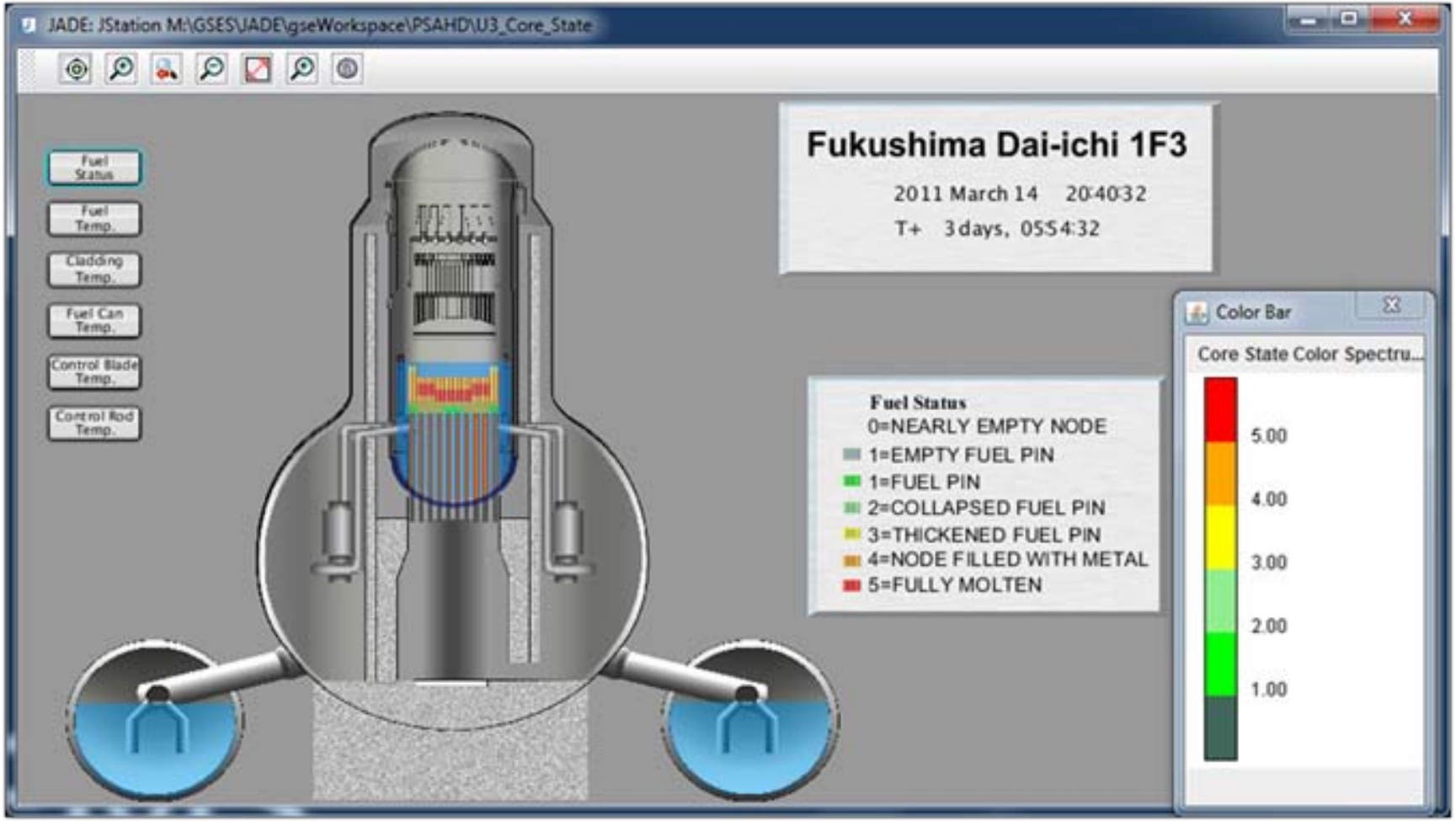
EPRI Example
Multiple Scenarios on Short Order



10,000 simulations in 3 hours on 448 cores

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EPRI with High Performance Computing

- "Modeling and simulation through high performance computing is here. EPRI can unlock new knowledge by solving tough problems with no computational constraints."

What computational resources do I need to solve this problem rather than what problem can I solve using this computer?

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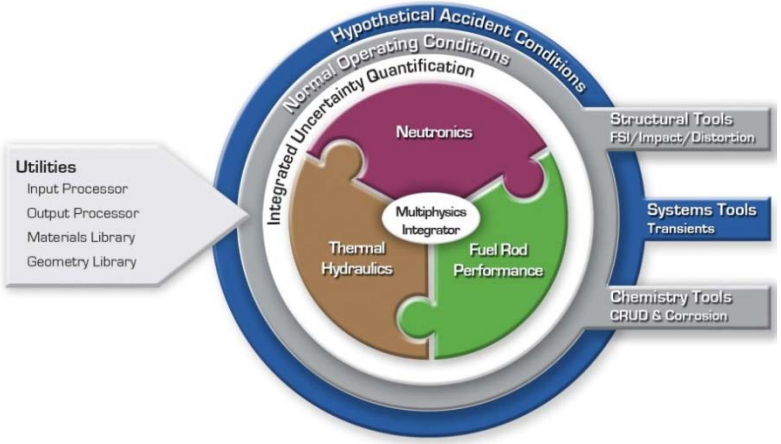
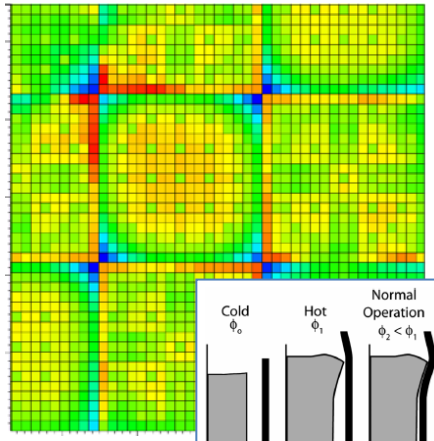
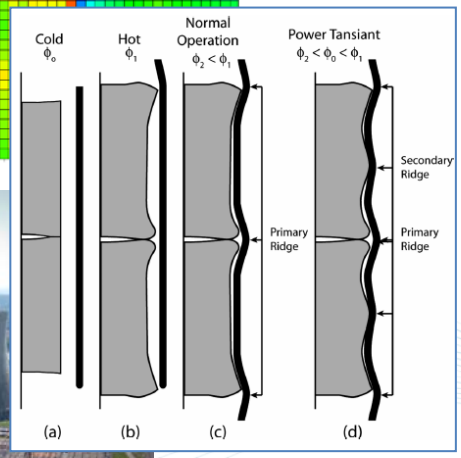
Together…Shaping the Future of Electricity

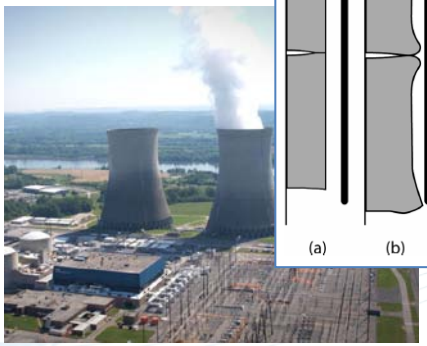
CASL Test Stands: From Plan to Execution

- Early deployment into industrial environment for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
- Status of initial deployment to core industry partners
  - ➢ WEC: Deployment during June 2013; focus on VERA simulation of AP1000 first core startup
  - ➢ EPRI: Deployment as of Dec 2013; new EPRI computing capabilities will be utilized to test VERA fuel (Peregrine) performance applications
  - ➢ TVA: Deployment planned for Q2 2014; lower plenum flow anomaly (LPFA)
- Early Test Stand deployment is already producing dividends for CASL and users
  - – Better code installation processes
  - – Input processing for heterogeneous cores
  - – Reductions in user problem setup times
  - – Core tilt analysis
  - – Analysis of new design features (e.g., tungsten rods)









External Test Stand Process

- Test Stand selection process
  - Proposal memo to CASL written by host organization describing scope, timing, goals, cost share, etc.
    - *A preliminary list of Test Stand ideas would be helpful to move the planning process ahead*
  - CASL reviews the host proposal to ensure all needed capabilities will be available
  - CASL develops a response memo discussing ability to meet the proposed Test Stand scope and schedule
  - Software components are deployed to host and Test Stand analyses are completed with limited CASL support
  - Host develops a report detailing lessons learned identified during testing
    - *The typical Test Stand duration is ~ 6 months, but the schedule can be adjusted*
- The list of institutions interested in hosting external Test Stands is growing
  - GE-H, Areva, B&W, GSE, Rolls Royce, Universities (for classrooms), other R&D programs
- The first External Test Stand deployment target is September 2014

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EPRI Test Stand Update

Brenden Mervin
Project Engineer

Industry Council Meeting
March 11–12, 2014

EPRI Test Stand Deployment

- **Scope**
  - VERA installation & verification
  - Training
  - Evaluation of Watts Bar 1 PCI during fuel cycle startup
  - Development of PCI margin screening and assessment workflow
  - MPS analysis

- **Status**
  - Test Stand was deployed on the new EPRI industry class HPC system during October 2013
  - Training and code assessment work is ongoing
  - Test Stand report anticipated during fourth quarter FY 14

Component	Included	May Be Included	Not Included	Comments
Physics Components				
COBRA-TF	X			Standalone with VERAIn input
Insilico	X			Sn/Spn with Scale/XSProc and VERAIn input
Coupled Insilico + COBRA-TF	X			Single assembly
Hydra-TH			X	
MPACT	X			
MAMBA-2D			X	
Peregrine	X			Standalone
MOOSE/Bison	X			Required for Peregrine
Tiamat (CTF + Insilico + Peregrine)			X	Not ready for use.
Coupled COBRA-TF + MAMBA-2D			X	Not ready for use.
Shift			X	
Infrastructure Components and TPLs				
Trilinos	X			
TriBITS	X			
VERAIn	X			Common VERA input parser
Dakota	X			With COBRA-TF examples (VUQDemos)
LIME	X			
DataTransferKit	X			
Other Required TPLs	X			As defined in the VERA Installation Guide.

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Phoebe – EPRI's High-Performance Computer

- Greek goddess of intellect and prophecy (not…
- Specifications:
  - Intel® Xeon® processors
  - 31 nodes
  - 496 compute cores (~250 iPhones)
  - 100 TB storage (~1,562 iPhones)
  - 2 TB memory (~2,000 iPhones)
  - 8 teraflops
  - QDR Infiniband
    - 2.5 Gbit/s (x150 faster 4G LTE)
  - Linux & Windows OS

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Installation & Testing

- VERA Installation
  - Process streamlined well
    - VERA Installation Guide
    - Installation scripts for TPLs
    - CASL Support
  - Still not error-proof
    - Architecture dependent issues
    - CASL support staff eager to help
- Testing
  - Simple in most cases
  - Peregrine test suite not integrated into VERA
    - Currently exists in MOOSE

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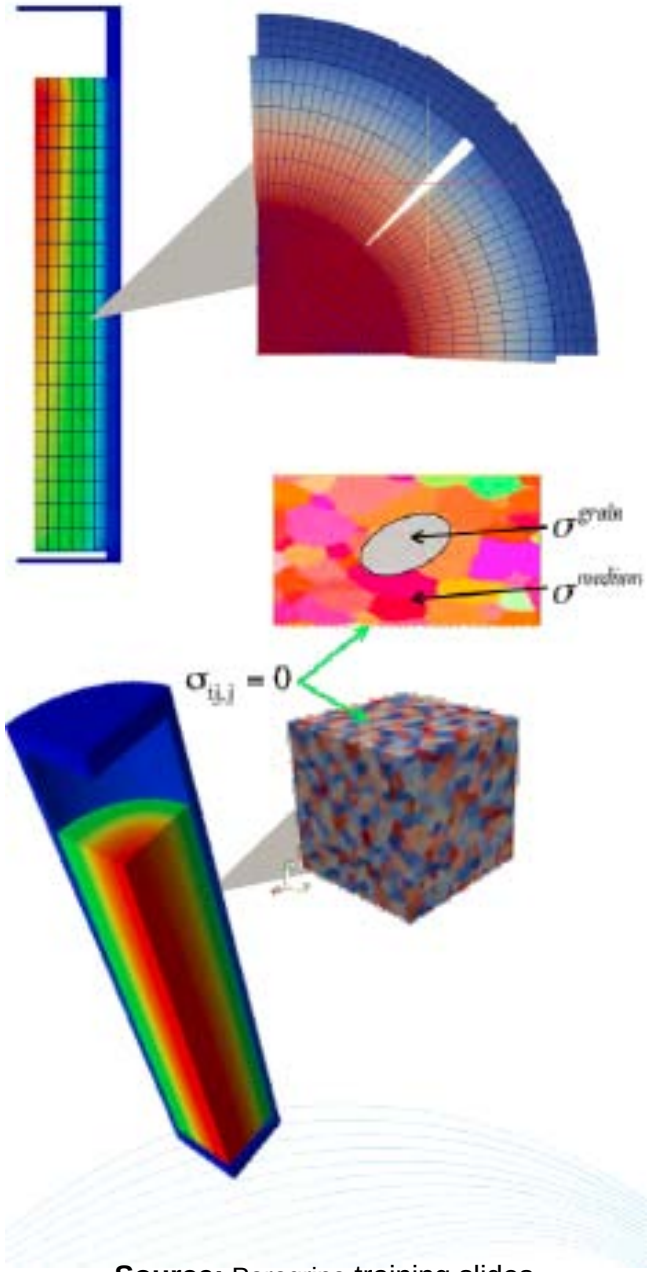
Peregrine Training

- Built upon the MOOSE/ELK/FOX framework as an extension of BISON developed by Idaho National Laboratory (INL)
  - Input/output (I/O)
  - Thermal transport
  - Mechanical solutions
  - Chemical transport
- Capabilities
  - Finite element (FE) framework
  - 2D and 3D modeling capabilities
  - Swelling/densification modeling
  - Irradiation creep/growth
- Under active development
  - Fuel cracking behavior
  - Fission gas release
  - Contact modeling
  - Friction modeling
- Uses Paraview for post processing



Source: Peregrine training slides

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Test Stand Scope

- Primary tasks
  - Perform comparisons between FALCON and Peregrine for key parameters using reactor data from Watts Bar
    - Start with a couple rods
    - Expand analysis to all rods in an assembly
- Extended tasks
  - Expand above analysis to all assemblies in the core
  - Perform analysis on a missing pellet surface (MPS) defect
  - Compare Peregrine results to PIE data available in an EPRI report

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Test Stand Schedule

#	Task	Estimated Completion Date
1	Input to DOE Reportable on Test Stands (L2.AMA.P8.01)	2/26/14
2	Falcon and Peregrine comparison for key parameters for two Watts Bar rods	3/7/14
3	Generalized analysis of all of the rods in a single assembly (three Watts Bar assemblies)	3/14/14
4	Develop calibrated PCI threshold value	3/21/14
5	Peak hoop stress associated with a MPS using the same FEM configuration as Falcon	3/28/14
6	Perform a core-wide analysis and develop criteria for determining the critical assembly/rod in a given cycle	4/15/14
7	Comparison of Peregrine results to PIE	4/22/14
8	Provide material summarizing EPRI Test Stand Experiences to CASL	4/30/14

- #6 requires additional Watts Bar data
- #7 requires data from Plant X (request has been sent)

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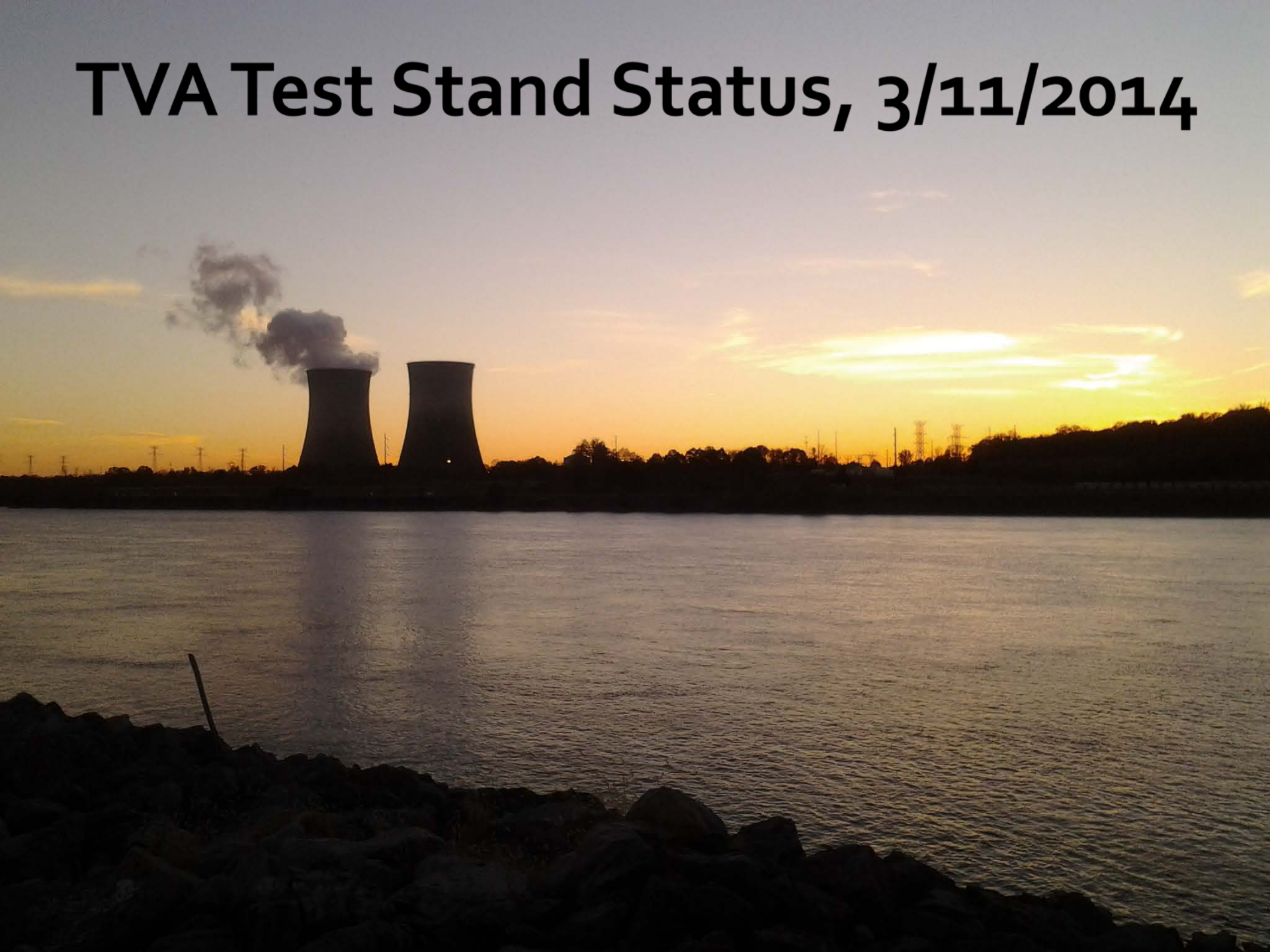
TVA Test Stand Status, 3/11/2014



TVA's CASL Test Stand Status

March 11, 2014

- TVA has selected Lower Plenum Flow Anomaly as our topic
  - Observed over many cycles at Watts Bar
  - Utilizes CASL CFD code Hydra-TH in a large scale demonstration
  - Planned to use coupled neutronics/channel flow with input from Hydra simulation
  - Memo sent to CASL detailing the test stand 12/13/13; waiting for CASL confirmation
- Exelon has agreed to provide industry independent review
- UT-C is supporting TVA in the area of mesh generation with their SimGrid toolset
- WEC has offered a full core geometry model of a 4-loop plant that we may use, depending on the modeling detail (it may be too complex for our needs)
- TVA has established simplified solid model geometry to test mesh & symmetry sensitivity, ability of code to simulate desired issue prior to implementing larger models

TVA's CASL Test Stand Status

March 11, 2014

- Meshing is in progress using available tools (Cubit, Hexpress, hand-meshing)
- TVA has signed the Hydra-TH licensing agreement
  - TVA has not yet executed a VERA T&E license
- TVA is working to establish required computing resources
  - Have investigated use of TVA T-Block. This will not be possible, as reconfiguring would require too much down time for other systems and would not produce an optimal engineering configuration.
  - EPRI declined our request to use their new computing cluster (may be possible later in 2014)
  - In the process of applying for a Titan allocation
- Work is on schedule

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Westinghouse Test Stand

Zero Power Physics Test Simulations for the **AP1000®** PWR

F. Franceschini – Fellow Engineer

Westinghouse Electric Company LLC

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Agenda

- Background (4 slides)
- Topics (6 slides)
- Results (10 slides)
  - Critical boron
  - Reactivity coefficients
  - Rod worth
  - Power distribution
- Usability (2 slides)
- Benefits (1 slide)
- Recommendations (1 slide)
- Conclusions (1 slide)

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Background

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Timeline

- Test Stand discussion (early 2013)
- Scope proposed in Westinghouse memo (April 2013)
- VERA deployment at Westinghouse (June 2013)
  - VERA built on dedicated compute cluster
  - VERA updates with new capabilities
- Technical analysis (July-Nov 2013)
  - Deterministic (VERA) plus Monte-Carlo (KENO)
- Analysis completed and documented (Jan 2014, Rev. 1 in Mar 2014)

First organization to host VERA Test Stand

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Personnel

- **Westinghouse:**
  - B. Oelrich, Manager, PWR Core Methods
  - K. Drudy, Manager, New Reactor Technology
  - F. Franceschini, Technical Lead
  - J. Kulesza, & G. Fischer, VERA build
  - L. Hampshire, J. Walsh, cluster configuration
  - J. Secker, D. Salazar
  - A. Graham, UM Intern, VERA simulations initial support
  - Westinghouse methods and core engineering personnel
- **CASL:**
  - J. Gehin ORNL - Physics Integration Focus Area Lead
  - R. Bartlett, M. Baird, ORNL - Installation and VERA code updates
  - A. Godfrey ORNL - Analysis Support

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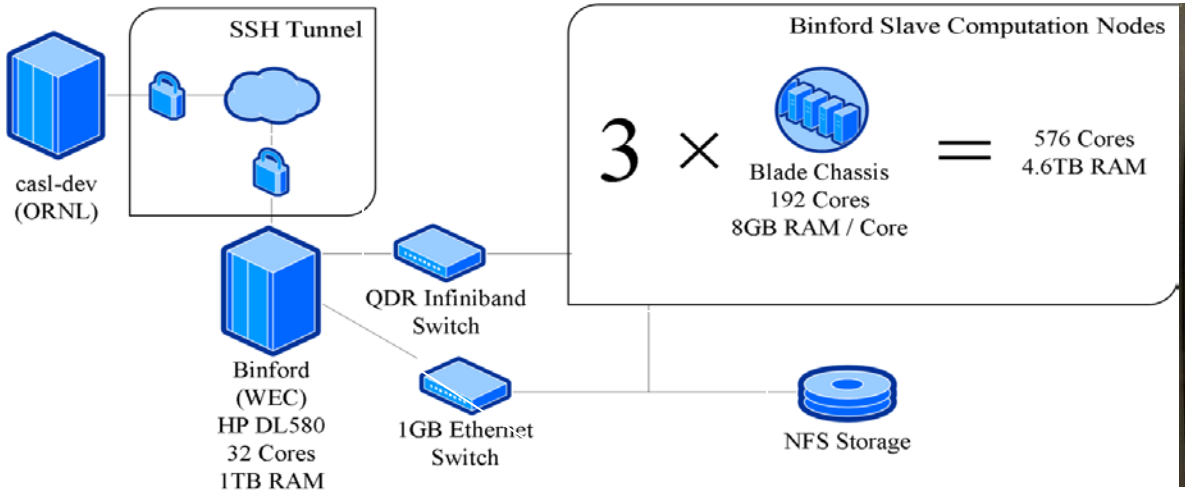
VERA Build

- VERA build at Westinghouse operational and exercised
  - 576 cores, 12 cores/ node, 96 GB/node (4.6TB total)



VERA ZPPT calculations performed on Westinghouse system

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Codes Used

- VERA with SP_N 3D flux solver
  - SP_5 with P_3 scattering in 23 energy groups
  - on-the-fly pin-homogenized XS with 1D transport calculations
  - SCALE B7.0-based 252-energy group library

- KENO-VI Monte-Carlo
  - Reference solution
  - Continuous energy
  - General geometry
  - Parallel capabilities
  - Scales well up to 200-300 cores

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Topics

AP1000 PWR First Core

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Topics

- Zero-Power Physics Tests for the **AP1000** PWR
- Advanced application of VERA
  - First-core
  - Heterogeneous fuel
  - MSHIM™ operation
  - IFBA

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AP1000 PWR First Core Design – Radial

	H	G	F	E	D	C	B	A
8	B	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	E 124 IFBA	C
9	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	B	E 88 IFBA 4 WABA	A
10	B	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	B	E 124 IFBA 8 WABA	C	
11	D 68 IFBA 12 WABA	B	D 68 IFBA 12 WABA	B	E 124 IFBA 8 WABA	C	A	
12	B	D 68 IFBA 12 WABA	B	E 124 IFBA 8 WABA	B	C		
13	D 68 IFBA 12 WABA	B	E 124 IFBA 8 WABA	C	C			
14	E 124 IFBA	E 88 IFBA 4 WABA	C	A				
15	C	A						

Region
IFBA
WABA

IT	M	M	SW	M	M	LW	M	LI
M	HI	H	M	H	H	M	M	L
M	H	HI	M	HI	HI	M	M	LI
SW	M	M	GT	M	M	GT	MI	L
M	H	HI	M	M	M	M	M	LI
M	H	HI	M	M	LW	M	M	L
LW	M	M	GT	M	M	M	M	LI
M	M	M	MI	M	M	M	MI	L
LI	L	LI	L	LI	L	LI	L	LI

High enriched fuel inboard like L^3P reload cycles.

Radial zoning in Cycle 1 to reduce spectral interface.

Mimics reload cycle to quickly establish equilibrium

Major Fuel Economic Advantage

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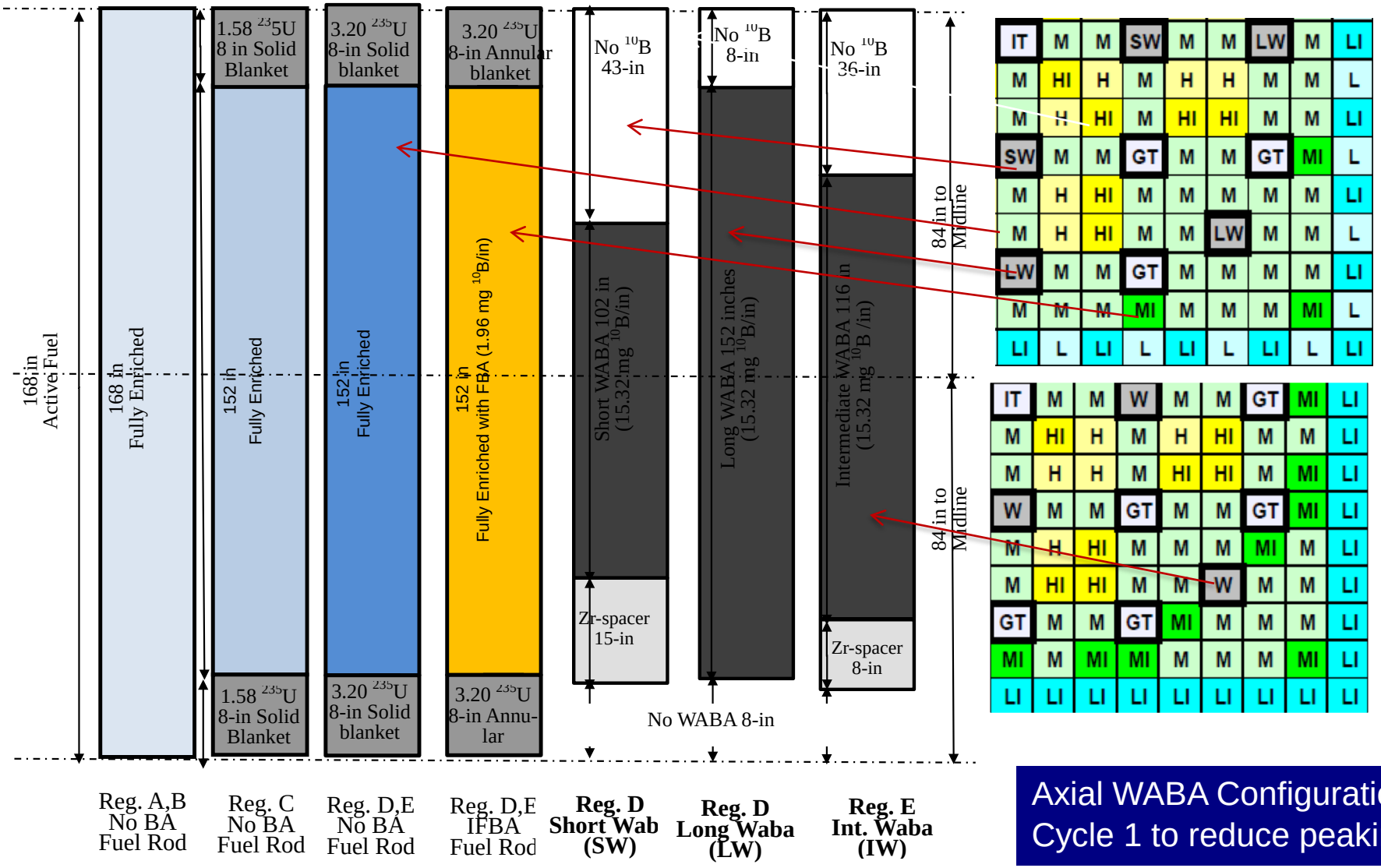
AP1000 PWR First Core Design – Axial



Axial WABA Configuration in Cycle 1 to reduce peaking.

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Control Rod Layout

Shutdown:

4 Banks / 32 RCCAs (Ag-In-Cd)

- Ensures adequate shutdown margin & trip reactivity

Axial Offset:

1 Bank / 9 RCCAs (Ag-In-Cd)

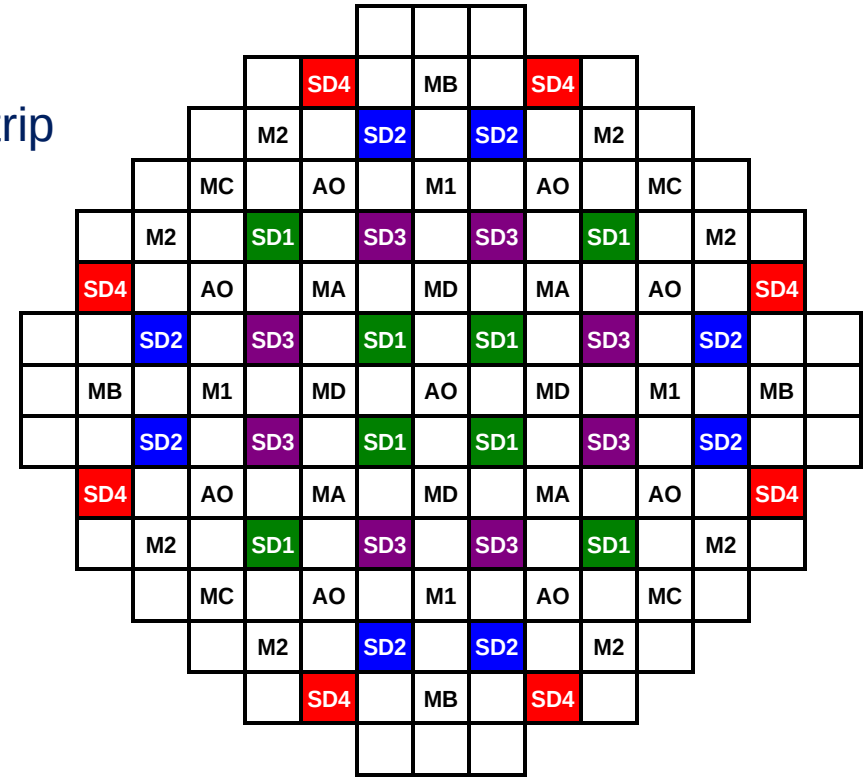
- Dedicated, high impact bank provides robust axial power shaping capabilities

MSHIM:

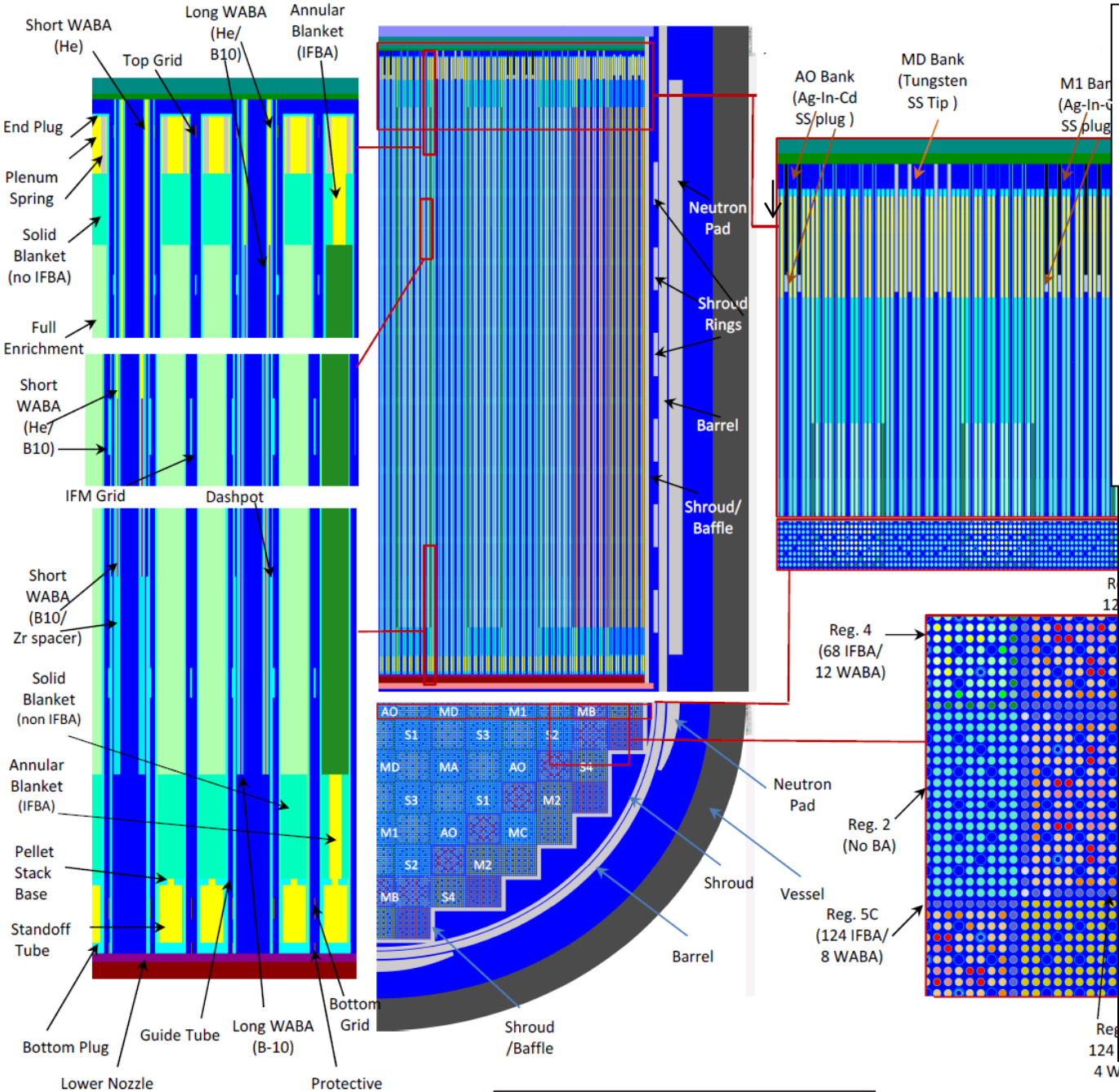
4 Banks / 16 GRCAs (Tungsten)

2 Banks / 12 RCCAs (Ag-In-Cd)

- Provides fine reactivity control while significantly reducing changes to soluble boron



Key to MSHIM Operating Strategy




```
axial 320E0I

  BOTPLUG
  BOTSTANDOFF  1
  PELLETBASE   2
  BOTBLK3      4
  BOTFUEL3     7
  TOPFUEL3    42
  TOPBLK3     44
  PLENUM      46
  ENDPLUG     46
  TOPGAP      46

axial 420E68I

  BOTPLUG
  BOTSTANDOFF  1
  PELLETBASE   2
  BOTBLK3      4
  BOTFUEL3     7
  TOPFUEL3    42
  TOPBLK3     44
  PLENUM      46
  ENDPLUG     46
  TOPGAP      46
```

```
rodmap  8waba4spacer
  -
  -   -
  -   -   -
  043 -   -   -
  -   -   -   -   -
  -   -   -   -   -   041
  041 -   -   -   -   -   -
  -   -   -   -   -   -   -
  -   -   -   -   -   -   -

rodmap  8waba4top
  -
  -   -
  -   -   -
  042 -   -   -
  -   -   -   -   -
  -   -   -   -   -   041
  041 -   -   -   -   -   -
  -   -   -   -   -   -   -
  -   -   -   -   -   -   -

rodmap  24thimbles
  -
  -   -
  -   -   -
  050 -   -   050
  -   -   -   -   -
  -   -   -   -   -   050
  050 -   -   050 -   -   -
  -   -   -   -   -   -   -   -
  -   -   -   -   -   -   -   -

axial   4W
                          41.2
      4spacer             61.6
      4waba              356.2
      4top               451.0
      20thimbles4wabas   466.6

axial   8W
                          41.2
      8spacer             61.6
      8waba              356.2
      8top               451.0
      16thimbles8wabas   466.6

axial  12W
                          41.2
      8waba4spacer        79.3
      12waba             338.4
      8waba4top          427.3
      12top              451.0
      12thimbles12wabas  466.6
```

```
  -   -

crd_map
  AIC
  -   AIC
  W   -   W
  -   AIC -   A
  AIC -   AIC -
  -   AIC -   A
  W   -   AIC -
  -   -

crd_bank
  AO
  -   S1
  MD  -   MA
  -   S3  -   S
  M1  -   AO  -
  -   S2  -   M
  MB  -   S4  -
  -   -

mat zirlo
mat zirc4
mat he
mat ifba
mat ss
mat ssspring
mat aic
mat tungsten
mat inc
mat waba
mat al2o3
```

```
!
  522 512 522 522 512 512 512 512
  521 521 521 521 521 521 511 521 511
lattice BOTFUEL5
  013
  512 513
  512 513 513
  012 512 512 012
  512 513 523 512 512
  512 513 523 512 512 012
  012 512 512 012 512 512 512
  522 512 522 522 512 512 512 512
  521 521 521 521 521 521 511 521 511
lattice TOPBLK5
  013
  531 531
  531 531 531
  011 531 531 011
  531 531 532 531 531
```

Westinghouse Non-Proprietary Class 3

3D Core KENO Model

Westinghouse

VERA Input

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Test Stand Simulations Performed

2D
- Single Lattice (20 types)
- Multi Lattice (Unrodded and Rodded)
- **Core with Reflector** (Various Reflectors)

3D Assembly
- Single Assembly (7 types)
- **Multi Assembly (Partial Rod Insertion)**

3D Core
- **HZP Critical Boron**
- **Rod Worth (11 Banks)**
- **Boron Worth**
- **ITC, DTC and MTC**
- **MSHIM Maneuver Bank Configuration**

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Results

Zero Power Physics Tests

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All-Rods-Out HZP Critical Boron

	KENO	VERA	VERA-KENO
k_{eff} cold dimensions, 1321 ppm	1.00066 ±1 pcm	1.00033	-33 pcm ±1 pcm
Boron Worth pcm/ppm	-9.6±0.08	-9.4	+0.2
Startup critical boron hot dimensions, instrumented	**1313**	**1310**	**-3 ppm**

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Temperature Reactivity Coefficients

	KENO	VERA	VERA-KENO
Doppler Temperature Coefficient (DTC) pcm/F	-1.54± 0.03	-1.72	-0.18
Moderator Temperature Coefficient (MTC) pcm/F	-1.12± 0.04	-1.50	-0.38
Isothermal Temperature Coefficient (ITC) pcm/F	-2.66± 0.05	-3.22	-0.56

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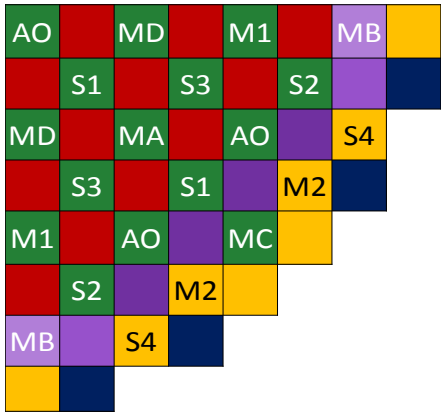
Rod Worth

		KENO	VERA-CS	
Bank	Material	Worth ± 2 pcm	ΔWorth (pcm)	ΔWorth (%)
MA	Tungsten	258	-1	-0.5
MB	Tungsten	217	-5	-2.1
MC	Tungsten	188	-2	-1.1
MD	Tungsten	234	0	0.0
M1	Ag-In-Cd	651	-4	-0.6
M2	Ag-In-Cd	887	3	0.4
AO	Ag-In-Cd	1635	-4	-0.3
S1	Ag-In-Cd	1079	0	0.0
S2	Ag-In-Cd	1096	-9	-0.8
S3	Ag-In-Cd	1124	0	0.0
S4	Ag-In-Cd	580	-3	-0.4
		RMS	**4**	**0.8**
		Max	**9**	**2.1**



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Results

Power Distribution Analysis

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2D Core - Midplane Radial Slice

Region	% Core	U235 AVG	U235 BLKT	IFBA Rods	WABA Rods
1	10%	0.74	-	0	0
2	31%	1.58	-	0	0
3	18%	3.20	1.58	0	0
4	**23%**	**3.77**	**3.20**	**68**	**8L+4S**
5A	**5%**	**4.34**	**3.20**	**88**	**4I**
5B	**3%**	**4.34**	**3.20**	**124**	**0**
5C	**10%**	**4.34**	**3.20**	**124**	**8I**

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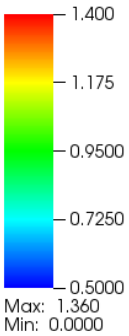
Power Distribution (KENO)

Assembly Power Distribution

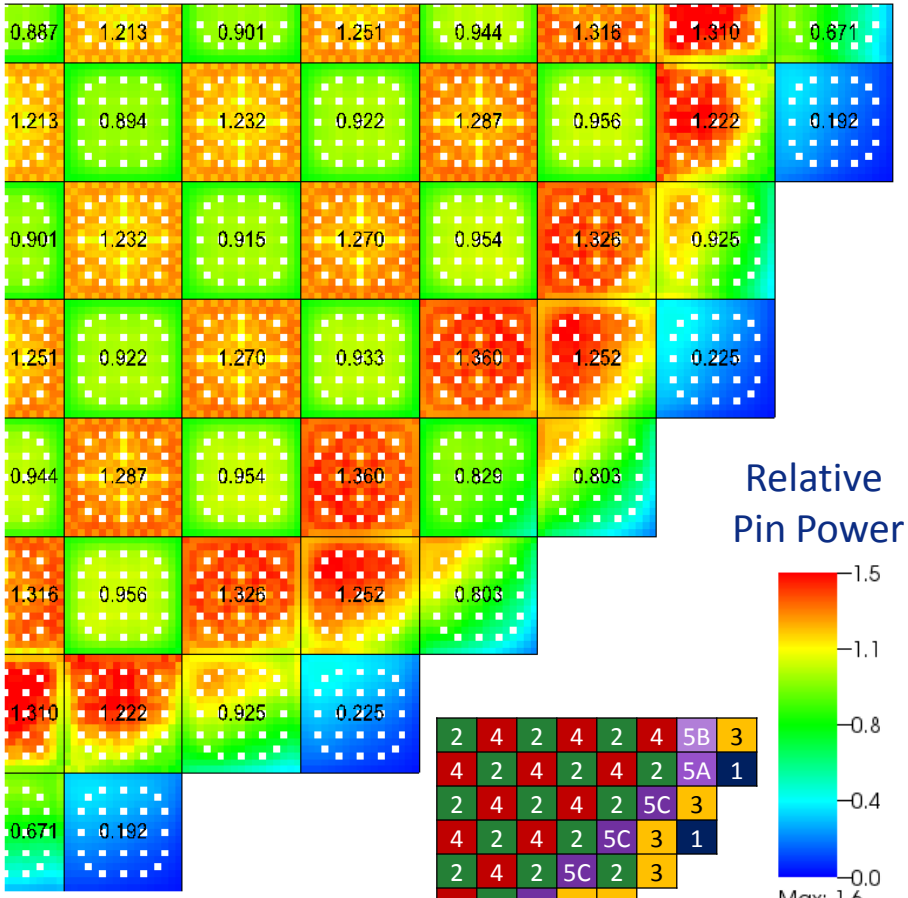
0.887	1.213	0.901	1.251	0.944	1.316	1.310	0.671
1.213	0.894	1.232	0.922	1.287	0.956	1.222	0.192
0.901	1.232	0.915	1.270	0.954	1.326	0.925	
1.251	0.922	1.270	0.933	1.360	1.252	0.225	
0.944	1.287	0.954	1.360	0.829	0.803		
1.316	0.956	1.326	1.252	0.803			
1.310	1.222	0.925	0.225				
0.671	0.192						

2	4	2	4	2	4	5B	3
4	2	4	2	4	2	5A	1
2	4	2	4	2	5C	3	
4	2	4	2	5C	3	1	
2	4	2	5C	2	3		
4	2	5C	3	3			
5B	5A	3	1				
3	1						

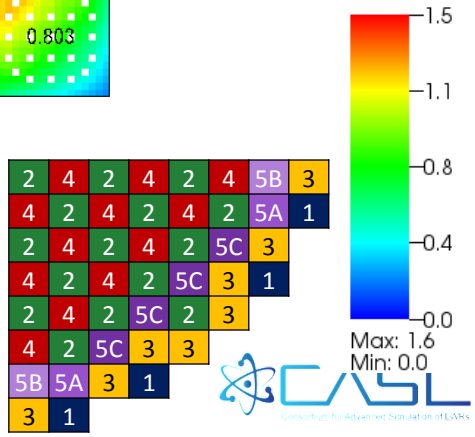
Relative Assembly Power



Pin Power Distribution



Relative Pin Power



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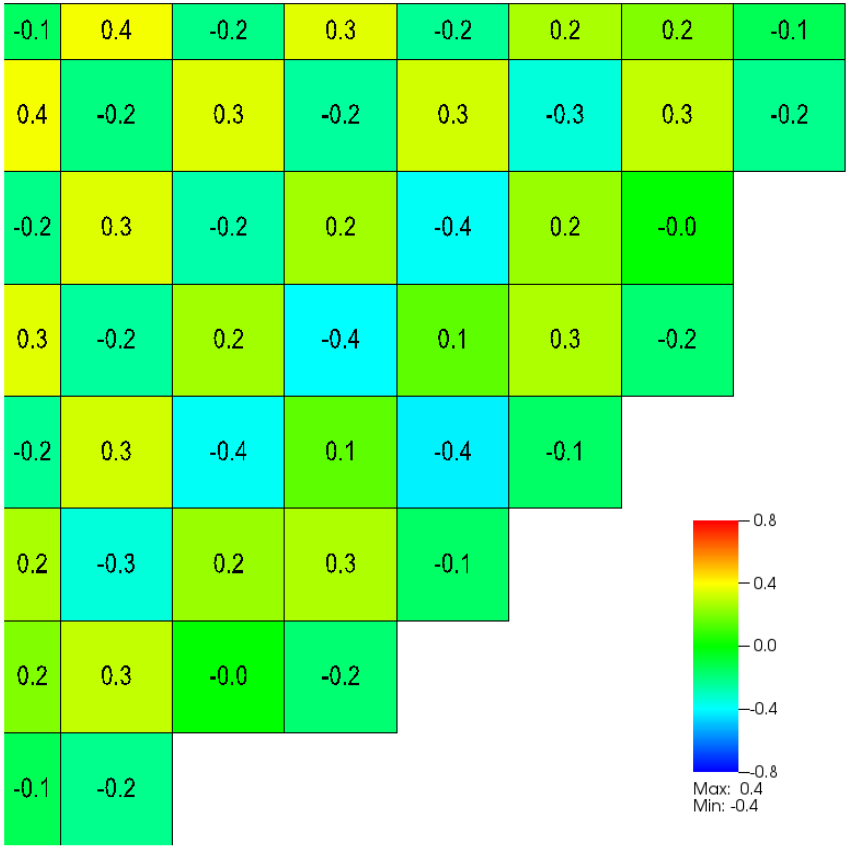
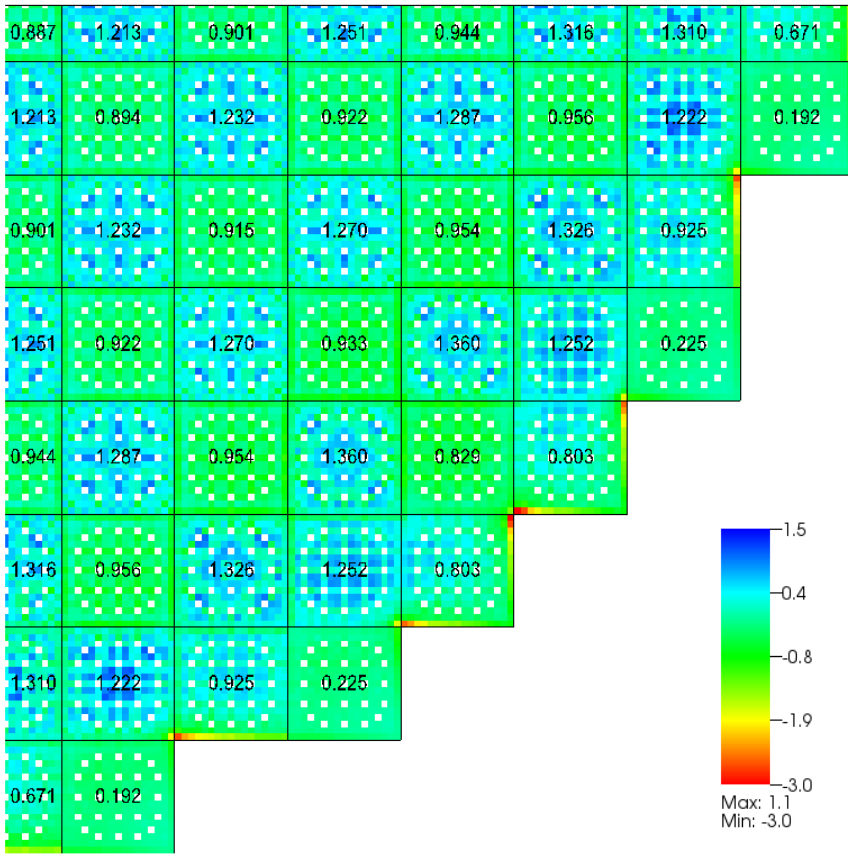
Power Distribution Comparison (VERA vs. KENO)

Delta **Assembly** Power
x100(VERA-KENO)



Delta **Pin** Power
x100 (VERA-KENO)



Delta k-eff : 0±1 pcm

Delta Assembly Power RMS/Max: <0.3/0.4%

Delta Pin Power RMS/Max: 0.4/3.0 %

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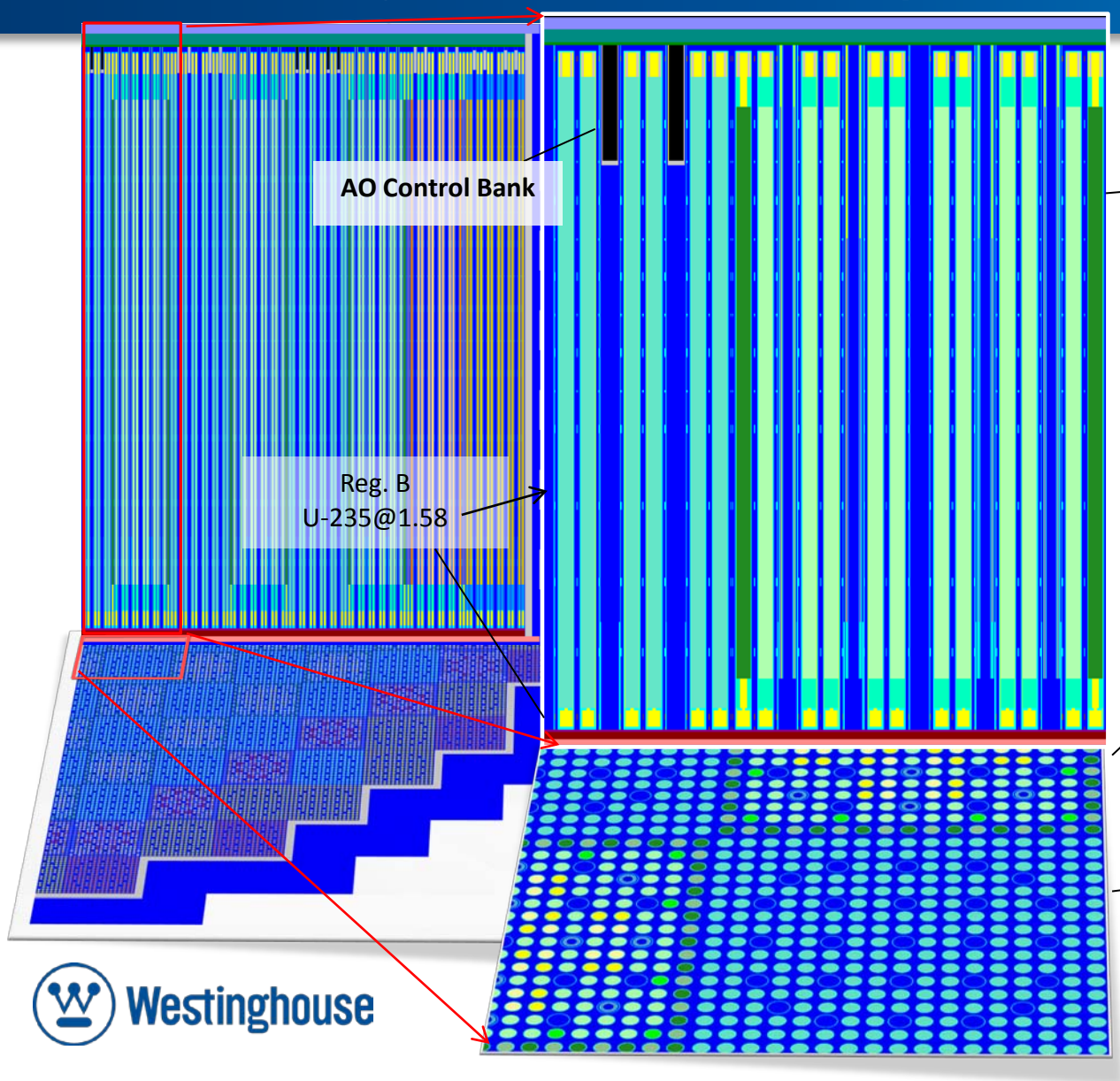
3x3 Assembly with Partial CR (KENO Model)



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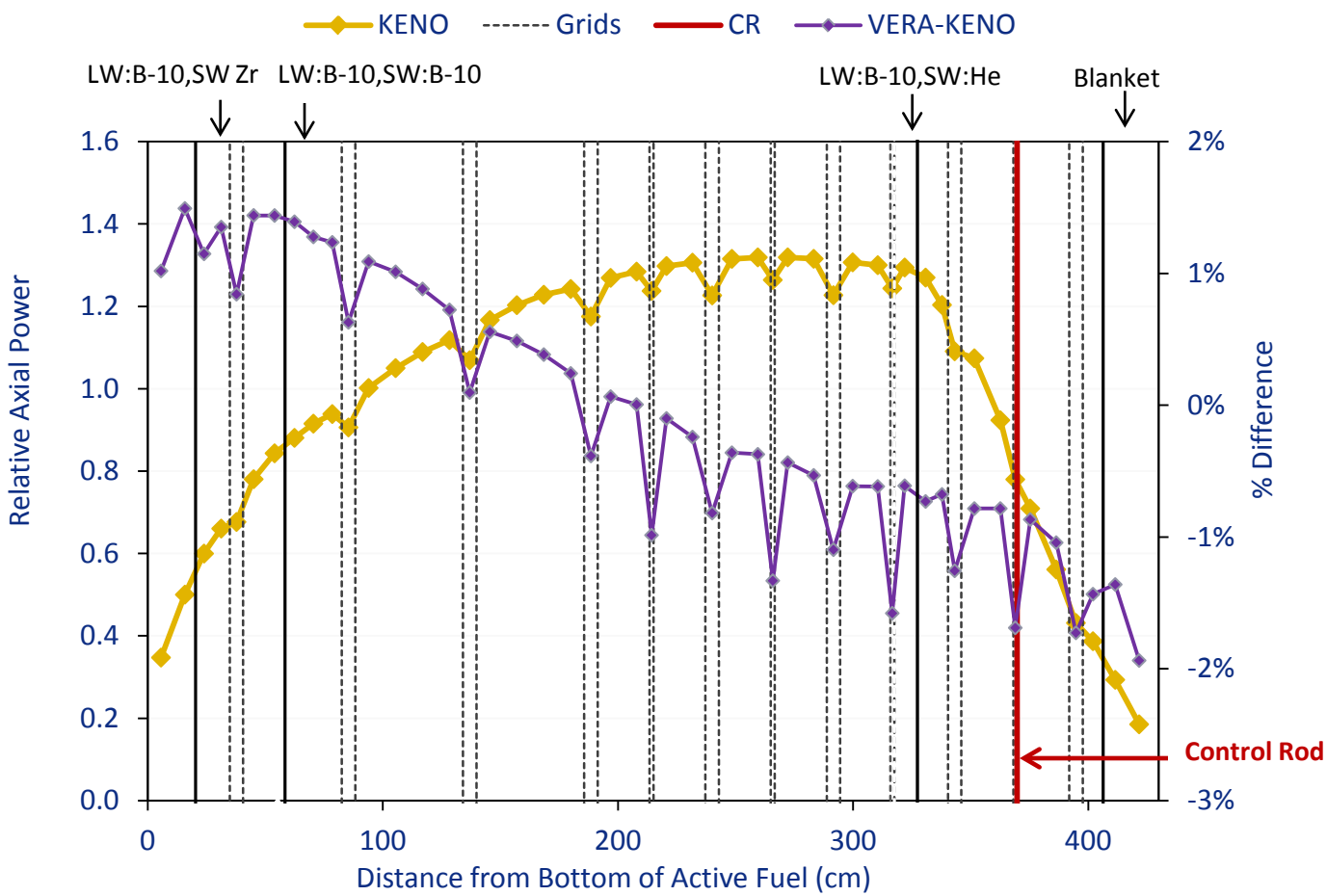
3x3 Assembly Results: Axial Power



Delta k-eff : -18±1 pcm

Delta Axial Offset: -0.7

Delta Power RMS/Max: 0.9/3.1%

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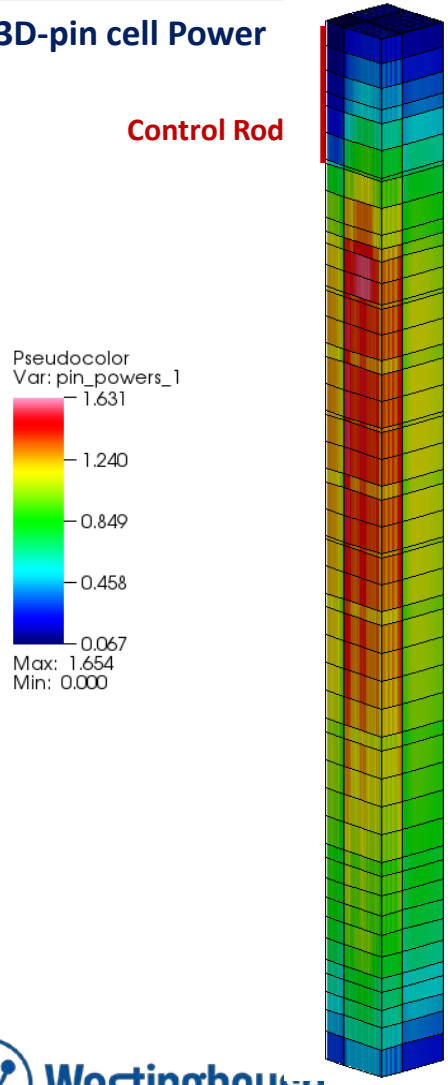
3x3 Assembly Results: 3D Power

3D-pin cell Power

Control Rod



3D-pin cell ΔPower 100x(VERA-KENO)

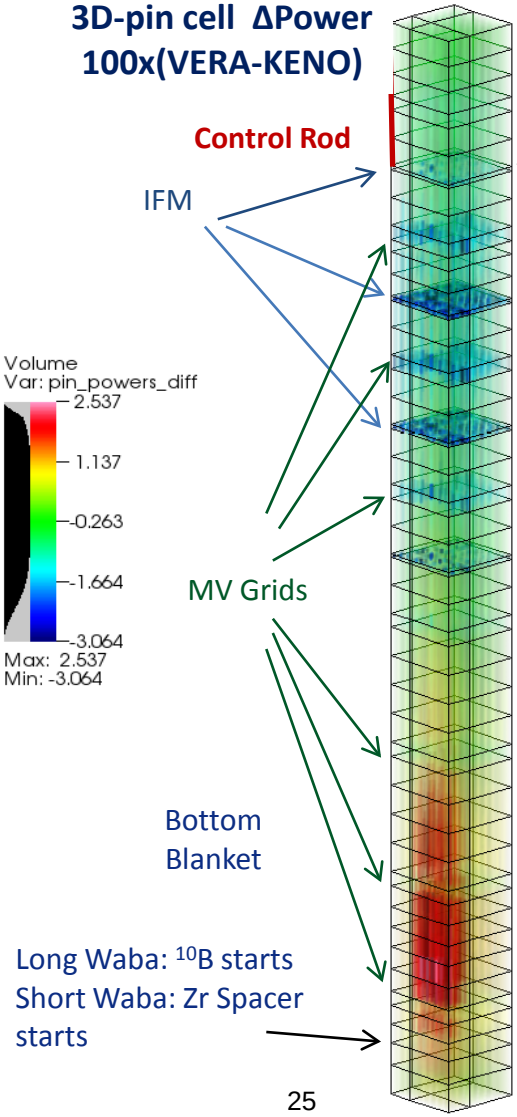
Control Rod

IFM

MV Grids

Bottom Blanket

Long Waba: ^{10}B starts
Short Waba: Zr Spacer starts

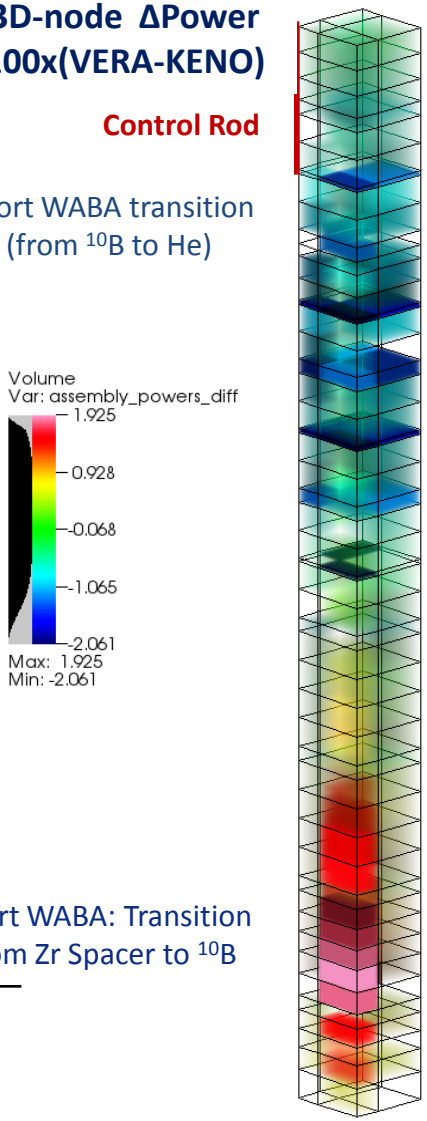


3D-node ΔPower 100x(VERA-KENO)

Control Rod

Short WABA transition (from ^{10}B to He)

Short WABA: Transition from Zr Spacer to ^{10}B



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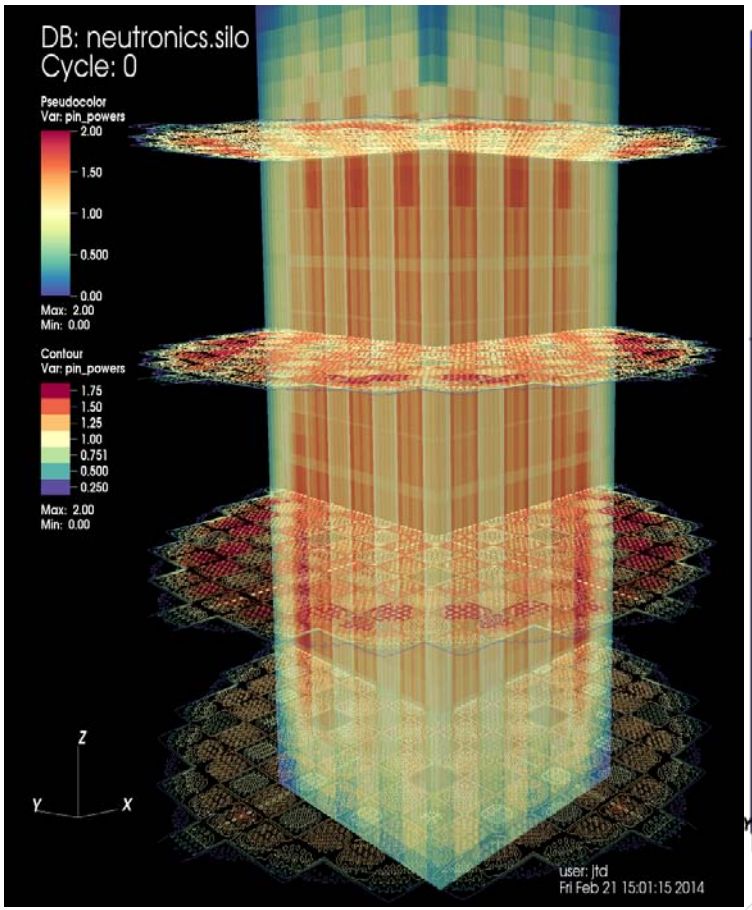
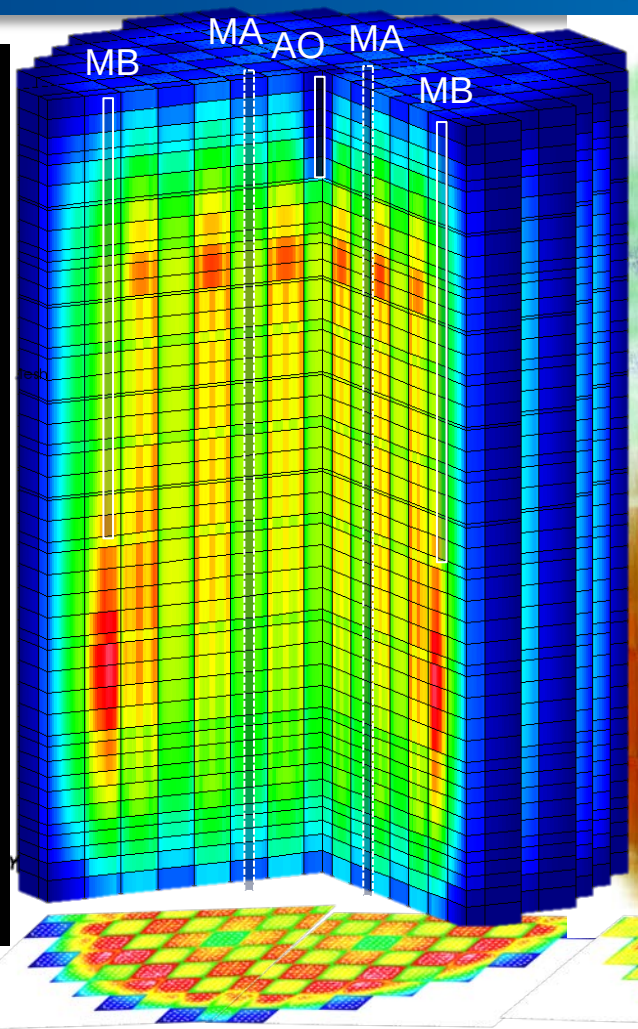
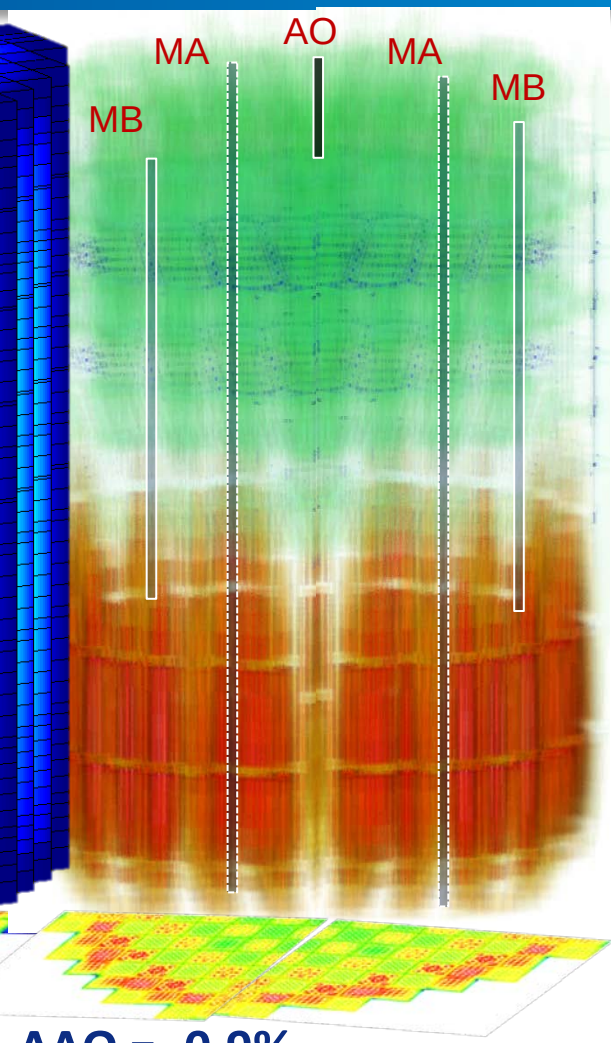
3D Core Power Distribution
(AO and M-Banks Inserted)

3D Core ΔPower
100x(VERA-SHIFT)







Δk-eff = -81 +/- 2 pcm Hot Spot ΔP = 1% ΔAO = -0.9%

RMS ΔP = 1.2% Max ΔP = 5.9%

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CASL

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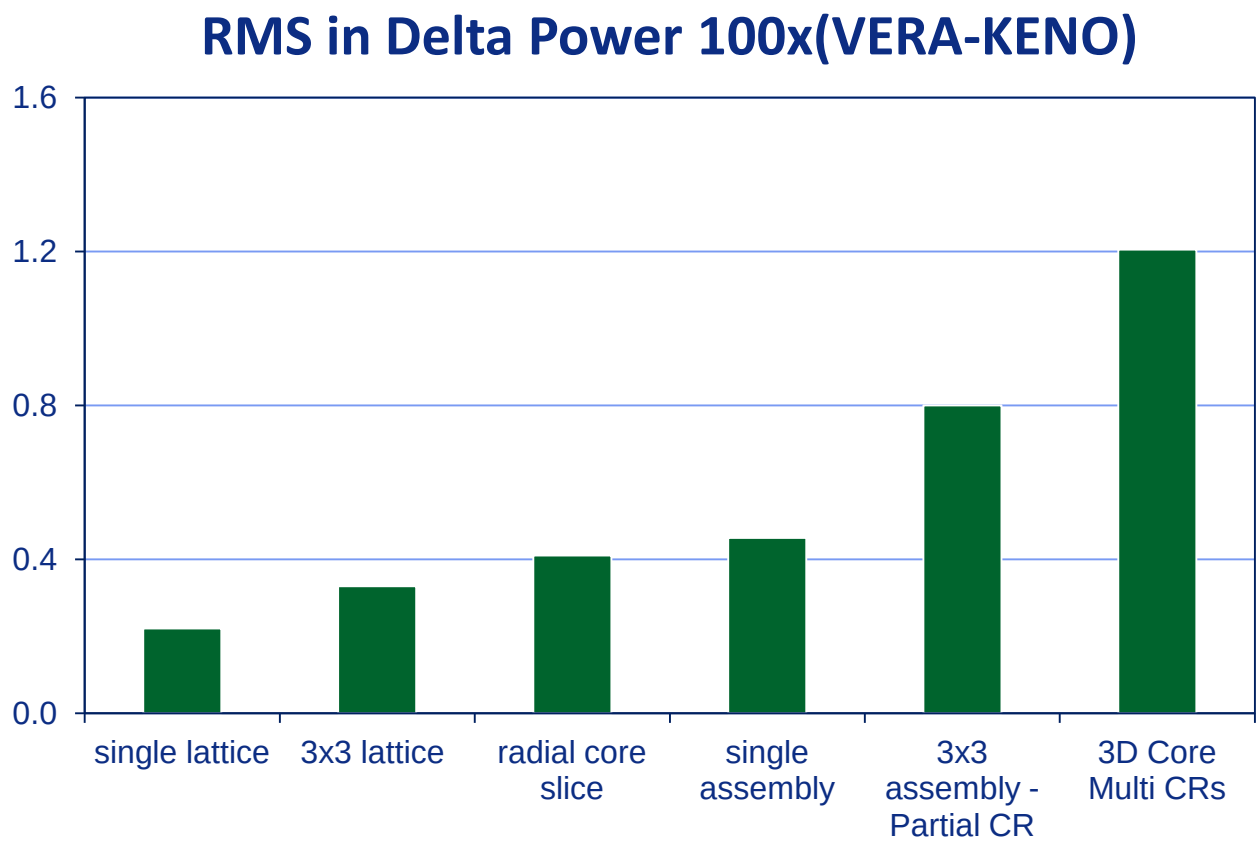
Power Distribution Summary



Overall Remarkable Agreement for VERA Including 3D Core with multi-CRs

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Usability, Benefits, Recommendations

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Computational Resources

	KENO (SHIFT for 3D Core)					VERA-CS SP_5P_3 23g				
	Particles (x10^9)	Pin Unc. %	Cores #	Wall Time	Core Hours	Cores #	Cells #	Core Hours	Wall Time	Memory
2D Lattice	1.1	0.02	312	~3.5h	1K	12	324	0.2	~1 min	<96 GB
3x3 Lattice	3	0.04	300	~10h	3K	12	3K	0.4	~2 min	<96 GB
2D Core	25	0.06	300	~6d	43K	144	86K	13	~5 min	<512 GB
3D Assembly	17.5	0.08	240	~3d	17K	64	0.2M	32	30 min	<512 GB
3D 3x3 Assembly	25	~0.1	180	~6d	26K	144	1.5M	96	40 min	<1.2 TB
3D Core (Eigenvalue)	25	0.38	180	6.5d	28K	320	6M	0.5K	100 min	<4 TB
3D Core (Pin Power)	1,000	<1%?	232K	5.5h	1.3M	4,096	24M	2.3K	34 min	<32TB

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Usability

- Intuitive single-input deck
- Similar to typical core simulators
- Stable execution
- Comprehensive features *for this application*
- Reasonable computational time *for this application*
- Post-processing scripts for comparison and visualization (VISIT)
- Needs a reference (Monte-Carlo and/or measurements)
- Impractical for coupled analysis
- Depletion under development
- No thermal expansion
- Simplistic reflector
- Limited documentation

Promising, applicable to this analysis but not a complete tool yet

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Benefits

- Enhanced confidence in **AP1000** PWR start-up predictions
- Generated high-quality benchmarks for code comparison
- Laid groundwork for cycle depletion calculations
- Expanded application of VERA to an advanced core
- Provided key feedback to guide future developments
- Provided framework for VERA build and update

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Recommendations

- **Mitigate computational resources**
- **Cycle depletion and shuffling**
- Expand capabilities
  - Thermal expansion
  - General reflector
  - Other fuel lattice configurations
- Improve output
- Improve documentation

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Reporting

- Test stand activity documented in public report
  - CASL-U-2014-0012-000

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Conclusions

- Relevant and engaging application of VERA to an advanced PWR first-core
- Remarkable agreement with Monte-Carlo
  - Critical boron and rod worth (excellent agreement)
  - Reactivity coefficients (some discrepancies)
  - Power distribution (very good agreement)
- Very positive and useful experience
- Enhances confidence in first-core start-up prediction
- Main concerns relate to expanding capabilities (coupling, depletion) and mitigating computational resources

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Acknowledgements

- Westinghouse: Jeff Secker David Salazar, Westinghouse PWR Methods group (Mohamed Ouisloumen and Larry Mayhue, Fellow engineers, Baocheng Zhang, Boyan Ivanov and Harish Huria, Principal Engineers), Keith Drudy, Bob Fetterman, Larry Hampshire, Joseph Walsh, Greg Fischer

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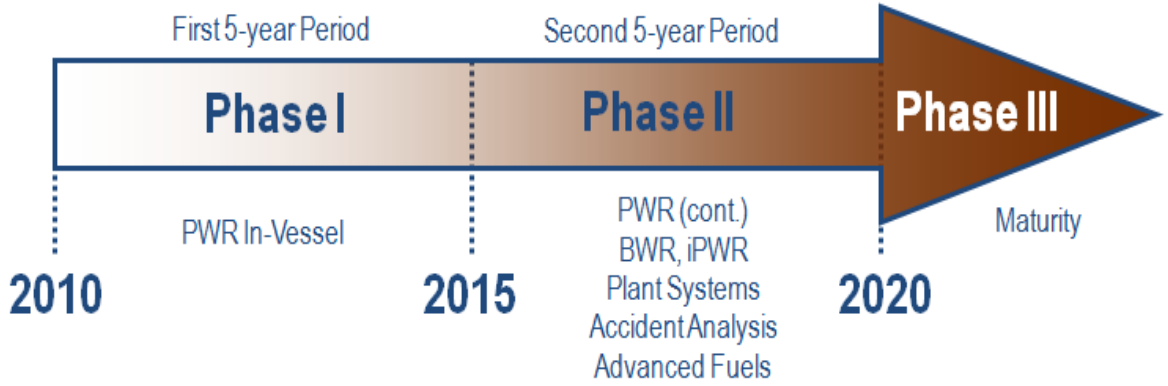
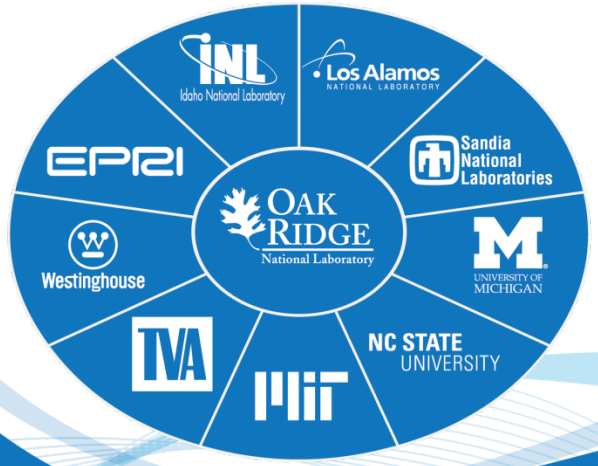
- The KENO-VI development and CE data teams at ORNL, including Kursat Bekar and Cihangir Celik





Phase 2 Technical Scope Determination

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Guiding Principles for Phase 2 Technical Scope Selection

- Top Priority: Deepen the active Challenge Problems in Phase 1 and support deployment to industry
- Industry Impact: Assure new Challenge Problems will be impactful if successful?
  - Supports power uprates, improved fuel utilization, and/or increased operational freedom
  - Extends PWR capabilities to other reactor types, e.g. BWRs and iPWRs
- Programmatic: Assure ModSim capabilities required can be developed
  - Technical challenges be overcome
  - Budget and time available adequate to accomplish
  - Capabilities required leverage capabilities being developed under Phase 1
- Science/Engineering Innovation
  - Better understanding of basic science
  - “Game changer" with respect to current industry methods

DOE-NE Phase Two Scope Guidance

CASL Phase 1 Results

Broaden

Other Reactors Scope

- Other PWR fuel forms
- BWRs
- New PWRs
- SMRs
- More . . . ?

Deepen

Phase 1 Reactors Scope

- Improve modeling and simulation products to better address existing challenge problems
- Extend modeling and simulation products to other PWR challenge problems
- Improve usability
- Extend and improve deployment
- More . . . ?

Firm scope constraints not evident at this time

Potential expanded scope for Phase 2

OPTIONS *(other combinations possible)*

A. Deepen the work on the active PWR Phase 1 CPs (limited structural)

B. Deepen capabilities for structural analysis beyond those available and apply to address PWR FAD, GTRF and seismic CPs

C. Broaden capabilities for iPWR regarding core simulator, coupling to system code, and technically support one Phase 1 CP Test Stand (e.g. PCI)

D. Broaden capabilities for BWR regarding core simulator with no specific CP addressed

E. Broaden capabilities for BWR regarding MCFD (constrained capabilities development factoring in across focus areas balance and staff resources)

F. Broaden capabilities for BWR regarding fuel performance to address PCI, CILC, PCI, RIA and LOCA (exclusive of core simulator development)

Remaining funding, if any, after activity selection could be utilized to address CFD natural circulation [including transport and chemistry], BWR specific CPs, and deeper dive into iPWR CPs, as budget allows

Possible Phase 2 Technical Scope - PWR

PWR Challenge Problems

- Deepening of work on seven CPs started in Phase I.
  - CIPS/CILC
  - PCI
  - GTRF
  - RIA
  - DNB (multiphase-CFD focus)
  - LOCA (fuel performance focus)
  - RIA Boron Precipitation during LOCA (with fibrous debris)
- FAD
- Seismic Response (fuel performance focus)
- Upper internals thermal stratification of coolant & related materials issues

Possible Phase 2 Technical Scope - BWR

- BWR Core Simulator

<u>BWR Challenge Problems</u>

- Extension of Phase I PWR CPs
  - CILC
  - PCI
  - Dryout (multiphase-CFD)
  - RIA
  - LOCA (fuel performance focus)
- Bypass Flow
- Channel Bow
- Shadow Corrosion
- Seismic Response (fuel performance focus)
- Stability
- Boron Precipitation during ATWS(with fibrous debris)
- Lower plenum flow mixing

Possible Phase 2 Technical Scope - SMR

- SMR Core Simulator

<u>SMR [of iPWR type]</u>

- Extension of Phase I PWR CPs
  - CILC
  - PCI
  - GTRF
  - RIA
  - DNB (multiphase-CFD)
  - LOCA (fuel performance focus)
- FAD
- Seismic Response (fuel performance focus)
- Stability (natural circulation)

Possible Phase 2 Technical Scope - Assorted

- Accident Tolerant Fuels
- Natural Circulation & Mixing (Normal Ops [NuScale] & Passive Safety Systems' Responses [all reactor types])
  - BWR boron mixing and distribution during ATWS
  - PWR & BWR ECCS injection and distribution (modeling with CFD)

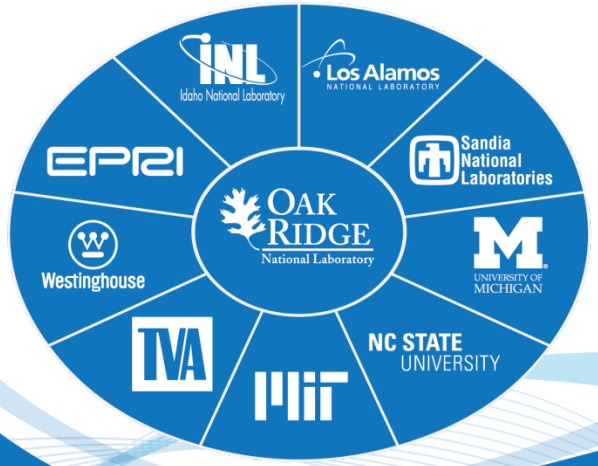
New CP Mini-Charters

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 INDUSTRY 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

Deployment Area



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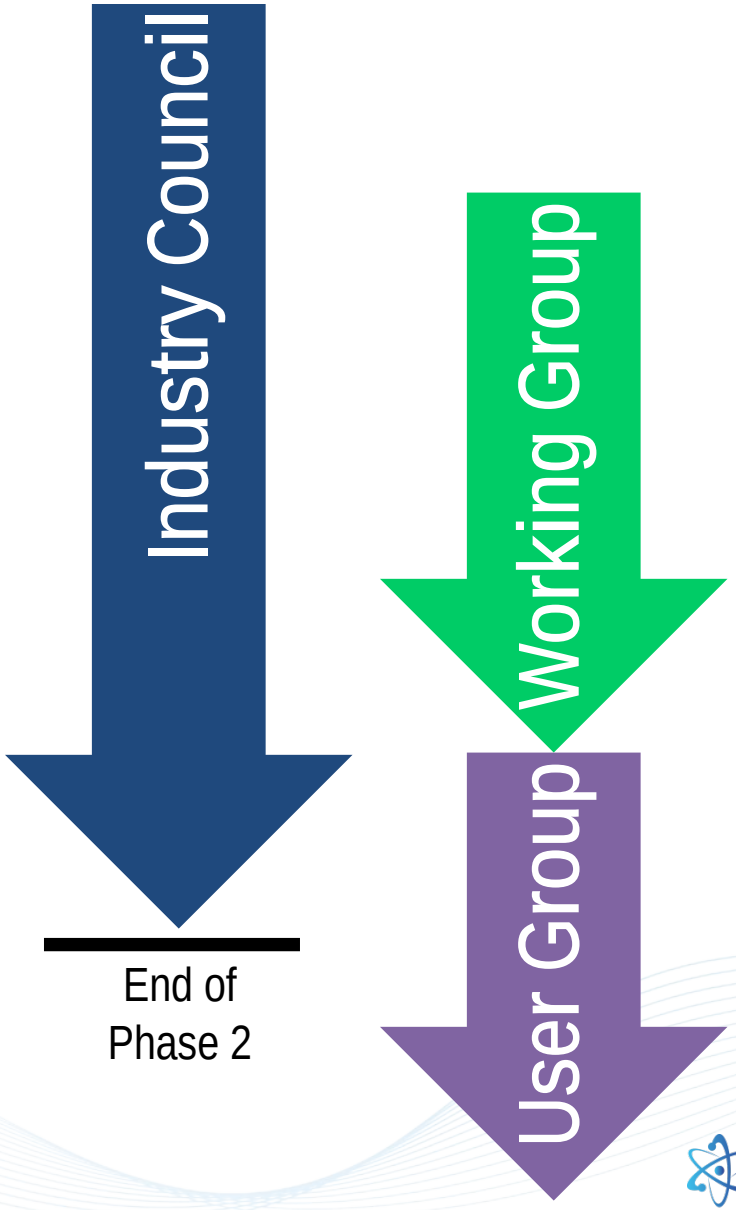
Management Structure
Establish a “Deployment” Area

The current concept…

- Lead and Deputy reports to the SLT
- Scope includes:
  - Industry Council
  - Modeling and Simulation Working Group that evolves to a User Group
  - Test Stands
  - VERA Release, Support, and Training
  - Software Licensing

Industry Council Continues with Expanded Outreach
Working Group Gears Up and Transitions to User Group

- Two distinct organizations:
  - Industry Council
    - CASL milestone focus
  - Modeling and Simulation Working Group / User Group
    - User experience focus
- General plan is for the User Group to take over from CASL after the hub is discontinued



Industry Council
Evolution

- Expand purpose
  - Current
    - "…provide critical two-way communications and information exchange…"
  - Expanded
    - Provide guidance/direction and functional requirements to CASL on the application of VERA to a problem that is relevant to industry (from initiation to completion)
- Change the leadership structure to include a member of the IC
  - For example - Industry Council is supported by a CASL team member (Executive Director) and chaired by a member of the Industry Council (Chairperson)
- Subcommittee of the Industry Council working on this
- Implement changes in September 2014

Modeling and Simulation Working Group / User Group
Value

- Members will be users of CASL products and receive product information /updates
- Members will receive software support for CASL products
- Members will receive periodic training
- Members will have opportunity to “pool” resources for software development
- Members will have opportunity to fund directed software development

Modeling and Simulation Working Group / User Group
Concept

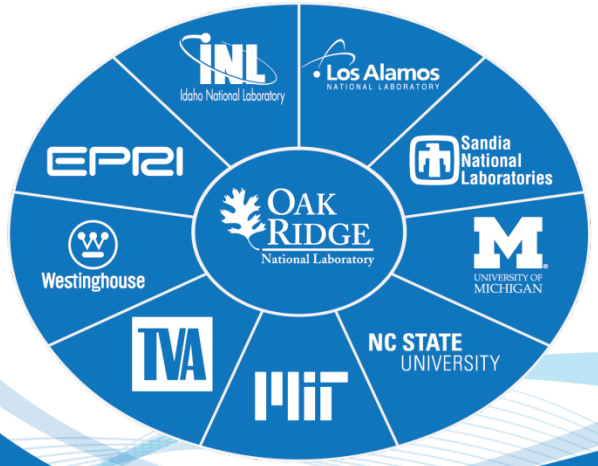
- CASL would like to more aggressively embrace potential users and researchers in the nuclear community during Phase 2 with and through VERA
- Modeling and Simulation “User” or “Working” Group consisting of industry and research community members that we would stand up in Phase 2
- This UG, if successful, could be one of the key entities to “lives on” after CASL
- Group would provide a community for sharing experience, and if able to generate and/or receive revenue (e.g., from DOE NE, CASL, user/license fees, etc.), help to continue development and on-going support of the CASL tools
- Periodic meetings
- Similar to other groups where the membership proposes projects. Then prioritizes projects to determine what work gets done.

VERA Interoperability

Jess C. Gehin
CASL, Physics Integration

Eric Volpenhein
CD-adapco

Industry Council Meeting
Electric Power Research Institute
Charlotte, NC
March 11-12, 2014



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interoperable |ˌintərˈäp(ə)rəbəl|

adjective

(of computer systems or software) able to exchange and make use of information.

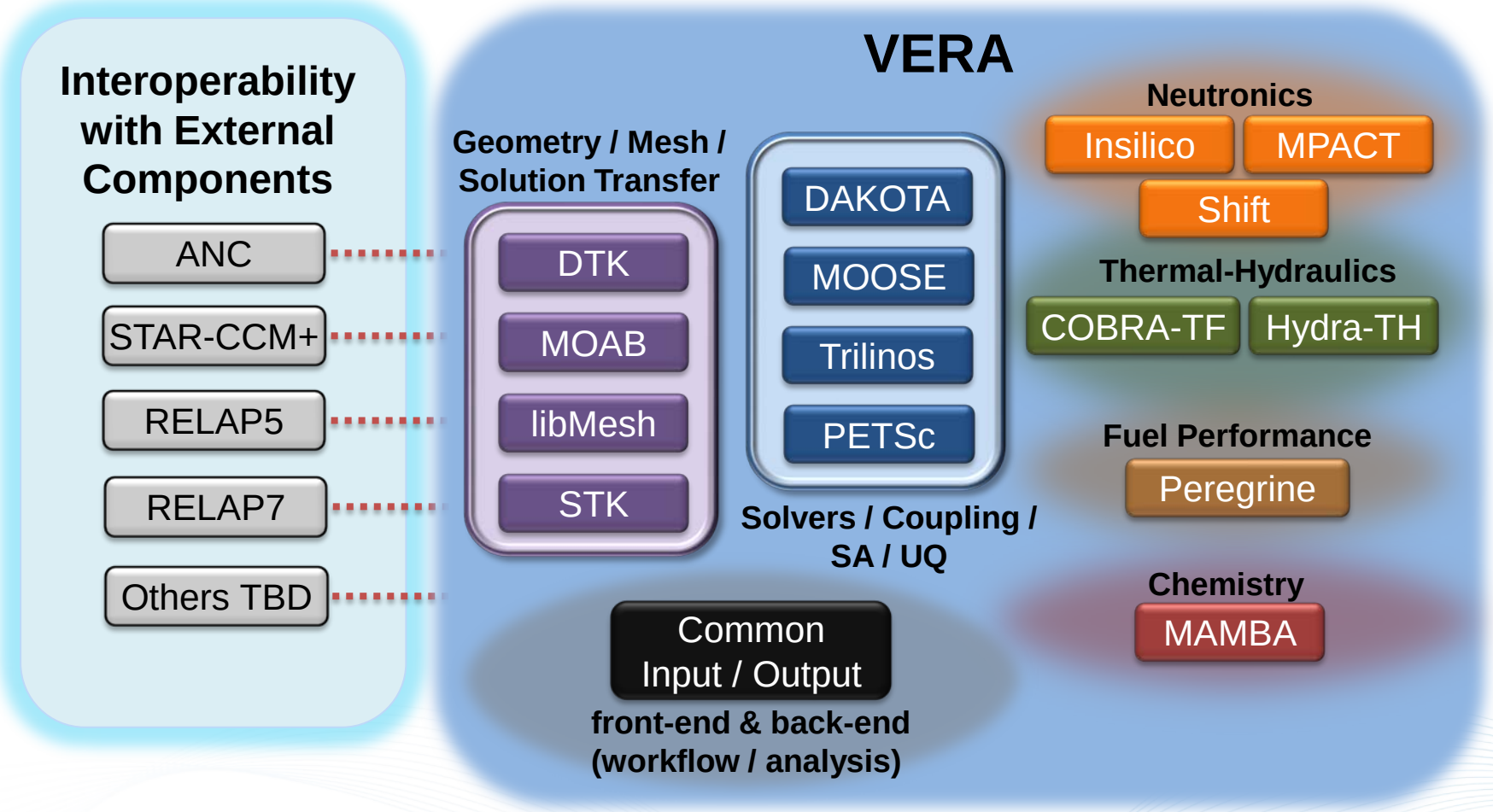
DERIVATIVES

interoperability |-ˌäp(ə)rəˈbilitē| noun

- For CASL purposes, *interoperability* refers to the process of working with software that is external to VERA
- Approaches for interoperability will be determined by needs for the software to work together
- Three primary scenarios for interaction with external codes / components
  1. Share data through data files (input, output, restart or other data formats)
  2. Software coupling and data transfer with external (potentially proprietary) components
  3. Use VERA components (or applications) in another environment
- We are currently focusing on #1 and #2

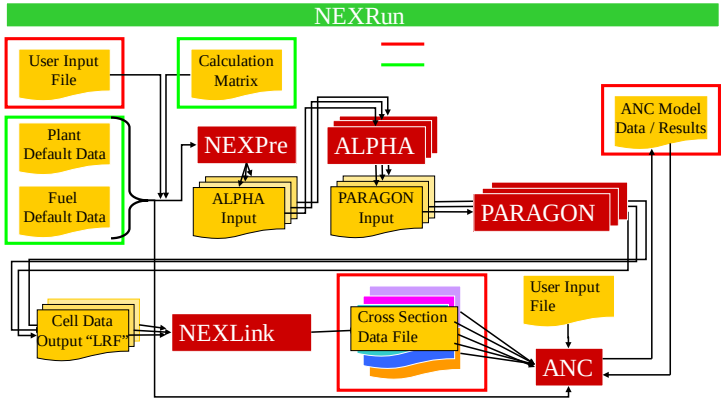
Virtual Environment for Reactor Applications (VERA)

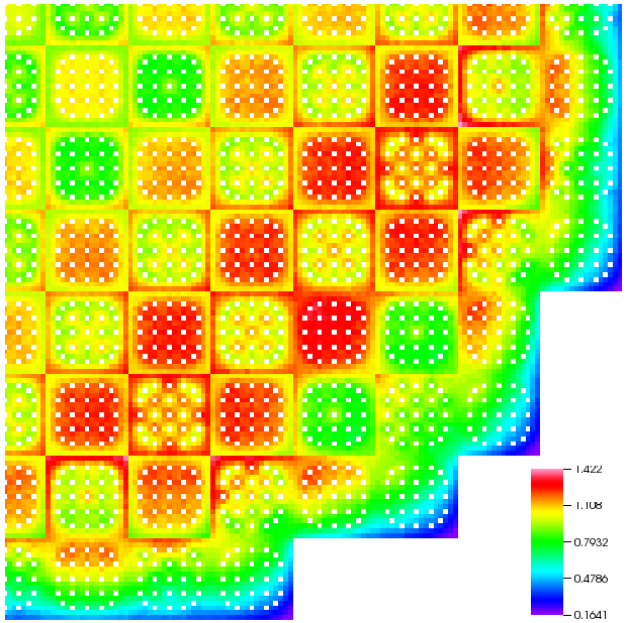
Planned Components



Planned Interoperability with ANC

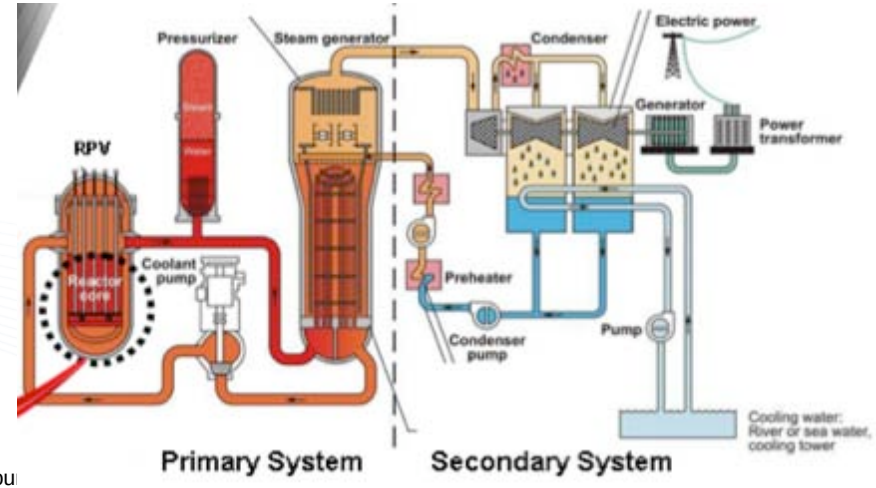
- A common need is for VERA to use results from existing core simulators:
  - Rod power histories for fuel performance, crud deposition analysis (Peregrine, Mamba)
  - Steady state and transient power distributions for thermal-hydraulics analysis (COBRA-TF)
  - Isotopic distributions for VERA-CS starting conditions at a particular cycle
- Currently working to use power distribution data from Westinghouse nodal core simulator ANC
- Data transfer is in the form of simple data files since data transfer is one direction and relatively small user VERA restart file format ("Type 1" interoperability)
- File transfer will be compatible with other industry codes
- Requires no (or minimal) changes to ANC and VERA to accommodate





Planned Interoperability with RELAP5/RELAP7

- CASL needs a reactor systems code to support challenge problems
  - Reactivity Insertion Accident – plant response to calculate peak pressure
  - Loss of Coolant Accident – provide LOCA conditions for fuel performance
- Initial activity in CASL to integrate with RELAP5
  - Model evaluator developed and demonstrated for RELAP5
  - Not coupled to other physics at that time
- Future activity will be to couple RELAP5 to CASL tools (COBRA-TF and HYDRA-TH) ("Type 2" interoperability)
- RELAP7 currently under development by LWR-S/NEAMS programs and will be a target for interoperability in the future.
  - RELAP7 is MOOSE-based and interoperability development will parallel that of integration of Peregrine



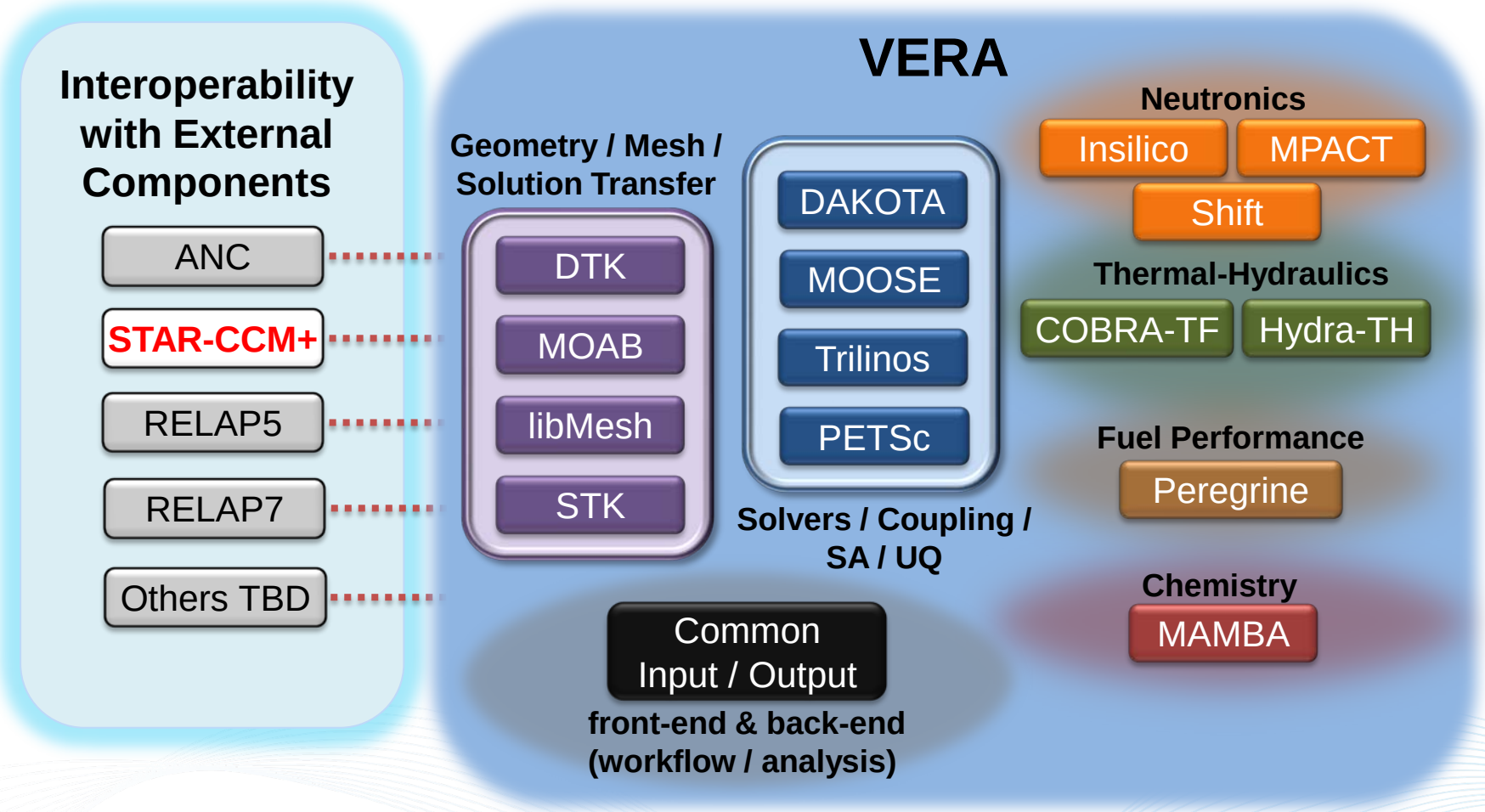
Interoperability with STAR-CCM+

- Commercial CFD codes provide substantial simulation capably that would be useful for VERA users to leverage
  - Existing models and experience in use of the codes
  - Develop example application of means of more tightly coupling with external codes
  - Can provide path way to other commercial physics codes using the commercially developed interfaces
- As discussed at last IC, CD-adapco is supporting development of interoperability capably with VERA and SHARP (NEAMS capability)
  - Addresses issues with early CASL work in coupling with STAR-CCM+ involving file-based transfers
  - Extensive work in model development
  - Identified needs for both CASL and NEAMS to provide tighter integration
- Engagement between CD-adapco, NEAMS and CASL on requirements for data and solution exchange
- Eric Volpenhein will provide a status update

Other Potential Interoperability Targets

- CASL is interested in interoperability with other software tools that:
  1. Support an identified need within CASL to meet our goals and objectives
  2. Are identified by VERA as a need or requirement
  3. To support CASL objectives of having broad impact with CASL products
- Of course, resources are limited, so we will have to be judicial in our choices.
- Initiated planning and discussions with ANSYS for interoperability with Fluent
- Considering need for interoperabilty with structural mechanics code
- Please discuss your interests with us to determine if it would be mutually beneficial to support interoperability of your software with VERA

VERA – STAR-CCM+ Interoperability



VERA / STAR-CCM+ Interoperability Timeline

Accepted by IF

Accepted by PDT

PDT Steering Committee

Mar 2013 → **Mar 2014**

Working Descriptioin

To Innoavation Form (IF)

Feasibility Assessment

Functional Requirements

Conceptual Design

MOAB Integration Project
Software Requirements Specification
Version 0.6
January 2014 Draft

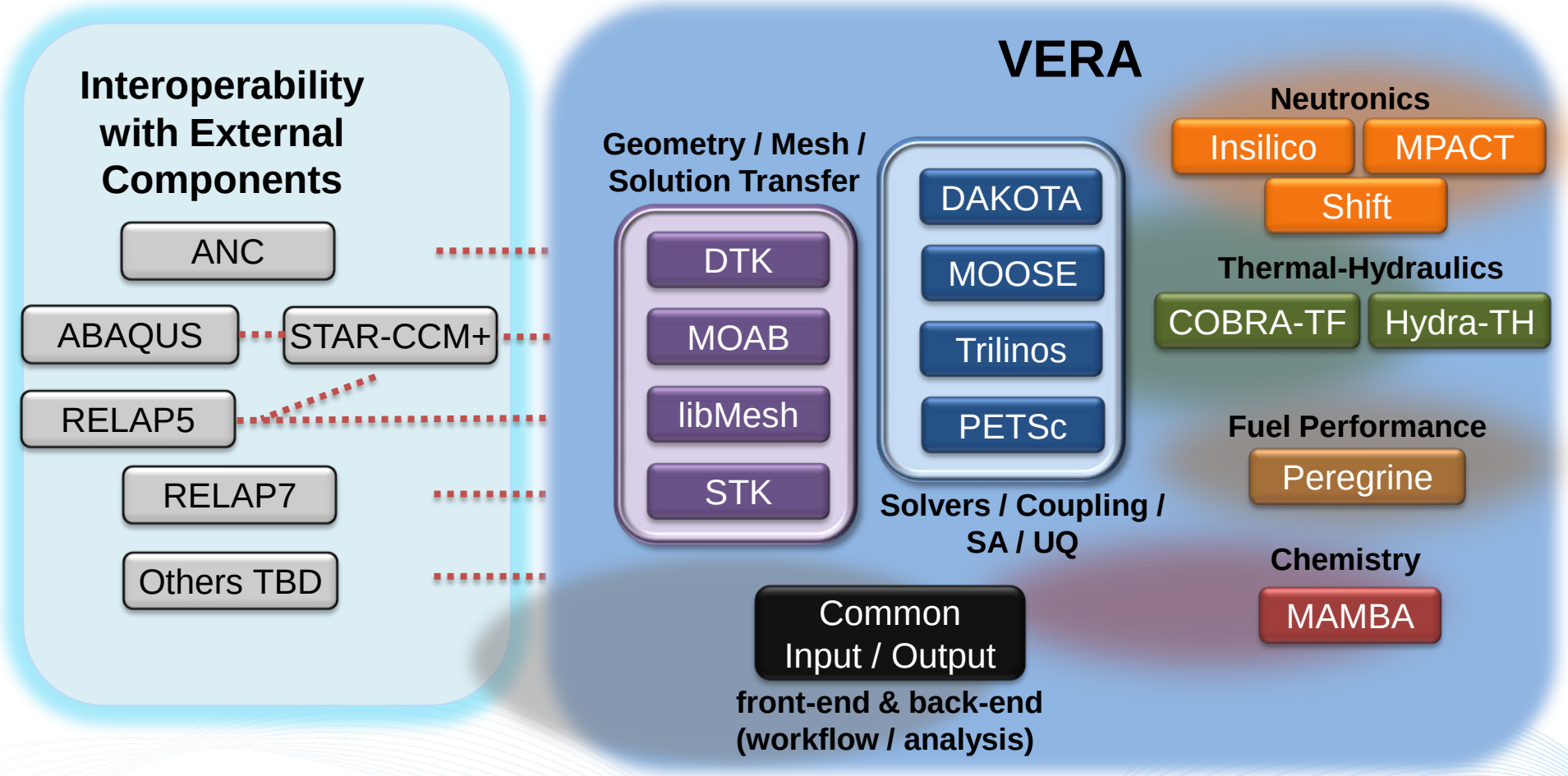
Highlights of STAR-CCM+ API for MOAB / DTK

- Enable efficient static and dynamic communication with MOAB / DTK:
  - Static
    - Two way mesh translation and results mapping
  - Dynamic
    - Mesh translation
    - Spatial and temporal data transfer, in memory, core-to-core
    - enhanced solution control via embedded call functions: Begin & End Simulation(Run), Begin & End Time-Step, Begin & End Iteration
- Future considerations:
  - Topological changes (mesh motion / morphing)
  - Additional solution controls
    - Time step do-over
    - Distress management
- Communication with external (to STAR-CCM+) code done via MOAB / DTK and / or User Programming

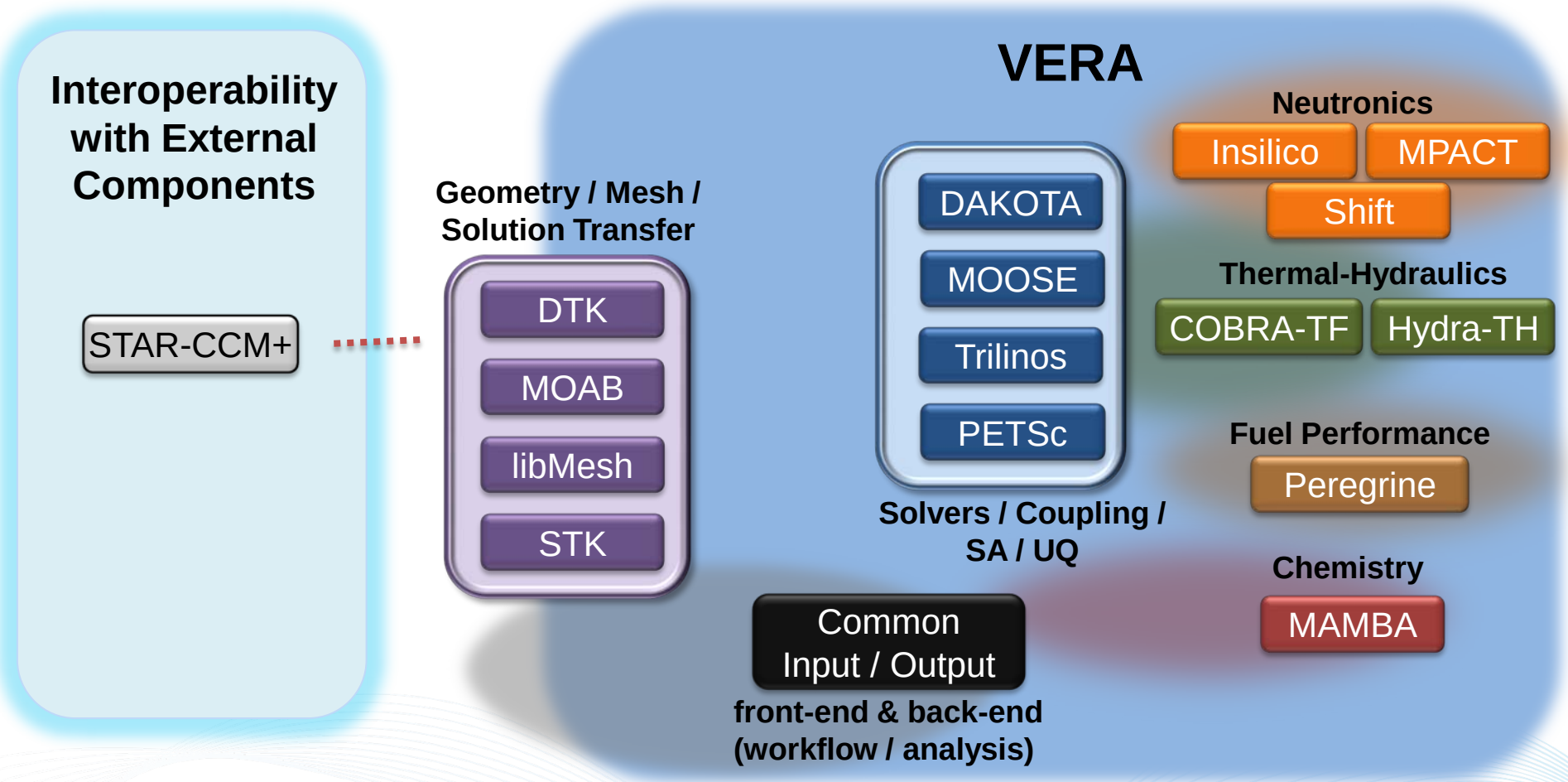
Requested STAR-CCM+ Release Schedule

2014	v9.02	v9.04	***v9.06***
	Feb	Jun	Oct

VERA – STAR-CCM+ Interoperability Collateral Connections



VERA-STAR-CCM+ Interoperability Collateral Uses



Modelling and simulation at EDF

Didier BANNER

CASL March 11-12 2014 Meeting

About EDF

World leader in electricity

From generation to trading and network management

1st nuclear fleet in the world

1st French renewable operator

International group with roots in Europe

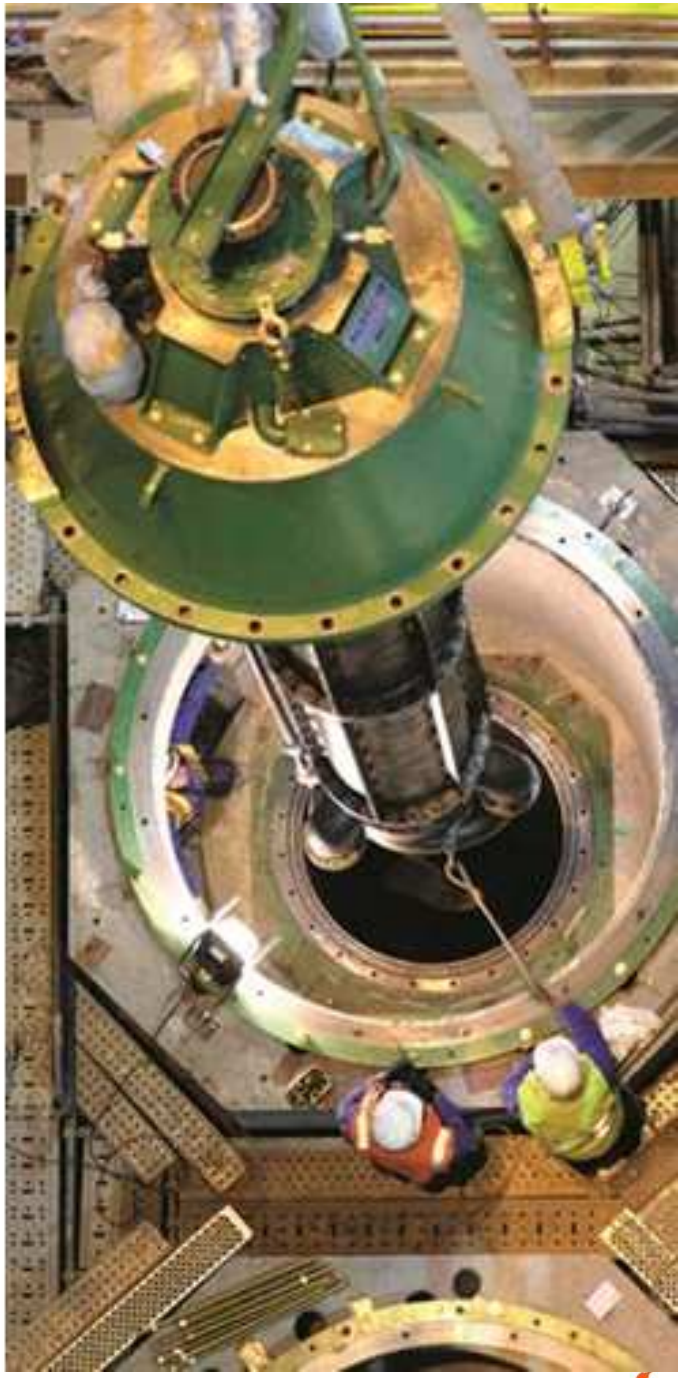
37.7 million
customers worldwide

628.2 TWh
electricity generation worldwide

156,168
employees worldwide

99.6 g of CO_2
per kWh generated
(CO_2 emissions from EDF Group electricity and heat generation)

€65.3 billion
in sales



Modelling and simulation at EDF

1. Strategy for simulation at EDF

2. A short walk through applications :
   General overview of simulation via applications

Modelling and simulation at EDF R&D

1. **Strategy for simulation at EDF**

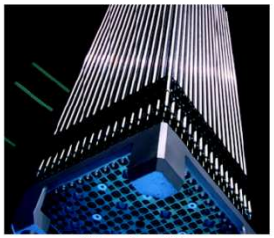
2. **A short walk through applications :**
   General overview of simulation via illustrations

Modelling and simulation what for ?

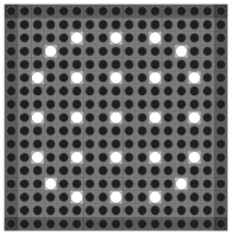
- **Justifying installations**
  - Identification of **new safety margin** allowing to extend lifetime of plants
  - Evolution of regulations and rules
  - Analysis of accidental situations non reproducible by experiments
- **Understanding physics or system response**
  - **Ageing** of materials and installations
  - Addressing the issue of uncertainties and identifying the prominent parameters
- **Qualifying and optimizing processes**
  - NDT methods
  - **Optimizing** materials

The need for a complete chain of skills and tools

1- Modelling :
from physics to equations

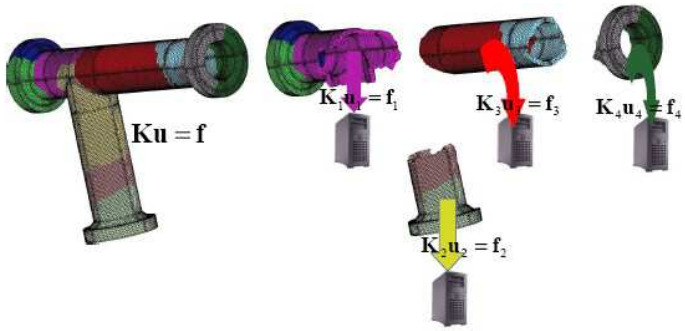


(b) Assemblage MOX

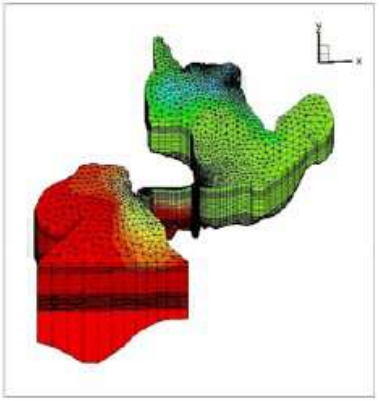


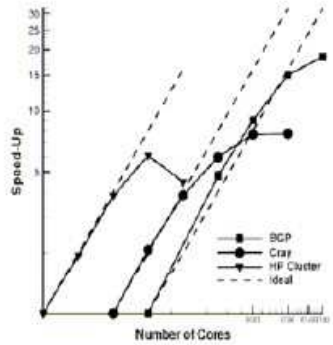
$$\frac{1}{v}\frac{\partial\phi(\vec{r},\vec{\Omega},E,t)}{\partial t} = -\left[\vec{\Omega}\cdot\vec{\nabla}+\Sigma(\vec{r},E)\right]\phi(\vec{r},\vec{\Omega},E,t)+ \frac{\chi(\vec{r},E)}{4\pi}\int dE'\,\nu\Sigma_f(\vec{r},E')\int d^2\Omega'\,\phi(\vec{r},\vec{\Omega}',E',t)+ \int dE'\int d^2\Omega'\,\Sigma_s(\vec{r},\vec{\Omega}'\leftarrow\vec{\Omega},E\leftarrow E')\phi(\vec{r},\vec{\Omega}',E')+Q_e(\vec{r},\vec{\Omega},E,t)$$

2- Analysing and coding :
from equations to algorithms and codes



3- Adaptation to computers architectures for HPC

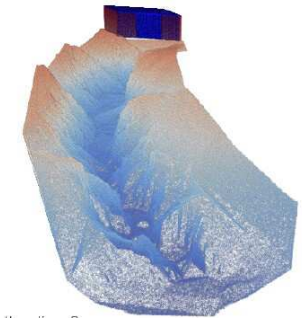


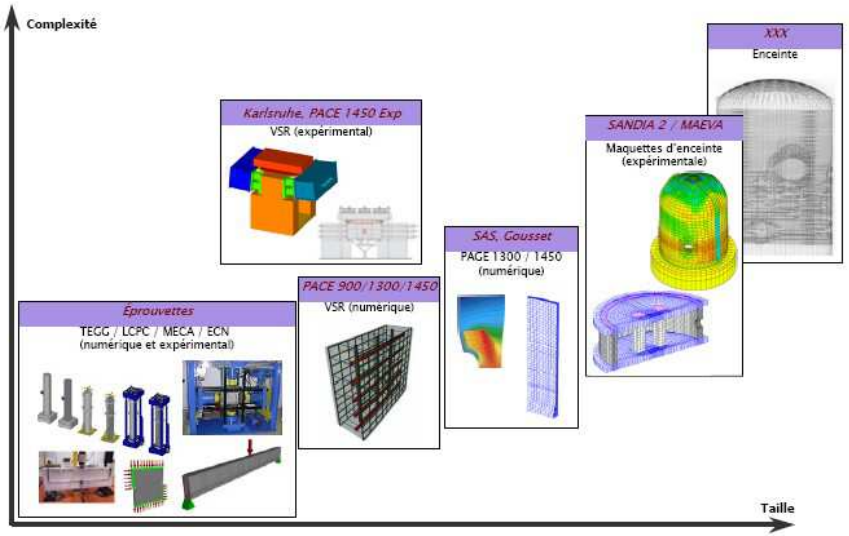


Chemistry-hydraulics of Berre Lagoon

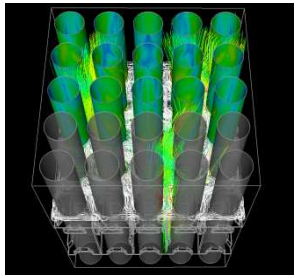
The need for a complete chain of skills and tools

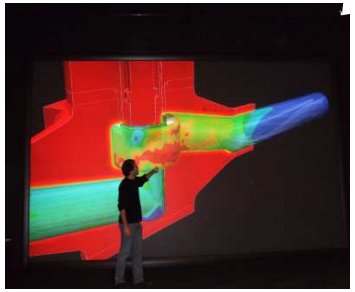
4- Validating and identifying :
on benchmarks and experimental campaigns, determination of physical parameters

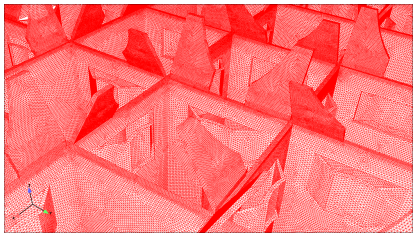




5-Pre and post processing :
Meshing, visualisation, error computation and mesh adaptation

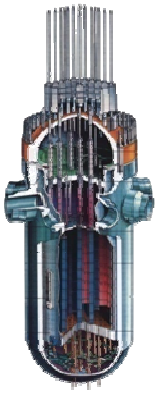


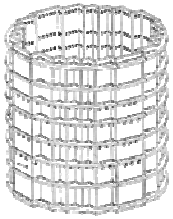


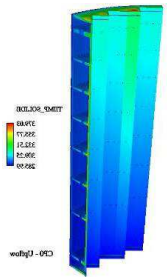


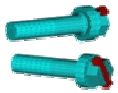
The need for a complete chain of skills and tools

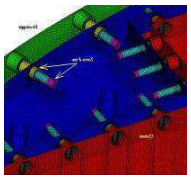
6- Building of methodologies :
probabilistic approach, coupled physics, multiscale analysis, best estimate analysis, data assimilation

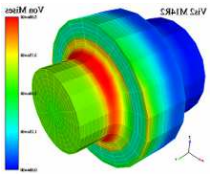


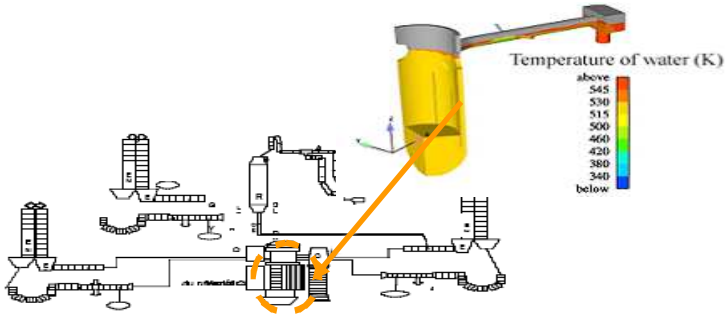


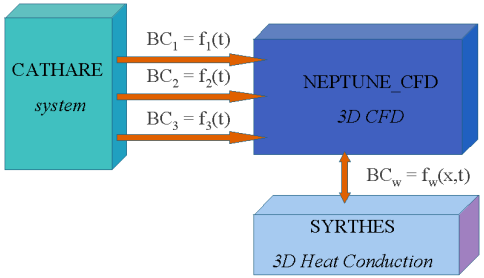




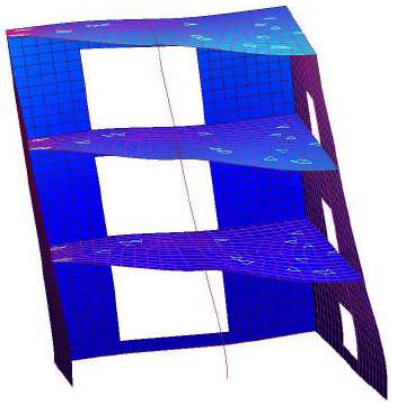








7- Qualifying :
determination of validity domains of methodology in real life applications



Simulation codes developed at EDF R&D

Aero Acoustics	Solid and structure Mechanics	Hydro dynamics	Fluid Dynamics	Material Simulation	Neutronics	Electro magn.	System Code	Th-meca fuel rod
Safari	ASTER	Telemac	Saturne/ Syrthes	Dy-Laki Moca	Coccinelle	Carmel	Cathare	Cyrano
	Euro plexus	Estel	Thyc	Micro megas	Cocagne			
		Mascaret	Neptune	VASP	Tripoli			

EDF codes

Non-EDF codes

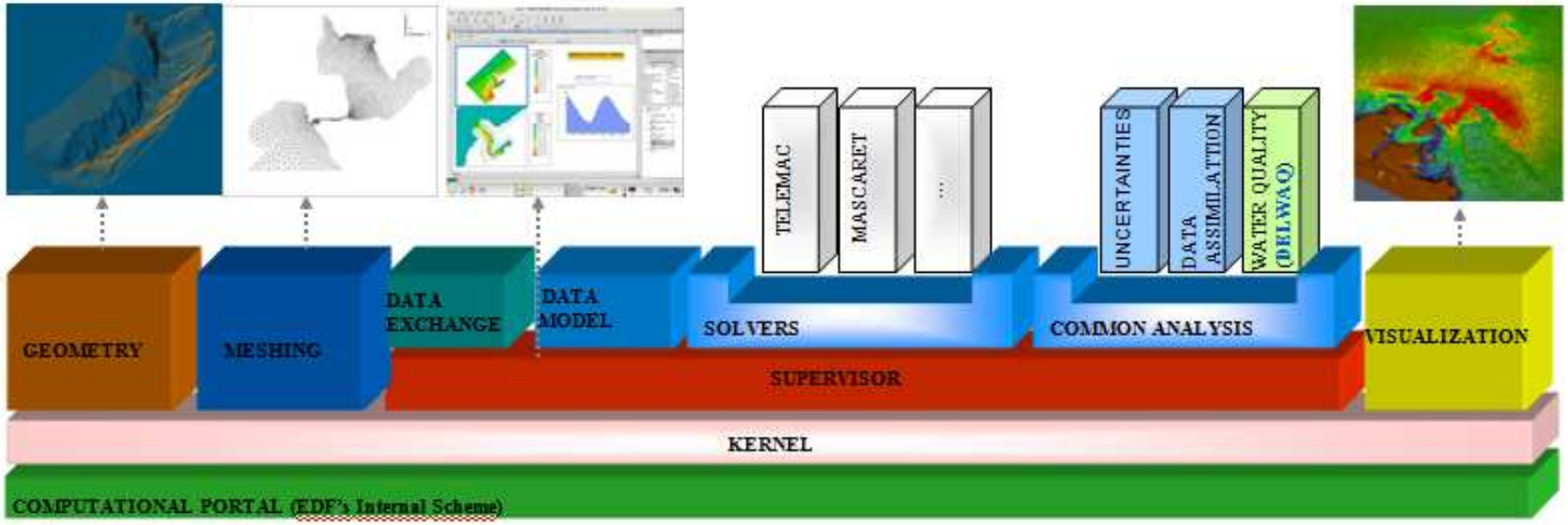
+ Simulation Platforms Salome, Pleiades, Hydroinfo, …

ISPRA	Delft BAW	CEA	ONERA	CERFACS	LIFL	CEA	CEA
CEA	CETMEF SOGREAH	Man chester	LMPGM	INRIA	LEEP		
GIREF	ENPC INRIA Bristol	LEA	CEA	CEA			

Development Partners

EDF

THE SALOME MODELLING ENVIRONNEMENT



SALOME

The choice of a significant effort on in-house codes development

- **Capitalization tool for**
  - Expertise
  - Methodologies
  - Linked tools : data bases and pre-post

- **Efficient technological transfer to BU or engineering divisions**
  - Ageing of materials and installations
  - Development of new overall methodologies

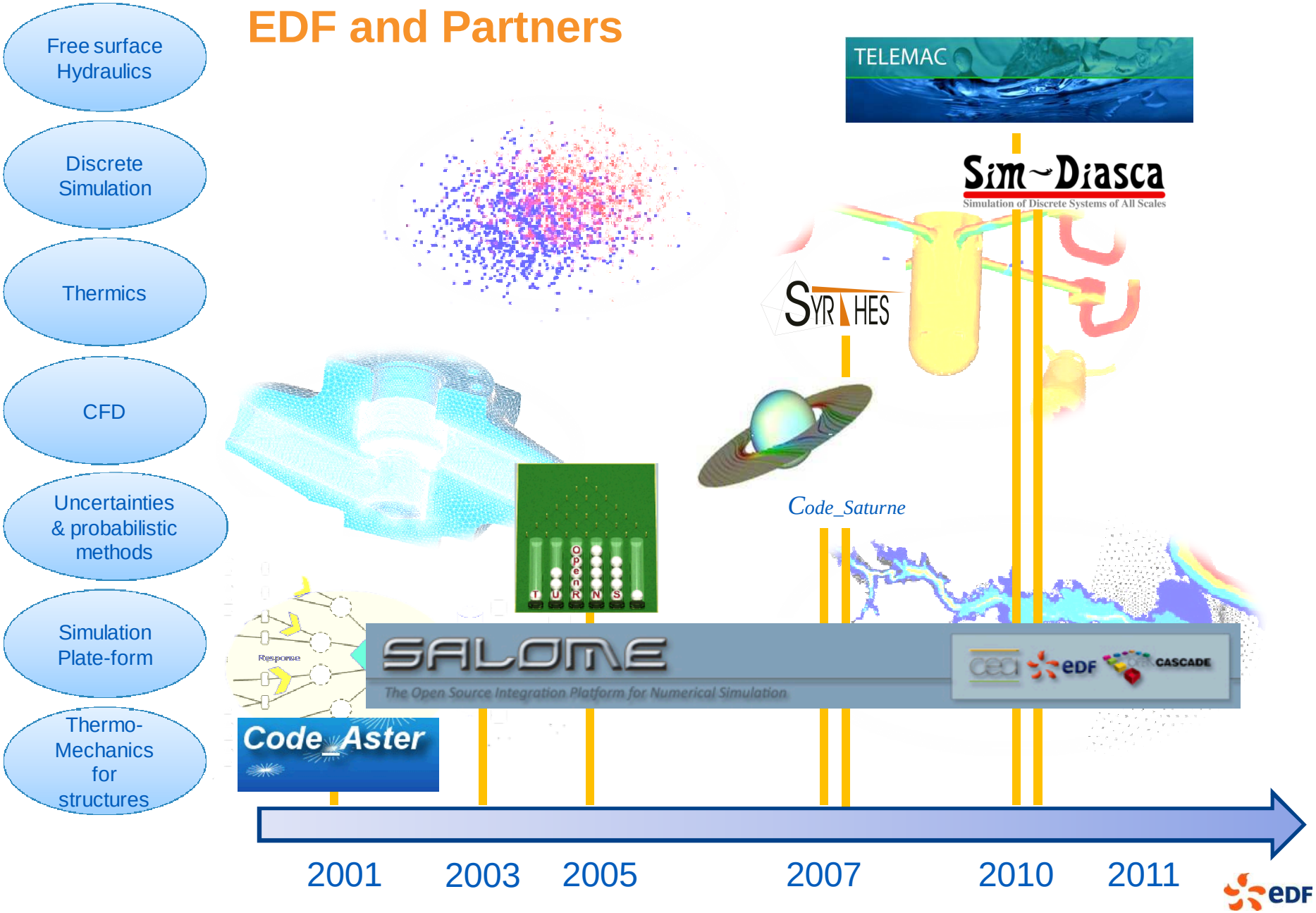
- **Non existing adequate commercial offer**
  - Specific physics or functionalities not addressed
  - Closed black-box solutions

The open source way for in-house developed codes and systems

Code_Aster, Code_Saturne, Telemac Open-Turns, Code_Carmel, Salomé

- **Improving the codes :**
  - By validation, bug detection,
  - Extension of validity domain or to new simulation domains
- **Sharing development effort**
  - Development induced in the community
  - Open codes can be coupled with other ones in multiphysics or multi purposes platforms
  - Sharing validation effort
- **Facilitating collaboration**
  - With academics (no licence, capitalisation tool, .)
  - With industrial partners (interaction with others codes,
- **Facilitating dissemination acceptance of methods**
- **Support to education**
  - For students and initial formation
  - Building a community of end-users

Open Source dissemination of softwares of EDF and Partners

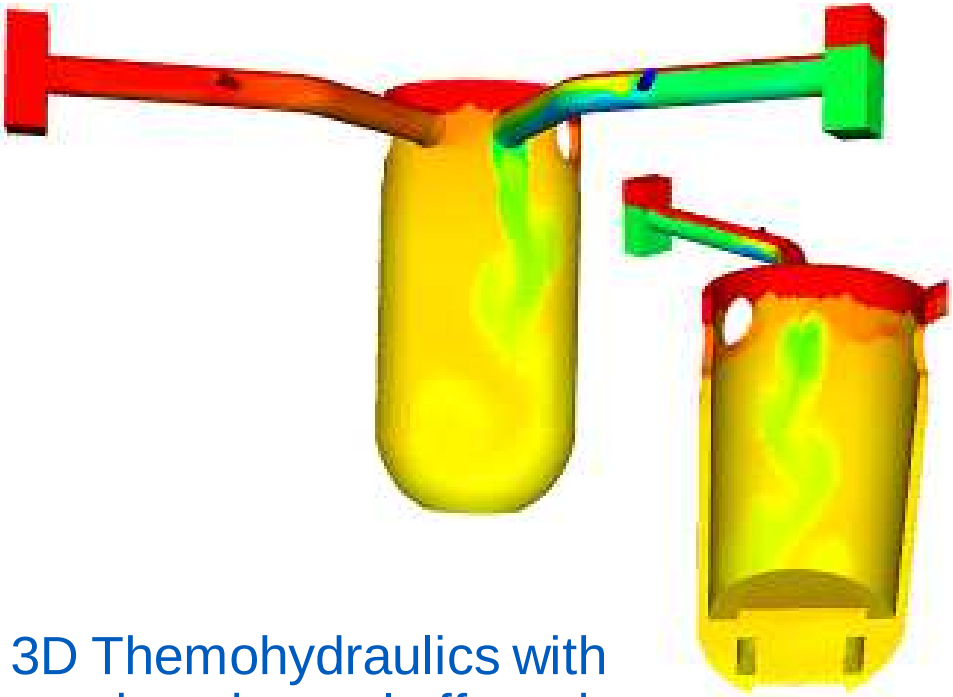


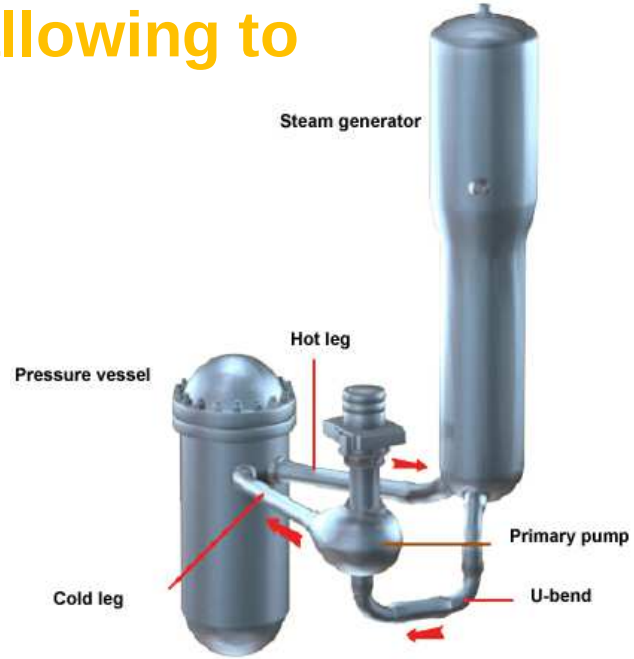
Modelling and simulation at EDF R&D

1. Policy and resources for simulation at EDF R&D

2. A short walk through applications :
   General overview of simulation via illustrations

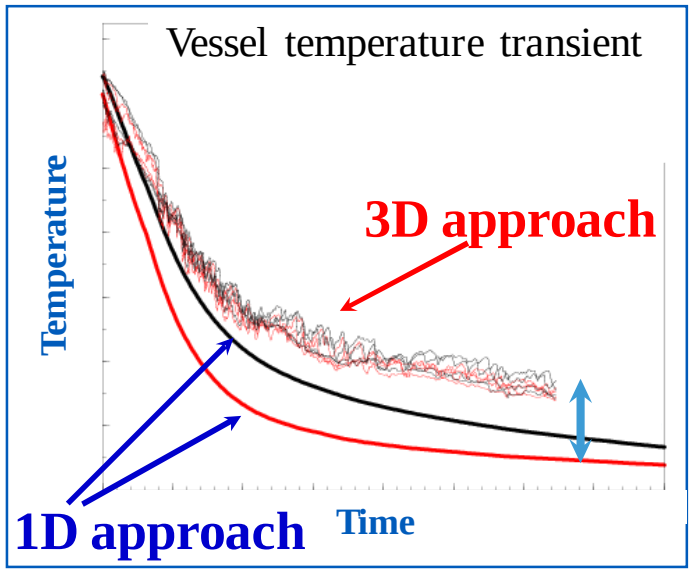
Identification of new safety margin allowing to extend lifetime of plants





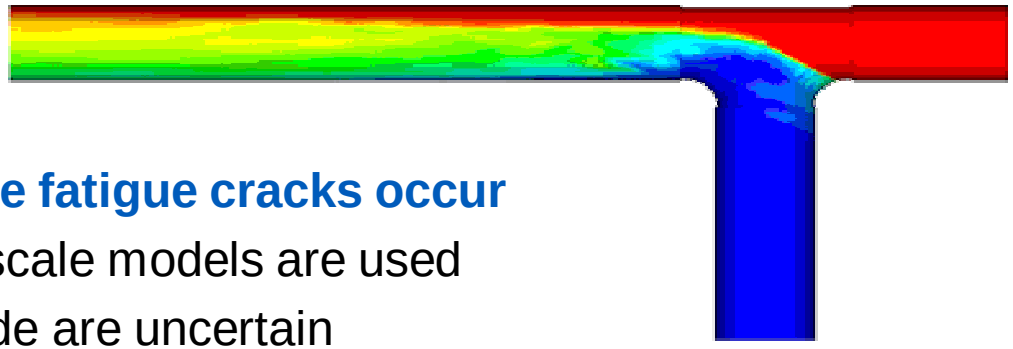
3D Themohydraulics with transient thermal effects in the vessel for a cold fluid injection

Coupled Code_Saturne and SYRTHES



Understanding system response
Addressing the issue of uncertainties

Cracking fracture by thermal fatigue in mixing hot/cold liquid zones

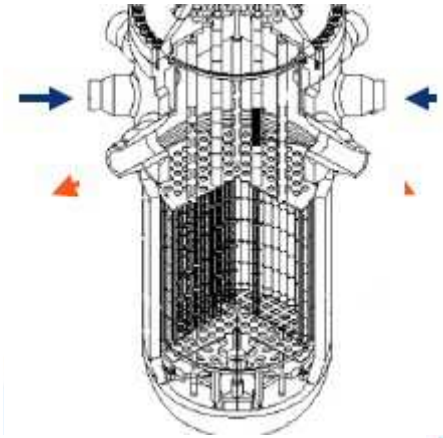


- Variable of interest: **Time before fatigue cracks occur**
- Both numerical simulation and scale models are used
- Input variables of simulation code are uncertain
- Goal of uncertainty analysis: **Explaining the differences between analytical and scale models**
  - Assessing the uncertainty over the variable of interest
    → qualify experimental tests
  - Sensibility analysis: which are the most "influent input variables" with respect to the uncertainty of model output?
    → prioritize R&D effort over the most influent variables
  - Result: need to better model mechanical fatigue behavior of the material

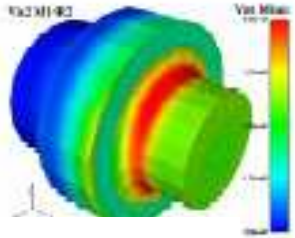
Coupled OpenTurns and Code-Aster /Saturne simulations

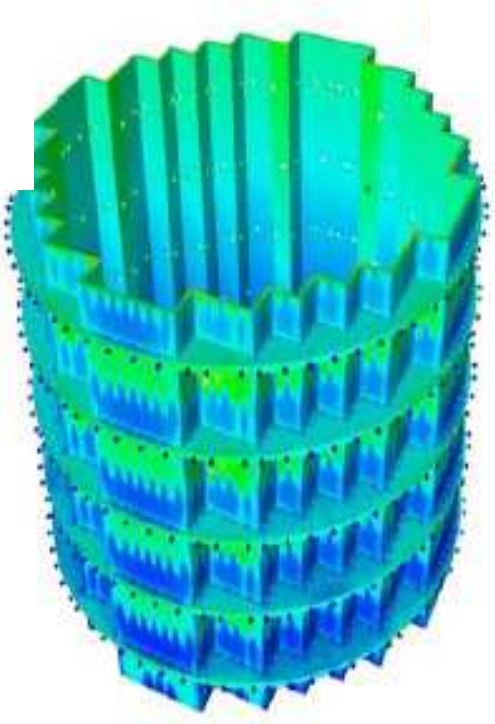
Identification of new safety margin allowing to extend lifetime of plants

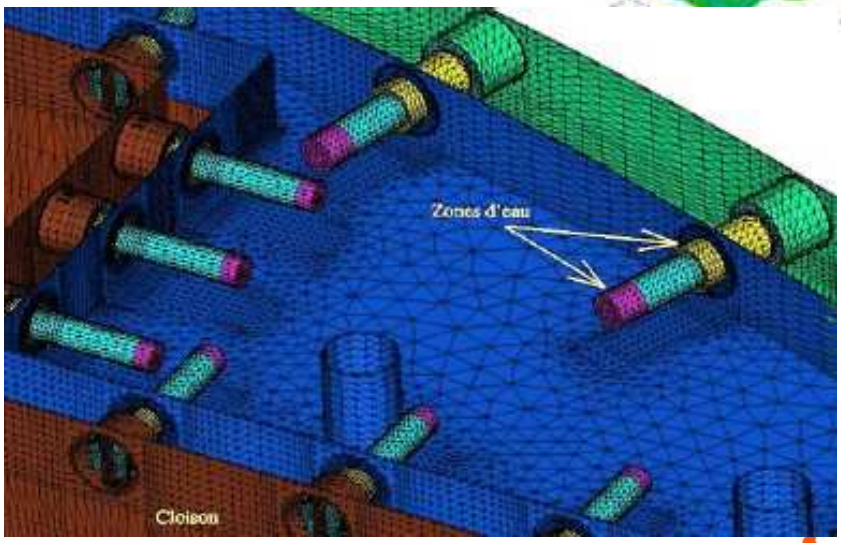
Identification of potential affectation of bolts by thermal and irradiation degradation



Code_Aster multiscale simulation

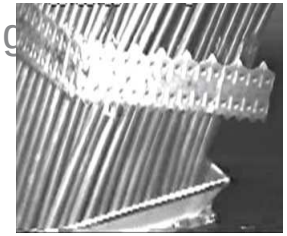


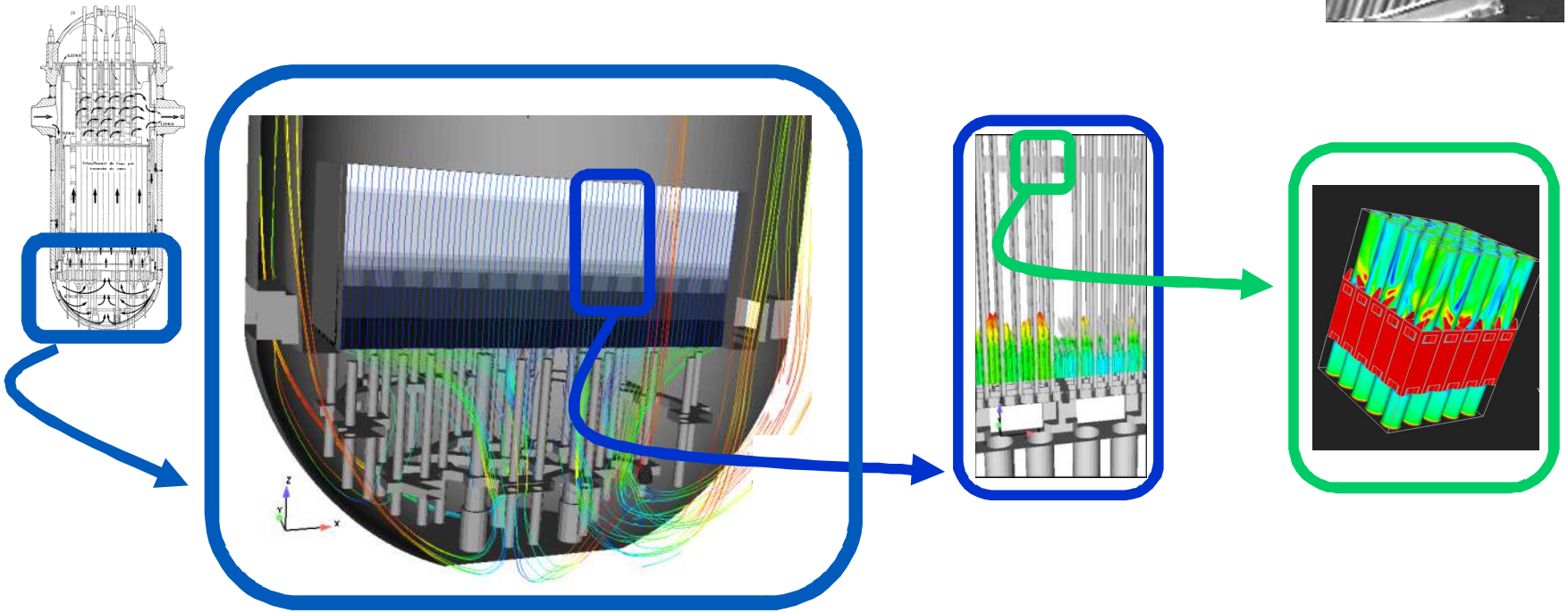




Fuel Assembly Vibration and Deformation

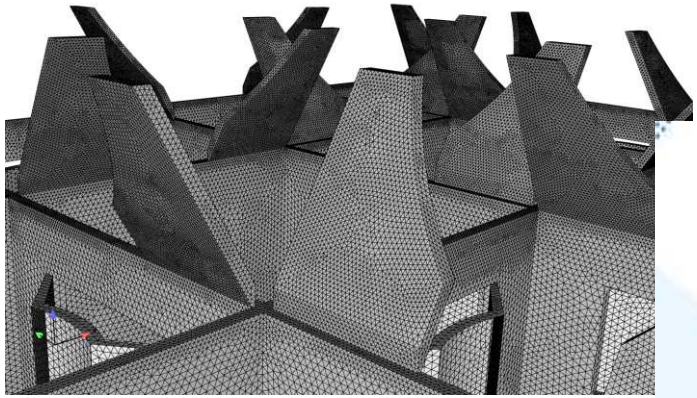
- Expertise of manufacturer solutions
- Effect of hydraulic loads on:
  - Progressively local approach from the vessel to the mixing g
  - Validation on experimental data at each stage

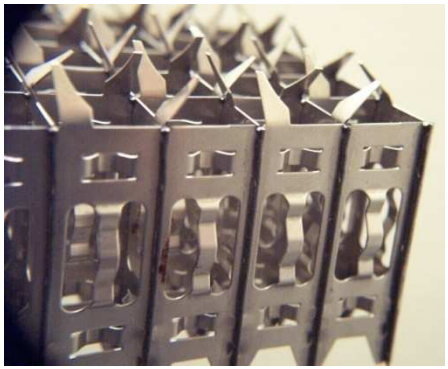


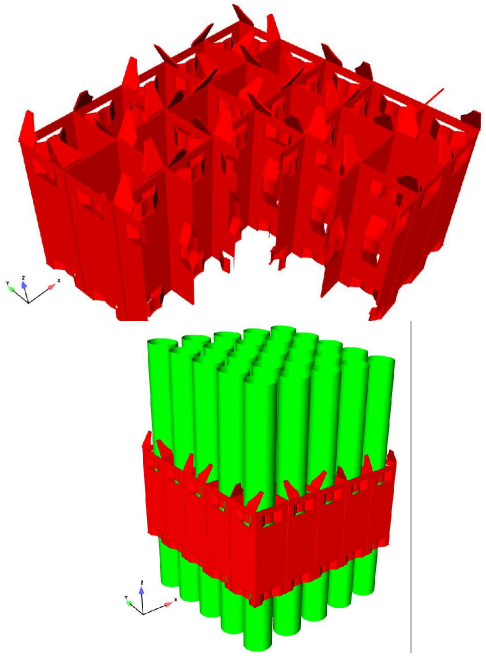


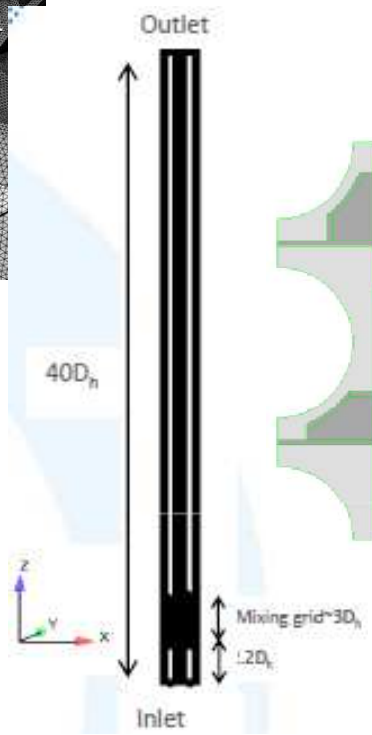
Understanding system response

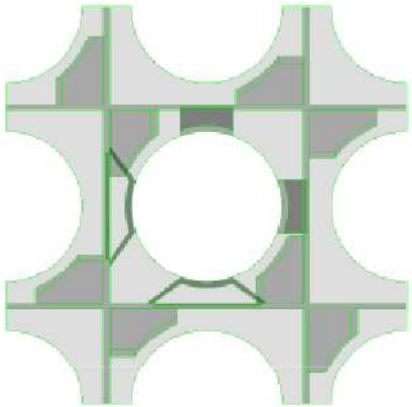
Computing PWR fuel rod vibrations with LES











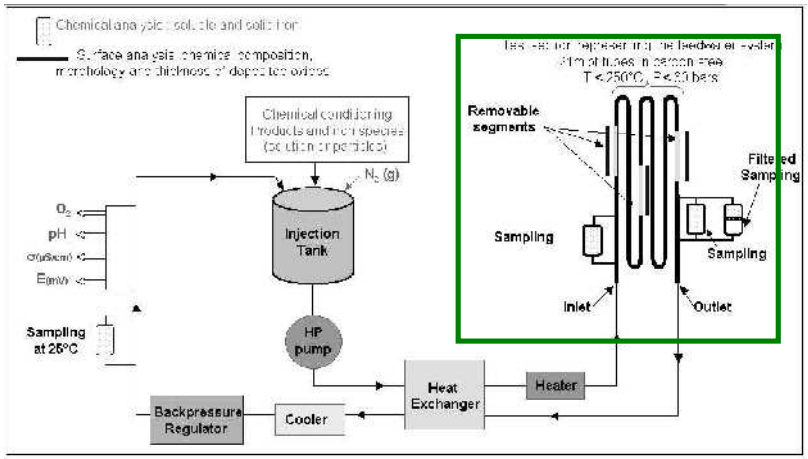
Code_Saturne LES

Understanding the physics : iron oxides deposition in a feedwater system

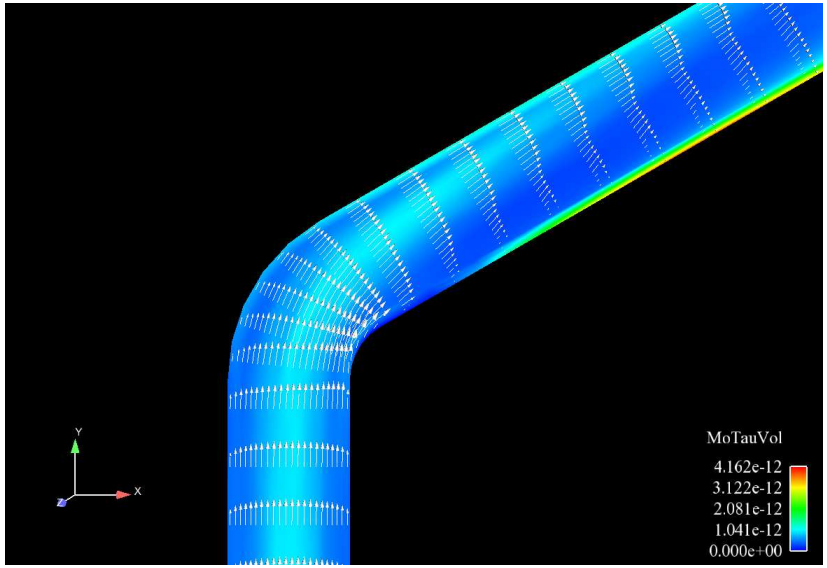
- <u>Industrial issues</u>: Understanding of the effect of chemical conditioning on the deposition of iron oxides in the feedwater system of the secondary circuit of PWR plants

- <u>Study content</u>: Simulation of the flow and the particle deposition on the test section of loop representing the feedwater system

- <u>Results:</u> Qualitative experimental observations are numerically reproduced:
  - More deposition in the bended sections
  - Sedimentation for particles diameter equal to 2 micrometers



Scheme of the loop; the test section (boxed) is composed of 21 m of tubes in carbon steel

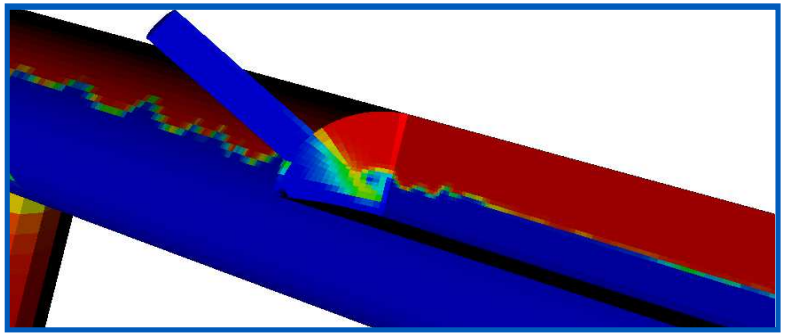


Particle volume fraction; near-wall accumulation is visible after the bend

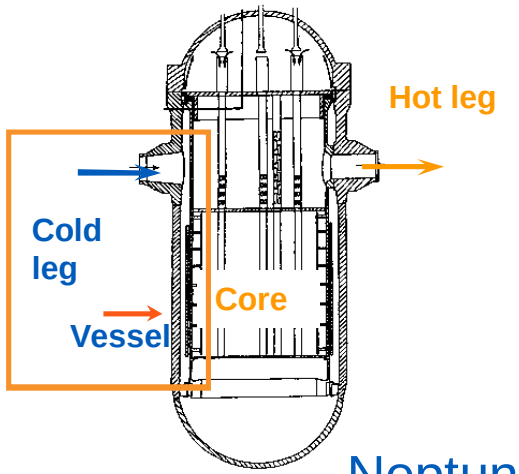
Identification of new safety margin allowing to extend lifetime of plants

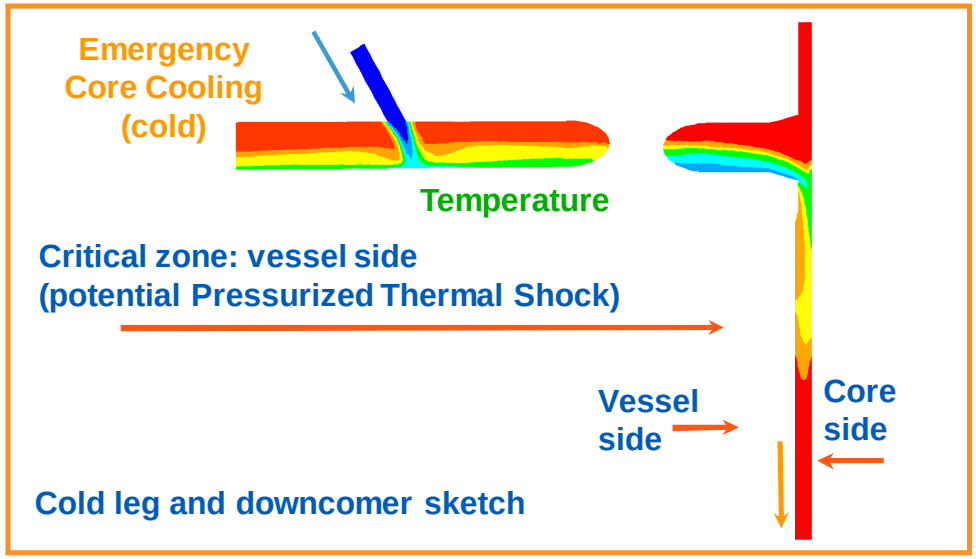
Justification of mechanical resistance to thermal shock under safety injection

3D two-phase CFD code with conjugate heat transfer



Free surface + Friction + Turbulence
Jet + Turbulence
Condensation + Turbulence
Coupled fluid –heat transfer in structures
Chained to fracture mechanics





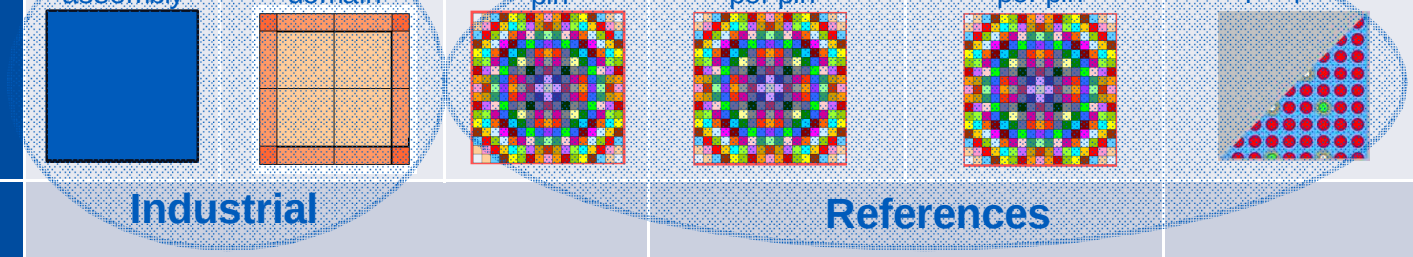
Neptune simulations

Nuclear Core Calculation Chains:
Three neutronic projects within EDF R&D

- **Three distinct projects, for three distinct time horizons**
- **CASSIOPEE:**
  - CASSIOPEE is EDF's operating core calculation chain for EDF's current **58 PWR fleet** and the forthcoming french **EPR**
  - The CASSIOPEE project:
    - maintains the CASSIOPEE core calculation chain
    - Evolves for the calculation of EPR cores
    - … until 2019 at least
- **F3C (Future Core calculation Chain) – ANDROMEDE:**
  - Industrializes new scientific calculation tools
  - Builds the new core calculation chain ANDROMEDE
  - … for operationnal services beginning in 2019
- **SIMUCŒUR2:**
  - Performs upstream research and development in neutronics
  - Capitalizes state of the art models and calculations schemes within the ANDROMEDE scientific calculation tools

ANDROMEDE neutronic core calculation schemes

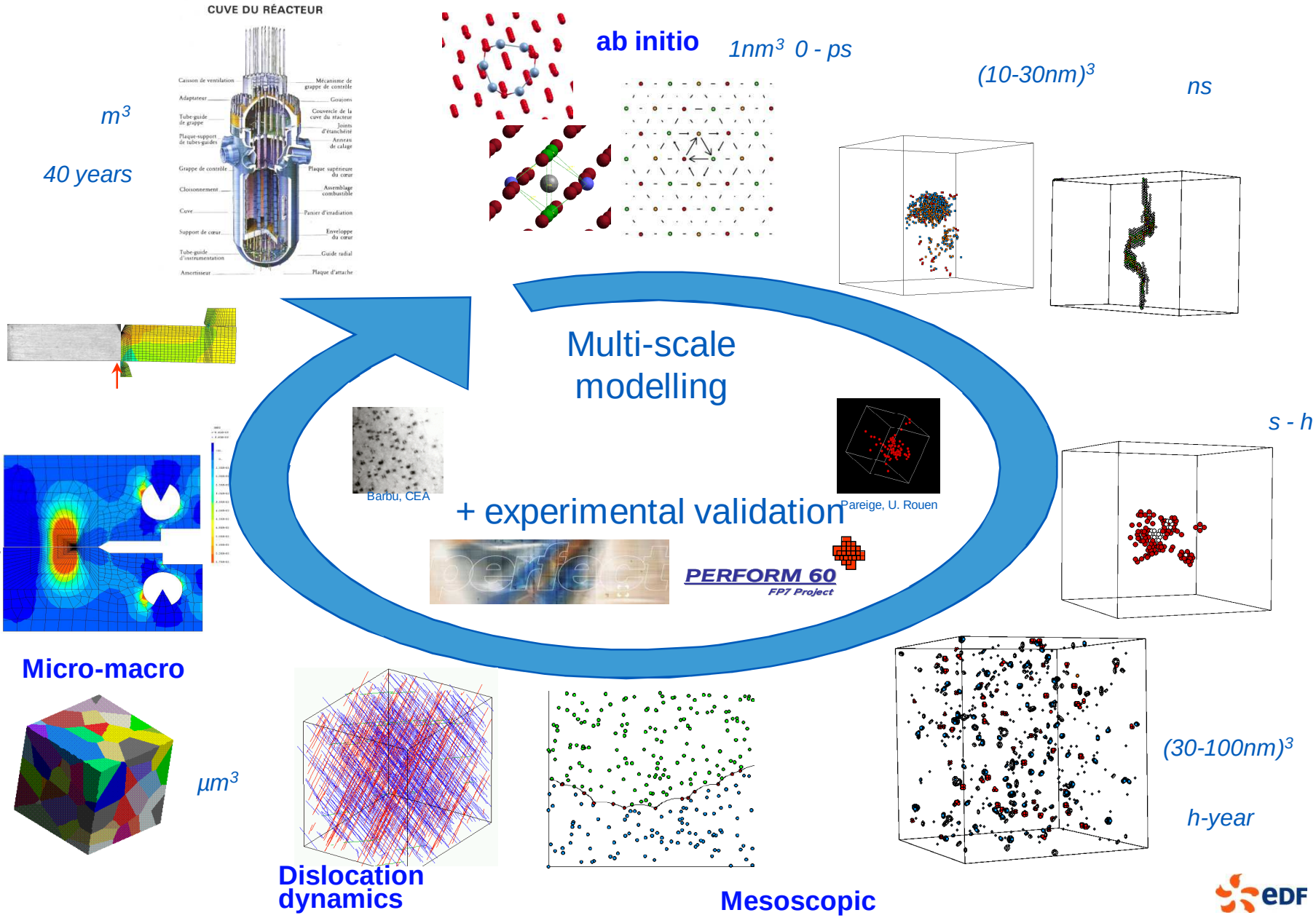
	DIFFUSION			SP_N (simplified transport)	S_N (transport)	MOC (transport)
Number of energy groups	2 groups			Multi-group (≈ 10g)		
Spatial nuclear data representation	assembly	Homogeneous per domain	… pin	Homogeneous per pin	Homogeneous per pin	Heterogeneous per pin
Full availability within ANDROMEDE	Industrial			References		
	Since 2012			**2016**		**???**



Precision

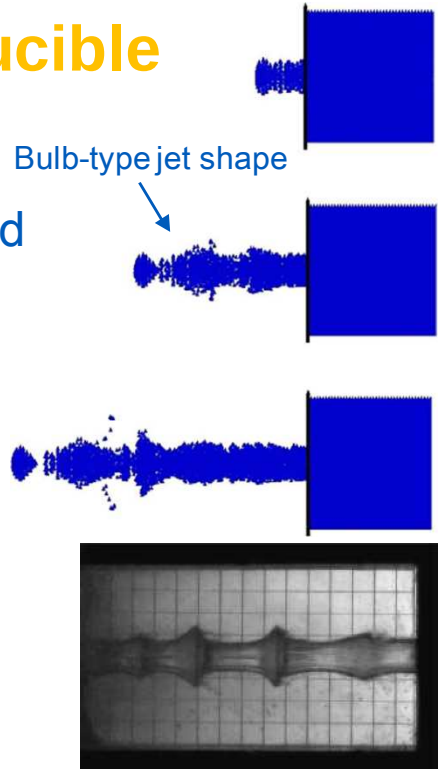
Computing time

Multiscale methodology : fracture mechanics analysis of the vessel taking into account irradiation embrittlement

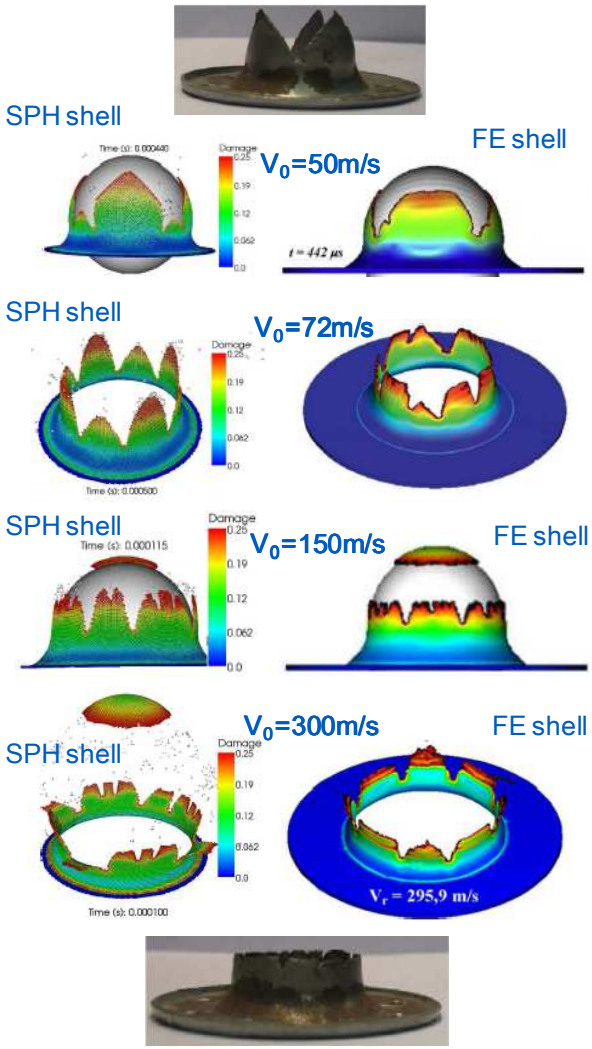


Analysis of accidental situations non reproducible by experiments : FSI problems with rupture

Assess the possibility of failure and leakage of shells filled with fluid

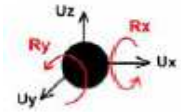


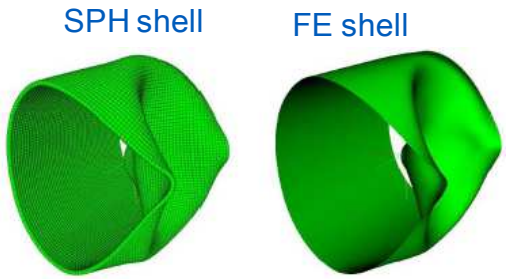
Perforation of a plate by a sphere



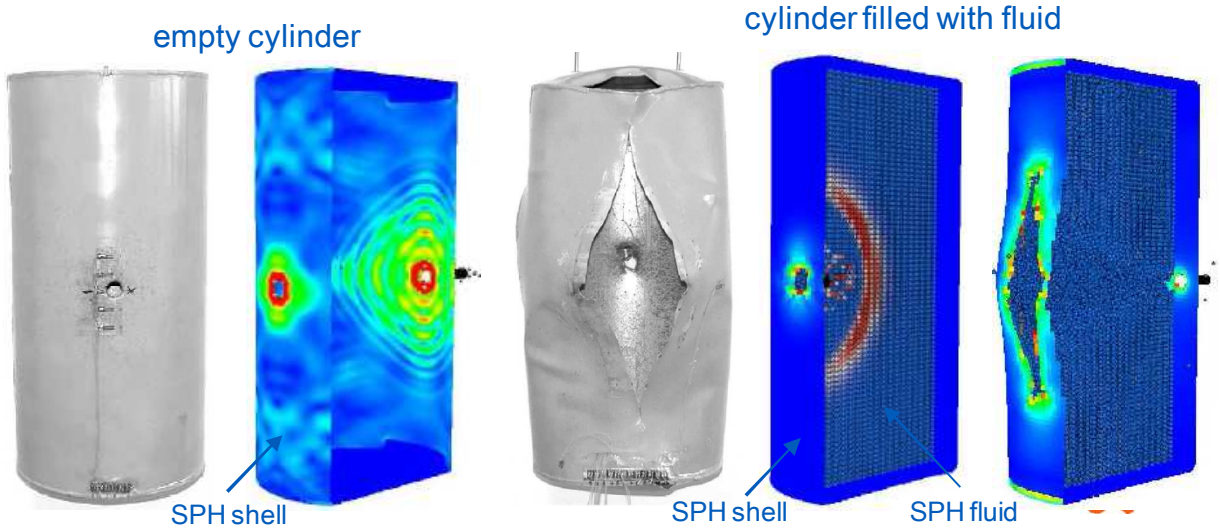
SPH FSI modelling = SPH shell + SPH fluid

Europlexus



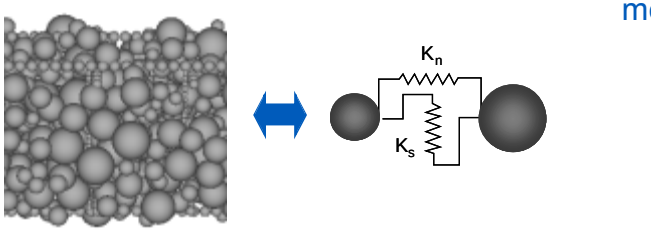


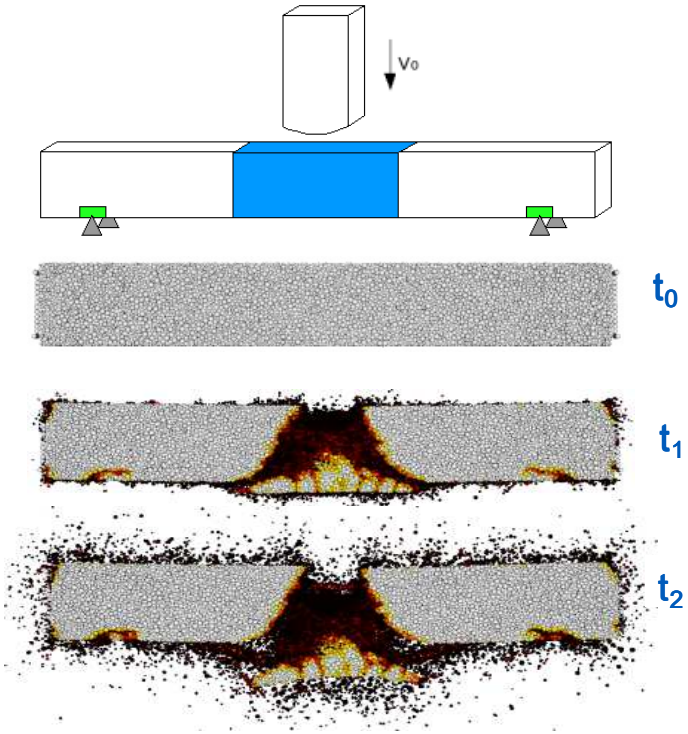
Non-linear dynamic fracture of a cylinder under a ball impact

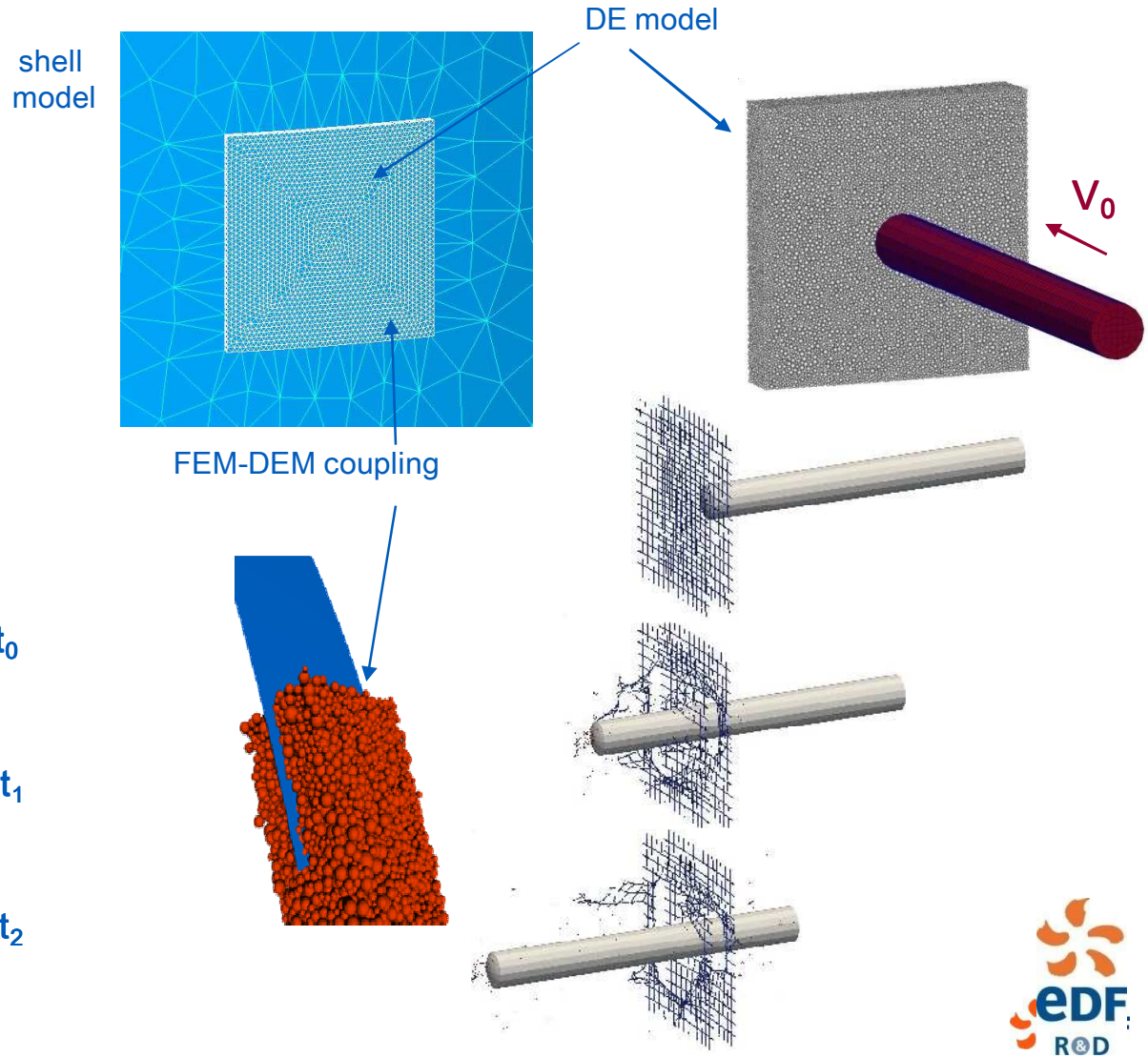


Analysis of accidental situations non reproducible by experiments : RC structures under severe impact

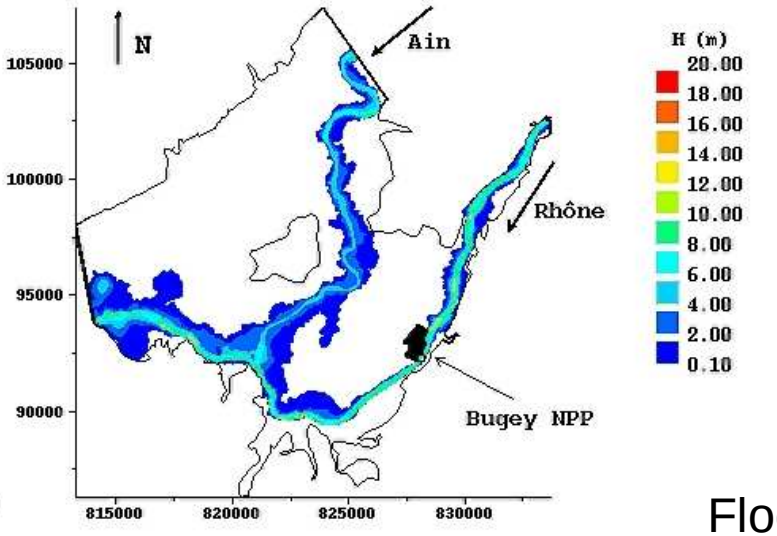
coupling FEM and DEM simulations in EUROPLEXUS

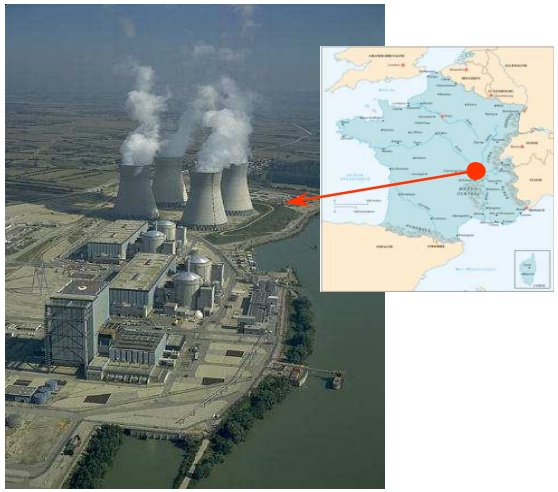


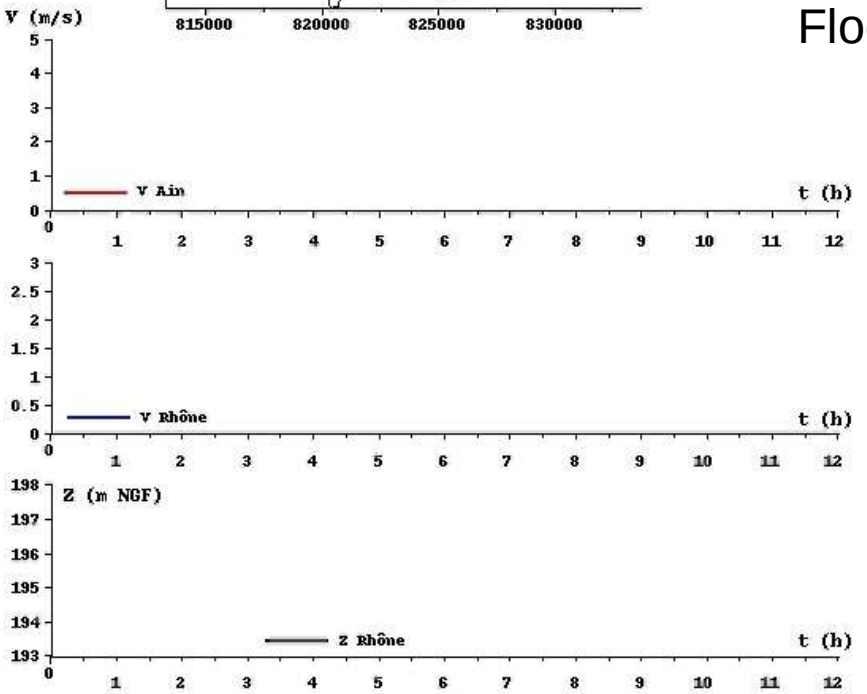




Analysis of accidental situations non reproducible by experiments : Floods analysis

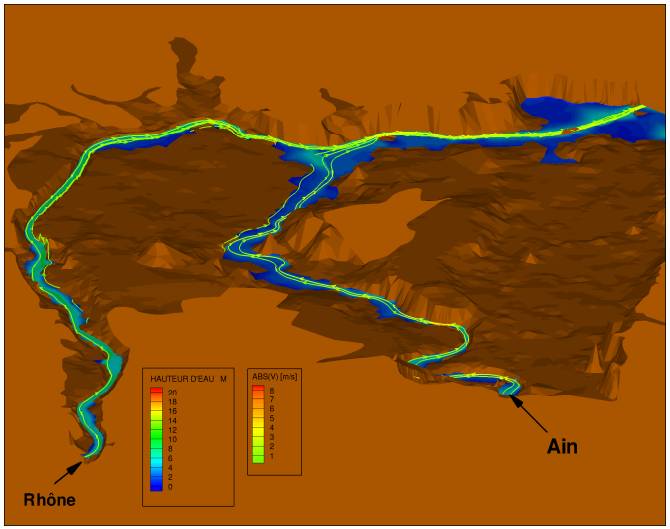






Flood level : Dam failure above the Rhone River

(TELEMAC detailed simulation for Bugey PP)



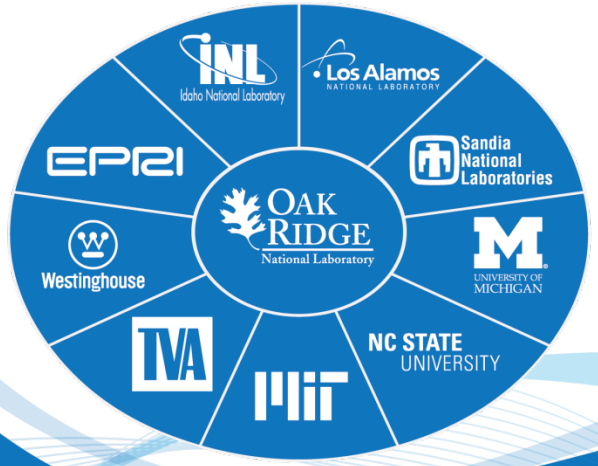
Thanks for your attention

Evolution of the Industry Council

Heather Feldman

March 11-12, 2014

Industry Council



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

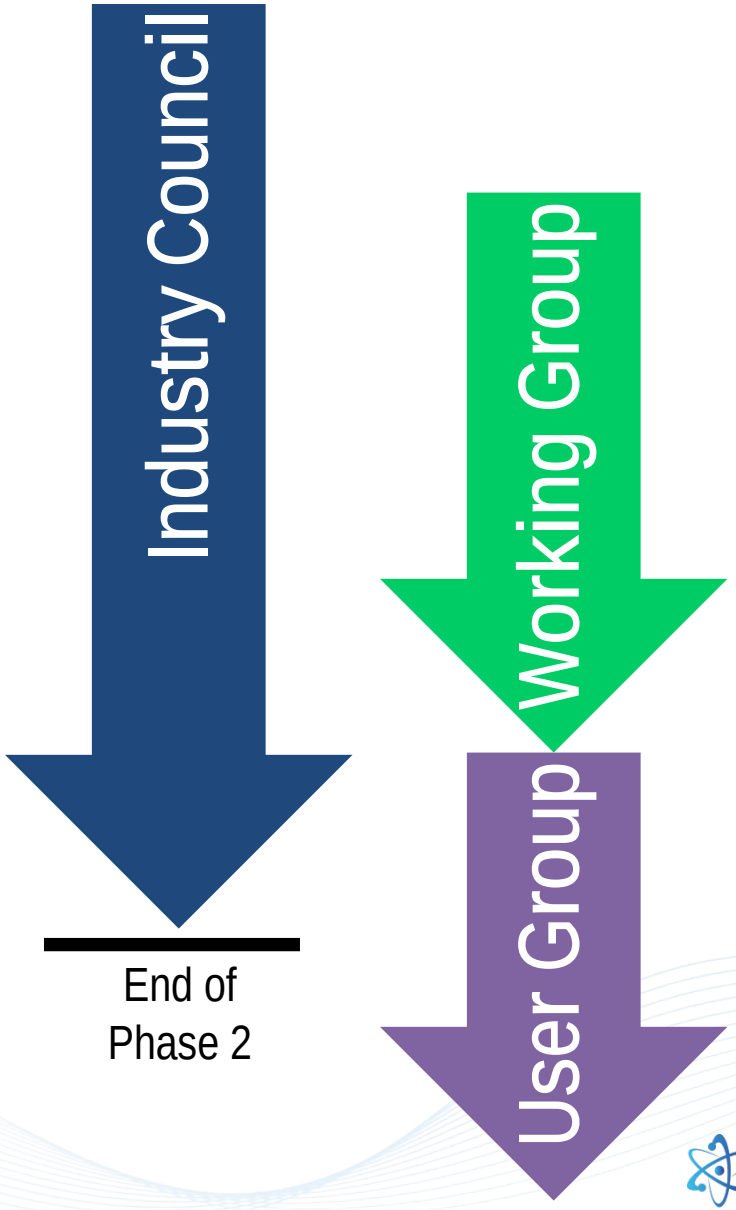
Management Structure
Establish a “Deployment” Area

The current concept…

- Lead and Deputy reports to the SLT
- Scope includes:
  - Industry Council
  - Modeling and Simulation Working Group that evolves to a User Group
  - Test Stands
  - VERA Release, Support, and Training
  - Software Licensing

Industry Council Continues with Expanded Outreach
Working Group Gears Up and Transitions to User Group

- Two distinct organizations:
  - Industry Council
    - CASL milestone focus
  - Modeling and Simulation Working Group / User Group
    - User experience focus
- General plan is for the User Group to take over from CASL after the hub is discontinued



Industry Council
Evolution

- Expand purpose
  - Current
    - "…provide critical two-way communications and information exchange…"
  - Expanded
    - Provide guidance/direction and functional requirements to CASL on the application of VERA to a problem that is relevant to industry (from initiation to completion)
- Change the leadership structure to include a member of the IC
  - For example - Industry Council is supported by a CASL team member (Executive Director) and chaired by a member of the Industry Council (Chairperson)
- Subcommittee of the Industry Council working on this
- Implement changes in September 2014

Discussion

- Is this the “right thing”?
- How do we do it?
- Subcommittees?