CASL Industry Council Meeting
September 10-11, 2013 – Oak Ridge, TN
Minutes

The seventh meeting of the Industry Council (IC) for the Consortium for Advanced Simulation of Light Water Reactors (CASL) was held on September 10-11, 2013; at Oak Ridge National Laboratory in Oak Ridge, TN. A joint meeting of the Science Council and the Industry Council was held the first day and chaired by Paul Turinsky (CASL Chief Scientist) and Heather Feldman (IC Chairman). The Industry Council meeting on the second day was chaired by Heather Feldman.

The meeting attendees and their affiliations are listed at the end of these minutes. Attendance was by invitation only. Industry Council representatives from 21 member organizations were invited. Fifteen members of the Industry Council attended representing 14 organizations. Two representatives from a non-member organization attended. Members of the CASL project team participated in the meeting including the program director, chief scientist, the quality manager, the project manager, focus area leads, and technical staff. The DOE-NE Director of Advanced Modeling and Simulation also participated during both days.

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

Doug Kothe began the Joint Science and Industry Council meeting with a warm welcome and extended his appreciation to the Industry Council and Science Council members for their active participate in CASL. Paul Turinsky provided an overview of the morning session and Heather Feldman provided an overview of the afternoon session.

Doug Kothe, CASL Director, provided an overview of the CASL project including: the CASL team, organization, the challenge problems, the milestones that are formally reportable to DOE in fiscal year 2013, and the status of VERA. Changes to the organization since March 2013 include: the evolution of the Virtual Reactor Integration (VRI) Focus Area to the Physics Integration (PHI) Focus Area, Jess Gehin is the Lead for PHI, Scott Palmtag is the Deputy for PHI, Zeses Karoutas is the lead for AMA, Rose Montgomery is a Deputy for AMA, Steve Hess is a Deputy for AMA, and John Turner is the Chief Computational Scientist. Doug noted the significant accomplishments during year 3 of CASL which include the deployment of a Test Stand to an industry partner, and the first and successful comparison of VERA results against data from an operational reactor. More details can be found on Slide 10 of the presentation. Paul Turinsky, CASL Chief Scientist, provided an overview of the Science and Technology Program. He started with a description of the enhanced capabilities that CASL will provide over current practices and then reviewed the high level differences for each technical area (i.e. thermal-hydraulics, radiation transport, etc). The challenge problems were presented from the perspective of the time scale, the spatial scale (e.g. core-wide, pin resolved), and the required

code coupling. The accomplishments for each of the Science and Technology Programs were presented:

- THM: 1) Development of robust, parallel solution algorithms for multiphase/multi-field CFD (Hydra-TH), and 2) Assessment of subcooled boiling and bubble flow closure relationships using experimental data & direct numerical simulation
- RTM: 1) Development of integrated cross-section generation/transport solver capability (Insilico), using Sn and newly developed SPn, and 2) 2D MOC/1D Diffusion code (MPACT) with convergence issue understood & addressed and developed full 3D MOC capability (MPACT-3D).
- MPO: 1) Crud: Enhanced thermodynamic understanding, thermochemical data base, & two-phase fluid flow in Crud & cladding oxidation models, 2) PCI; Development, validation and benchmarking of fuel performance code (Peregrine) along with advanced viscoplastic self consistent cladding deformation model, and 3) GTRF: Cladding wear model development based upon experimental data & micro-scale modeling.
- VUQ: 1) Development and assessment of advanced MCMC methods for data assimilation, 2) Verification of numerical discretization aspects for the large phase space associated with neutron transport models, and 3) Assessment of CASL codes' SQA and code verification practices, along with validation data needs.
- PHI: 1) Development of parallel data transfer capability for multi-processor/multi-core architectures (DTK), and 2) Multiphysics integration of Neutronics (Insilico SPn)-Fluids (Cobra-TF)-Fuel Performance (Peregrine) = VERA-CS.

The status of the component SQA and verification practices for all of the codes was provided. Paul concluded with a summary of items that he perceives to be technical challenges. Doug and Paul's presentation is included as Attachment 1.

Zeses Karoutas, CASL AMA FA Lead, presented the status of the challenge problem charters and implementation plans. CASL is currently working on operational challenge problems: CRUD-induced power shift (CIPS), CRUD-induced localized corrosion (CILC), grid-to-rod fretting failure (GTRF), and pellet-clad interaction (PCI), and on safety challenge problems: departure from nucleate boiling (DNB), cladding integrity during (LOCA), and cladding integrity during (RIA). The operational challenge problem on fuel assembly distortion (FAD) has been deferred to a future date (limited planning and scoping has been done to date). The scope of the safety challenge problems on reactor vessel integrity and reactor internals integrity has been moved to the DOE-funded Light Water Reactor Sustainability (LWRS) program. A Challenge Problem Integrator is assigned to each of the challenge problems and is responsible for driving critical applications, products, and outcome across the focus areas. Zeses provided a high-level overview of the charters and implementation plans as well as the overall progress on the challenge problems. Zeses's presentation is included as Attachment 2.

Mark Christon, THM FA Lead, presented a detailed review of the Thermal-Hydraulics Methods Focus Area. The scope of the THM FA is focused on Computational Fluid Dynamics and excludes COBRA-TF, which is the responsibility of PHI. The tagline for the THM area is "advanced thermal-hydraulics models and simulation tools for nuclear energy applications".

THM is developing a scalable, implicit CFD code (called Hydra-TH) for turbulent, multiphase flow which includes new closure models. Key accomplishments over the last year include:

- Level 1 Milestone "CFD Turbulence Force Calculations and Grid-to-Rod Fretting Simulation": Hydra-TH velocities were compared with experimental results and showed good agreement; Hydra -TH results were used as input to the Westinghouse grid-to-rod fretting code (VITRAN). The resulting workrates compared favorably to workrates obtained using the existing method to obtain the thermal-hydraulics input.; The scope of these studies included 3x3 and 5x5 bundles, two types of mesh, and numerous size meshes.
- Level 3 Milestone "Computational Performance Assessment of Hydra-TH": The performance on Hydra-TH on a real geometry, V5H grid, showed trend in the expected direction. THM is working with NVIDIA on ways to speed up the calculations.
- Level 2 Milestone "Demonstration and Assessment of Advanced Modeling Capabilities for Multiphase Flow with Sub-cooled Boiling": THM demonstrated that fully implicit projection algorithms can be used as a means to retain an implicit solution while increasing the minimum acceptable time step for solution stability.; THM demonstrated the multiphase flow Hydra-TH capabilities in a V5H geometry.; They also verified the in-situ drag closure.

THM closure model work is using interface tracking method/direct numerical simulation (ITM/DNS) and fundamental experiments to inform a closure model for multiphase flow with sub-cooled boiling. Mark noted that Hydra-TH is available for download (the link is in the presentation and authentication is required). There have been more 20 downloads since January of 2013. Mark's presentation is included as Attachment 3.

During the working lunch, Nam Dim, presented his work on identifying the validation needs to support the CASL Challenge Problems. CASL subject matter experts responded to a survey that Nam used to identify validate data needs. Since CASL is developing a coupled suite of codes that involve a wide range of temporal and length scales, the validation needs are different than that for an existing engineering code. Nam noted that new experiments and instrumentation are needed especially at the micro scale. He presented a high-level overview of the identified gaps. Nam's presentation is included as Attachment 4.

The VERA Description, Status, and Plans presentation was divided into three main topics:

- Introduction of the Physics Integration (PHI) Focus Area (Jess Gehin, PHI FA Lead)
- VERA Results – Watts Bar Zero Power Physics Test (Andrew Godfrey)
- VERA Results – Single Assembly Coupled Physics (Scott Palmtag, PHI FA Deputy).

Jess provided an overview of the PHI Focus Area whose role is to integrate the CASL virtual reactor physics being developed throughout CASL. The VERA development approach is three pronged: develop a base capability which is referred to as the "core simulator" (neutronics – thermal-hydraulics – fuel performance coupling), integrate challenge problem modeling capability, and develop for usability by making VERA usable on industry class computing resources and with easy to use input and output capabilities. Ten Progression Problems drive development of the core simulator. CASL recently completed Progression Problem 5 which is a physical reactor hot zero power physics test and Progression Problem 6 which is hot full power beginning of life assembly. Progression Problem 6 is the first problem that that involves

coupling of physics, in this case neutronics and thermal-hydraulics. Jess concluded the overview of PHI with an overview of the Fiscal Year 2014 plans which include: completion of the 10 progression problems, integration and coupling of Peregrine (fuel performance) and MAMBA (coolant chemistry), VUQ integration, development of common output, and Test Stand support. Andrew Godfrey then gave a detailed presentation on Progression Problem 5 "Watts Bar 1 Cycle 1 Zero Power Physics Tests". The report is available on the CASL website (http://www.casl.gov/ – R&D – Publications – Technical Reports). CASL would like feedback from the Industry Council on this report. Zero power physics tests are performed prior to initial power escalation for each fuel cycle to confirm that the core is loaded as designed. Tests include: initial criticality, control rod bank reactivity worth, differential soluble boron reactivity worth, and isothermal temperature reactivity coefficient. This analysis used Insilico 3D SP_N for 3D neutronics transport analysis. The runtime was 33 minutes on Titan for quarter-core eigenvalue calculation without thermal-hydraulics feedback. The Insilico results were compared with a numerical reference solution (KENO-VI) and a current industry solution (NEXUS). The initial criticality, control rod bank reactivity worth, and differential soluble boron reactivity worth results from VERA agreed well with KENO and NEXUS. The VERA results for isothermal temperature reactivity coefficient seem to be too negative and further investigation is warranted. Scott Palmtag presented the current status of Progression Problem 6, which is hot full power beginning of life assembly. To address this Progression Problem, Insilico (cross-sections, neutron transport) to COBRA-TF (fluid flow and fuel/clad temperatures) coupling is required. Scott presented coupled results for boron concentration and power level. The next Progression Problem is "Hot Full Power Beginning of Cycle Physical Reactor with Xenon". The next coupling this will be developed is Insilico (cross-sections, neutron transport) to COBRA-TF to Peregrine (fuel performance). David Brown (TVA) noted that VERA needs to model a variety a fuel assembly types and reactor types beyond the Westinghouse 17x17 design that was used in the Progression Problems. CASL noted that some relevant information is in "VERA Requirements Document – Revision 1" (CASL-U-2011-0074-002) which is available on the Industry Council website. The presentation is included as Attachment 5.

The meeting attendees then walked over the to the Virtual Office, Community and Computing (VOCC) lab. April Lewis (VOCC Lab Director) provided an overview of the capabilities. Heather Feldman reviewed the five demonstrations and the meeting attendees rotated through the five demonstrations. The five demonstrations were:

- Immersion Room (THM) – Bubble Model
- F-5 (AMA) – Fibrous Debris Project
- Waldo (MPO) – Crud build up and fuel performance
- I-DEATE Stations 4&5 (PHI) – NiCE demo – VERA usability/workflow
- I-DEATE Station 6 (PHI) – Exploration of VERA Results, VERA input / demo, COBRA-TF activities

The presentation is included as Attachment 6.

The meeting was adjourned for the day.

The next morning the Industry Council and Science Council held separate meetings. Heather Feldman opened the Industry Council meeting with an overview of the Industry Council scope, members, website, and action items. The Industry Council website contains links to resources including minutes and presentations (http://www.casl.gov/IndustryCouncil.shtml). No new members joined the Industry Council since the March meeting. DS/Simulia has expressed interest in CASL and the Industry Council and attended the meeting as a guest. During the review of Action Items, the Industry Council requested the document for Validation Data associated with the presentation given by Nam Dim during lunch on the first day of this meeting. The Industry Council expressed interest in an overview presentation by the CASL VUQ Focus Area at the next Industry Council meeting. Then Heather reviewed the meeting agenda. To prepare for the Round Table later in the day, Heather noted CASL documents that are planned to be provided to the Industry Council and noted that the next meeting is scheduled for March 2014. The meeting dates and location have not been finalized. The presentation is included as Attachment 7.

Doug Kothe (CASL Director) presented an overview of Test Stands. Test Stands, a mechanism for beta testing VERA outside of the in-house development process, are a key component of the deployment process. Host organizations self-fund a portion of the Test Stand activities and the scope is agreed upon by CASL and the host organization. The first three Test Stands will be deployed to partner organizations:

- Westinghouse: deployed in June 2013, focus on neutronics of the AP-1000®
- EPRI: to be deployed by December 2013, focus on fuel performance (pellet-cladding interaction)
- TVA: to be deployed in 2014, list potential topics provided to CASL, leading topic is Watts Bar 1 lower plenum flow anomaly

Then the current plan is the deployment of a Test Stand at a Non-Partner Organization. CASL is engaged in on-going discussions with Industry Council members that have expressed interest in hosting a Test Stand which include: AREVA, GSE Systems, ANSYS, mPower, and Rolls Royce. CASL has visited AREVA and GSE Systems and has received a list of potential simulation topics from AREVA. Doug concluded his presentation with a summary of the lesson learned on Test Stand deployment. Fausto Franceschini (Westinghouse) reviewed the scope and results to date for the Westinghouse Test Stand. A follow-on presentation is planned for the March Industry Council meeting. The presentation is included as Attachment 8.

Matt Sieger (CASL QA Manager) reviewed the results of the survey "VERA End User Uses and In-House Requirements" with the Industry Council to ensure a complete and correct understanding of the responses. The results are summarized in the presentation which is included as Attachment 9. Matt indicated that CASL will provide a response to the survey and update on QA deliverables and expectations at the March Industry Council meeting.

Heather Feldman gave a status update from the Value Proposition subcommittee. CASL has an objective to deliver technology and products that are used and useful by industry to effectively provide safe and cost-effective electricity from nuclear power for benefit of the U.S. public. During the March 2013 Industry Council meeting, John Gaertner (former CASL Industry

Council Chairman) provided a strawman for assessing the value of the CASL solutions to the U.S. public. Following the meeting, a subcommittee was formed and members include: Bill Arnold (mPower), Heather Feldman (EPRI), Steve Hess (EPRI), Rose Montgomery (TVA), Bob Oelrich (Westinghouse), Jeff Secker (Westinghouse), and Scott Thomas (Duke Energy). The subcommittee met four times. The value assessment is currently focused on the CRUD Challenge Problems (CIPS and CILC) from the perspective of the industry. The value is being assessed starting from the CASL solutions which go to intermediate customers then through objective measures to capture the benefit to the U.S. public. Each subcommittee member ranked the value for a given solution, customer, objective measure combination. The results were inconsistent. Therefore, the subcommittee will be making adjustments. Heather also noted the starting place for CIPS and CILC history. The subcommittee will be meeting in September to continue to work to assess the value. Contact Heather Feldman if you are interesting in joining the subcommittee. The presentation is included as Attachment 10.

During lunch, Doug Kothe (CASL Director) presented "Thoughts on Phase II". Phase I ends in July of 2015. The time table for Phase II includes discussing and finalizing scope between October and December of this year, preparing a renewal proposal between January and March of 2014. The DOE review and decision is expected to occur in the April to July 2014 timeframe. Doug noted ideas for expanding the scope beyond PWR in-vessel. High level scope options include: reactor types other than currently operating PWRs, beyond the reactor vessel and contents to the nuclear power plant, lifecycle of current and advanced nuclear fuel, and support for severe accident analysis. CASL has engaged the Board of Directors in discussions on scope for Phase II. Doug outlined the draft process for defining the scope. The process includes discussions with the current industry partners and potential industry partners, presentation to the current partners, possible presentation to the industry council, and presentation to the Board of Directors. Doug mentioned possible Phase II Challenge Problems. The draft high level scoping priority is currently (from highest to lowest priority): complete the seven challenge problems that are currently being worked along with deployment to industry, expand to BWRs, complete the three challenge problems that were planned for Phase I but not initiated. There was a group discussion on the potential funding for Phase 2, it was stated that the Council expected the same level of funding but the group suggest going for a higher amount to address expand the effort to BWR's and other Challenge Problems. Doug's presentation is included as Attachment 11.

John Turner (CASL Chief Computational Scientist) discussed VERA Interoperability and Standardization. The Industry Council confirmed to John that the three primary scenarios for interaction with external codes and components are:

- share input and output file formats
- replace VERA components with different (potentially proprietary) components to produce new applications
- use VERA components (or applications) in another environment

VERA uses a common input to provide data to all of the individual codes within VERA. It is in a format that is user friendly and is similar to current industry workflows. There is a write up on this that will be made available to the Industry Council in late 2013/early 2014. John noted that

since CASL is coupling together various codes and used the coupling of neutronics to thermal-hydraulics as an example. CASL is currently working on VERA common output. CASL is currently working with Independent Software Vendors (ISVs) in two ways: commercial tools are used in the CASL project where appropriate and CASL is collaborating with ISVs. For example, CASL has had discussions with ANSYS on workflow tools and with GSE Systems as a potential Test Stand candidate. The initial coupling efforts with Star-CCM+ have now evolved into a deeper discussion of application programming interfaces (APIs) to facilitate closer coupling which was further discussed in the next presentation. John's presentation is included as Attachment 12a.

Eric Volpenhein (CD-adapco) provided an overview of how STAR-CCM+ has interfaced with VERA, the associated limitations, and the current plan to overcome those limitations. Eric noted that coupling STAR-CCM+ to VERA is win-win-win for CD-adapco, CASL, and CD-adapco's clients. STAR-CCM+ is currently coupled to VERA by iterative file exchange. To overcome the limitations of this method, CD-adapco is planning to develop an API for MOAB (Mesh-Oriented Database). Heather noted that this is a great example of VERA interoperability and CASL-Industry Council member engagement. The presentation is included as Attachment 12b.

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:

- THM area
    - Impressed with progress
- Test Stand
    - Impressed with progress
    - Not surprised by the installation challenges noted by Westinghouse
    - Critical to get Test Stands deployed
- Value Proposition
    - VUQ is important because it will define how good VERA is and the scope of use
    - VERA will be used to address problems that we don't yet know exist
- Phase II
    - Extending VERA to BWRs could be a huge effort.
    - FAD and incomplete rod insertion are very important to the industry
- Expand beyond a Westinghouse 17x17 reactor and fuel design. Need to ensure the VERA can model other designs and design features. This should be included in the CASL planning documents.
- Establish credibility with VERA. This can be done by solving relevant industry problems with existing tools and with VERA and then showing why VERA is better.
- One members expressed interest in seeing CRUD prediction results compared with data.
- Settle in and select methods that will be used.
- Interested in using VERA to understand the impact of uncertainty (slight variability) of inputs on solution.

- Looking forward to VERA solutions of more complex problems that could demonstrate the value of high fidelity coupled solutions (vs the industry practice).
- The importance of the gaps in validation data should be discussed.
- A measure of success for VERA will be how easy the tool is to use (e.g. input file, output file, installation)
- Lower plenum flow anomaly occurred after units replaced an impeller on a RCP. As more units are replacing impellers, this will affect many units. The industry needs a tool to model these physics which appear to be related to the pump start up sequence after impeller replacement.

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

1. 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.
2. Heather Feldman to provide IC members with the HUB lessons learned document "what went right" once it is received from Alex Lazelere (DOE-NE).
3. Industry Council members to contact Heather Feldman to join the Value Proposition subcommittee.
4. 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.
5. 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).
6. Heather Feldman will provide the Industry Council with the following documents:
    a. CASL Program Plan
    b. Industry Workflows and Use Cases document
    c. Document on Validation Data effort
    d. VERA Common Input document

Bill Weber (Acting Chairman of the Science Council) provided a report out from the Science Council meeting. Bill noted that work in the CASL project is progressing along well. The Science Council did not have any significant findings during this meeting.

Alex Lazelere made some closing remarks. He said that the comments he heard during the joint Science and Industry Council meeting were similar to those heard during the DOE Annual Review. The comments included: define the product at the end of Phase 1, do a few things very, very well (rather than a lot of things so-so), and be clear about what activities are in what phase. Alex acknowledged the good team and good leadership of the CASL project.

The next in-person meeting of the Industry Council will be in March 2014 and a webcast is planned for January. Topics for the March 2014 meeting include: Deployment; Test Stand: WEC results, EPRI status, TVA status; VERA End Use Requirements; VUQ update (depending on FA Lead availability); Value Assessment, Grid-to-Rod Fretting, and CRUD problems.

The meeting was adjourned at approximately 3:00 pm on September 11.

Prepared: September 17, 2013
Distributed to Industry Council for Review: September 17, 2013
Finalized: September 27, 2013

By Heather Feldman, Industry Council Chair

Attendance

	Name	Institution	Sept 10	Sept 11
1.	Marc Adams	NVIDIA	Y	N
2.	Bill Arnold	mPower	Y	Y
3.	David Brown	TVA	Y	Y
4.	Alan Copestake	Rolls Royce	Y	Y
5.	Tom Cully	Dassault Systems SIMULIA Corporation	N	Y
6.	Heather Feldman	EPRI	Y	Y
7.	Fausto Franceschini	Westinghouse	Y	Y
8.	Steven Freel	GSE Systems	Y	Y
9.	Alex Larzelere	DOE	Y	Y
10.	Chris Lewis	AREVA	Y	Y
11.	Walt Schwarz	ANSYS	Y	Y
12.	Scott Simonson	Bettis/Naval Nuclear Propulsion Program	Y	N
13.	Russell Stachowski	Global Nuclear Fuels	Y	Y
14.	Tyrone Stevens	Exelon	Y	Y
15.	Ian Stevenson	Dassault Systems SIMULIA Corporation	Y	Y
16.	Eric Volpenhein	CD-adapco	Y	Y
17.	Zen Wang	GSE Systems	Y	N
18.	Phillip Finck	INL	Y	N
19.	Richard Lahey	RPI	Y	N
20.	Elmer Lewis	NWU	Y	N
21.	Finis Southworth	Areva	Y	N
22.	James Tulenko	UFL	Y	N

	Name	Institution	Sept 10	Sept 11
23.	William Weber	UTK/ORNL	Y	N
24.	Jeff Banta	ORNL	Y	Y
25.	Mark Christon	LANL	Y	N
26.	Nam Dinh	NCSU	Y	N
27.	Jess Gehin	ORNL	Y	N
28.	Steve Hess	EPRI	Y	N
29.	Zeses Karoutas	WEC	Y	N
30.	Doug Kothe	ORNL	Y	N
31.	April Lewis	ORNL	Y	N
32.	Rose Montgomery	TVA	Y	Y
33.	Vincent Mousseau	SNL	Y	N
34.	Scott Palmtag	Core Physics	Y	N
35.	Matt Sieger	ORNL	Y	Y
36.	Paul Turinsky	NCSU	Y	N
37.	John Turner	ORNL	Y	Y
38.	Brian Wirth	UTK	Y	N
39.	Keith Bradley	ANL	Y	N
40.	Weiju Ren	ORNL	Y	N
41.	Hyung Lee	Bettis	Y	N

CASL Science / Industry Council Meeting

Agenda

September 10-11, 2013

Location: Oak Ridge National Laboratory

Tuesday, September 10

Joint Industry and Science Council Meeting (Building 5100, Room 128, JICS Auditorium)

8:00	Check In (Building 5200, Visitor's Center)	
8:30	CASL technical accomplishments past 12 months (PoR6 and PoR7)	Doug Kothe Paul Turinsky
10:00	*Break*	
10:15	Challenge Problems – Charters, Implementation Plans, Results	Zeses Karoutas & Challenge Problem Integrators (as available)
11:15	Progress Made in THM Focus Area	Mark Christon
12:15	Working Lunch – Validation Data Needs Assessment	Nam Dinh
1:15	VERA: Description, Status, Plans	Jess Gehin
2:30	*Break*	
3:00	(CASL VOCC Facility, Building 5700) VOCC Laboratory Demonstrations of selected applications of VERA 1. Immersion Room (THM) – Bubble Model 2. F-5 (AMA) – Fibrous Debris Project 3. Waldo (MPO) – Crud build up and fuel performance 4. I-DEATE Stations 4&5 (PHI) – NiCE demo – VERA usability/workflow 5. I-DEATE Station 6 (PHI) - Exploration of VERA Results, VERA input / demo, COBRA-TF activities	 April Lewis Heather Feldman Mark Christon Zeses Karoutas Brian Wirth Jay Billings John Turner
4:45	Adjourn	

Wednesday, September 11

Industry Council Meeting (Building 5100, Room 128, JICS Auditorium)

8:30	Welcome and Introductions	Heather Feldman
9:00	Test Stands – Overview – Westinghouse Perspective Presentation	 Doug Burns Fausto Franceschini
10:30	Break	
10:45	Survey - VERA End User Uses and In-House Requirements	Matt Sieger
11:15	IC Project – VERA Value Proposition	Heather Feldman
11:45	Working Lunch – Thoughts on Phase 2 (2015-2020) Scope	Doug Kothe
12:45	VERA Interoperability – Overview – CD-adapco Perspective Presentation	 John Turner Eric Volpenhein
1:30	Break	
Joint Industry Council/Science Council Meeting (Building 5100, Room 128, JICS Auditorium)		
1:45	*Science Council Joins Industry Council* Industry Council Round Robin **(opportunity for individual IC members to comment)**	All Industry Council Members
2:45	Industry Council Action Items	Heather Feldman
3:00	Science Council Out Briefing of Major Findings	Bill Weber (Acting Chair)
3:45	Adjourn	

Wednesday, September 11

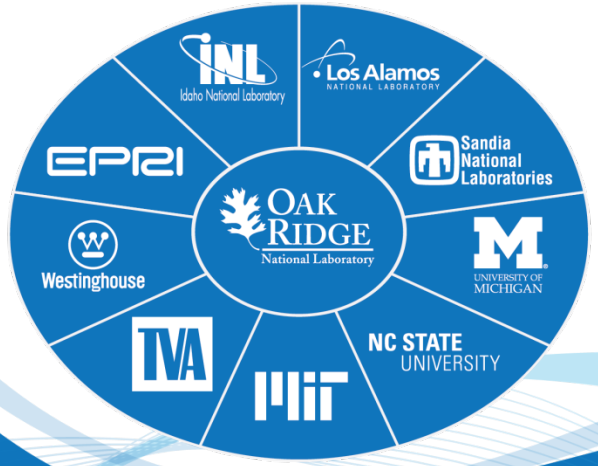
Science Council Meeting (Building 5700, VOCC Lab, ICREATE)

8:00	Update on FY14 S&T Plans and Beyond (Phase 2)	Doug Kothe/Paul Turinsky
8:45	Charge to Science Council regarding S&T Annual Review	Bill Weber (Acting Chair)
9:00	Report on RTM FA Annual Review & Planning Meeting	Tom Evans
9:20	Report on THM FA Annual Review & Planning Meeting	Mark Christon
9:40	Report on MPO FA Annual Review & Planning Meeting	Brian Wirth
10:00	Break	
10:20	Report on VUQ FA Annual Review & Planning Meeting	Vince Mousseau
10:40	Report on VRI/PHI FA Annual Review & Planning Meeting	Jess Gehin
11:00	Report on AMA FA Annual Review & Planning Meeting	Steve Hess
11:20	Breakout Meetings with Focus Area Leads	Science Council and FA Leads
12:00	Science Council Working Meeting on S&T Annual Review Preparation, *working lunch*	Science Council
1:30	Break – Walk to Building 5100	
Joint Industry Council/Science Council Meeting (Building 5100, Room 128, JICS Auditorium)		
1:45	*Science Council Joins Industry Council* Industry Council Round Robin **(opportunity for individual IC members to comment)**	All Industry Council Members
2:45	Industry Council Action Items	Heather Feldman
3:00	Science Council Out Briefing of Major Findings	Bill Weber (Acting Chair)
3:45	Adjourn	

Summary of Recent Accomplishments

CASL: Consortium for Advanced Simulation of Light Water Reactors

Doug Kothe (ORNL), Director
Paul Turinsky (NCSU), Chief Scientist
CASL Joint Science / Industry Council Meeting
Sep 10, 2013



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

The CASL Team

Core partners

Oak Ridge National Laboratory

Electric Power Research Institute

Idaho National Laboratory

Los Alamos National Laboratory

Massachusetts Institute of Technology

North Carolina State University

Sandia National Laboratories

Tennessee Valley Authority

University of Michigan

Westinghouse Electric Company

Individual contributors

ASCOMP GmbH

CD-adapco

City College of New York

Florida State University

Imperial College London

Rensselaer Polytechnic Institute

Texas A&M University

Pennsylvania State University

University of Florida

University of Tennessee – Knoxville

University of Wisconsin

Notre Dame University

Anatech Corporation

Core Physics Inc.

Pacific Northwest National Laboratory

G S Nuclear Consulting, LLC

University of Texas at Austin

University of Texas at Dallas

Core partners: Unchanged

Contributing partners:
3 additions, 1 removal

CASL Organization

Oak Ridge National Laboratory
Thom Mason, Laboratory Director
Nuclear Science and Engineering Directorate
Jeff Binder, Associate Laboratory Director

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Science Council
Bill Oberkampf, Chair

Industry Council
Heather Feldman, Chair

Director
Doug Kothe
Deputy Director Doug Burns
Chief Scientist Paul Turinsky

Board of Directors
Dale Klein, Chair

Outreach
Education Program Director
Mike Doster
Communications Coordinator
Mark Uhran

Chief Computational Scientist
John Turner

Operations Management

Collaboration & Ideation	**Project Management**
April Lewis	Jeff Banta
Quality	**Finance**
Matt Sieger	Victoria Shope
Partnerships	**Legal**
Jeff Cornett	Jud Hightower

Technical Focus Areas

Materials Performance & Optimization
Lead Chris Stanek
Deputy Brian Wirth

Validation & Uncertainty Quantification
Lead Vince Mousseau
Deputy Brian Williams

Advanced Modeling Applications
Lead Zeses Karoutas
Deputy Steve Hess
Deputy Rose Montgomery

Radiation Transport Methods
Lead Bill Martin
Deputy Tom Evans

Thermal Hydraulics Methods
Lead Mark Christon
Deputy Emilio Baglietto

Physics Integration
Lead Jess Gehin
Deputy Scott Palmtag

Operations Support
Technology Control
Sam Howard
Contracting Authority
Jo Ann Fitzpatrick
Justin Keck
Virtual Office, Community, and Computing (VOCC)
Teresa Robison, A.J. Iurelli, John Shaw
Safety Officer
Jeff Banta
Web Design
Cindy Latham
Information Technology
Ken Barker, George Smith
Administrative
Linda Weltman

Product Integrators

Challenge Problems
Lead Zeses Karaoutas

CRUD	Jeff Secker
GTRF	Zeses Karoutas
PCI	Rob Montgomery
RIA	Gregg Swindlehurst
LOCA	Gregg Swindlehurst
DNB	Yixing Sung

Validation Data
Nam Dinh

CASL
Consortium for Advanced Simulation of LWRs

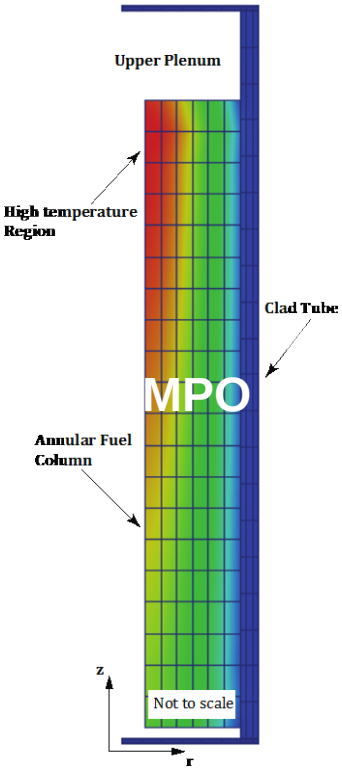
Challenge Problems

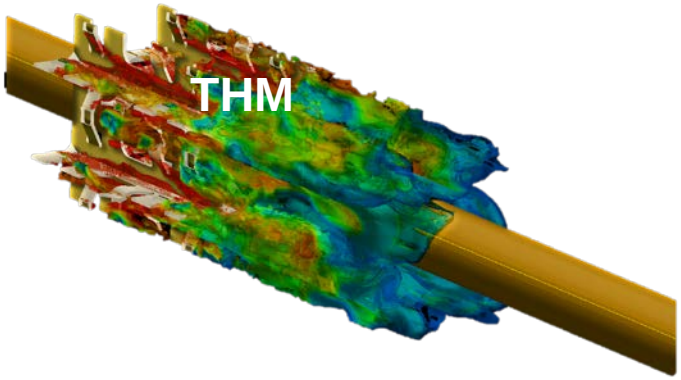
Product Integrators are in place and driving metrics, products, and plans

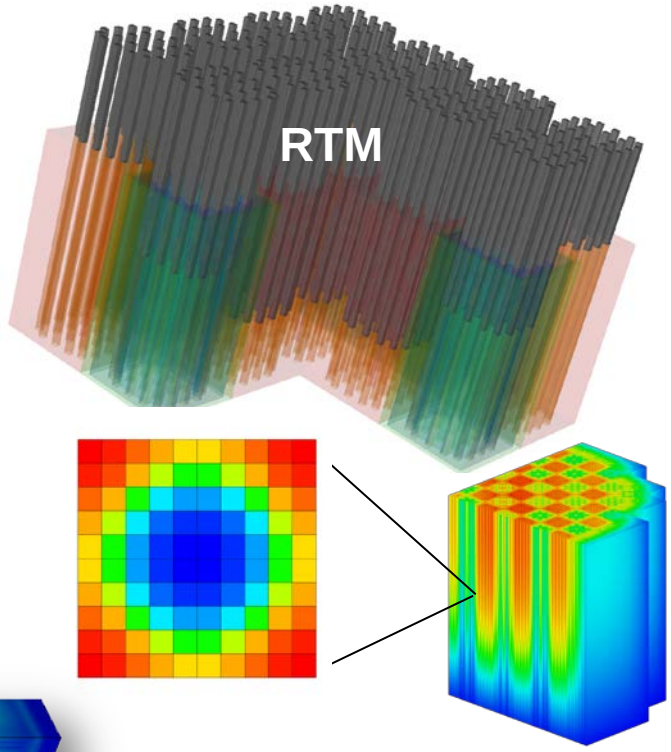
CP	Description and Impact	Simulations Gaps and Drivers
Crud-induced power shift; crud-induced localized corrosion	High uncertainties in crud source, thickness, boiling surface area, and margin to fuel leakage affect fuel management and thermal margin in many plants, limiting power uprates	More accurate, higher resolution models for boiling surface area, crud deposition, boron uptake and cladding oxidation rate for each rod in core, with boron feedback in neutronics
Grid-to-rod fretting	Rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation affect wear, especially for fuel near the core shroud	Reliable predictions of grid to rod gap, turbulent flow excitation, and resulting rod vibration and wear at any location in core
Pellet-clad interaction	Cladding creep-down onto pellets, followed by pellet expansion, creates local cladding stresses at pellet imperfections, resulting in clad failure sometimes assisted by SCC	Sufficient 3D geometric detail of fuel rod material property changes; pellet growth, cracking and fission product release; cladding stresses, creep, fracture and SCC attach; fuel-cladding binding; and coupling to neutronics and T-H
Fuel assembly distortion	Forces from radiation-induced growth and fluid flow may cause distortion and alter power distributions, challenge fuel handling, retard control rod insertion, and restrict plant operation	Fully 3D structural models of fuel assemblies accounting for material property changes, growth and creep; coupled with neutronics and TH
Reactor vessel and internals integrity over reactor lifetime	Damage from radiation results in increased temperature for onset of brittle failure and higher failure probability due to thermal shock stresses with safety injection for RV, and damage from radiation, thermal & mechanical fatigue render upper internal package more susceptible to distortion under blow-down or seismic loads.	3D prediction of temperature, force, stress, fluence and resulting material property changes of reactor internal structures and vessel; and solid mechanics prediction of vessel fracture and internals distortion
Departure from nucleate boiling	Local clad surface dryout, affected by detailed flow patterns and mixing, cause dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures	3D subchannel and CFD tools to model detailed flow patterns downstream of mixing grids for single and two-phase flow, coupled to detailed pin-resolved radiation transport and fuel performance models for application to DNB transients (e.g., RIA, Loss of Flow)
Cladding integrity during a reactivity insertion accident and loss of coolant accident	Physical changes during transient (e.g., swelling and burst, oxidation mechanics), leading to clad failure followed by fuel dispersal	Enhanced fuel rod models, with improved predictive capability for normal operations to obtain fuel initial conditions at initiation of accident simulation, and transient fuel rod behavior

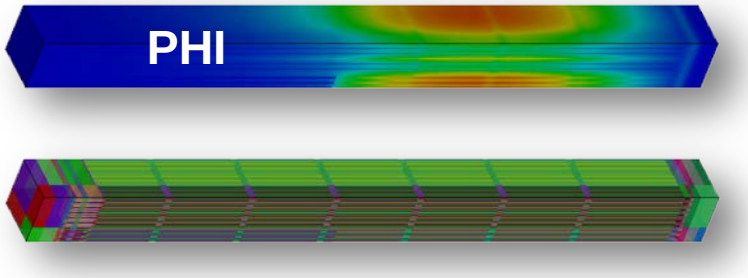
- FAD: Defer until mechanics plan and capability in place thru GTRF execution
- Lifetime Extension (integrity): Leverage scope in LWR Sustainability Program

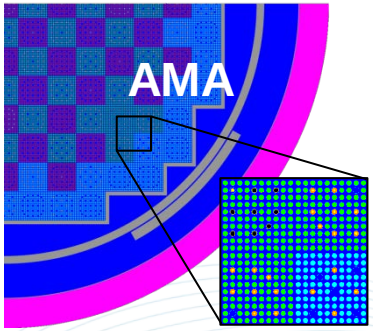
Good Technical Progress in Every Focus Area

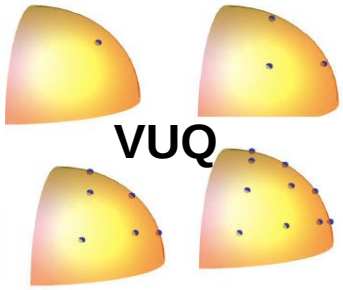












More detail: 2013 Round Table proceedings

Our 2010 L1 Milestone Roadmap

Framed by demonstrable, value-added Challenge Problem M&S capabilities

Year	VERA Capability	L1 Milestone Category	L1 Milestone
1	Initial core simulation using coupled tools and models	CRUD	Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate quantities relevant to CRUD initiation and growth
		GTRF/FAD	Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting
2	Detailed phenomena modeling in fully coupled VR	CRUD	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness
		GTRF/FAD	Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration
3	Assembly simulation with rod fretting and upscaled materials models	CRUD	Model boron uptake from reactor coolant into CRUD on fuel rods
		GTRF/FAD	Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods
		Safety	Initial modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		OR	Initial modeling of reactor operation; qualify with operational data
4	Initial predictive reactor modeling in coupled VR	CRUD	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape
		GTRF/FAD	Calculate fuel rod material wear resulting from GTRF
		LE	Model reactor vessel fluence and material property changes that result in material degradation and limit vessel performance
5	Predictive reactor simulation coupled to physical plant	CRUD	Analyses to mitigate CRUD formation and minimize CIPS
		GTRF/FAD	Analyze grid geometry and spring materials to mitigate material changes and wear
		Safety	Improved modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		LE	Model mechanical and thermal stresses and fatigue that result in material failures of core internals
		AF	Demonstrate the impact of new fuel forms (clad materials, fuel materials, and fuel geometries) for use in current reactor core configurations
		OR	Improved simulation of reactor operation; qualify with operational data

FAD (fuel assembly distortion) and LE (lifetime extension) descoped; rest of CP scope remains relevant and on track

We are here

We have worked with our Product Integrators in developing specific metrics (*minimal, acceptable, end game*) for measuring our CP progress

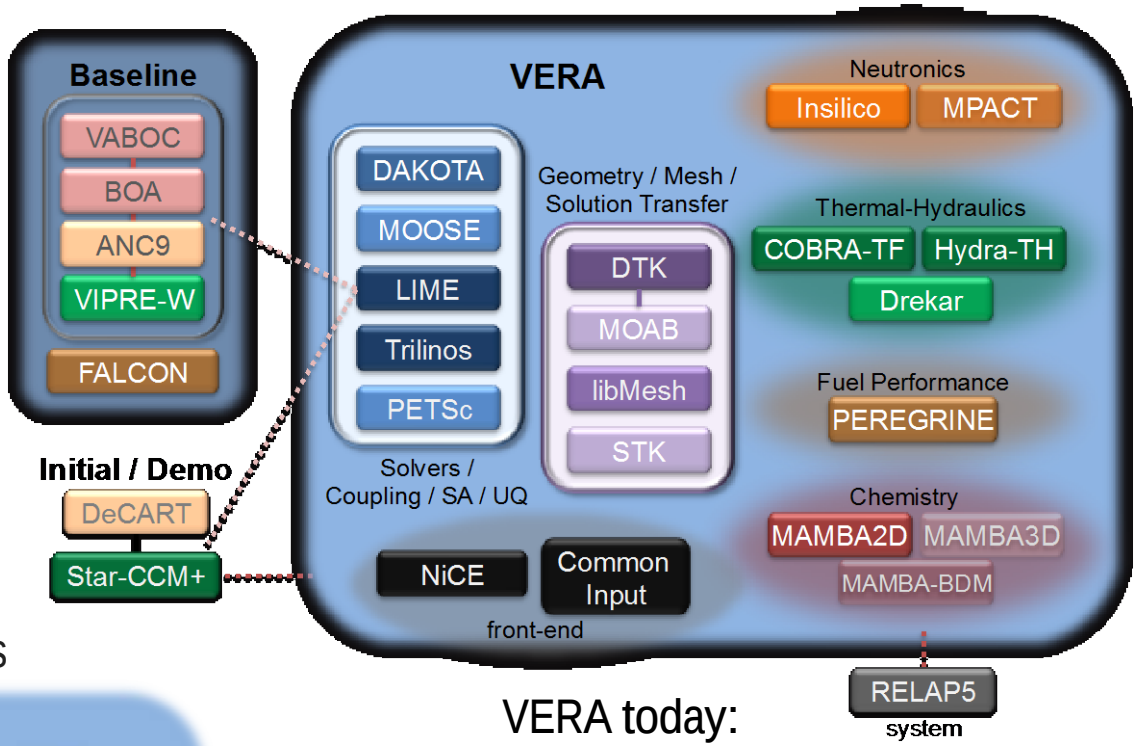
FY13 CASL Milestones Formally Reportable to DOE

Milestone ID	Milestone Description	Planned Finish Date	Actual Delivery Date	Status
CASL.001	Demonstration of advanced pin-resolved method of characteristics (MOC) capabilities for neutron transport	12/21/2012	12/21/2012	Completed
CASL.002	DNB Relevant Experimental Data Collection and Modeling with CASL Tools	03/29/2013	03/28/2013	Completed
CASL.003	Operational Reactor Model Demonstration with the VERA Core Simulator	06/07/2013	06/7/2013	Completed
CASL.004	Peregrine: Validation and Benchmark Evaluation of Integrated Fuel Performance of Halden Test Reactor Data and Falcon	06/28/2013	06/28/2013	Completed
CASL.005	Initial demonstration of Peregrine integration into the VERA Core Simulator	07/31/2013	07/31/2013	Completed
CASL.006	Issue an updated CASL Program Plan	07/31/2013	07/31/2013	Completed
CASL.007	Demonstration & assessment of an advanced modeling capabilities for multiphase flow with subcooled boiling	08/30/2013	08/30/2013	On Track
CASL.008	Uncertainty quantification and data assimilation (UQ/DA) study on a VERA component for CRUD analysis	08/30/2013	08/30/2013	On Track
CASL.009	Multiphysics modeling of CRUD deposition on PWR fuel	09/30/2013		On Track
CASL.010	VERA Release	09/30/2013		On Track
CASL.011	Demonstration of neutronics coupled to thermal-hydraulics for a full-core scenario using VERA.	09/30/2013		On Track
CASL.012	Determine extent structural analysis amplifies (or damps) differences in pressure forces between different CFD codes for analysis of GTRF phenomenon.	09/30/2012	12/12/2012	Completed

- Coverage of CASL Challenge Problems and important Focus Area capability development
- Consistency where appropriate with original 2010 proposal plan (e.g., operational reactor milestone)
- FY12 delayed milestone delivered 3 months later
- All reportable milestones delivered to date have been provided as evidence
- Other outstanding milestones on track but not without risk (e.g., full core coupling)

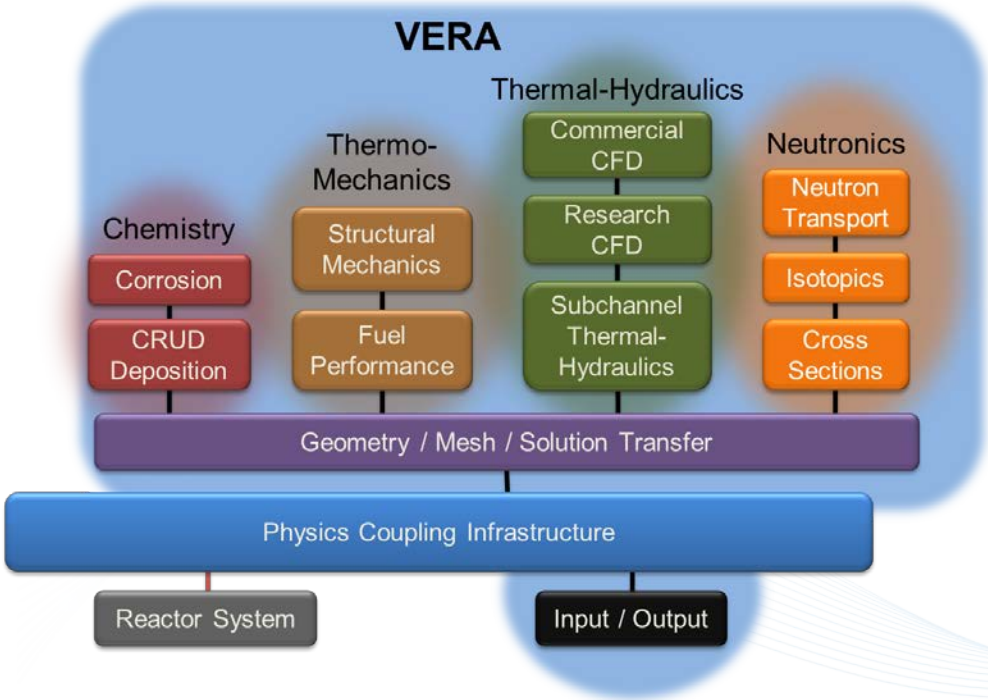
Virtual Environment for Reactor Applications

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



VERA today: Version 3.1 (August 2013)

Required functional capabilities



VERA 3.1 Profile

Table 1.1: VERA Infrastructure Components.

Component	Description	Activity	Integration	Capability
LIME	Coupling			
Common Input	Usability			
DTK	Solution transfer			
MOOSE	Framework			
DAKOTA	SA / UQ			

Table 1.2: VERA Core Simulator Components.

Component	Description	Activity	Integration	Capability
SCALE / XSProc	Cross sections			
Insilico	Pin-homogenized neutronics			
COBRA-TF (CTF)	Subchannel Thermal-Hydraulics (T-H)			
DAKOTA + CTF	Subchannel T-H with SA / UQ			
CTF + Insilico	Coupled neutronics and T-H			
MPACT	Pin-resolved neutronics			
Peregrine2D	Fuel performance			
Tiamat	CTF + Insilico + Peregrine2D			

Table 1.3: Other VERA Components.

Component	Description	Activity	Integration	Capability
RELAP5-3D	Reactor System			
Drekar	CFD			
Insilico + Drekar	Coupled neutronics and CFD			
Hydra-TH	CFD			
MAMBA2D	CRUD			
CTF + MAMBA2D	CRUD			

Table 1.4: VERA Physics Components Under Development.

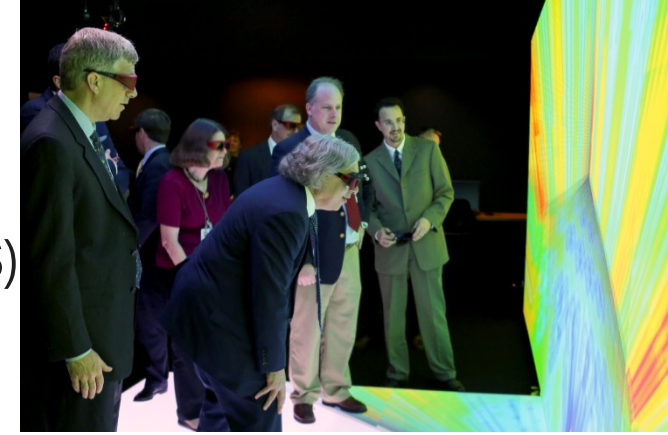
Component	Description	Activity	Integration	Capability
CTF + MPACT	Coupled pin-resolved neutronics and T-H			

Table 1.5: VERA Baseline Components.

Component	Description	Activity	Integration	Capability
ANC 9.5	Nodal neutronics			
VIPRE-W	Subchannel Thermal-Hydraulics (T-H)			
DAKOTA + VIPRE-W	Subchannel T-H with SA / UQ			
ANC9.5 + VIPRE-W	Coupled nodal neutronics and T-H			
ANC9.5 + VIPRE-W + BOA	Coupled nodal neutronics, T-H, and CRUD			

- Substantial infrastructure and component development, integration, and coupling progress since August 2012
- VERA today: 5 infrastructure and 11 physics components (5 coupled), constructed with >8M lines of source code in >35K files, housed in 18 software repositories and 184 packages
- Continuous integration is supported with >500 nightly tests
- We are continuously improving our release process, build system, testing harness and coverage, documentation, support model, and product definition and maturity

CASL at Year 3



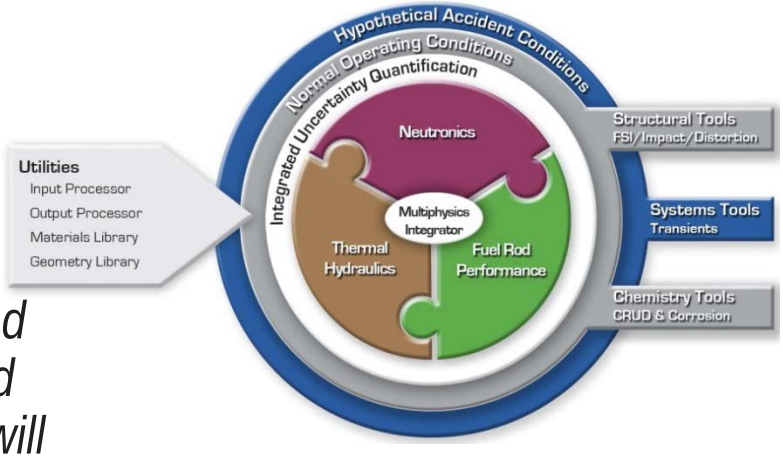
- ✓ First VERA Test Stand deployed to industry for application to WEC Gen III AP1000 design (4 now under construction in US)
- ✓ First and successful comparison against operational reactor data (Watts Bar 1 zero power physics tests)
- ✓ Challenge Problem solution metrics and VERA products defined and driving development and application to real operational PWR core scenarios
- ✓ VERA: multi-physics integrator functional for coupling multiple applications (neutronics, T-H, fuel, CRUD, UQ) to address feedback effects not currently reflected in the industry analytical approach
- ✓ VERA: baseline industry physics capabilities integrated to demonstrate increased fidelity of the coupled approach for a direct industry comparison point.
- ✓ VERA-CS: progressed thru 6 (almost 7) core physics benchmark problems required for real industry use
- ✓ Continued targeted development of advanced simulation components: UQ, neutron transport, multiphase CFD, CRUD deposition/corrosion, fuel performance, structural dynamics

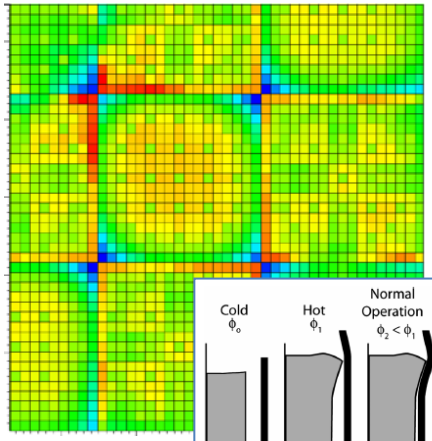
Scientific Output thru Jun 2013

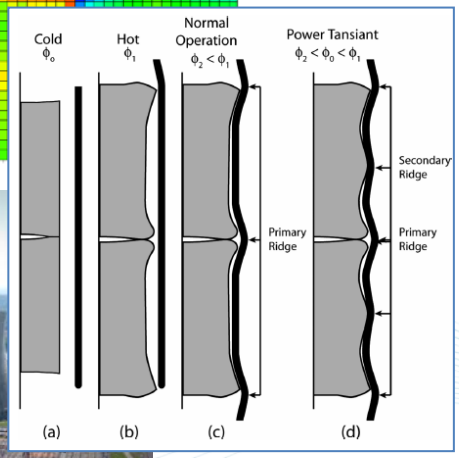
- 81+ journal articles
- 328 conference papers
- 28 technical reports
- 51+ invited talks
- 382 milestone reports
- 216 programmatic reports

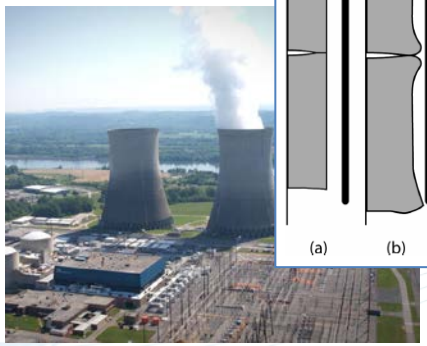
CASL Test Stands: From Plan to Execution

- Early deployment into industrial environment for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
- Excerpt from 2010 Proposal: "*… interactive VR 'test stands' will be set up to provide industry-led design and analysis teams with opportunities to test, evaluate, and begin to apply the VR. … A beta version(s) of the VR will be applied and compared with the reference case and plant data. The VR will also be measured against all the challenge problems …*"
- Status of initial deployment to core industry partners
  - WEC: Deployment scheduled Jun 2013; focus on VERA simulation of AP1000 first core startup
  - EPRI: Deployment planned for Dec 2013; new EPRI computing capabilities will be utilized to test VERA fuel (Peregrine) performance applications
  - TVA: Deployment planned for Spring/Summer 2014; focus currently under discussion





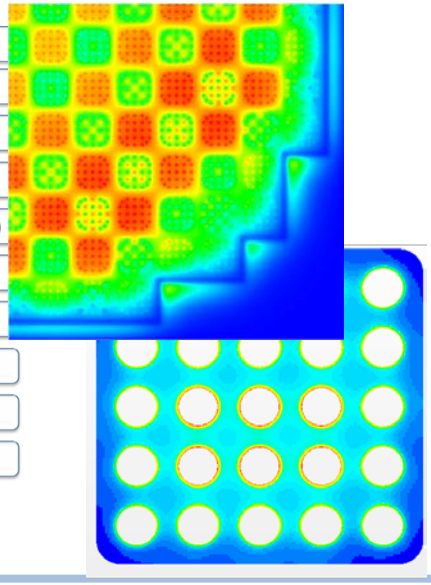




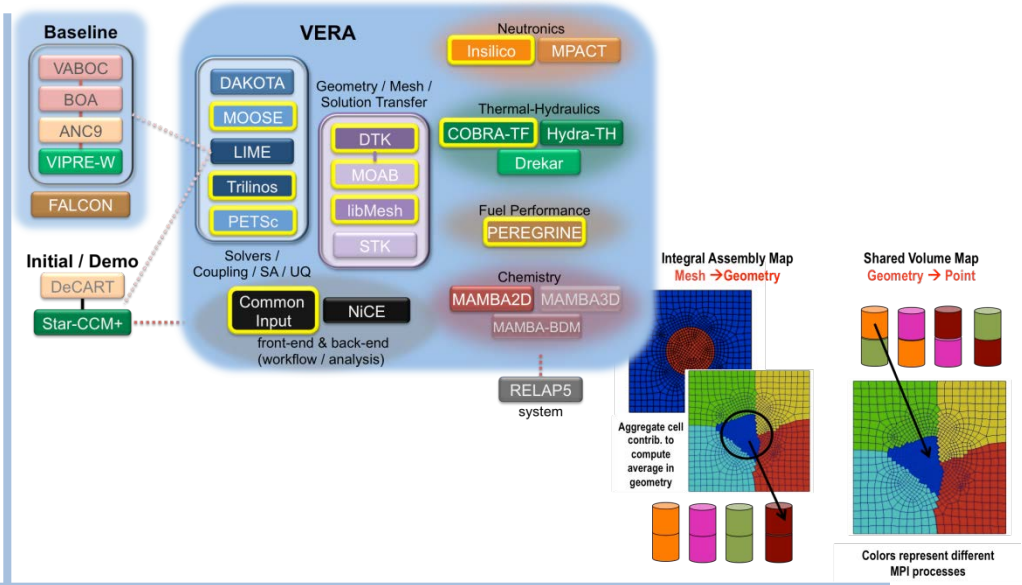
Technical Execution This Past Year

Advanced Modeling Applications

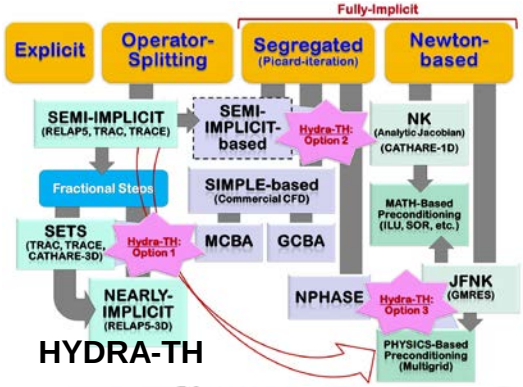
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- **#5 Physical Reactor Zero Power Physics Tests (ZPPT)**
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical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

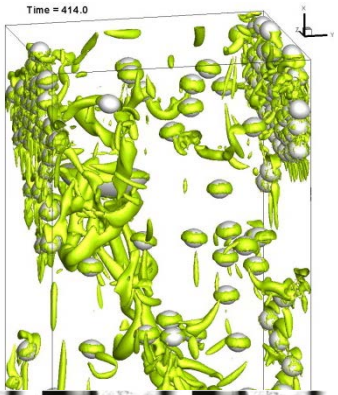


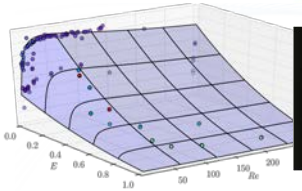
Virtual Reactor Integration

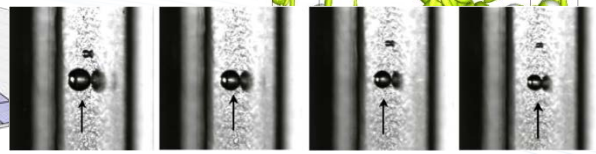


Thermal Hydraulic Methods

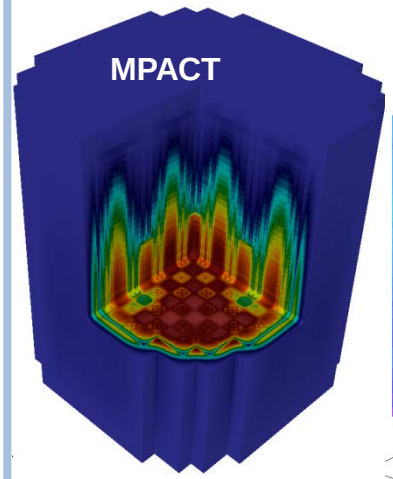


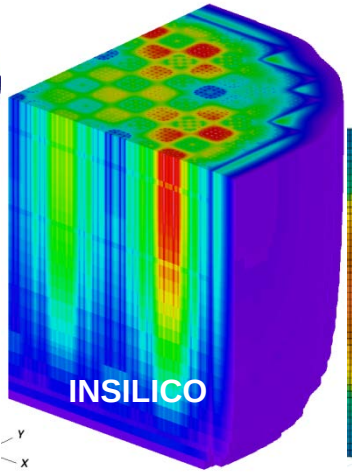


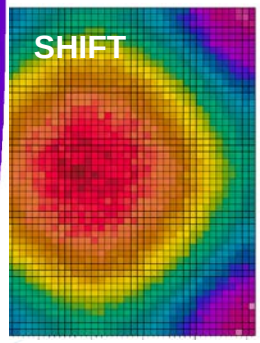




Radiation Transport Methods

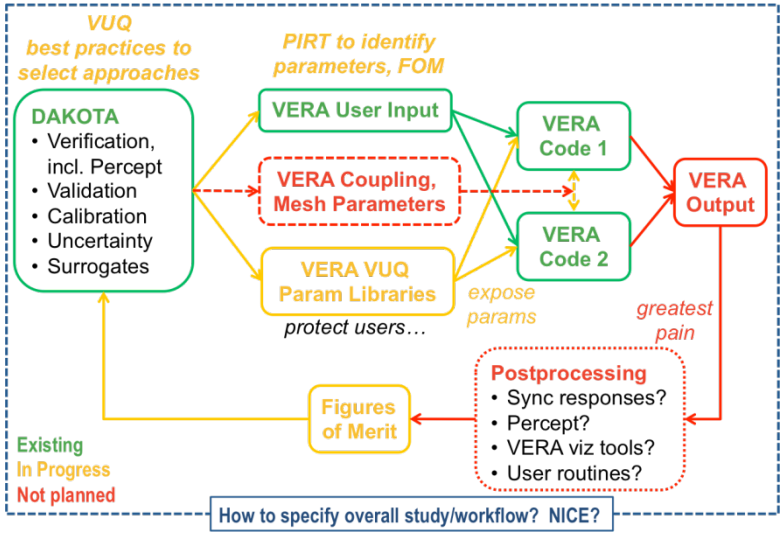






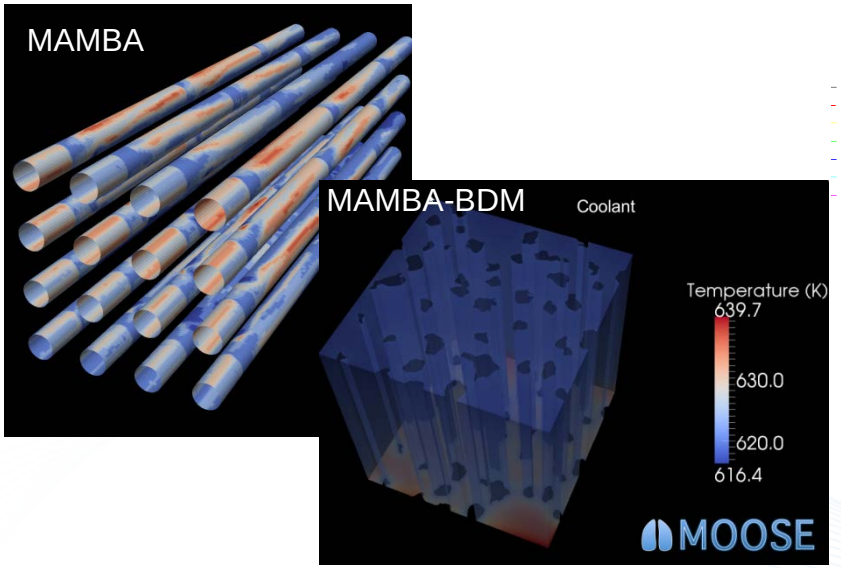
Technical Execution This Past Year

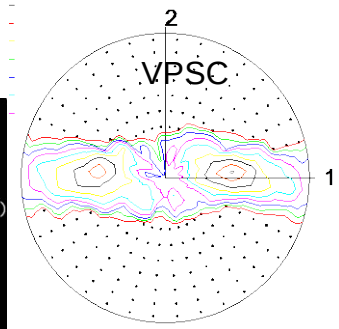
Validation & Uncertainty Quantification

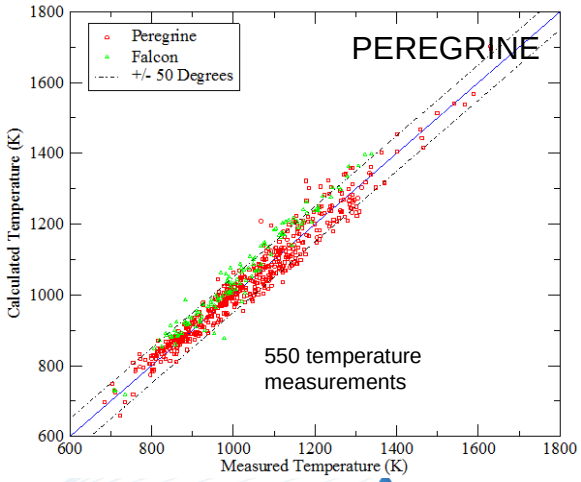


VOCC

Materials Performance and Optimization







CASL S&T Program

- S&T Capabilities Needed for Challenge Problems
- M&S Current Practice versus CASL Practice
- FY13 Highlighted Accomplishments (to date)
- FY13 Annual Review S&T Relevant Comments

Lots to cover, so let's get on with it!

What enhanced capabilities over current practices will CASL provide?

Predictive capabilities

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

Phase-space resolution

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

VUQ practices

- Verification & validation
- Data assimilation
- Uncertainty quantification

Computational resource utilization

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

High level differences of current versus CASL capabilities

Fluids (HYDRA-TH)

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

Radiation Transport (MPACT & INSILICO)

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

High level differences of current versus CASL capabilities

Fuel Performance (PEREGRINE)

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

Crud Chemistry (MAMBA & MAMBA-BDM)

- Current Practice: 2D with limited chemical species & experimentally derived models' parameters
- CASL Practice: 2D and 3D with expanded chemical species, experimentally & micro modeling derived models' parameters, and enhanced mass/energy transport

Multiphysics (VERA)

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

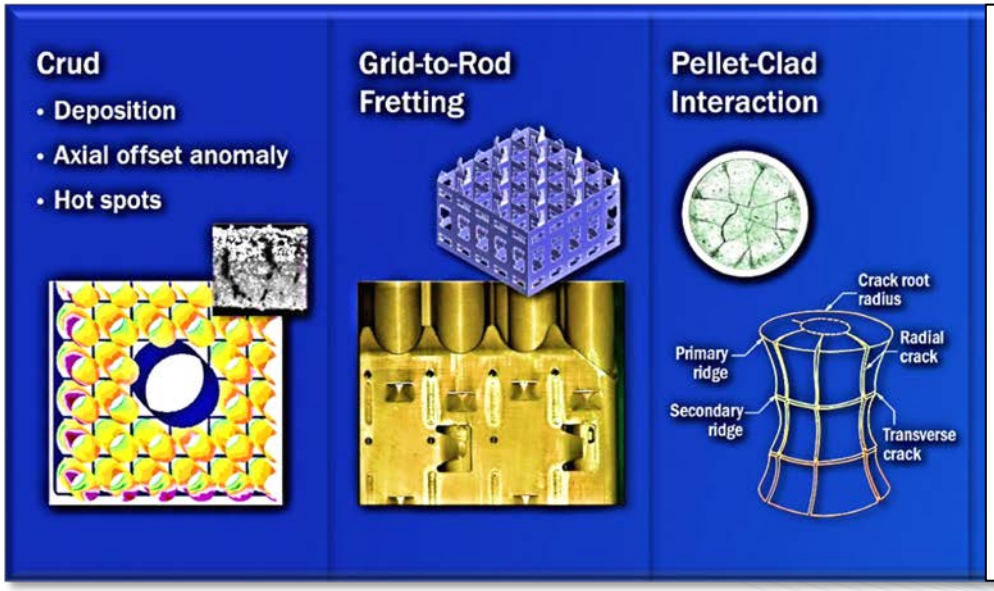
CASL Challenge Problems

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



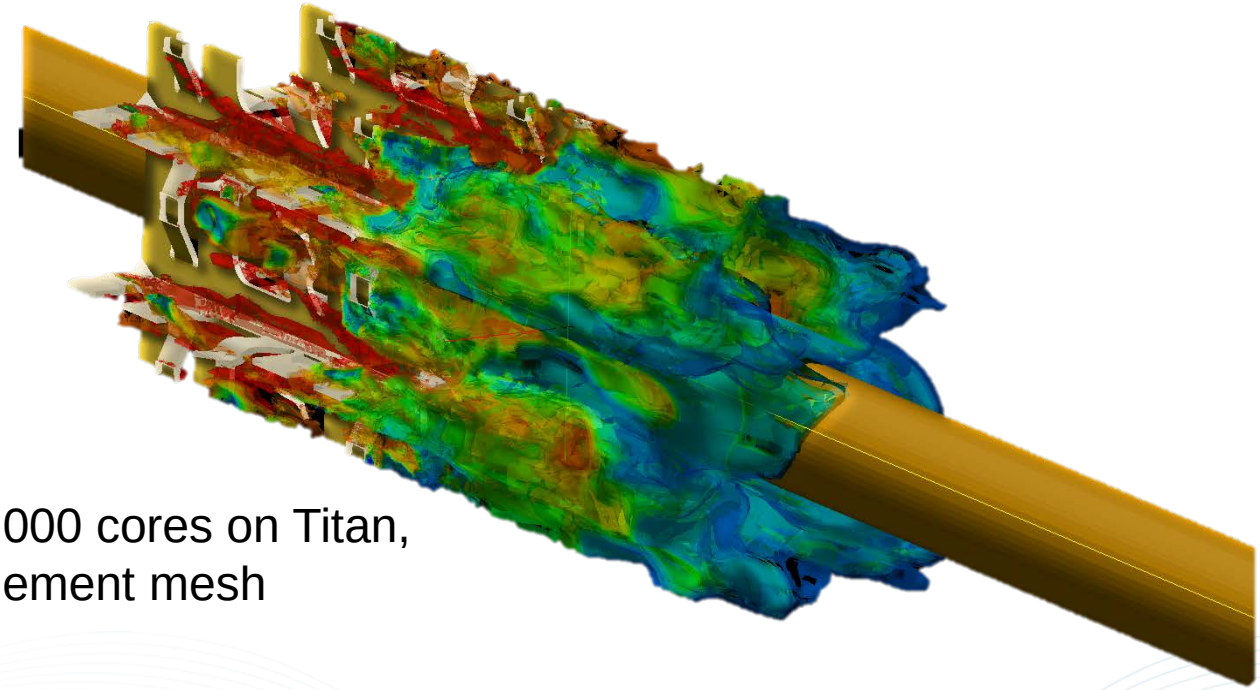
Operational Challenge Problems

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
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

S&T Program: FY13 Highlighted Accomplishments (to date)

- Thermal-Hydraulic Methods (THM)
  - Development of robust, parallel solution algorithms for multiphase/multi-field CFD (Hydra-TH)
  - Assessment of subcooled boiling and bubble flow closure relationships using experimental data & DNS (energy partitioning, wall effect lift & drag force, bubble departure characteristics)



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

More details to come during
THM focus area presentation

Hydra-TH: MCFD 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

S&T Program: FY13 Highlighted Accomplishments (to date)

- Radiation Transport Methods (RTM)
  - Development of integrated x-section generation/transport solver capability (Insilico), using Sn and newly developed SPn
  - Refactored 2D MOC/1D Diffusion code (MPACT) with convergence issue understood & addressed and developed full 3D MOC capability (MPACT-3D)

$$\theta_{opt} = \begin{cases} \frac{2}{2-c} & , \quad \frac{2}{\sqrt{3c}} < \Sigma_t \Delta_z \ , \\ \frac{3(\Sigma_t \Delta_z)^2}{2+3(1-c)(\Sigma_t \Delta_z)^2} & , \quad \Sigma_t \Delta_z \leq \frac{2}{\sqrt{3c}} \ , \end{cases}$$

$$\rho = \begin{cases} \frac{c}{2-c} & , \quad \frac{2}{\sqrt{3c}} < \Sigma_t \Delta_z \ , \\ \frac{2}{2+3(1-c)(\Sigma_t \Delta_z)^2} & , \quad \Sigma_t \Delta_z \leq \frac{2}{\sqrt{3c}} \ . \end{cases}$$

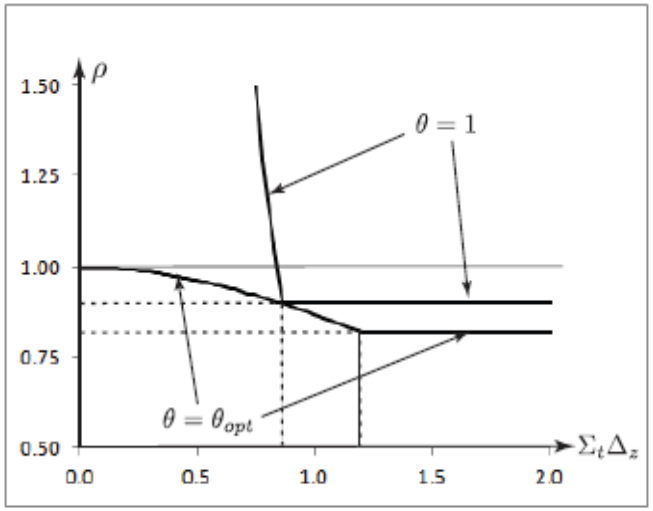
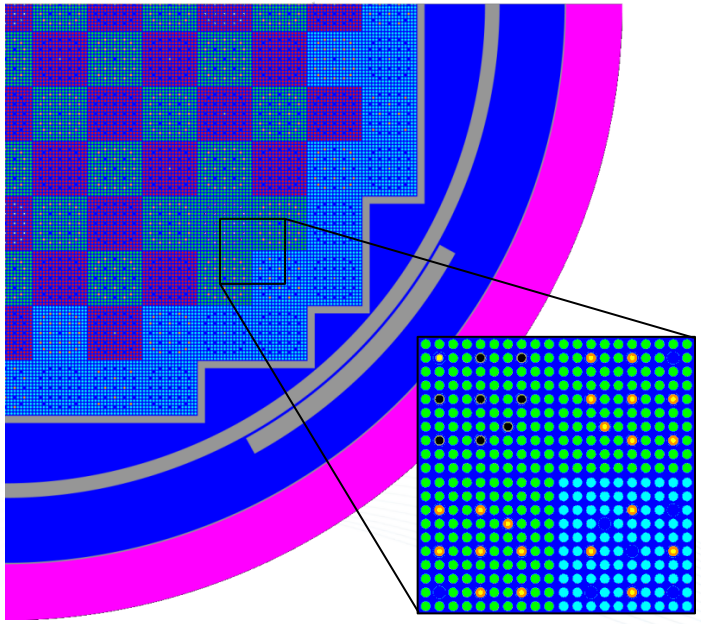


Figure 2: Spectral Radius ρ vs Axial Optical Thickness $\Sigma_t \Delta_z$ for $c = 0.9$

Insilico (SPn): Need for Low Order Transport

- 3D pin-resolved transport is very computationally expensive
  - A single state point calculation for a full/quarter core model with reasonable fidelity may require most (if not all) of a Titan-class computer for hours
- Multiphysics (T/H, depletion, etc.) simulations require numerous transport calculations
  - Run time of resolved transport makes this intractable
  - Goal for SP_N is to be cheaper than transport, more accurate than diffusion



DENOVO

Shift

EXNIHILO

INSILICO

Insilico (SPn) Performance Results – 3D Assembly

- 23 energy groups
- SP_5, P_1 scattering
- 4x4 mesh per pin, 2 in. axial mesh (143,325 cells)
- 9.9 million total unknowns
- 36 compute cores

Eigen solver	Preconditioner	Iterations	Time (s)
Power Iteration	ILUT	861	5126
Arnoldi	ILUT	21	2608
Davidson	ILUT	1515	1610
Davidson	ML	316	745
Davidson	MGE(ILU)	47	300

- Denovo S_N (LD) runtime on same problem with coarse quadrature is around 1.5 hours

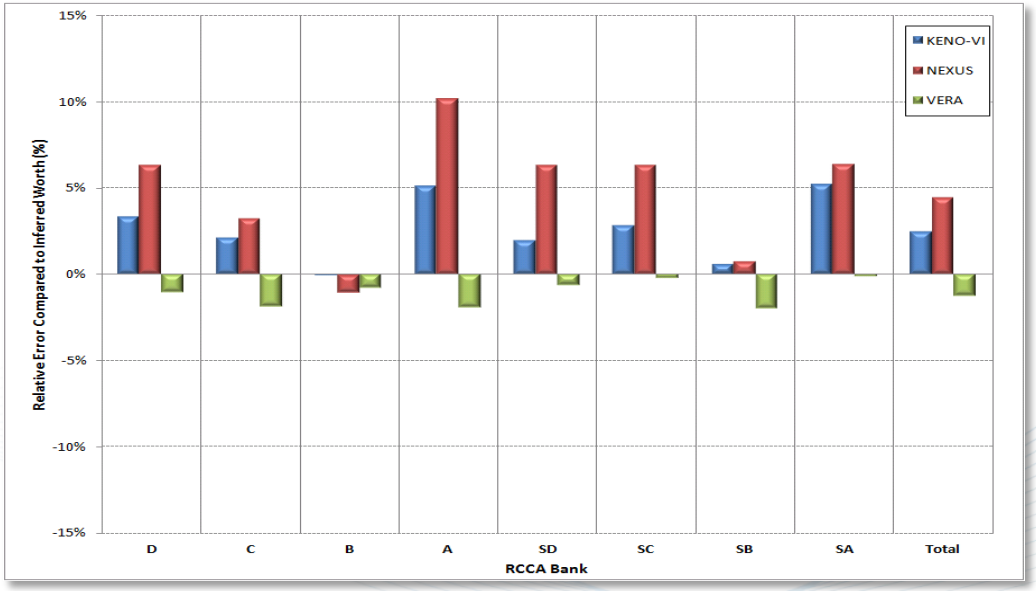
Application of Insilico SPn method to Watts Bar Unit 1 – Cycle 1 HZP Startup Physics Test

Table 2: WBN1 Cycle 1 Initial Criticality Results

Result	k-effective	Reactivity Difference (pcm)	Effective Critical Boron Difference (ppmB)†
Measured	1.00000	--	--
CE KENO-VI	1.00014 ± 0.00005	14 ± 5	1 ± 1
NEXUS	0.99793	-208	-21
VERA	1.00122	122	12

† calculated using the calculated ARO DBW for each code, to the nearest ppmB

Figure 21: WBN1 Cycle 1 Control Bank Worth Deviations



Application of Insilico SPn method to Watts Bar Unit 1 – Cycle 1 HZP Startup Physics Test

Table 6: WBN1 Cycle 1 Differential Boron Worths

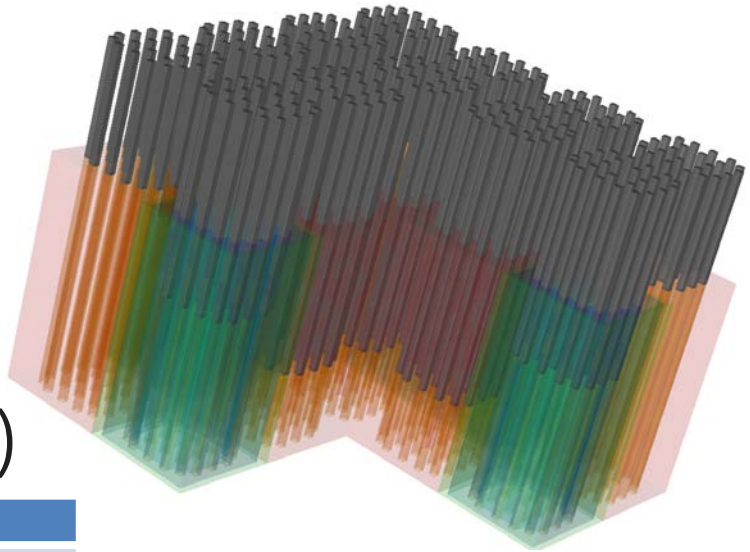
Result	DBW (pcm/ppmB)	Difference (pcm/ppmB)
Measured	10.8	--
CE KENO-VI	10.1	-0.7
NEXUS	10.0	-0.8
VERA	10.1	-0.7

Table 7: WBN1 Cycle 1 Isothermal Temperature Coefficients

Result	ITC (pcm/°F)	Difference (pcm/°F)
Measured	-2.2	--
CE KENO-VI	--	--
NEXUS	-2.6	-0.4
VERA	-3.8	-1.6

Except for ITC, results look encouraging

MPACT 2D/1D Results: C5G7 3-D Benchmark



- OECD transport benchmark
  - Heterogeneous geometry

- Original Benchmark
  (Full height assembly without rods)

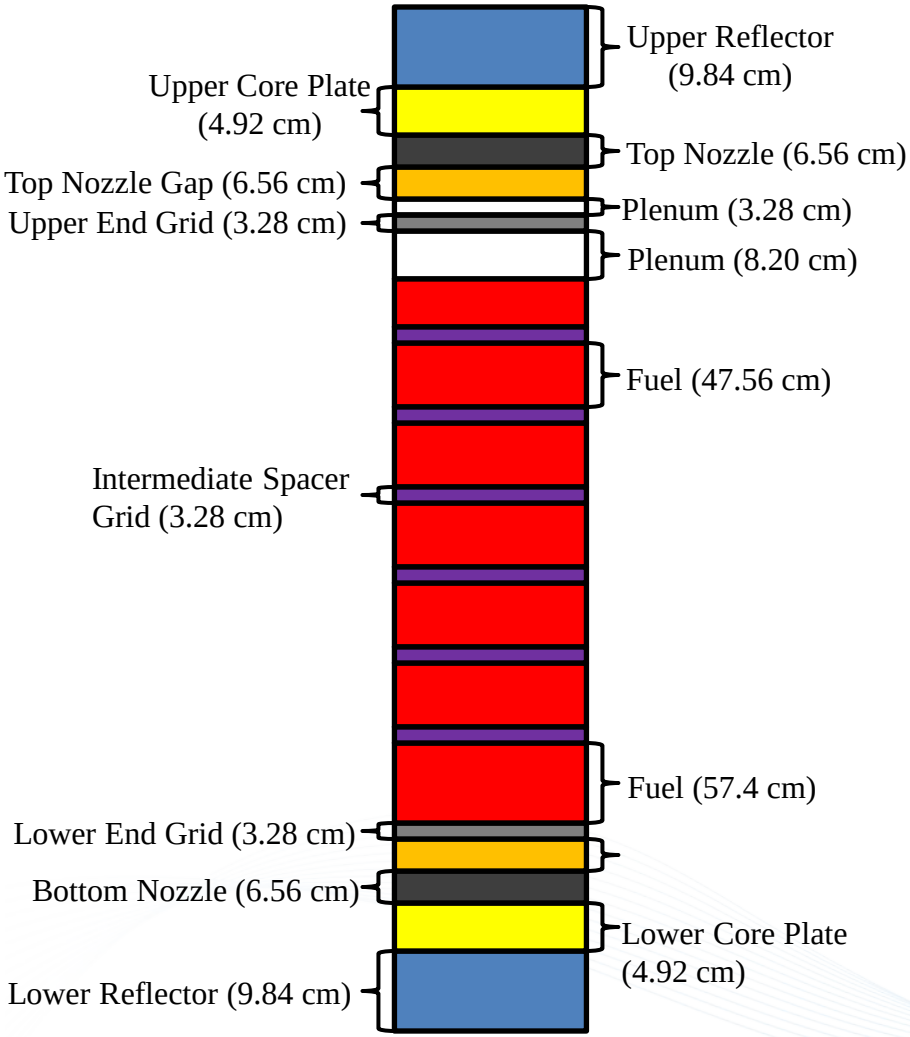
		Axially Integrated Powers				
	keff	min	max	Inner UO2	MOX	Outer UO2
MPACT	1.18390	0.24	2.49	491.62	211.80	140.10
Error	-9	2.38%	-0.41%	-0.26%	0.16%	0.36%

- Extended Benchmark (Reduced height with rods)

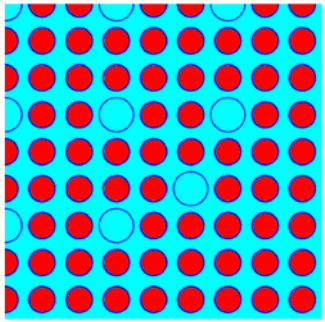
			Axially Integrated Powers					Slice Power Errors				
		keff	min	max	Inner UO2	MOX	Outer UO2	Slice	max	Inner UO2	MOX	Outer UO2
Rodded A	MPACT	1.12744	0.26	2.25	461.13	221.62	151.63	1	-0.1%	-0.2%	-0.8%	-1.0%
	Error	62	--	0.05%	-0.02%	-0.04%	0.15%	2	-1.0%	-0.8%	-0.6%	-0.6%
								3	2.6%	3.7%	3.7%	2.9%
Rodded B	MPACT	1.07751	0.35	1.83	395.24	236.73	187.30	1	-0.7%	-0.6%	-0.5%	-0.6%
	Error	26	--	-0.16%	-0.04%	0.05%	0.00%	2	-0.2%	0.4%	-0.7%	-0.4%
								3	3.7%	3.1%	3.6%	2.6%

MPACT-3D Results: PWR Assembly

Axial Description



Radial Description



Problem Size Parameters

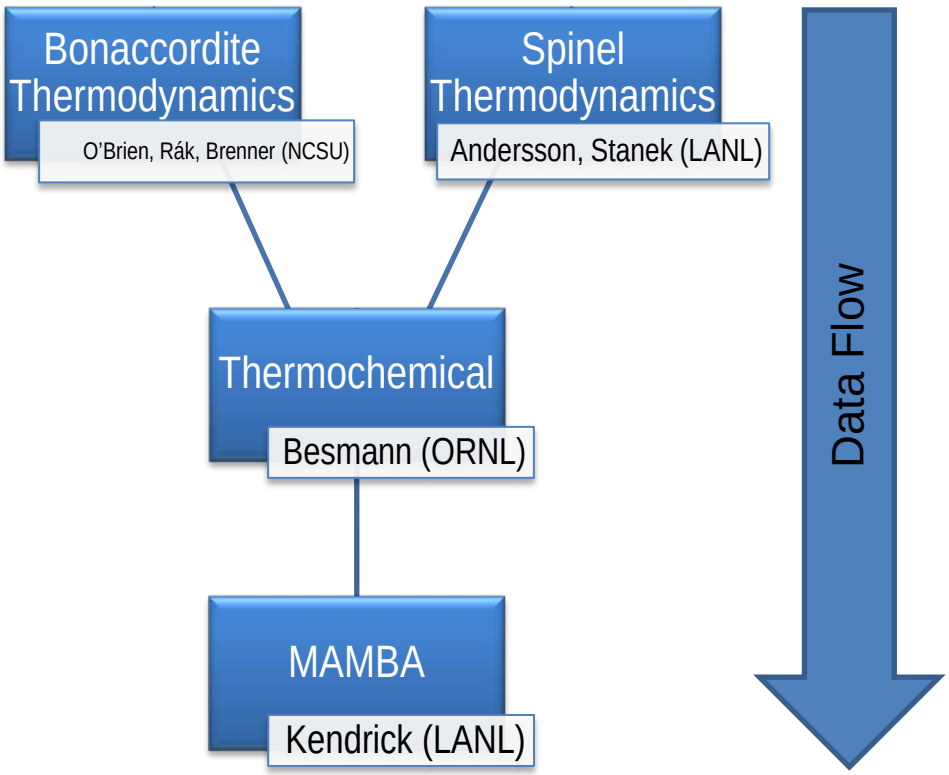
	3-D MOC	2-D/1-D
# of Segments	55,952,023,038	28,981,236
# of Rays	2,238,077,088	407,008
# of Regions	3,697,984	157,496
Directions per octant	36	64

3-D MOC and 2-D/1-D Comparison

	3-D MOC	2-D/1-D
k_{eff}	1.17180	1.17323
No. of Iters.	7	18
Processors	16704	368
Run Time	2103 s	630 s

S&T Program: FY13 Highlighted Accomplishments (to date)

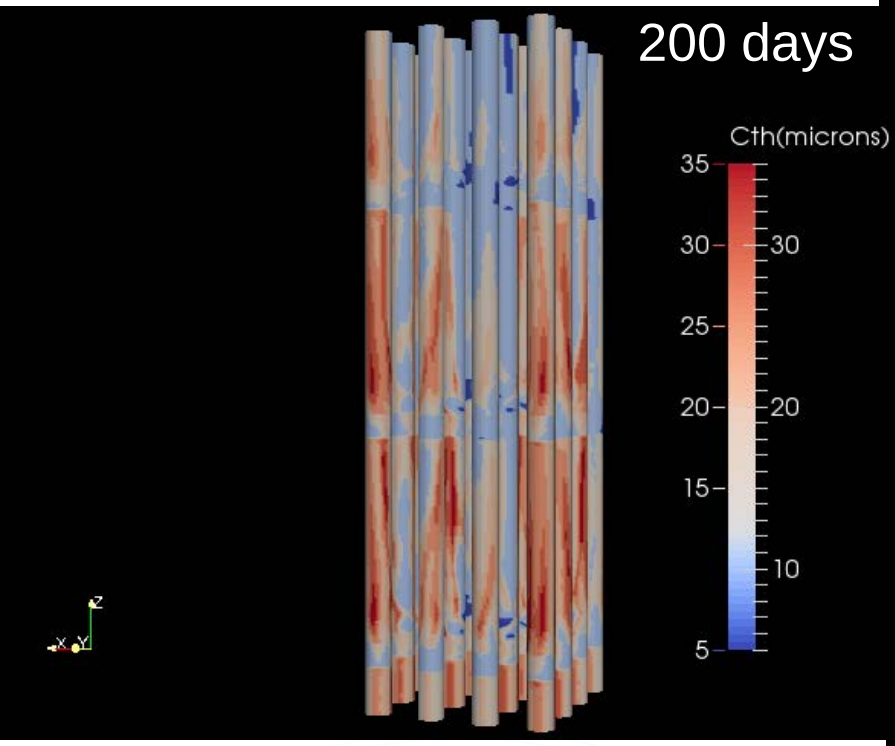
- Materials Performance & Optimization (MPO)
  - Crud: Enhanced thermodynamic understanding, thermochemical data base, & two-phase fluid flow in Crud & cladding oxidation models
  - PCI; Development, validation and benchmarking of fuel performance code (Peregrine) along with advanced viscoplastic self consistent cladding deformation model
  - GTRF: Cladding wear model development based upon experimental data & micro-scale modeling

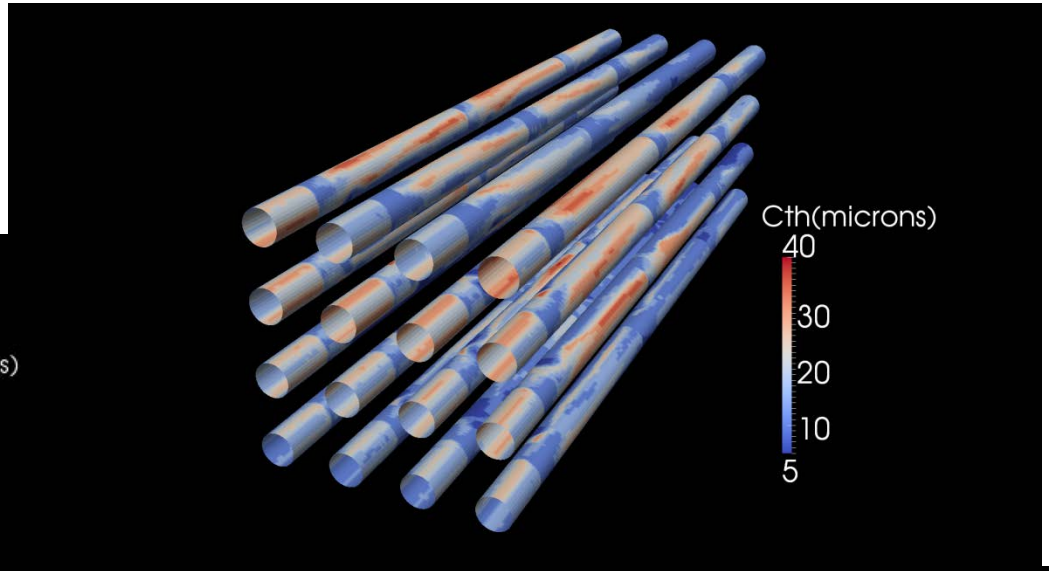


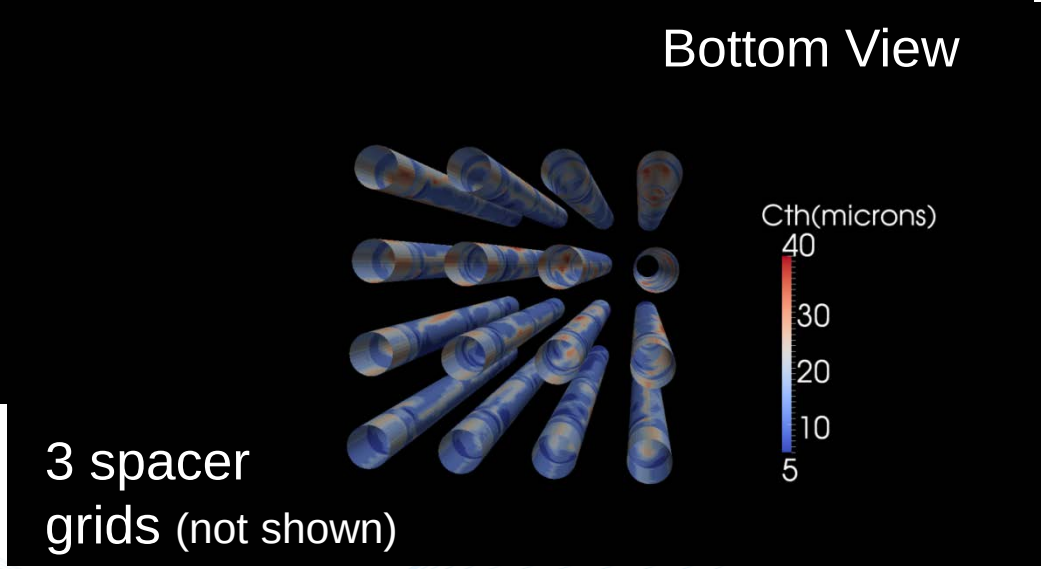
MAMBA & MAMBA-BDM: Crud Chemistry with Heat & Mass Transfer

- Attributes
  - Utilizes LANL ChemPac and INL Moose
  - 2D or 3D capability
  - Initial model parameters, e.g. Ni/Fe ratio, taken from the EPRI BOA code
  - Increased number of chemical reactions and associated reactants and products treated
  - Detailed models of physics, e.g. chimneys, crud porosity & structure, two-phase Darcy flow, solubility, & zirconium oxidation
- Current Activities
  - Continuing microscale modeling, e.g. DFT, to understand thermodynamics and chemical properties
  - Coupling to other physics in support of CIPS (sub-channel) & CILC (CFD)
  - Ongoing interactions with EPRI BOA activities

Crud: Initial high resolution crud simulations of a 4x4 subassembly using STAR-CCM+ / MAMBA (with fixed power)

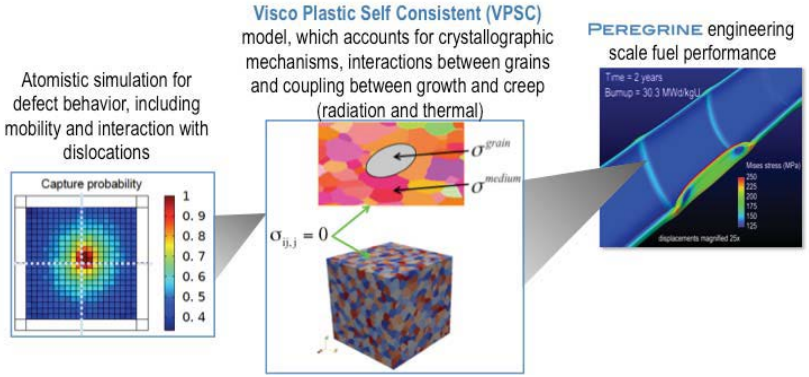






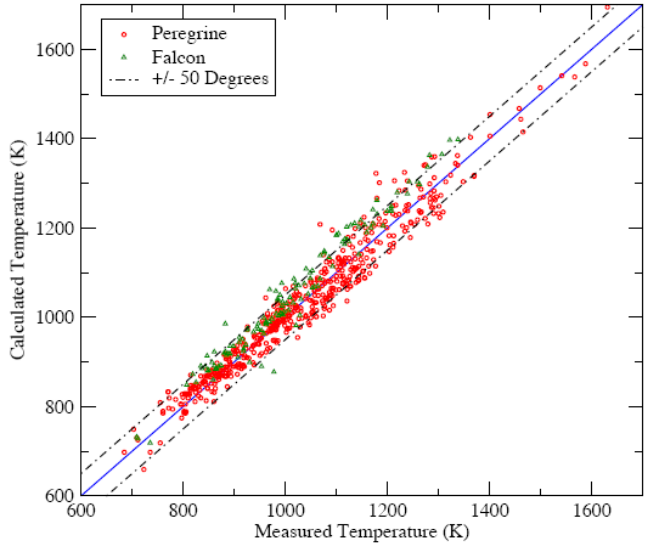
3 spacer grids (not shown)

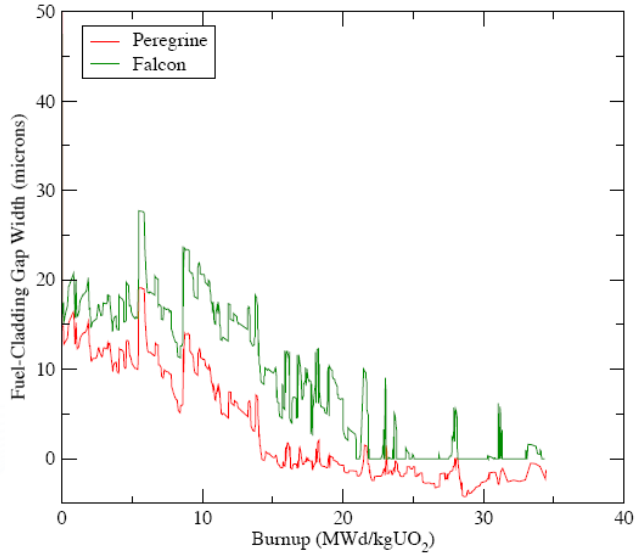
Peregrine: Fuel Performance (material, thermal & mechanical coupled behaviors)

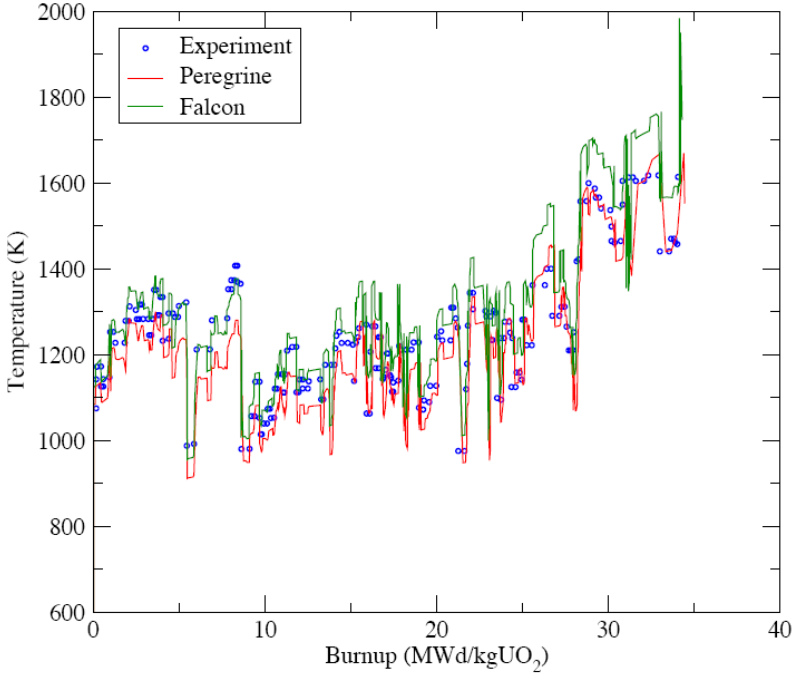


- Attributes
  - Built using INL Moose/Bison
  - 2D or 3D capabilities
  - For initial implementation borrowed physics models from EPRI FALCON fuel performance code
  - Continuous enhancements of physics models using micro/mesa scale modeling with CASL focus on zirconium based alloy cladding and NEAMS focus on UO2 pellet
- Current Activities
  - Development of viscoplastic self consistent model to address cladding deformation
  - Micro/meso scale modeling many phenomina, e.g. pellet cracking and relocation, fission gas retention and release, gap thermal conductance, pellet-clad mechanical contact (including improved advanced creep and growth models) and cladding oxidation and hydride formation and growth
  - Validation against experimental data & comparisons against FALCON predictions

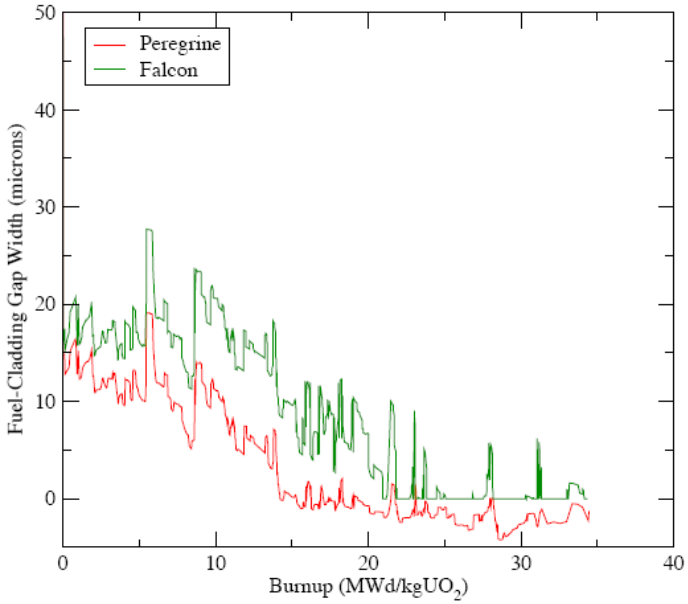
Peregrine predictions versus experimental data (Halden & Riso) & Falcon predictions

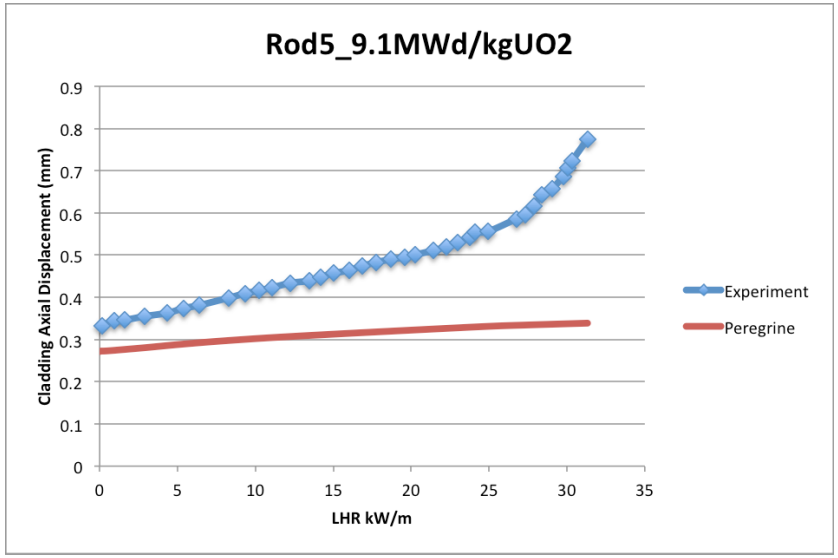


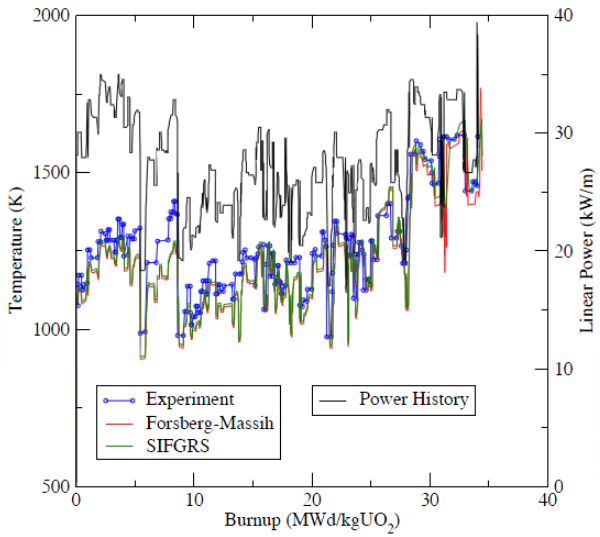


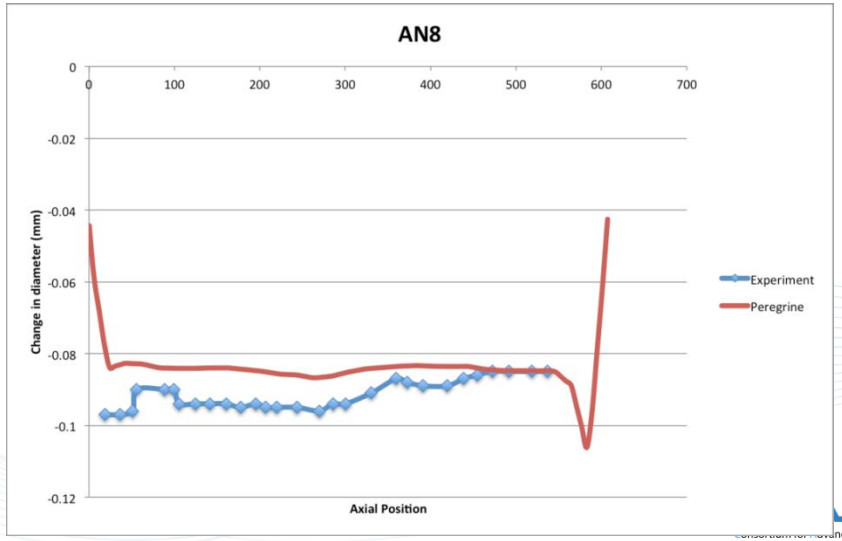


Peregrine predictions versus experimental data (Halden & Riso) & Falcon predictions









GTRF Related Developments

- Attributes Requiring Assessment
  - Fluid forces on fuel rods
  - Gap opening between fuel cladding – spacer grid support (spring & dimples) and associated material property changes
  - Fuel rod structural mechanics response
  - Cladding wear under spacer grids in a high velocity flow field
- Current Activities
  - Prediction of fluid forces on fuel rods (completed with Hydra-TH)
  - Assessment of appropriateness of utilizing beam model to capture fuel model structural response used to drive detailed fuel cladding – spacer grid support model to predict wear
  - Several projects on fretting wear model development and gap opening model

GTRF structural mechanics modeling – addressing wear

Full rod structural dynamic simulation

Input:

- CFD pressure load history
- Gap size (irradiation creep + wear) and/or preloads; 1-D contact stiffness
- Rod conditions: creep down;
- Grid conditions: growth;
- pellet/clad contacts; gaps

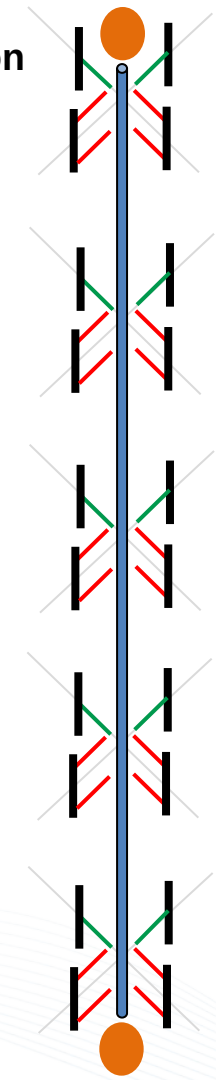
Output at discrete contact locations:

- History of contact forces, slip distances, work rates, etc.

Rod-model output:

Spatial distribution and history of

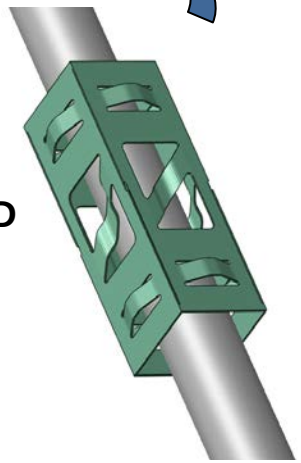
- Deflection, velocity, acceleration
- Rotation, rotational rate, angular acceleration
- Shear force, moment



Output:

- History of contact forces, slip distances, work rates, wear depths on 2-D contact domains;
- Enables updating of surface geometry based on evolving scar profiles; can be introduced as modifications of rod gap conditions for subsequent runs.

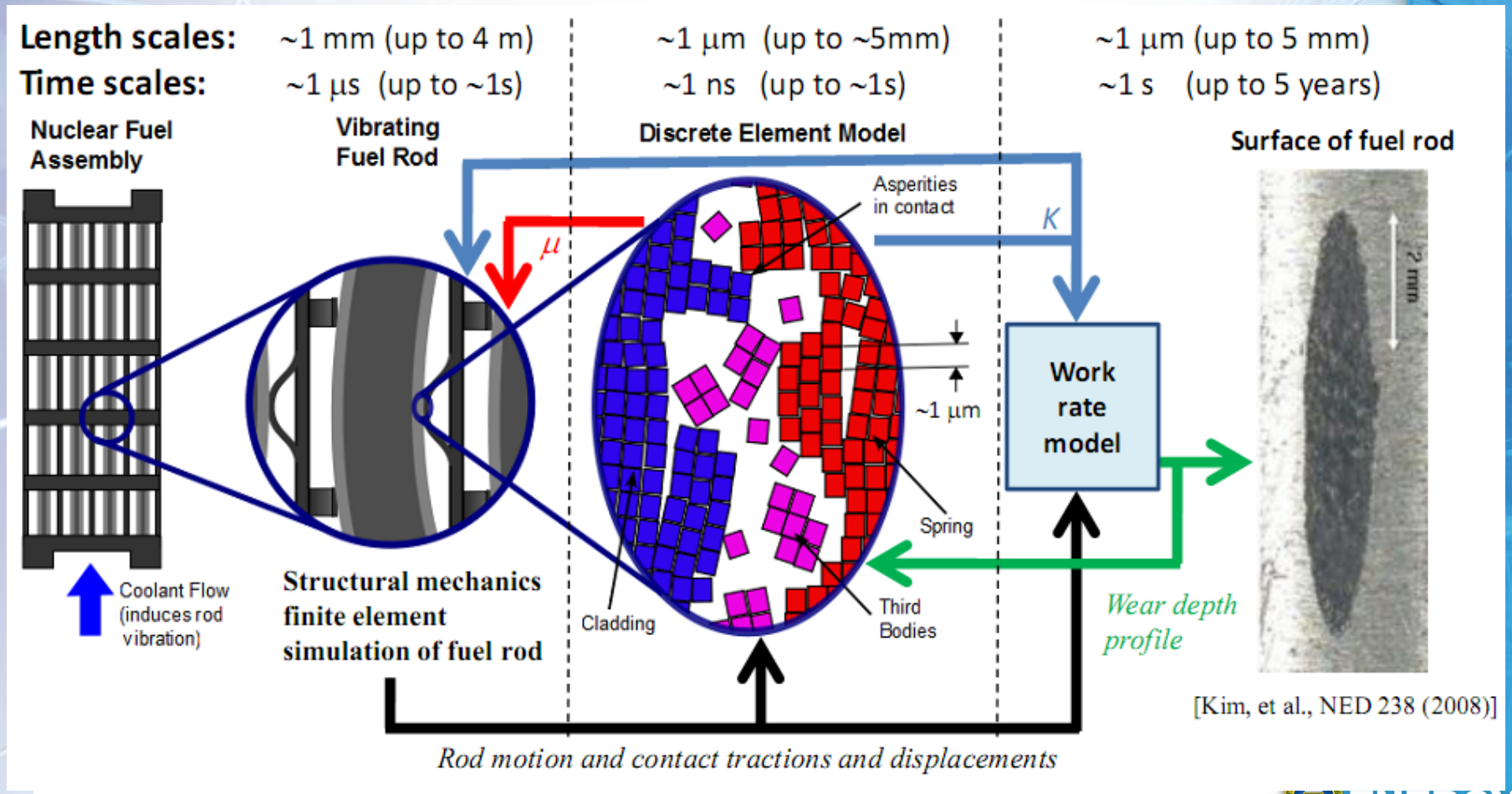
Single cell grid, 3D grid/rod contact interaction and wear



Input:

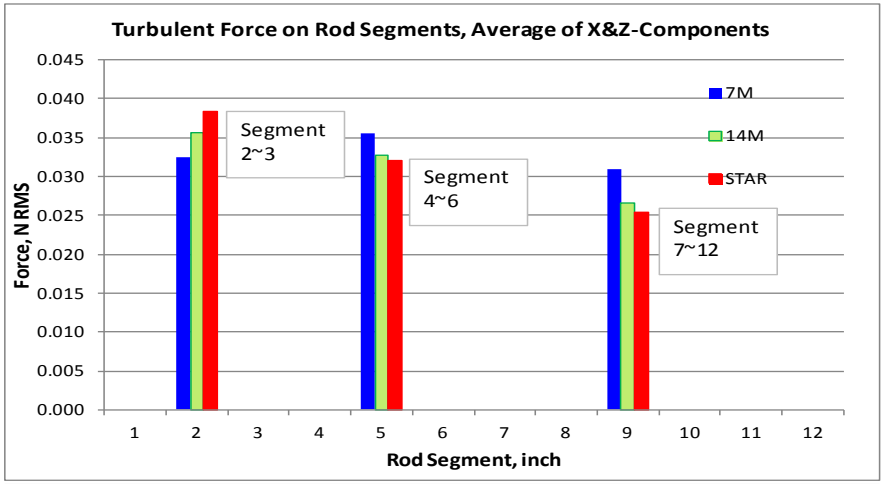
- Gap size (irradiation creep + wear) and/or preloads
- Initial wear depths
- Time variation of rod moment and/or rotation; transverse displacement or force

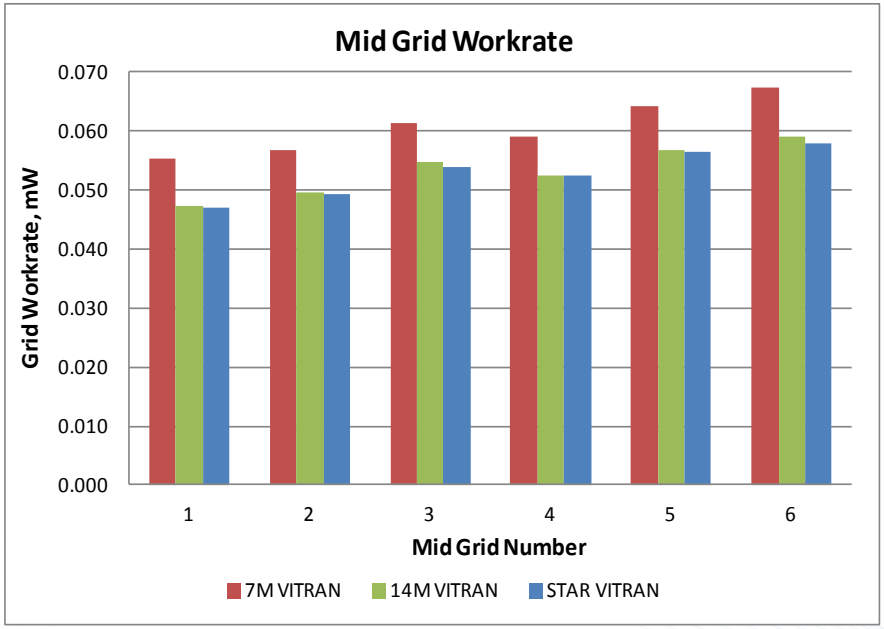
Summary of the CASL Team's Multi-Scale Modeling Approach to GTRF*

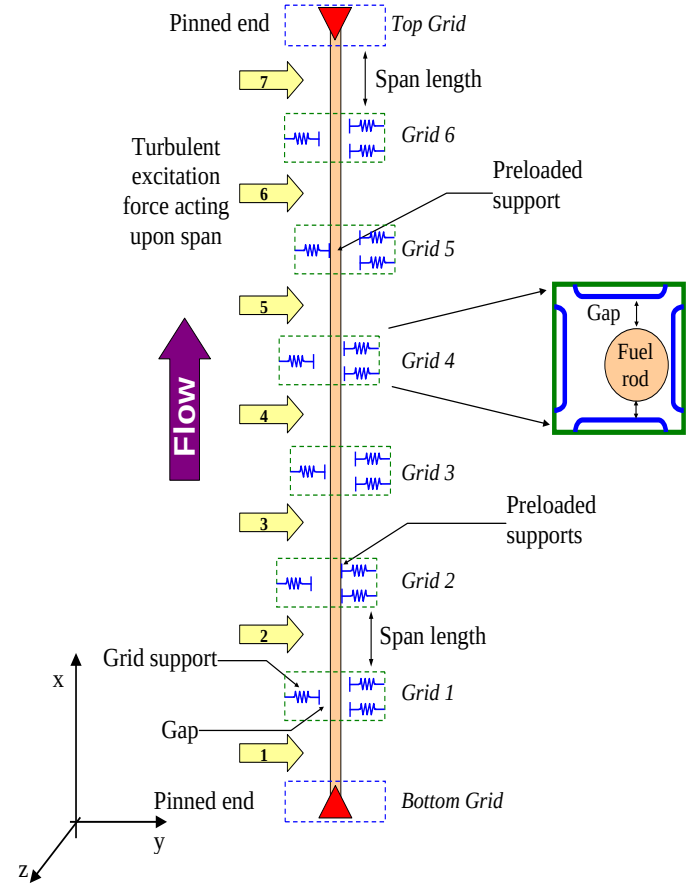


* Blau, Hayrapetian, and Demkowicz (2013) in ASTM STP 1563, in press.

GTRF: Coupling Computed Fluid Turbulent Forces to Fuel Rod Vibration Model



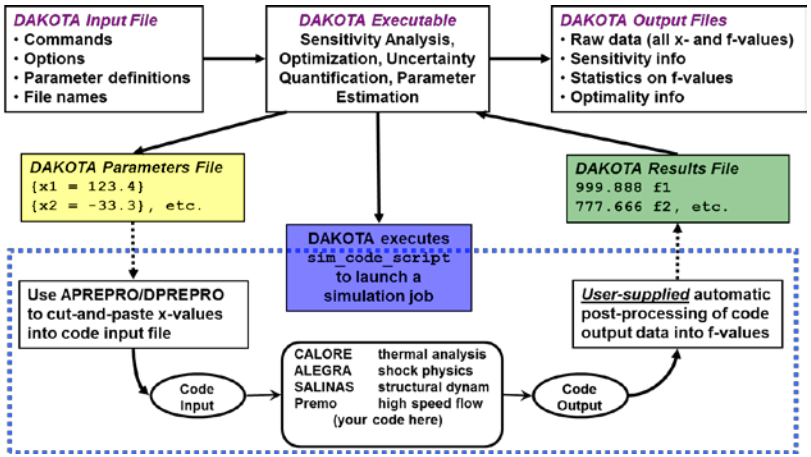




Grid	14M VITRAN	STAR VITRAN	Differences
1	0.04731	0.04691	-0.86%
2	0.04963	0.04917	-0.93%
3	0.05473	0.05392	-1.51%
4	0.05253	0.05246	-0.13%
5	0.05662	0.05659	-0.05%
6	0.05895	0.05797	-1.70%

S&T Program: FY13 Highlighted Accomplishments (to date)

- Validation & Uncertainty Quantification (VUQ)
  - Development and assessment of advanced MCMC methods for data assimilation
  - Verification of numerical discretization aspects for the large phase space associated with neutron transport models
  - Assessment of CASL codes' SQA and code verification practices, along with validation data needs



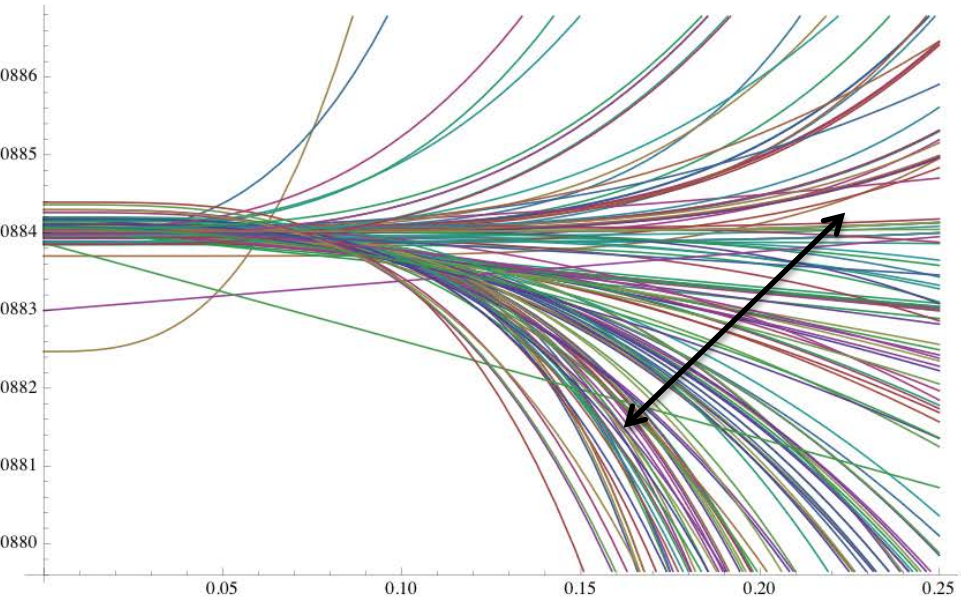
Loose coupling of DAKOTA to a generic application

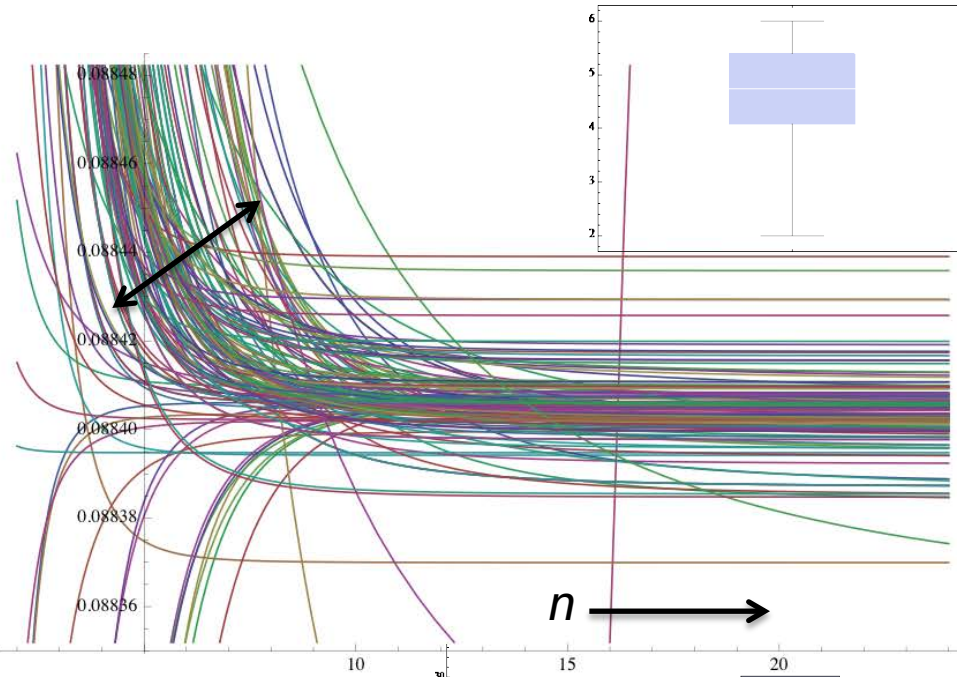
Dakota: Data Assimilation & Uncertainty Quantification

- Attributes
  - Builds upon existing SNL Dakota code
  - Nonintrusive approach 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
  - Integration into Dakota of capabilities that have been developed
  - Identification of validation data needs, availability and desired new experiments

Verification: Denovo (Sn) Downscatter Problem

- There are significant numbers of outliers. These are "ignored" effectively.

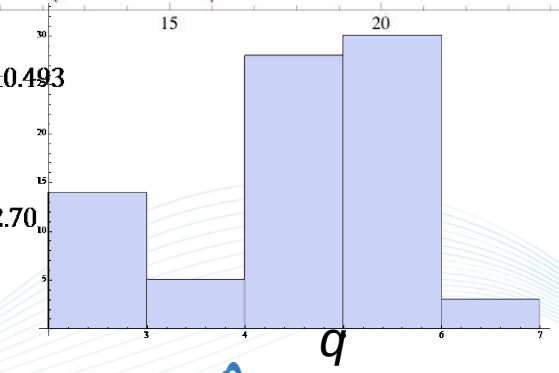




RMR space-angle LD+LS $\Phi = 0.0881292 \pm .000107 + Ah^{3.840\pm2.017} + B/n^{3.100\pm0.493}$

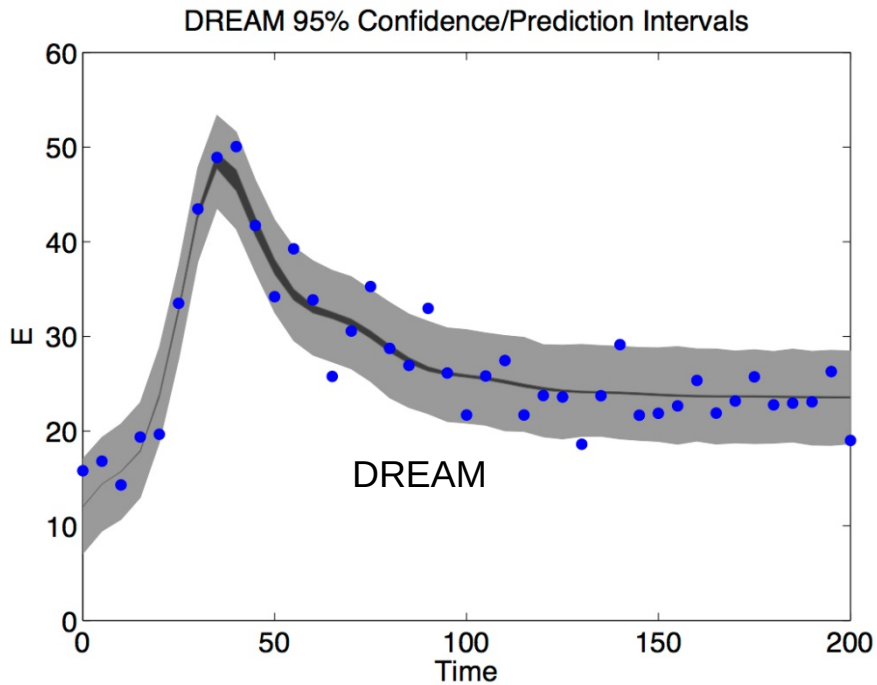
RMR angle for LDFE $\Phi = 0.0883713 \pm 0.0000002 + B/n^{4.985\pm2.70}$

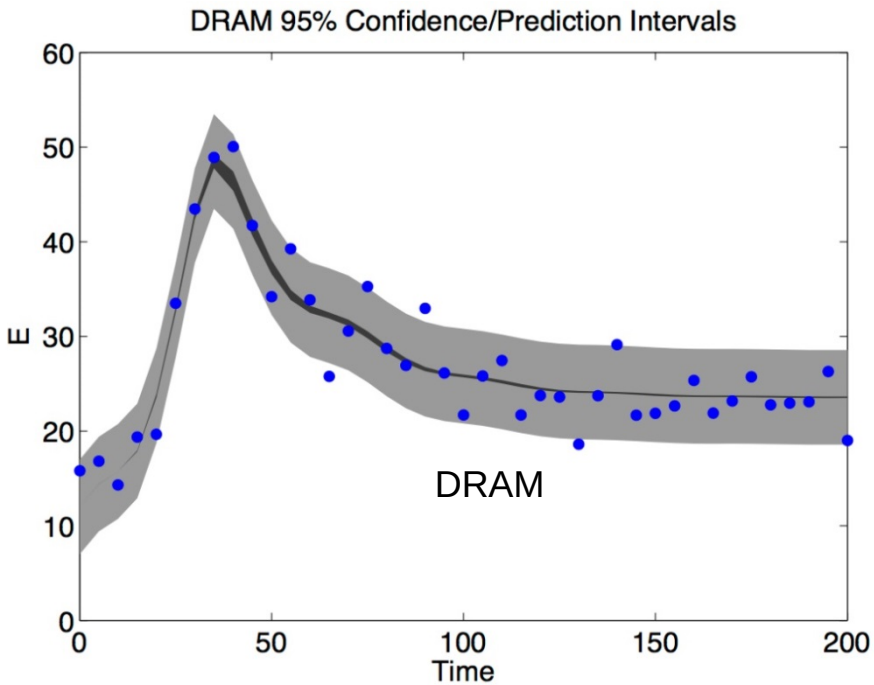
GCI angle for LDFE $\Phi = 0.088322 \pm 0.000148 + B/n^{10.825}$



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

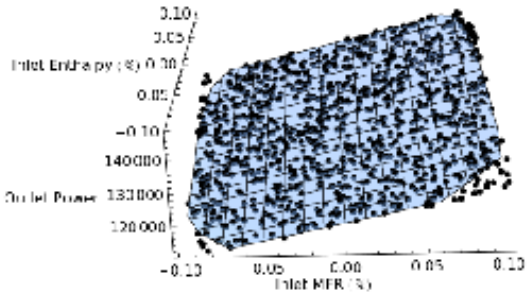
Test case with 16 parameters



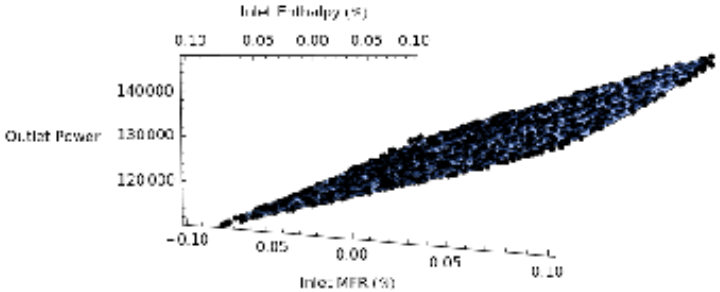


Application to the Cobra-TF code

First generate surrogate model (GP model)



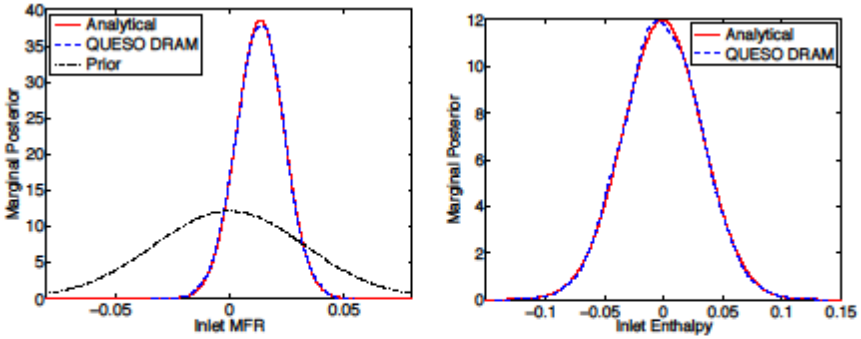
(a) Front View



(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

Survey of Component SQA & Verification Practices

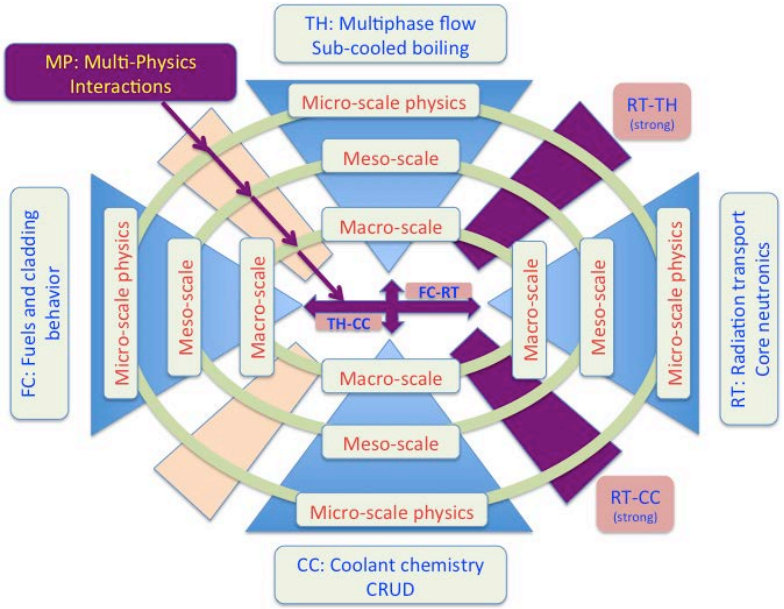
	COBRA-TF	Hydra-TH	Denovo	MPACT	Peregrine	MAMBA	MAMBA-BDM	DTK	Dakota
SQA Standard									
SQA Plan									
Life cycle									
Requirements									
Design									
Code standards									
Code reviews									
Configuration control									
Automated builds									
Unit testing									
Regression testing									
Test reporting									
Test coverage									
Defect tracking									
User manual									
Installation manual									
Developers manual									
Tutorials/examples									
Release management									
Theory manual									
Numerical analysis									
Verification problems									
Formal code verification									

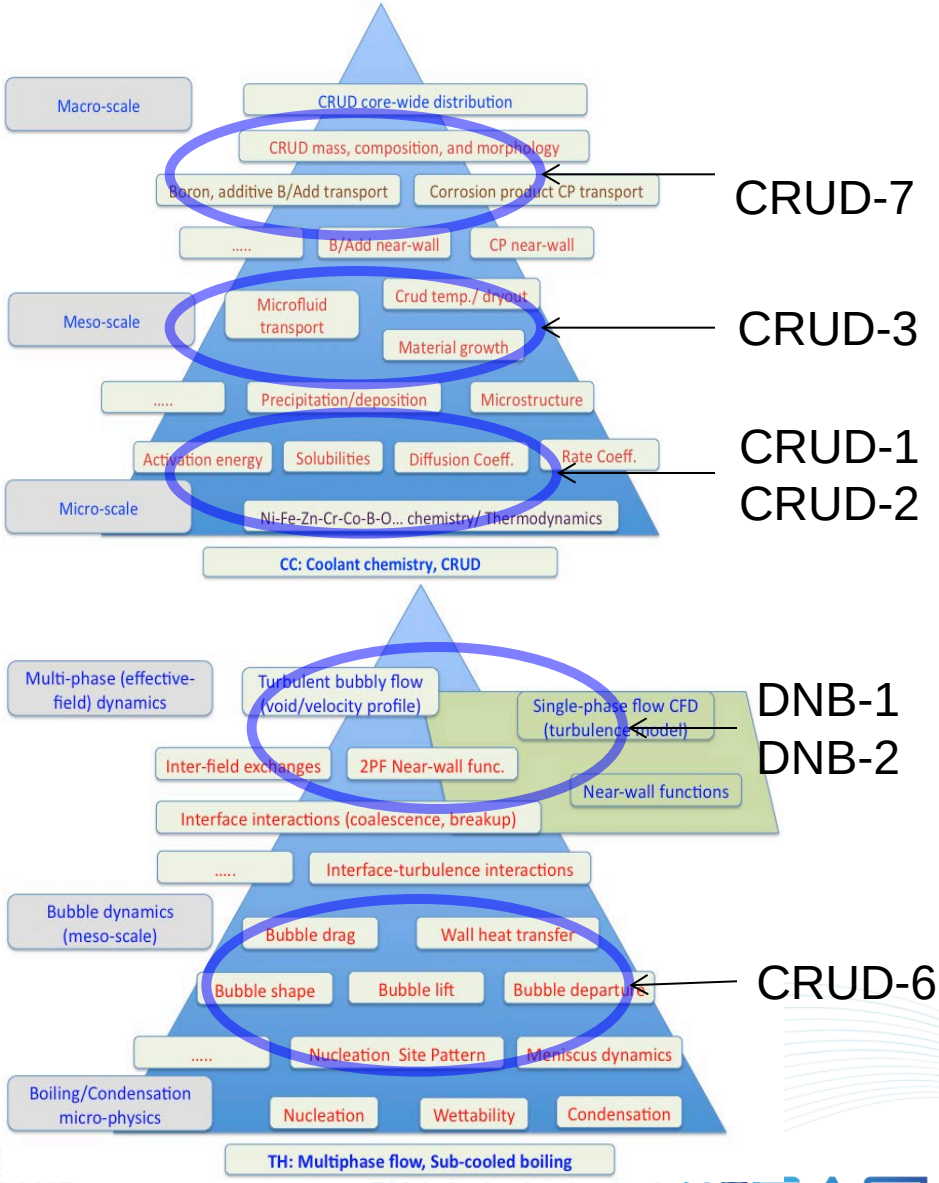
Needs Work

Opportunities for Improvement

Acceptable

Validation Data: CRUD Multi-Physics, Multi-Scale Pyramid

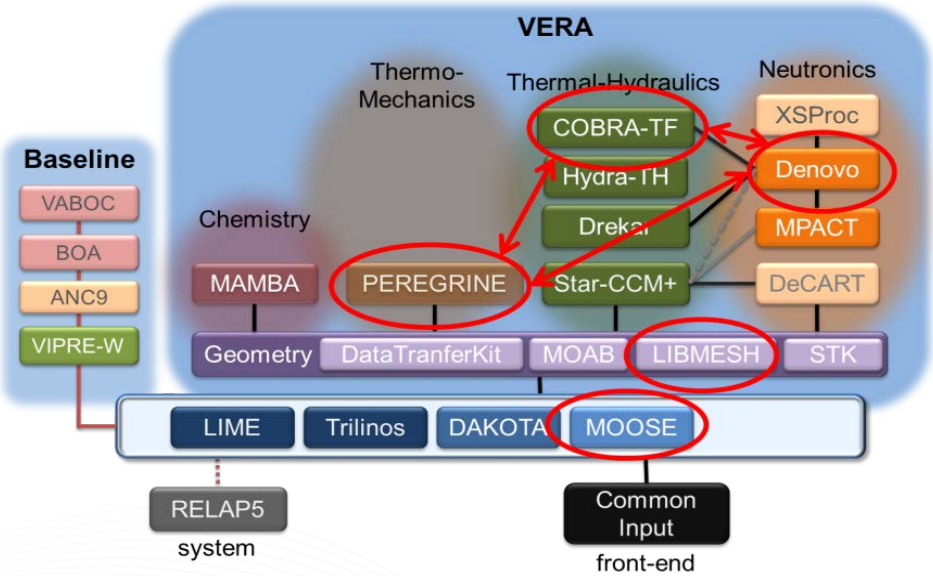




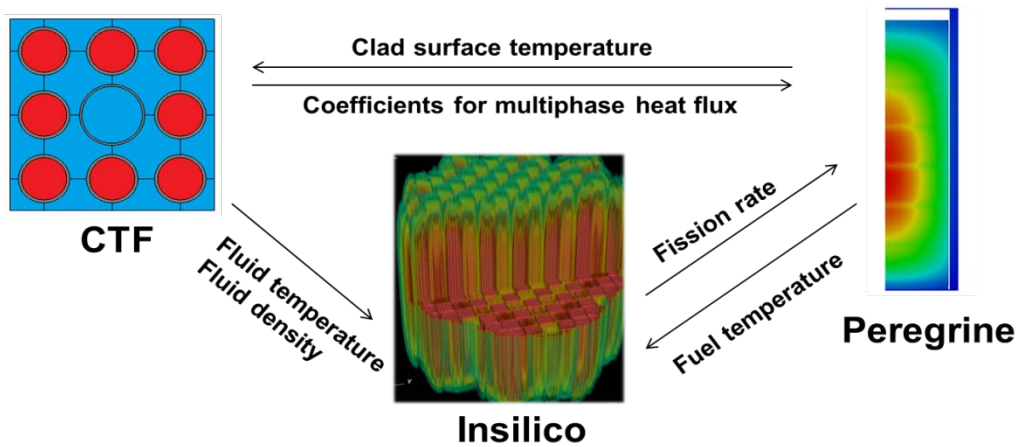
To be presented during working lunch

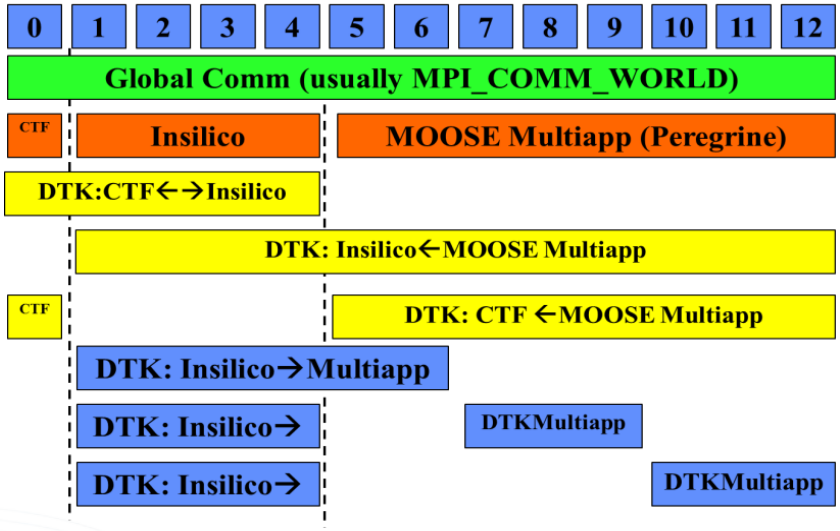
S&T Program: FY13 Highlighted Accomplishments (to date)

- Virtual Reactor Integration (VRI) *[now Physics Integration (PHI)]*
  - Development of parallel data transfer capability for multi-processor/multi-core architectures (DTK)
  - Multiphysics integration of Neutronics (Insilico SPn)-Fluids (Cobra-TF)-Fuel Performance (Peregrine) = VERA-CS



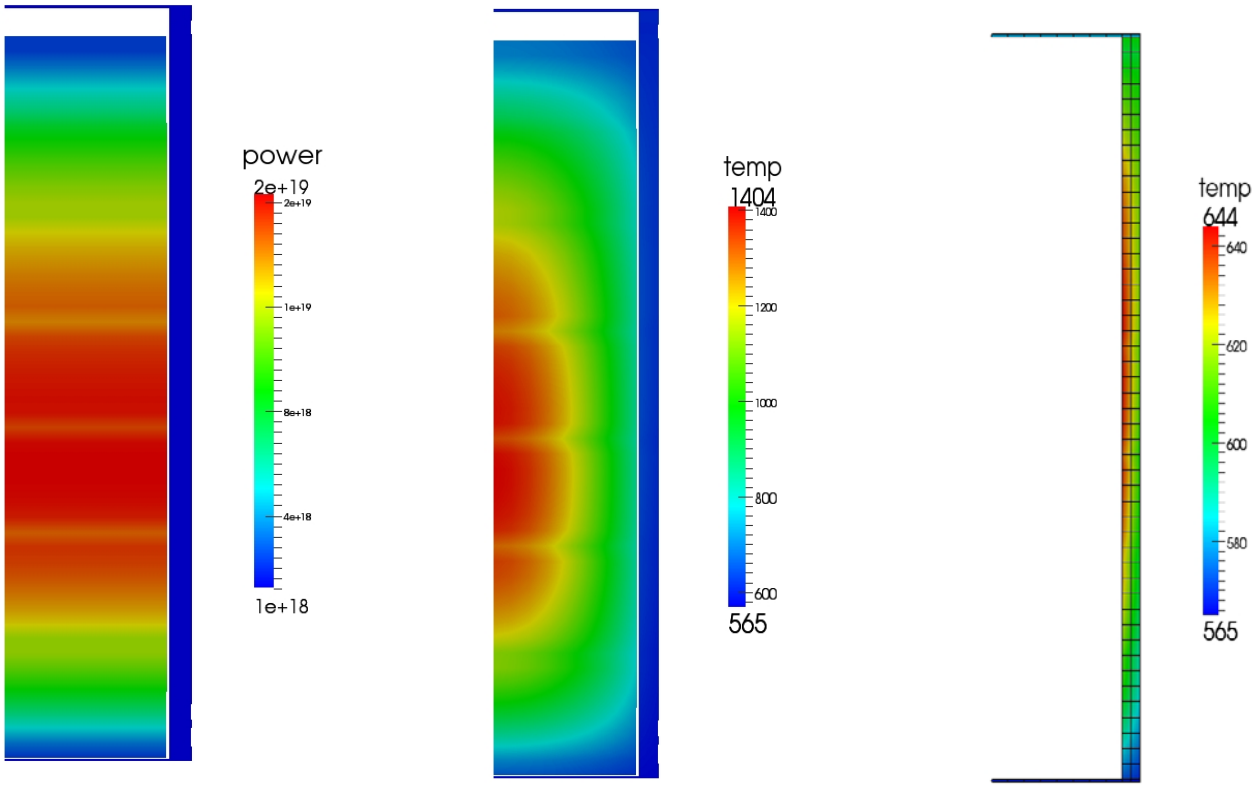
Progression toward VERA-CS multiphysics capability





Using DTK in support of multiphysics integration

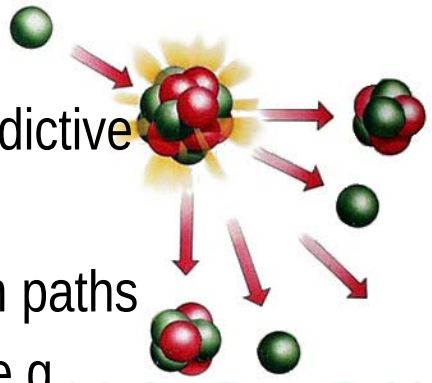
VERA Integration: Application to a single fuel assembly



Much remains to be improved upon regarding computational efficiency

Technical Items Likely To Prove Challenging to Address (under time & budget constraints)

- RTM: Full-core, pin-resolved radiation transport using deterministic approach with acceptable wall times
- THM: ~~Multiphase turbulence modeling and closure relationships selection, generation and validation~~; DNS/ITM bubble nucleation, coalescence and condensation
- VRI: “Tight” multiphysics coupling development; different physics time scales; software complexity & usability, structural mechanics
- VUQ: Multiphysics & multiscale uncertainty quantification (particularly epistemic errors) and data assimilation
- MPO: Predictive (minimum free tuning parameters) CRUD predictive capability; microscale informed macroscale
- AMA + Other FAs: Meshing complex geometries; CPs’ solution paths that are realizable within computational resource capabilities, e.g. clock time

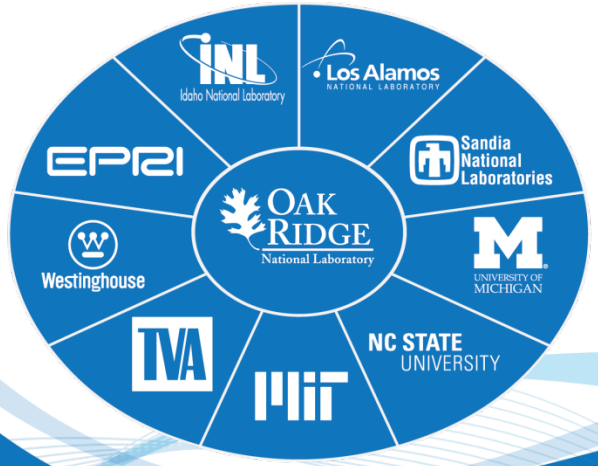


Plans to address range from under development to firm

Challenge Problem (CP) Status

Zeses Karoutas (WEC), Overall CP Product Integrator

CASL Industry Council Meeting
Oak Ridge National Laboratory
September 10-11, 2013



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

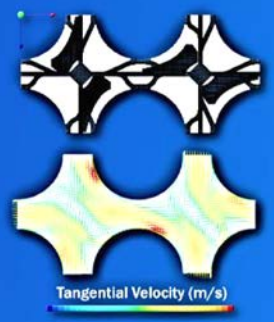
Outline

- CASL Challenge Problems
- Challenge Problem Integrators (CPIs)
- CASL VERA Tools
- High Level CASL Plan to Address Challenge Problems
- Discussion of Charters/Plans/Solutions
- Overall Status

CASL Challenge Problems

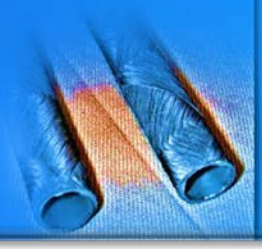
Key operational & safety relevant reactor phenomena that limit performance

Departure from Nucleate Boiling

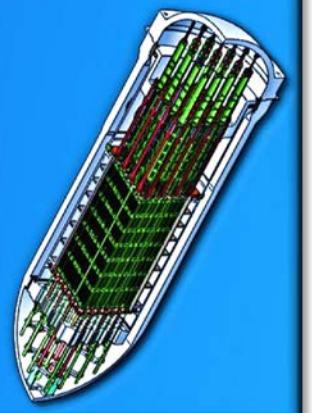


Cladding Integrity

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



Reactor Vessel and Internals Integrity

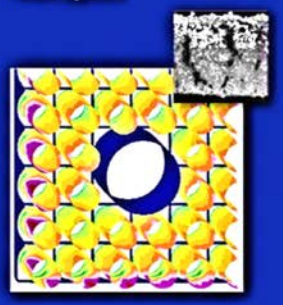


CASL is committed to delivering simulation capabilities for

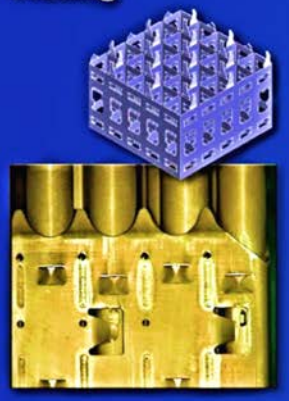
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

Crud

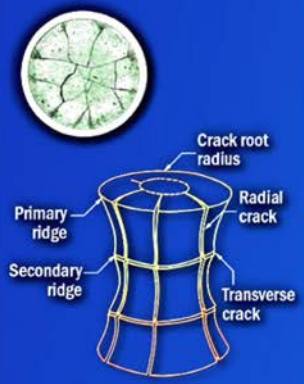
- Deposition
- Axial offset anomaly
- Hot spots



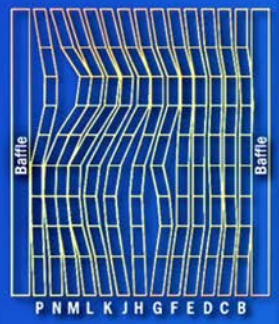
Grid-to-Rod Fretting



Pellet-Clad Interaction



Fuel Assembly Distortion



CASL Challenge Problems

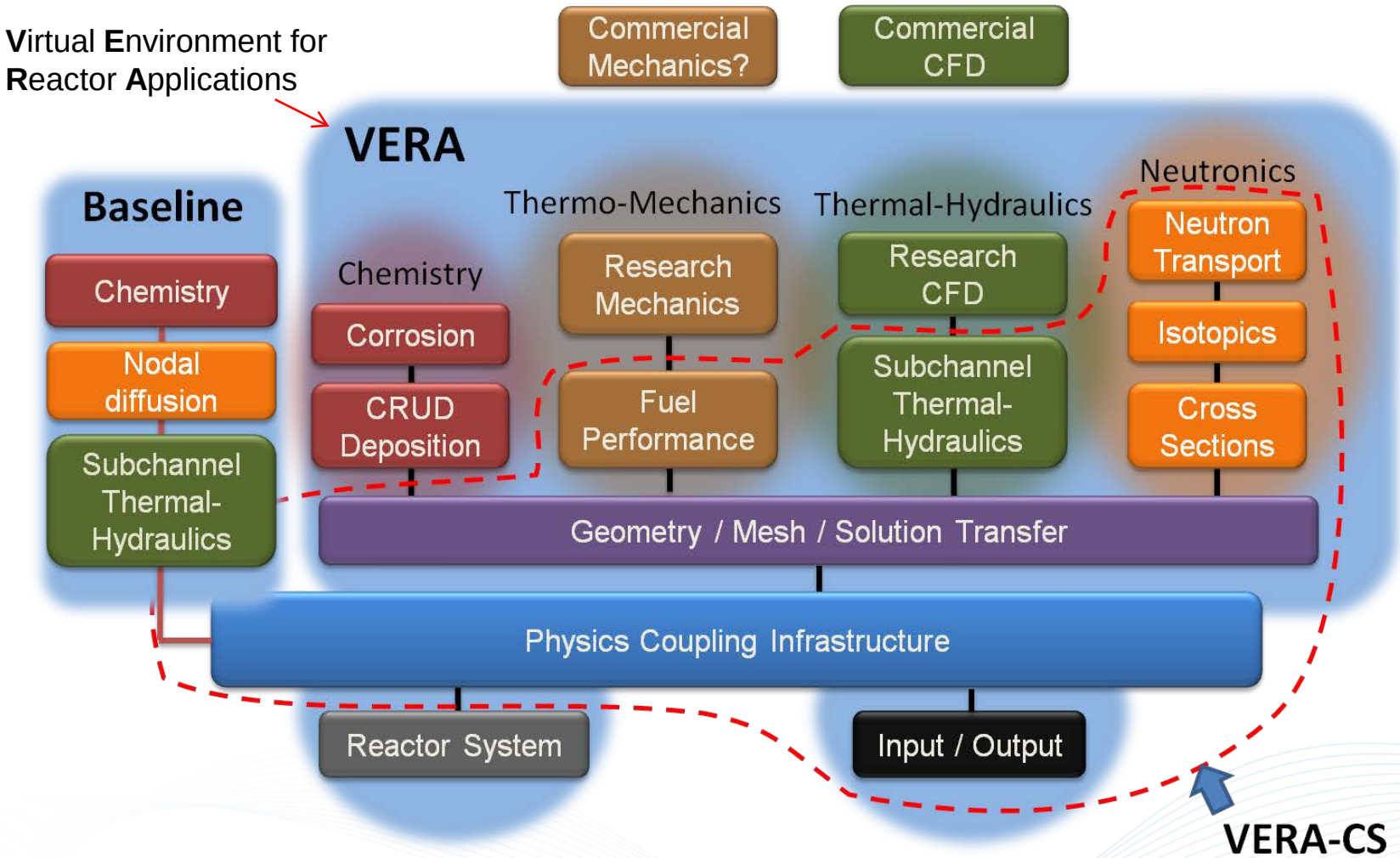
		Power uprate	High burnup	Life extension
Operational				
CRUD-induced power shift (CIPS)	J. Secker	✕	✕	
CRUD-induced localized corrosion (CILC)	J. Secker	✕	✕	
Grid-to-rod fretting failure (GTRF)	K. Yueh/TBD		✕	
Pellet-clad interaction (PCI)	R. Montgomery	✕	✕	
Fuel assembly distortion (FAD)	Future	✕	✕	
Safety				
Departure from nucleate boiling (DNB)	Y. Sung	✕		
Cladding integrity during (LOCA)	G. Swindlehurst	✕	✕	
Cladding integrity during (RIA)	G. Swindlehurst	✕	✕	
Reactor vessel integrity	LWRS	✕		✕
Reactor internals integrity	LWRS	✕		✕

Product Integrators Defined for Each Challenge Problem with Charters & Implementation Plans

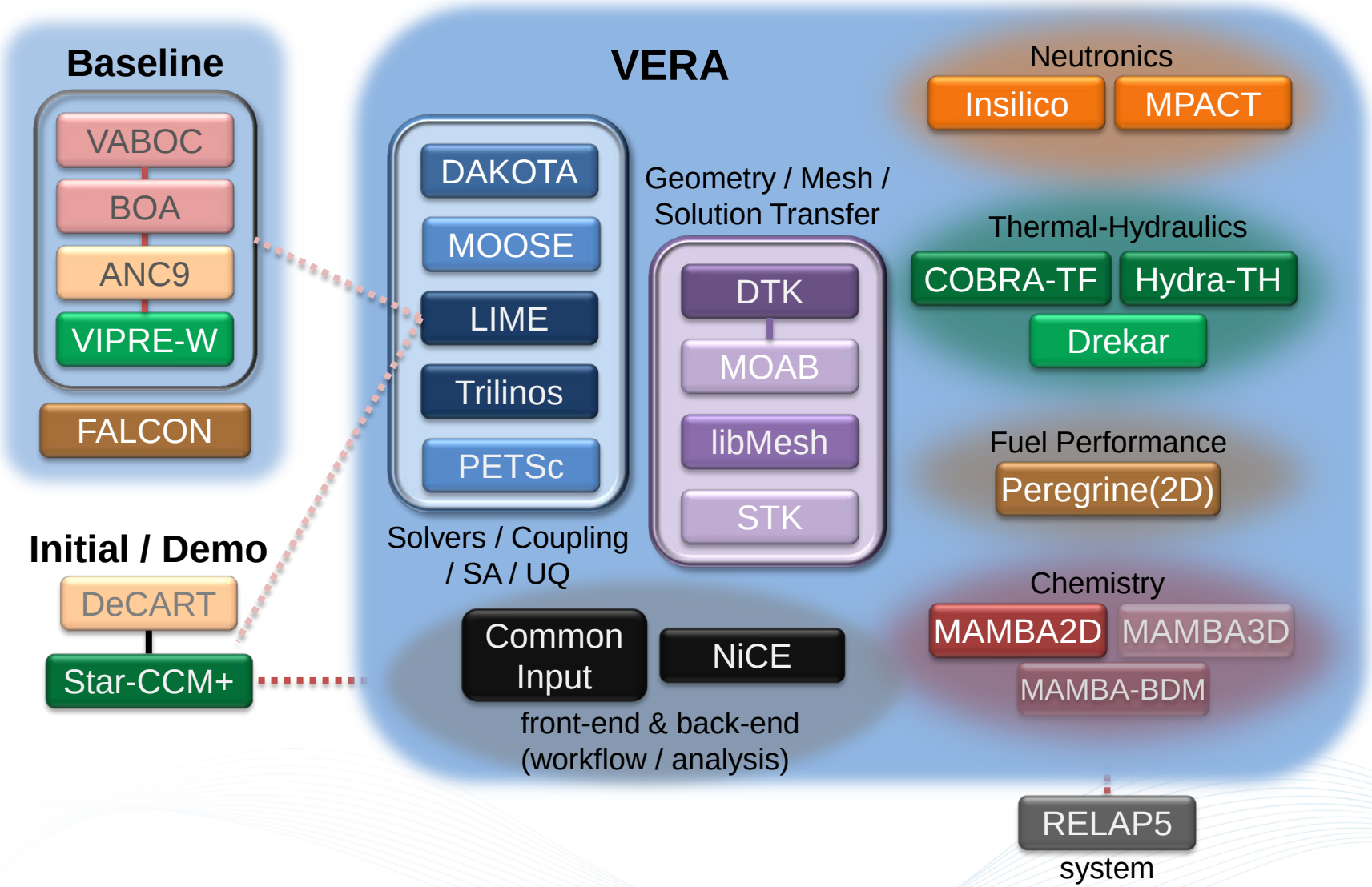
Challenge Problem Integrators

- Introduce Product Integrators over a year ago to work across FAs to assure challenge problems are addressed
- Responsibilities include driving critical applications, products, & outcomes that cross FA boundaries
- Each Product Integrator prepare a charter and implementation plan for Challenge Problem
- Define minimum, acceptable and ultimate end game levels of success
- Complete charters and implementation plans this fiscal year and make brief presentation at DOE annual review
- Complete overall Challenge Problem Integrator report including charter and implementation plans in this fiscal year

CASL VERA Tools



VERA 3.1 snapshot (07/2013)



High Level CASL Plan to Address Challenge Problems

PCI*

- Predict Core Wide PCI Margin with **PEREGRINE2D** - Plant data
- Zoom in and Predict MPS PCI leaker with **PEREGRINE3D** -Hot Cell, Halden, & Plant data

CRUD*

- **CIPS:** Predict Boron Uptake with **MAMBA2D** -Plant CIPS data
- **CILC**: Predict Crud thk & corrosion with **MAMBA3D** use STAR/HYDRA-TH single phase heat transfer multipliers -WALT loop,& Seabrook CILC data

VERA-CS*

Insilico-MPACT/ COBRA-TF/PEREGRINE
(full depletion for all rods in core)
Watts Bar 1 Physics Data, etc

RIA*

• Predict PCMI Margin using **PEREGRINE2D** –CABRI & NSRR data, Apply to Reactor core

LOCA*

•Predict PCT – Oxidation Margin using **PEREGRINE2D** & System Code **RELAP5** –FLECHT,APEX, Halden, Studsvik Data, Apply to Reactor Core

DNB*

- Predict DNB Margin for RIA – Apply to Core
- Predict Mixing & DNB with CFD using **STAR/HYDRA-TH** 1 and 2 phase flow - PIV,LDV, boiling, T/C mixing & DNB data

GTRF*

- Predict Minimum GTRF Margin in Core using **PEREGRINE2D** –gap, **STAR/HYDRA-TH**-excitation force, **BEAM** tool –vibration/wear –PIV, LDV, Vibration, Wear, Plant PIE wear data

*** For Each Challenge Problem Apply DAKOTA using Coupled Tools for UQ**

Challenge Problems – Charters/Plans/Solutions

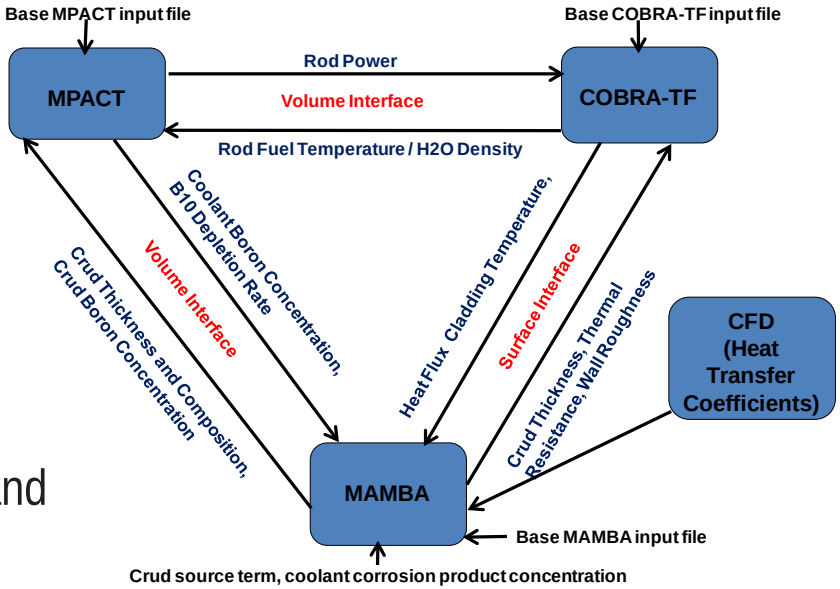
Responsibilities of CP Product Integrator

- For each CP prepare a charter
  - Description of CP to be solved
  - Current industry practice
  - Desired industry path forward
  - Definition of success (minimal, acceptable, end game)
- For each CP prepare an implementation plan
  - Simulation capabilities required (focus area interactions)
  - Simulation applications
  - Validation data and qualification data availability
  - Development plan & associated schedule (role in planning, tracking, reviewing)
  - Risks
- Summarize Solutions
  - Compare with current state in industry (particularly regarding uncertainties)
- Expected accomplishments by Aug 2014

CRUD - Definition of Success

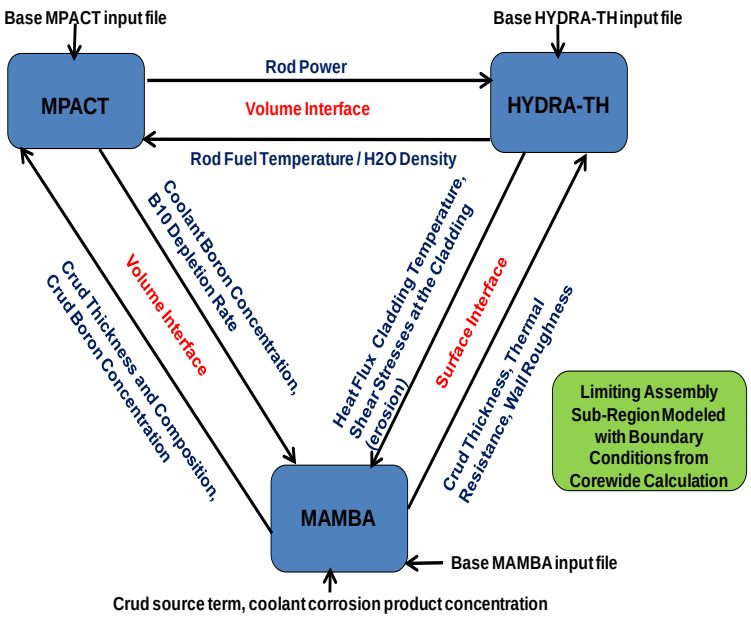
- Minimal – Couple current industry codes
- Acceptable – Implement higher fidelity CASL neutronics and T-H models and extend crud models to 3D, couple codes, calibrate and assess compared to available crud validation data; Use advanced linked codes to improve current industry codes/methods
- Ultimate end game – Accurately predict CIPS and CILC risk for actual cores. Use the detailed understanding of the phenomena gained from implementation of the advanced models to develop technology to reduce or prevent crud deposition on fuel
- Planned level of achievement – Achieve "Acceptable" level after the first 5 years of CASL, with the exception of improving prediction of crud source term (outside of Phase 1 CASL scope (outside of vessel)

Model Needs for CIPS



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

Model Needs for CILC



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

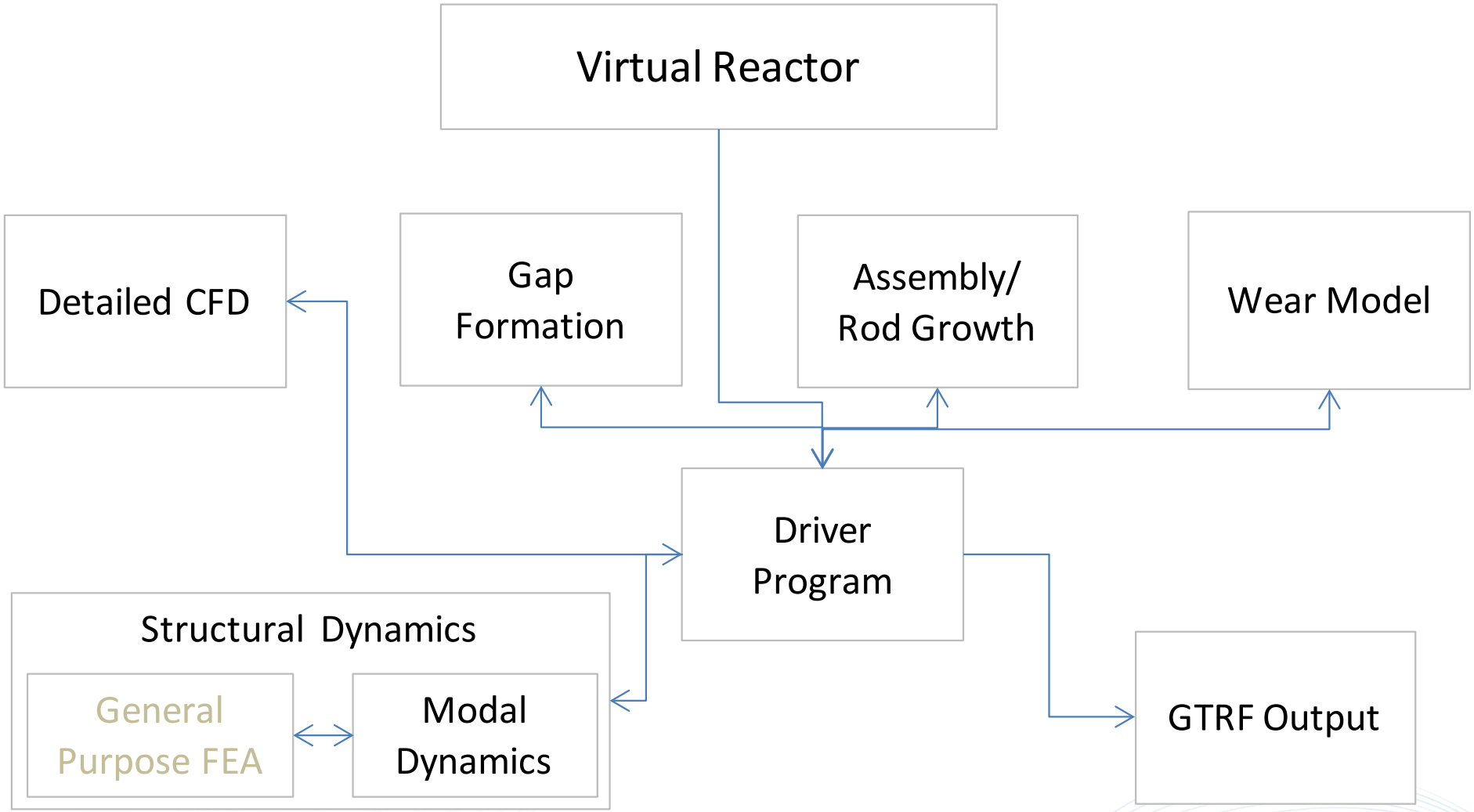
Crud Modeling Summary

- Crud charter and implementation plan issued
- Baseline tools (ANC/VIPRE-W/BOA) successfully coupled
  - Multiple cycles of Watts Bar, Vogtle modeled (quarter core, 3D)
  - Results demonstrate the importance of boron feedback
- Advanced crud model development (MAMBA, MAMBA-BDM) and application continues
- Initial coupling of advanced models completed
  - DeCART/STAR-CCM+/MAMBA applied to single rod
  - STAR-CCM+/MAMBA applied to 4x4 rod array
  - Move to MPACT/HYDRA/MAMBA and MPACT/COBRA/MAMBA next
- 2013 milestones
  - Application of advanced tools for crud deposition on PWR rods with CIPS/CILC
  - Model Seabrook Cycle 5, compare sub-channel to CFD based T-H
- 2014 plans – couple MPACT/COBRA-TF/MAMBA and MPACT/HYDRA-TH/MAMBA and apply to Watts Bar/Vogtle

GTRF - Definition of Success

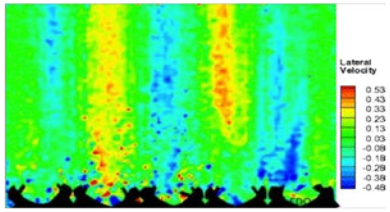
- Minimum level
  - Standalone calibrated physical models and GTRF modules
- Acceptable Level
  - Integrated use of modules to demonstrate predictive capabilities of package
  - Individual elements are being utilized by the industry but integration bring capability to beyond the current state
- Ultimate End Game Level
  - Fully integrated and automated software
    - Offer input flexibility to cover major plant design features
    - Full core 3D thermal-hydraulics
- Planned Level of Achievement by 2014
  - Physical models and key modules with partial integration

Development Plan – Modular Approach

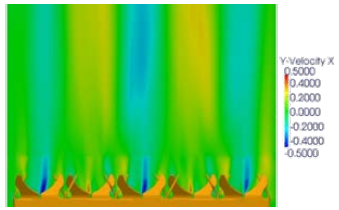


GTRF Summary

- GTRF charter issued (CASL-U-2013-0151-000) and implementation plan of core modules defined
  - Inclusion of secondary effects being considered



Texas A&M experiments

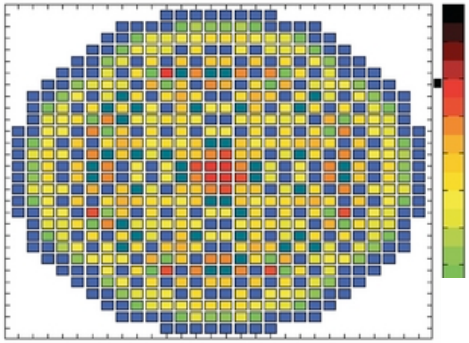


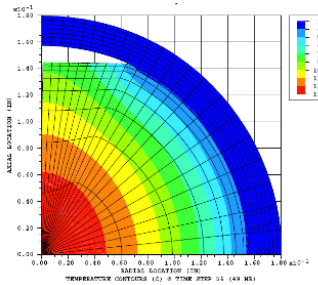
Hydra-TH calculations

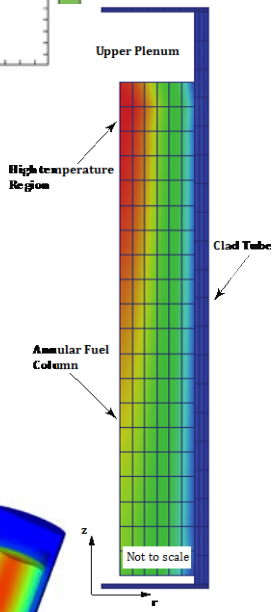
- Progress are being made in key areas
  - Material physical models for in-core performance - lacking calibration data
  - Hydraulic simulation strategy – results consistent with experimental
  - Evaluate structural dynamic approaches – two methodologies being evaluated
- Need for further experimental data for model calibration and validation

PCI - Definition of Success

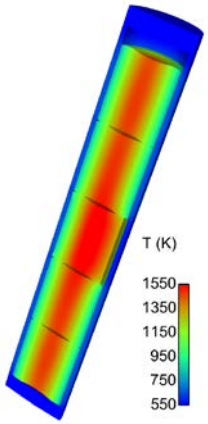
- **Minimal:** Use coupled neutronics/thermal-hydraulics/fuel performance to calculate axi-symmetric cladding stress distribution throughout the core.
  - Compare to empirical failure threshold stress (e.g. XEDOR/Powerplex)







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

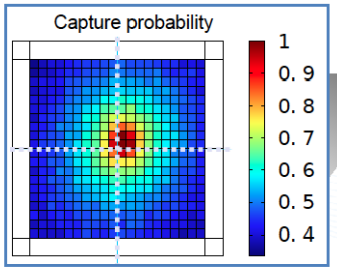


Goal: Methodology for PCI Failure Probability Assessment

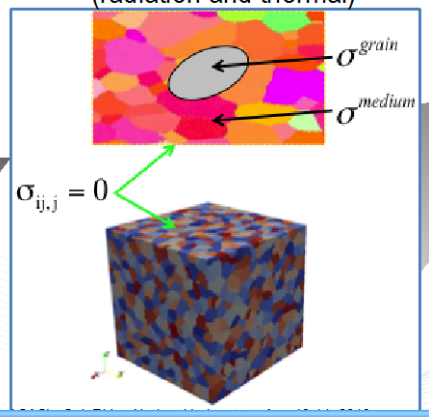
PCI - Measures of Success (con't)

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

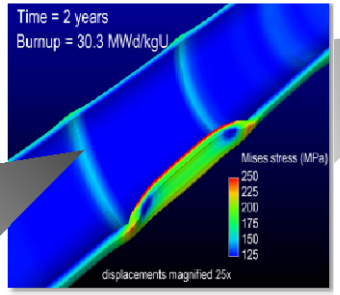
Atomistic simulation for defect behavior, including mobility and interaction with dislocations

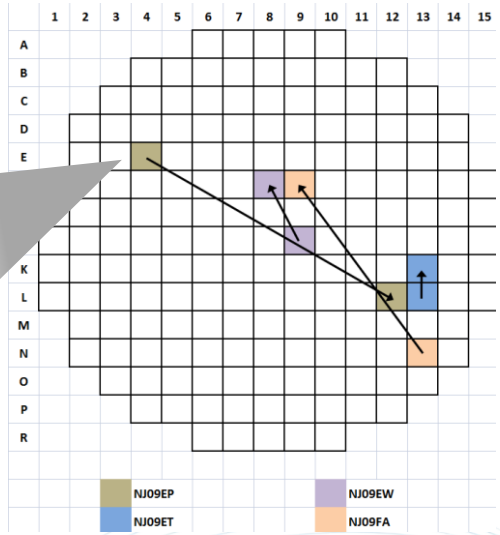


Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)



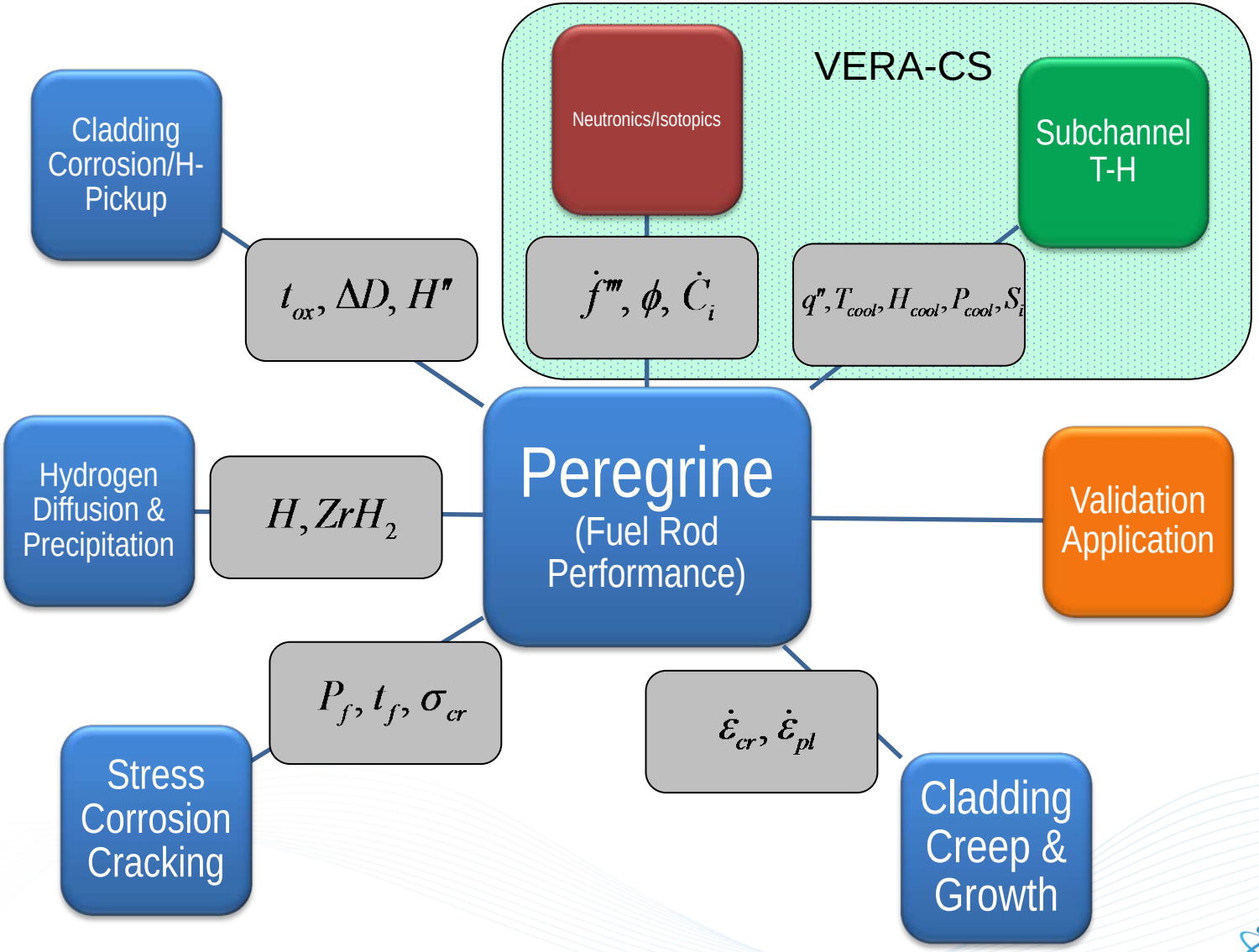
Peregrine engineering scale fuel performance



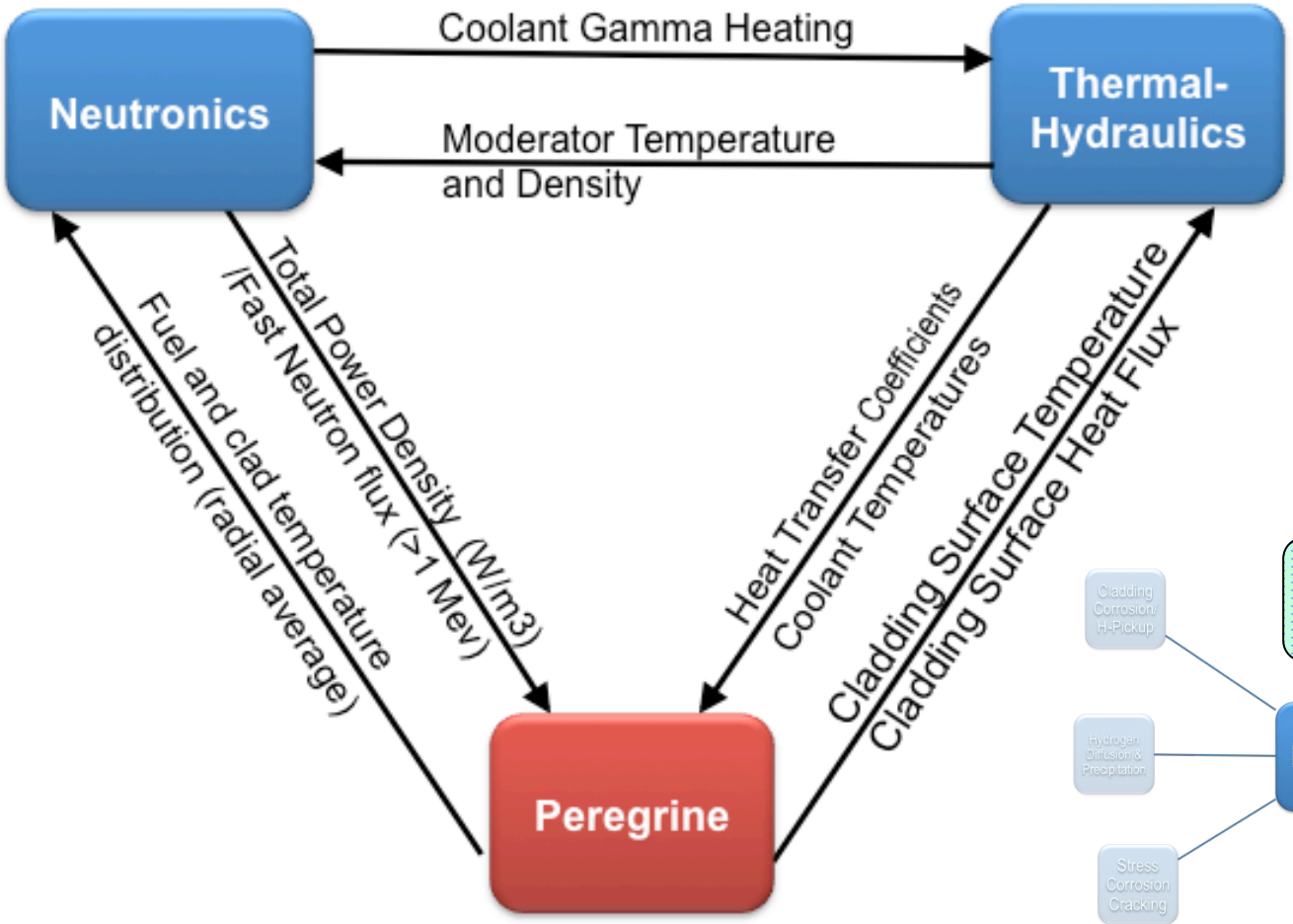


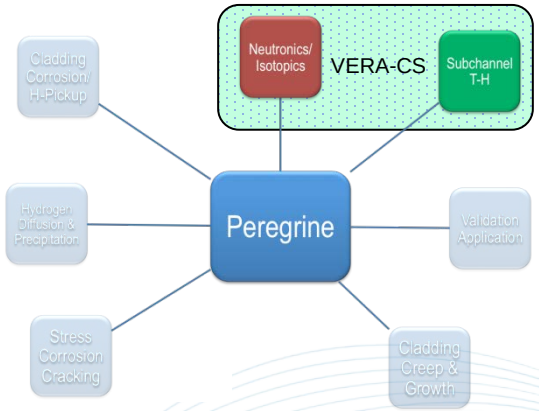
Challenge will be sufficient validation

Peregrine Interface with other MPO (blue) and Virtual Reactor Activities



Interfaces to couple Peregrine with Neutronics and Thermal-Hydraulics (VERA-CS)





First Steps to Assembly and Core-Wide Fuel Performance Calculations

PCI Modeling Summary

- Axisymmetric core-wide stress calculation – early 2014
  - Coupled neutronics (pin resolved powers), thermal-hydraulics and fuel performance with depletion and xenon effects
- Local stress calculation – mid 2014
  - 3-D cracked pellet simulation with mechanistic cladding creep and fission product interaction
- Integrated methodology – late 2014
  - Core wide to pellet scale simulation with failure assessment

Aggressive Schedule to Achieve Impact

DNB - Definition of Success

- **Minimum:** Subchannel and CFD modeling and simulation (M&S) with VUQ enhancement on data analysis to improve fuel design and existing codes for DNB analysis

- **Desirable:** High fidelity M&S with VUQ enhancement for fuel design optimization and margin quantification to DNB prevention

- **Ultimate End Game:** Integrated multi-physics and science based M&S of higher fidelity and VUQ capabilities as the new industry standard for LWR fuel thermal failure prevention

Acceptable Levels and Goal Defined

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

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

- Safety margin quantification in accident analysis
  - Multi-scale and multi-physics M&S capabilities
  - Technical basis for DNB-related fuel failure (e.g., DNB during Reactivity Insertion Accident (RIA))
  - Control and optimization of fuel cladding surface morphology and properties during reactor operation

M&S for Fuel Design and Safety Analysis

DNB Challenge Problem Summary

- Charter with path forward and levels of success defined
- Implementation plan with milestones planned in FY14
- Good progress in POR6/7 on VERA T/H code development, data collection, and initial application
- FY14 milestones focus on new VERA T/H code applications and data analysis using advanced VUQ method
- Work being planned for FY15 and beyond

DNB CP Work in Good Progress

RIA – Definition of Success

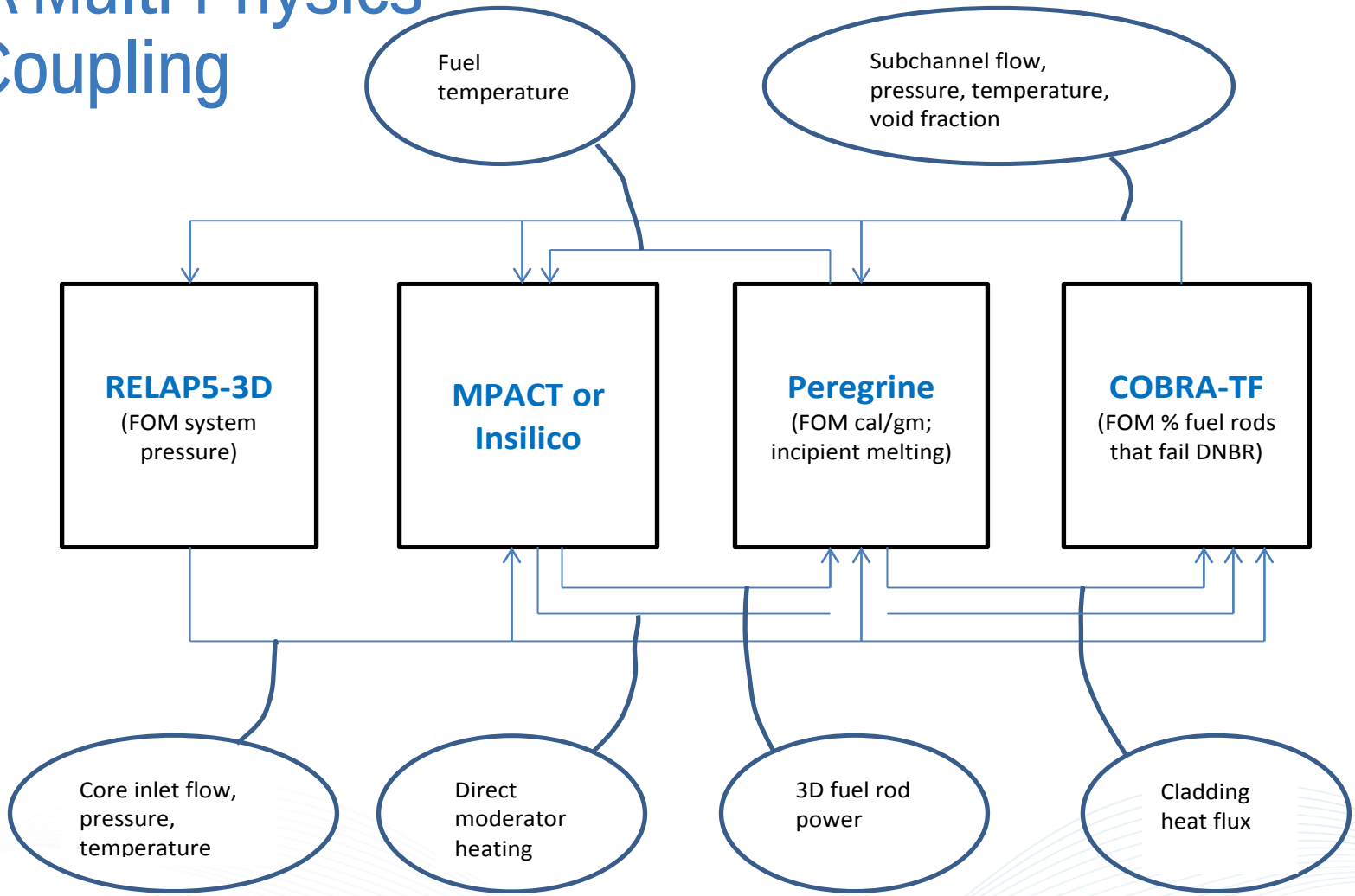
Minimum: Multiphysics capability with VERA components of at least equivalent fidelities to current industry practices with enhanced VUQ capabilities

Desirable: Multiphysics capability with VERA components of higher fidelities than current industry practices with enhanced VUQ capabilities

Ultimate End Game: Multiphysics capability composed of nearly all science based VERA components (reduced experimental validation / obtain understanding of risk/design margin)

RIA CP Implementation Plan

VERA Multi-Physics RIA Coupling



RIA CP Summary

- Charter completed – scope defined
- Implementation Plan draft completed – need to determine resource requirements and integrated schedule
- Technical work status
  - Insilico + COBRA-TF + Peregrine coupled
  - RELAP5-3D brought into VERA but not yet coupled
  - Peregrine capabilities progressing as planned
  - MPACT transient formulation developed and about to be implemented
- VERA components with tight coupling will provide
  - Higher fidelity RIA modeling compared to current industry
  - First time all RIA physics included (best-estimate + uncertainty)
  - Margin for plant uprates and burnup extension
  - Best analytical tool to address regulatory issues

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			

Significant Progress

Planning & Scoping

Good Progress

Not Started

Summary

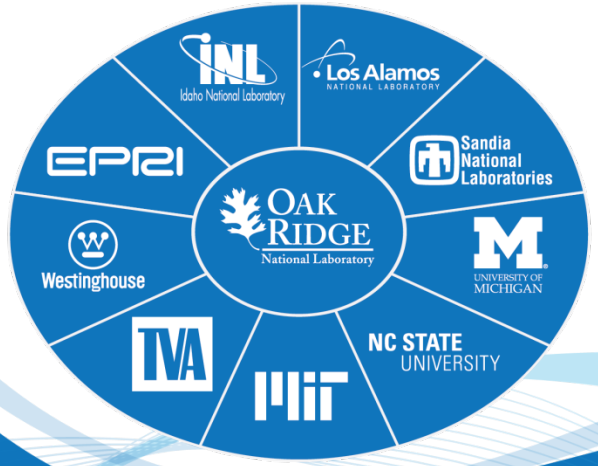
- Use of Charters and Implementation plans really helping us:
  - Improve communication across Focus Areas on what development is needed to address challenge problems
  - Define how to couple and apply VERA tools for challenge problems
  - Establish success targets
  - Identify innovation relative to current practice
  - Identify data needed for validation of tools
  - Help establish benefit of using CASL tools

- Expect to make significant progress in applying VERA tools for PWR challenge problems in Phase 1 and then apply for other applications towards 2020 (BWRs, iPWRs, other PWRs problems, etc)

Thermal Hydraulics Methods Focus Area

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

CASL Science/Industry Council Meeting
Oak Ridge National Laboratory
September 10-11, 2013

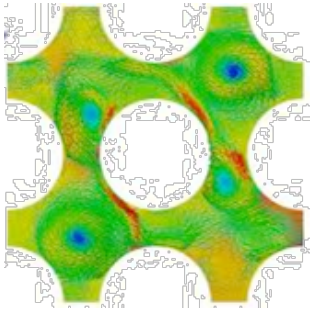


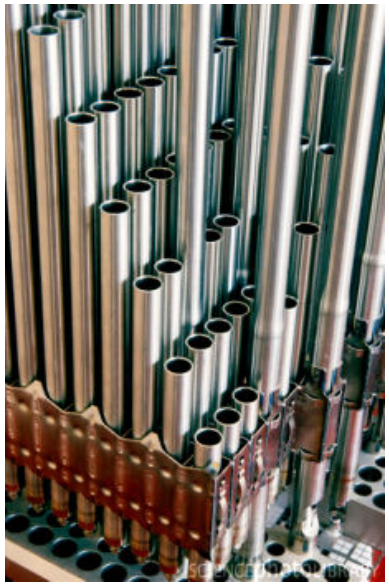
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

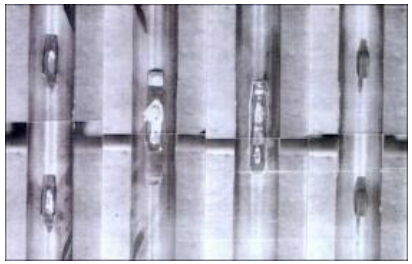
CASL
Consortium for Advanced Simulation of LWRs

CASL Thermal-Hydraulics applications range from FSI to reacting chemistry, and multiphase flows

- Grid-To-Rod Fretting (GTRF)
- Departure from Nucleate Boiling (DNB)
- CRUD-Induced Power Shift (CIPS)
- CRUD-Induced Localized Corrosion (CILC)

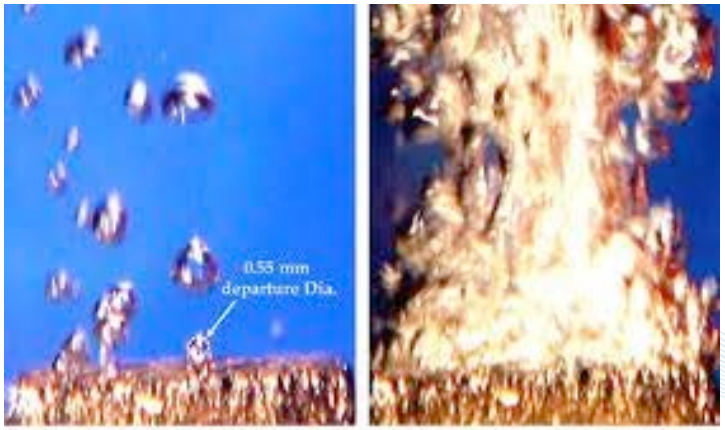






A largely metaborite 7.5 cm "rock" found in a reactor residual heat removal system

DNB: The point at which the heat transfer from a fuel rod rapidly decreases due to the insulating effect of a steam blanket that forms on the rod surface with a concomitant temperature increase.



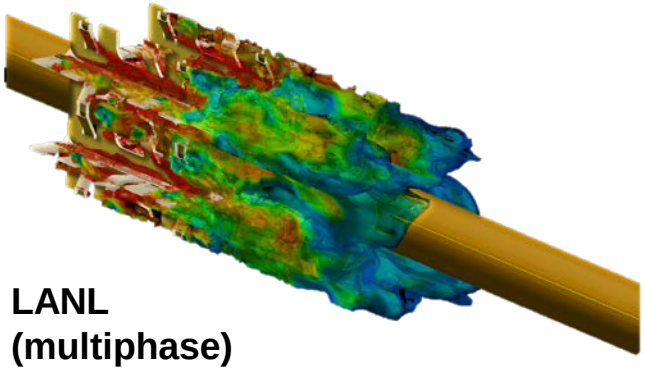
(a) 0.2 W/cm^2, ΔT_{sat} = 0.8 K (b) 10.0 W/cm^2, ΔT_{sat} = 7.9 K

Thermal Hydraulics Methods

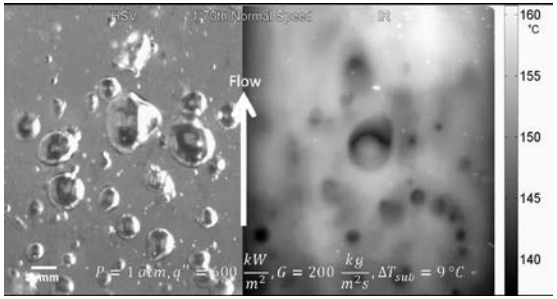
Advanced T-H Models and Simulation Tools for NE Applications

Objectives and Strategies

- Deliver next-generation T-H simulation tools to VERA, interfaced with the latest VUQ technologies, and accommodate tight coupling with other physics
- Computational Fluid Dynamics (CFD): Deliver scalable, verified and validated CFD tools
- Closure Modeling (CLS): Exploit micro-scale simulation results and experimental data for CFD closure models and validation based on new physical understanding
- Leveraging capabilities of THM teams to deliver state-of-the-art models and methods for T-H simulation



LANL (multiphase)



MIT

Requirements Drivers

- Customers & Stakeholders: SLT, AMA, MPO, PHI are the primary customers/stakeholders
  - Also important input from Westinghouse, EPRI, TVA, etc.
- Advances in THM needed to attain the fidelity required for detailed investigation of CASL Challenge Problems
- Key Requirements:
  - Scalable implicit algorithms for turbulent multiphase flow, from microscale through component length scales
  - Ability to mesh and analyze complex geometries
  - Sub-grid models that are focused on specifics of Challenge Problems
- Leverage capabilities from NE, Office of Science, NNSA, and Universities

Milestones and Impact

- 1 L1, 1 L2, and supporting 7 L3 CFD and 10 L3 CLS milestones
- THM Workshop focused on coordinating research efforts, organizing requirements for DNS/Experimental data and improving V&V/UQ efforts
- Use the capabilities developed to gain new insight into the CASL Challenge Problems
- Position 3-D CFD capability for DNB and future research on LOCA simulations

Feedback from THM Science Council Representative for FY13 Efforts Reported at THM Workshop

"In my opinion there has been a very impressive turn-around in CASL's THM program. Indeed it appears that the new management team (i.e., Mark Christon and Emilio Baglietto) have a clear understanding of what it will actually take to develop a CMFD model for the evaluation of subcooled nucleate boiling in PWR fuel rod bundles …", R. Lahey

2012 Review Comment

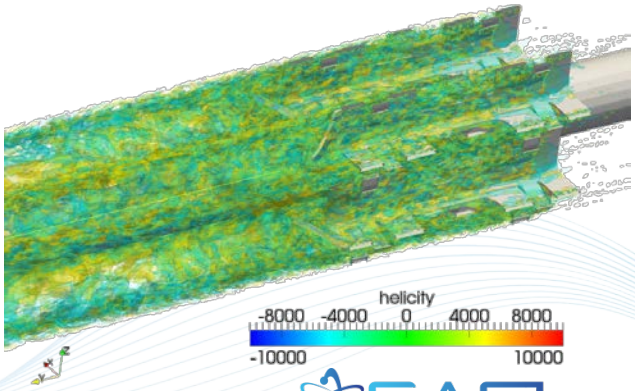
- Comment
  - In his report on a CASL workshop held in December of 2011 Science Council member Richard Lahey has presented several criticisms of the project's thermal-hydraulics modeling effort. He believes that many of the experiments being done at CCNY and MIT are of limited value to CASL. As discussed above, he proposes an experiment that he believes is sorely needed. In addition, he states that much of the work being done to support the analytical T-H needs of CASL is uncoordinated and duplicative. Finally, he maintains that it will take a very significant effort to develop from scratch a robust and reliable multiphase fluid dynamics solver for VERA. These are serious concerns expressed by an expert who is much more familiar than I am with the project's T-H modeling efforts. I agree with Lahey that multiphase fluid dynamics is an exceedingly difficult problem that warrants more attention. ... project leadership should scrutinize this area closely during the coming years.

THM Workshop Comments & Recommendations:

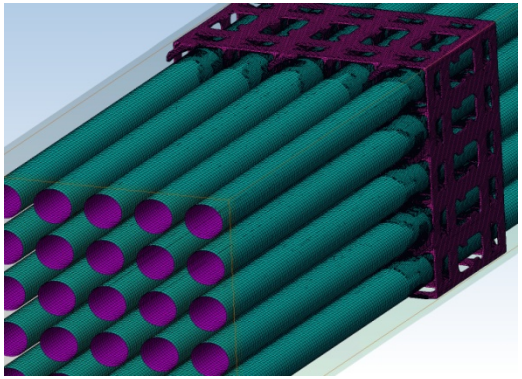
- Boiling experiments are well-focused and relevant to improved heat-flux partitioning model development
- Need to redirect "device-scale" experiments to focus on original CASL needs for rod-bundles
- Subchannel efforts may be a distraction for the THM team and development of multiphase capabilities
- DNS/ITM simulations need to move towards large bubble-number simulations and liquid-phase turbulence for improved multiphase turbulence closures
- Analytical work on force closures will be directly relevant to Hydra-TH development
- V&V efforts show no "surprises" with Hydra-TH, but V&V efforts are premature for the multiphase flow capabilities

L1 CFD Turbulence Force Calculations and Grid-to-Rod Fretting Simulation Highlights

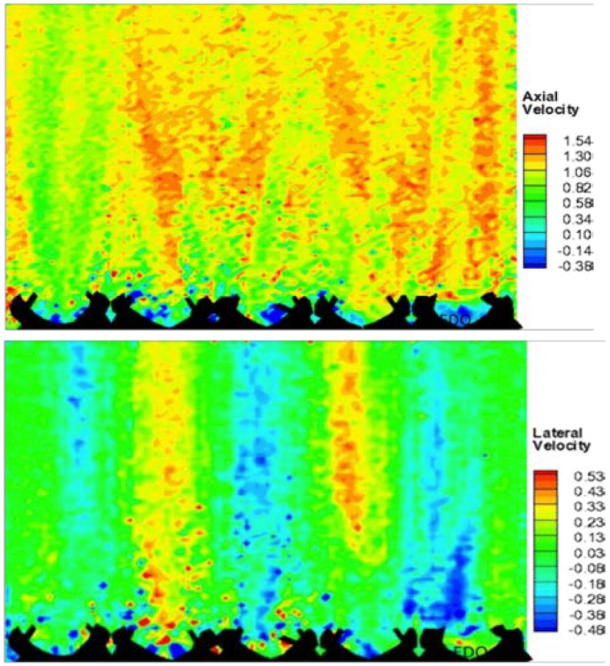
- Purpose
  - Understand the turbulent flow physics in rod bundles
  - Collect turbulence statistics for future use
  - Validate Hydra-TH with 5x5 rod bundle data
  - Collect baseline LES data for development GTRF models
  - Assess Cubit & Spider meshes
  - Provide input data for VITRAN analyses
- 3x3 rod bundle calculations:
  - Cubit (thex): 672k, 1M, 3M, 6M, 12M
  - Hybrid: 2M, 7M, 14M, 27M, (30 and 47M preliminary)
- 5x5 rod bundle calculations:
  - 14M, 96M hybrid meshes



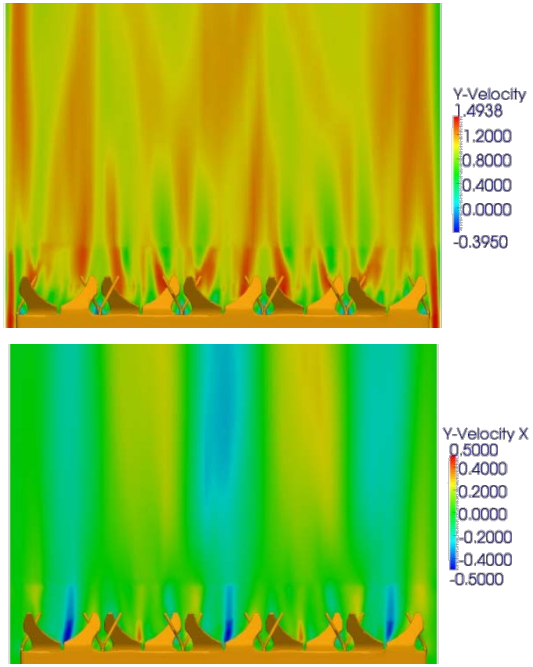
5x5 V5H study shows good agreement with experimental data



- Predicted mean peak velocities within 5% of experiments

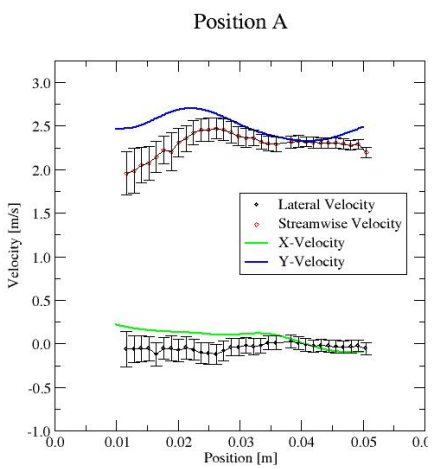


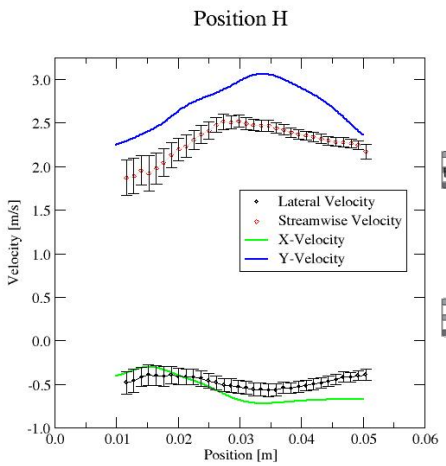
Texas A&M experiments

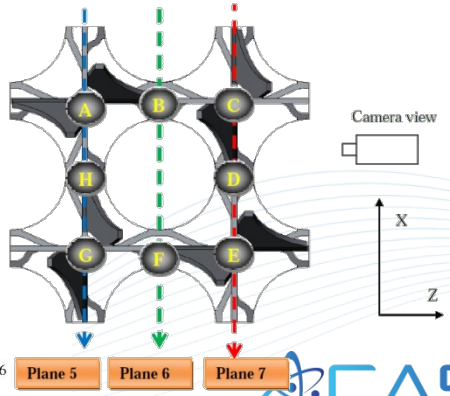


Hydra-TH calculations

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

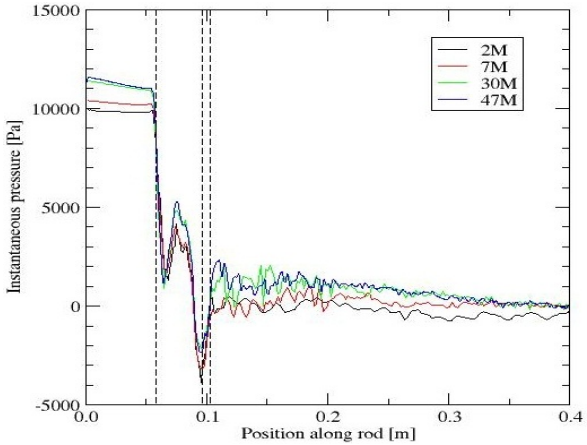


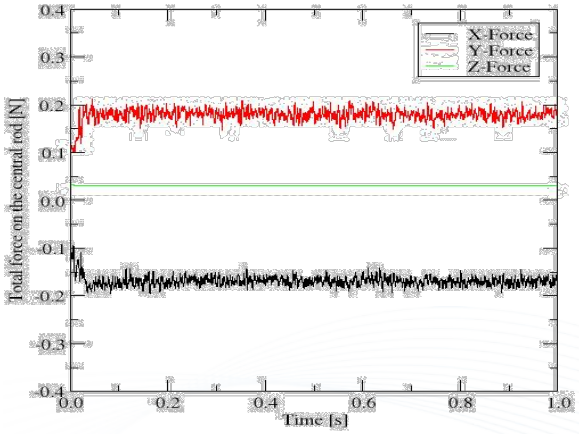


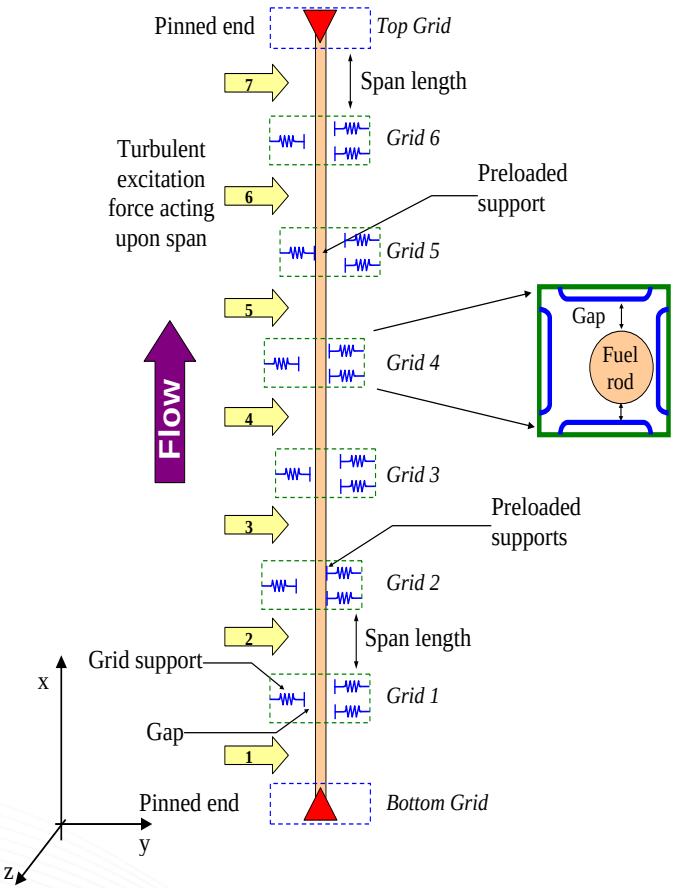


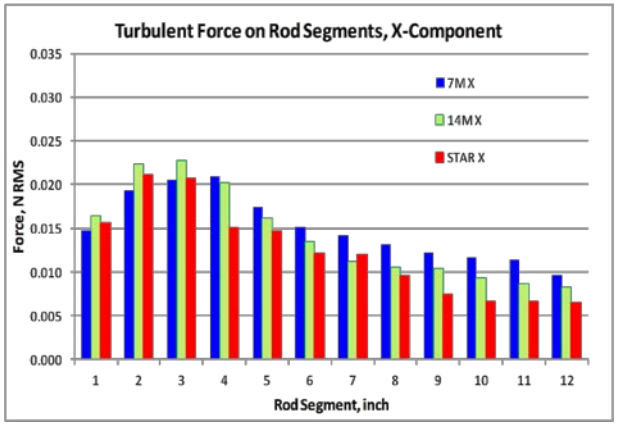
Large-Eddy Simulations Used to Drive Modal Dynamics and Wear Work Rate Calculations using VITRAN

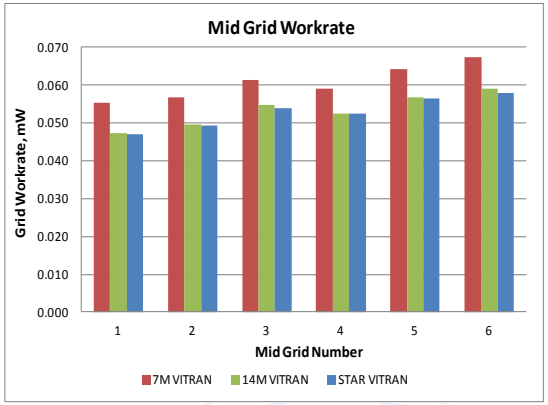
- Pressure Profiles and Rod Forces are extracted from Hydra-TH for the 3x3 Rod Bundle
- The data are used as input to VITRAN to compute rod acceleration/displacement
- 7 to 14M meshes required for reasonable fidelity in design analysis ~ 8 – 24 hour calculations









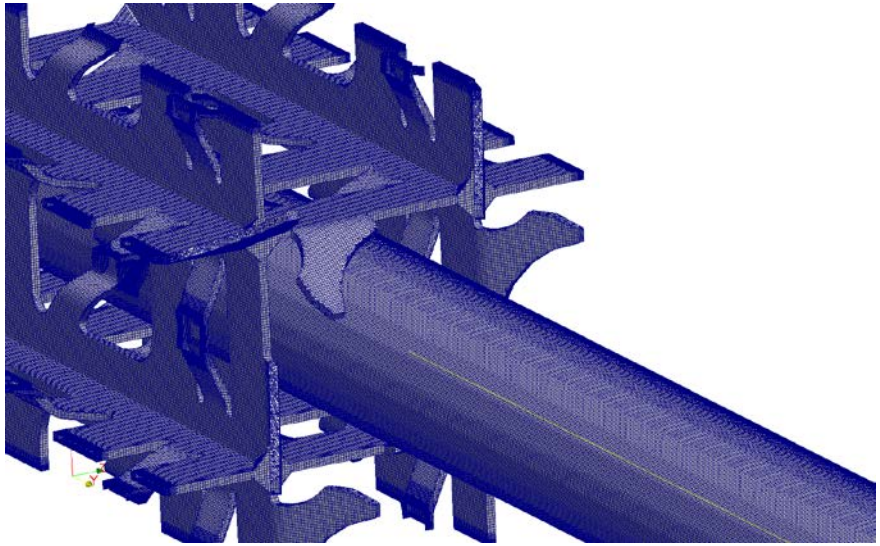


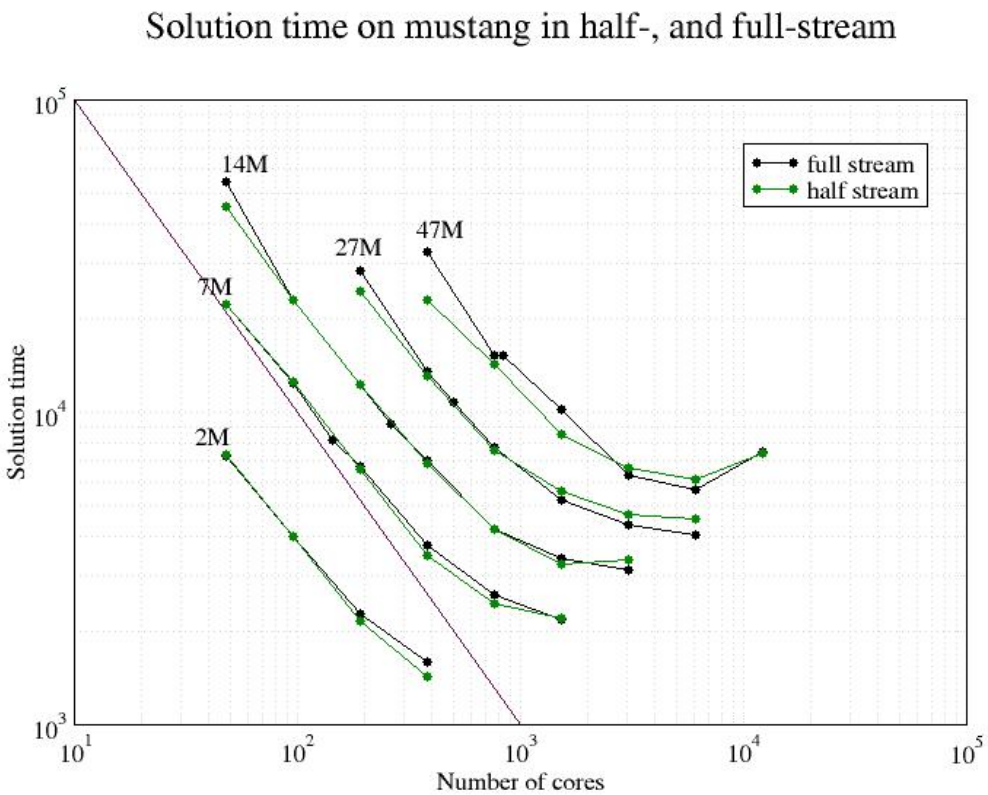
2% difference between CCM+ and Hydra-TH wear work-rates

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

Some performance numbers using the V5H 3x3 rod bundle

- Mustang – AMD 6176 Opteron 24 cores per node





Titan early profiling studies

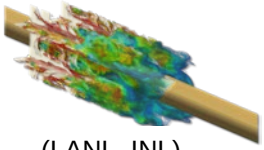
- 1024 nodes, 8 FP cores ea.
- 1.8 – 3.2% of peak FLOPs rate for AMD's

L3:THM.CFD.P7.03: Computational Performance Assessment of Hydra-TH

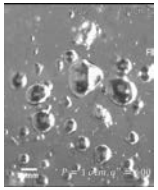
- *NVIDIA Tesla K20s delivered to LANL & ORNL*
- *Beginning to work with NVAMG library*

L2 - Demonstration and Assessment of Advanced Modeling Capabilities for Multiphase Flow with Sub-cooled Boiling

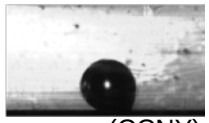
- A 'tour de force' effort used to coordinate/integrate research among the broad and diverse set of researchers in THM
- Primarily supports DNB Challenge Problem, but also positions THM for future applications



(LANL, INL)

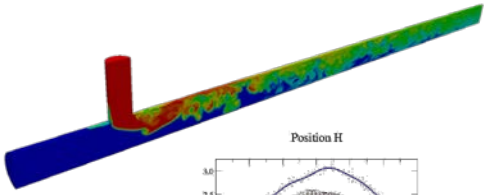


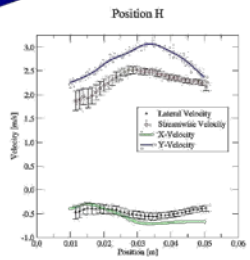
(MIT)



(CCNY)

(TAMU
)





Experiments

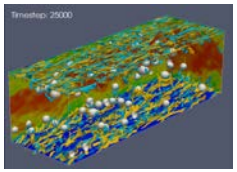
- Fundamental Understanding
- Code Validation
- Multiphase Closure Models

Algorithms & Architectures

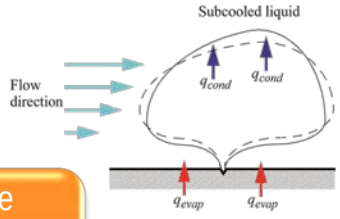
- Advanced CFD Algorithms
- Multiphase Solution Methods
- Advanced Architectures – NVIDIA nvAMG Library

V&V, Uncertainty Quantification

- Intrusive VUQ Algorithms
- Multiphase Model Sensitivities
- CFD Verification



(NCSU)



(Notre Dame)

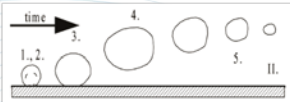
DNS - Interface Tracking

- Fundamental Understanding
- Multiphase Closure Models
- Code Validation

VERA -CFD (Hydra-TH)

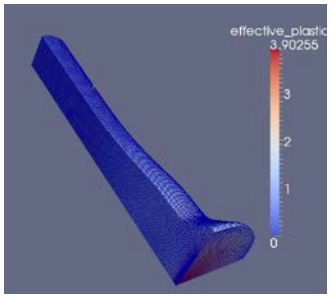
Multiphase Closure Models

- Mechanistic Subcooled Boiling
- Refined momentum closures
- Integrated lift/drag forces

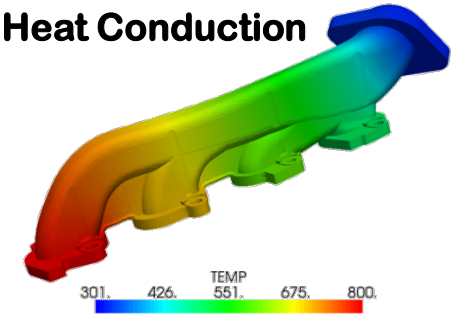


The Hydra Toolkit for Multi-Physics

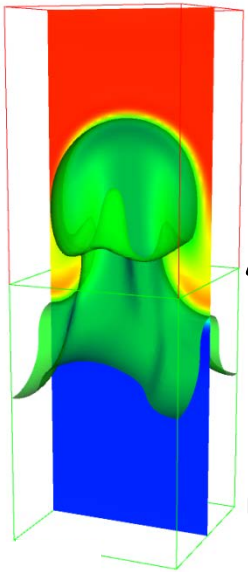
Lagrangian Hydrodynamics



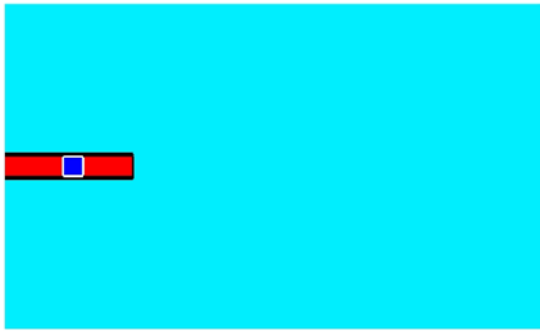
FEM/FVM Heat Conduction



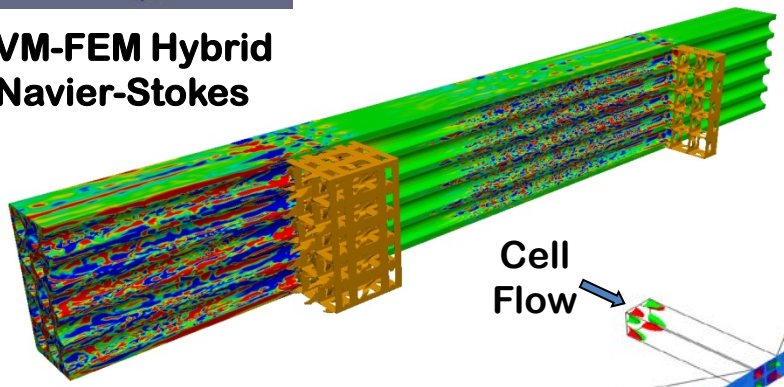
FVM Compressible w. Front-Tracking



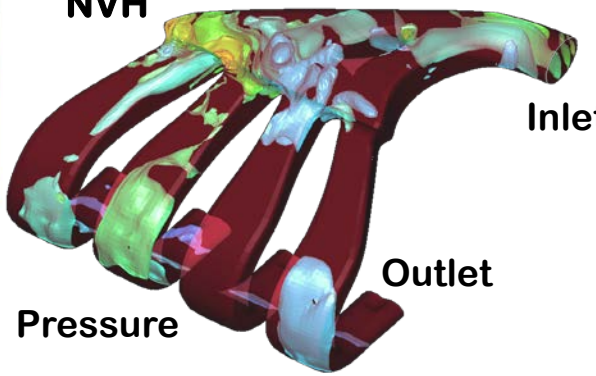
FVM Compressible w. Level Sets



FVM-FEM Hybrid Navier-Stokes

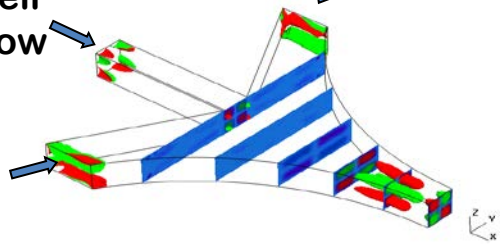


Automotive NVH

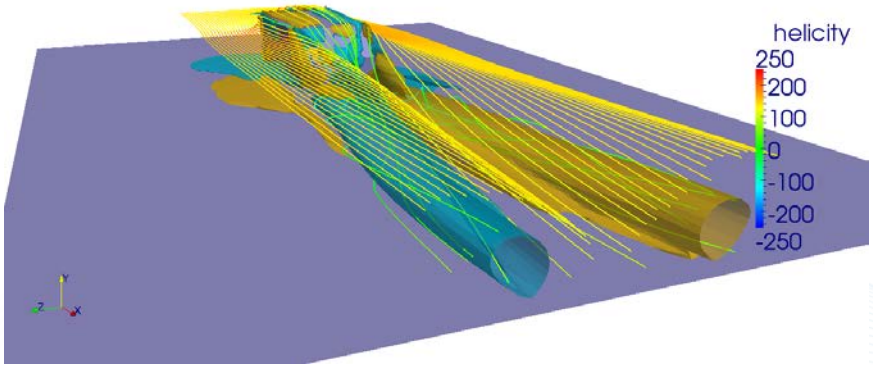


Carrier

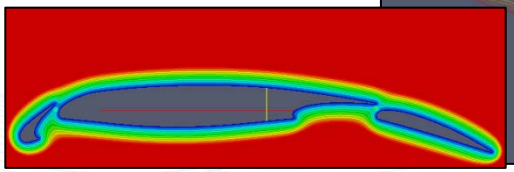
Cell Flow

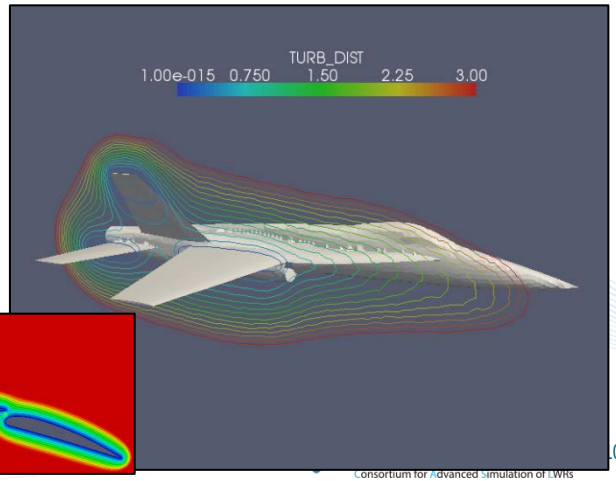


Rigid-Body Dynamics



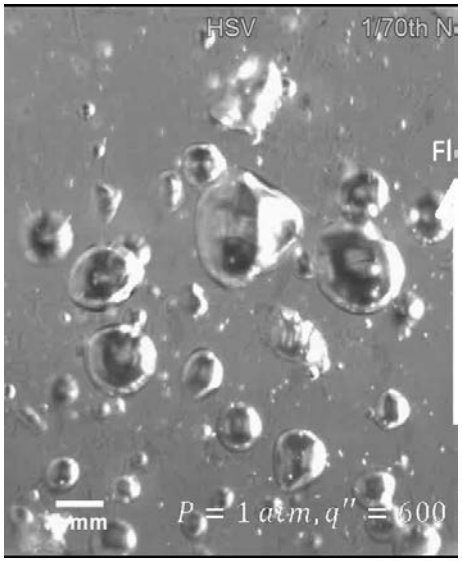
Flow Cytometry

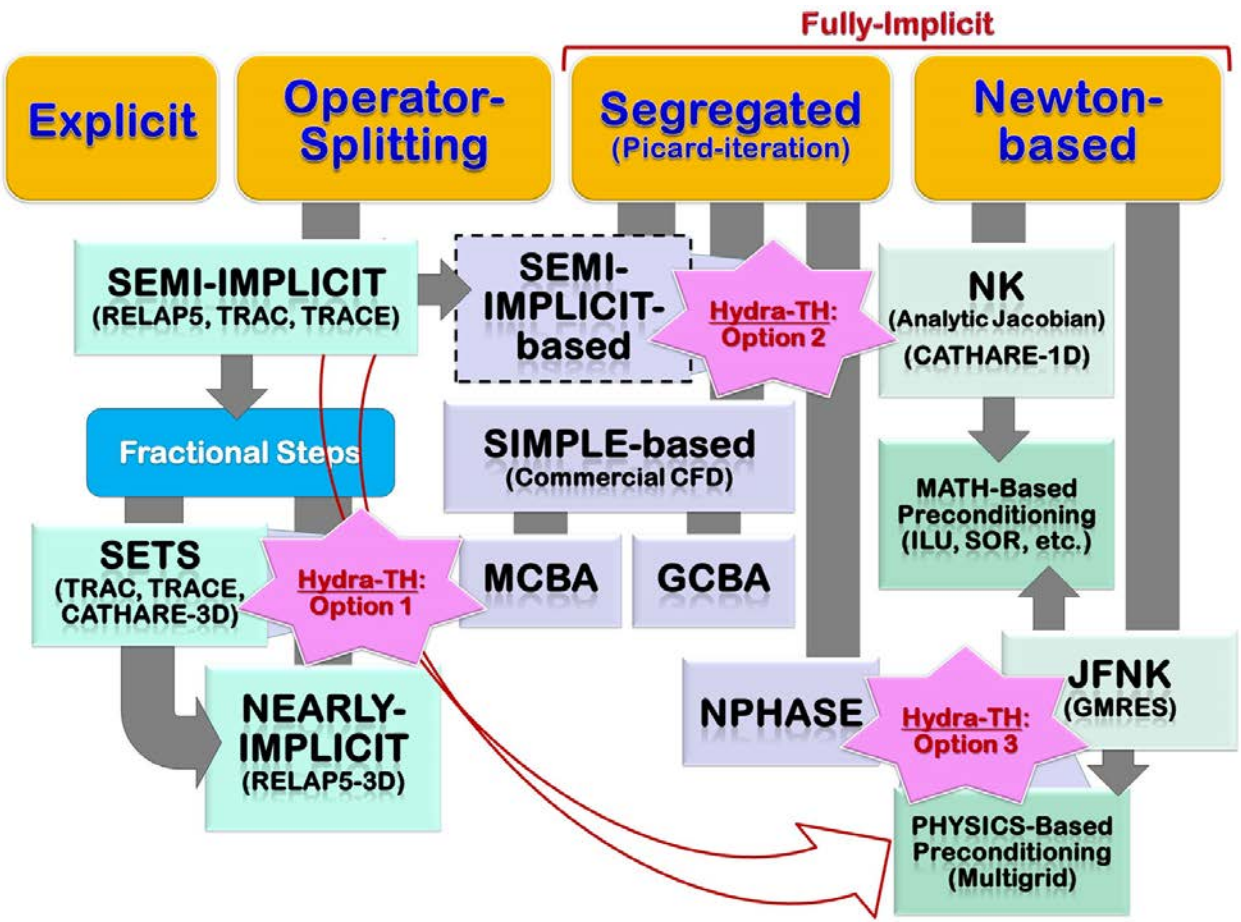




Single and Multiphase flow algorithms and the Hydra multiphase flow strategy/roadmap

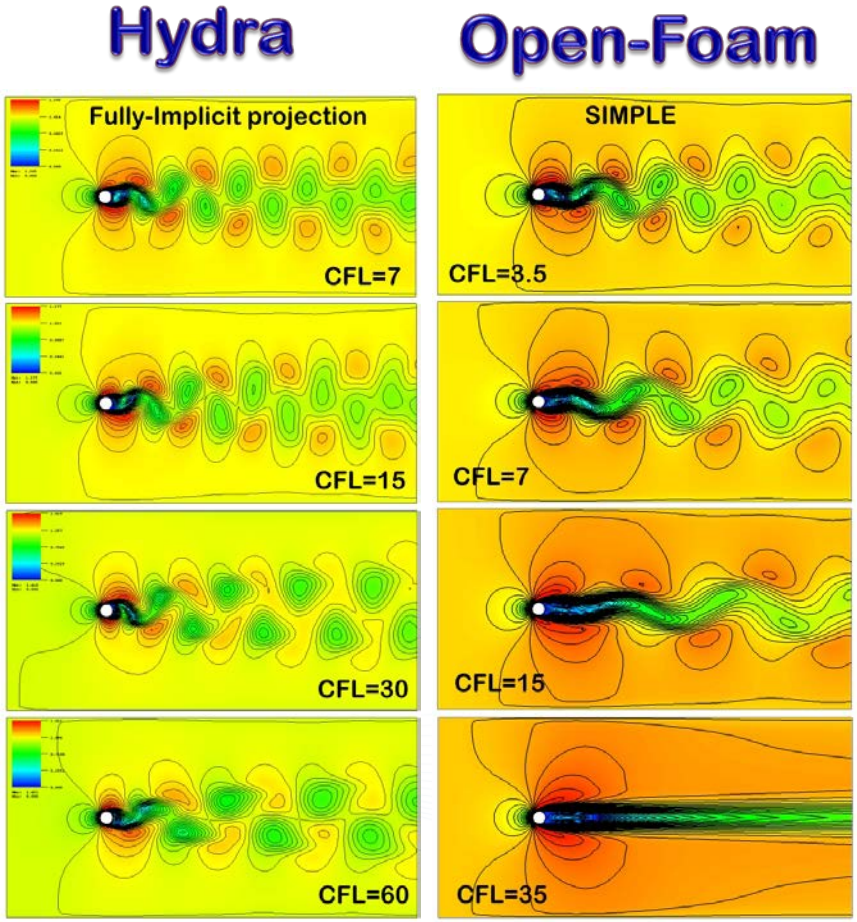
- Fully-implicit projection algorithms
- “Option 1” with momentum transfer (drag)
- “Option 3” – Fully-implicit w. physics-based preconditioning

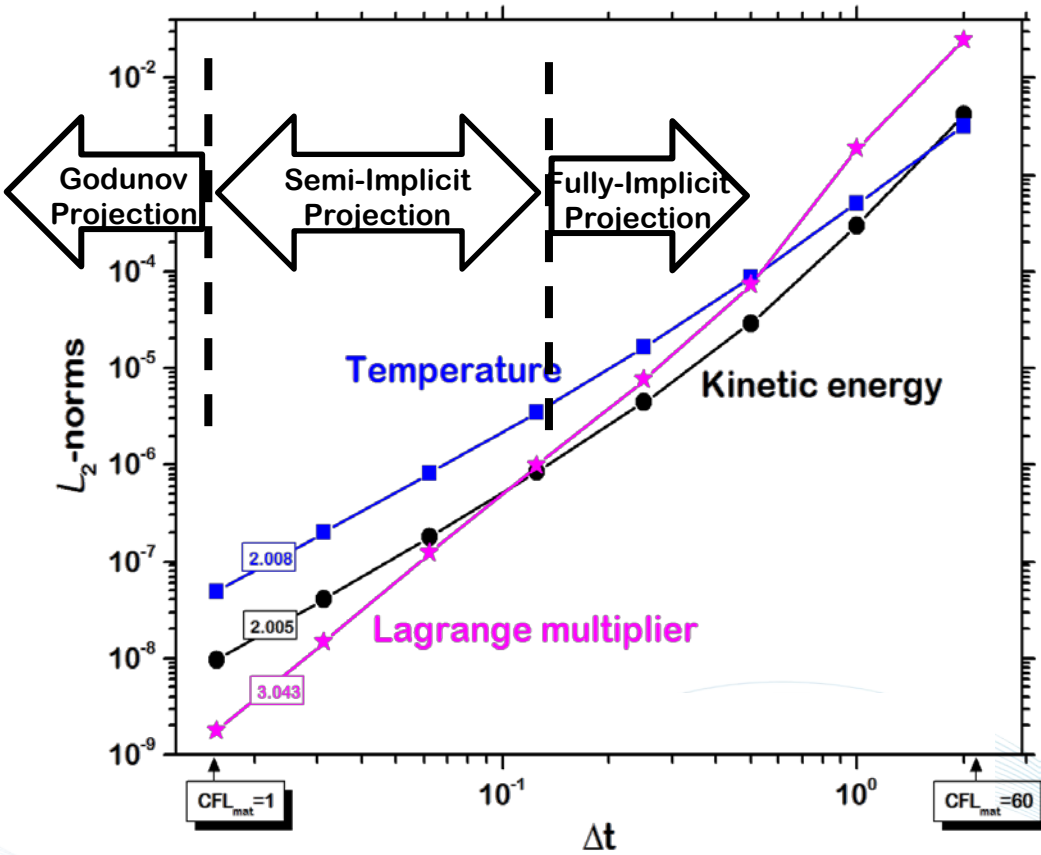




Fully-Implicit Algorithms based on Projection Methods

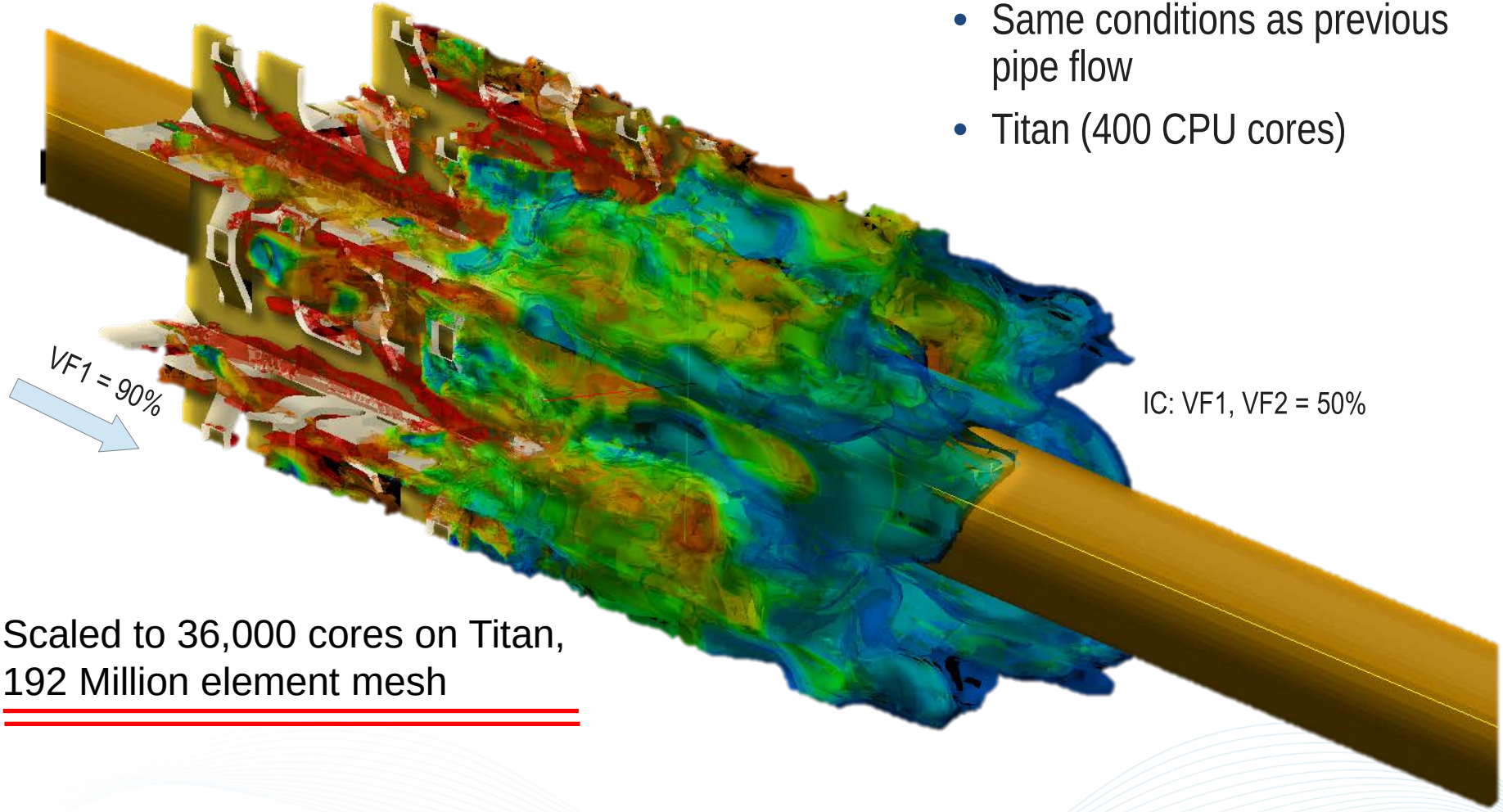
- Projection method acts a physically-based preconditioner providing an approximate factorization of the discrete Navier-Stokes Equations





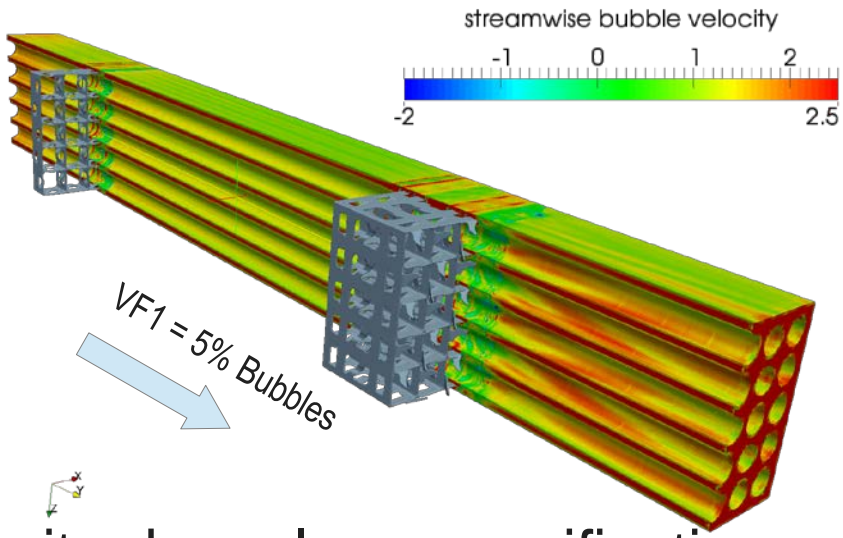
MultiPhase Flow – Complex Geometry, Reactor Flow Conditions

- V5H GTRF 3x3 2M cells
- Same conditions as previous pipe flow
- Titan (400 CPU cores)



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

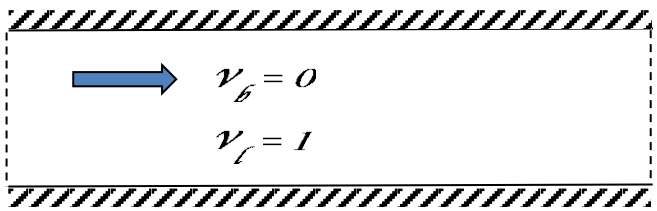
MultiPhase Flow in 5x5 Rod-Bundle



- "Option-1" Calculation w. Drag
- V5H 5x5 Spacer – 14M Cells
- Re=28,000 (TAMU Exp. Cond.)
- 100:1 water/air density ratio

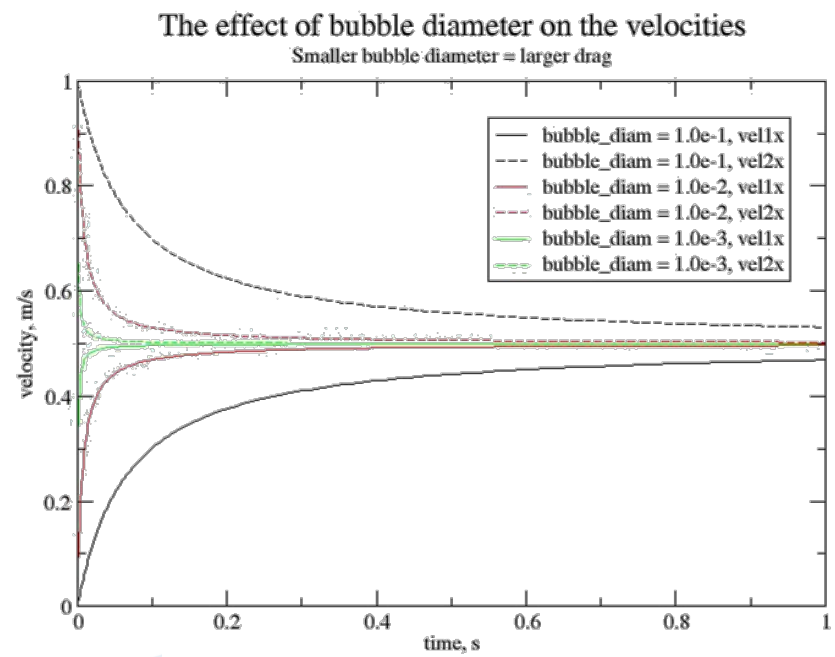
Verifies force anti-symmetry and momentum conservation!!

- In-situ drag closure verification



$$\mathcal{F}_D = -\frac{3}{4}\frac{C_D}{D_b}\alpha_l \rho_l \left\| v_b - v_l \right\| \left(v_b - v_l \right)$$

$$C_D = \begin{cases} \dfrac{24}{Re_b}\left[1 + 0.15\, Re_b^{0.687}\right] & 0 < Re_b \le 1000 \\ 0.44 & Re_b > 1000 \end{cases}$$



Hydra-TH Deployment, Support & Impact

- Early deployment of Hydra-TH was requested by a number of users, e.g., Jin Yan at Westinghouse, AMA
- Hydra-TH by Licenses (> 20 users) since January 2013
  - LANL – 1 (ASC user)
  - NCSU – 2
  - ORNL – 2
  - INL – 2
  - SNL – 2 (developer)
  - MIT – 1
  - U. Michigan - 3
  - AECL – 2
  - Ashton University (UK) - 2
  - Westinghouse – ~6 (requires binary distribution)
  - License agreements pending at Texas A&M, Kitware, …
- User support, code distribution, porting issues have diluted Hydra-TH multiphase development efforts in FY13
- E-mail support: hydra-th-users@lanl.gov, Downloads: get-hydra.lanl.gov
- Considering code distribution via Kitware…

2012 Review Comment

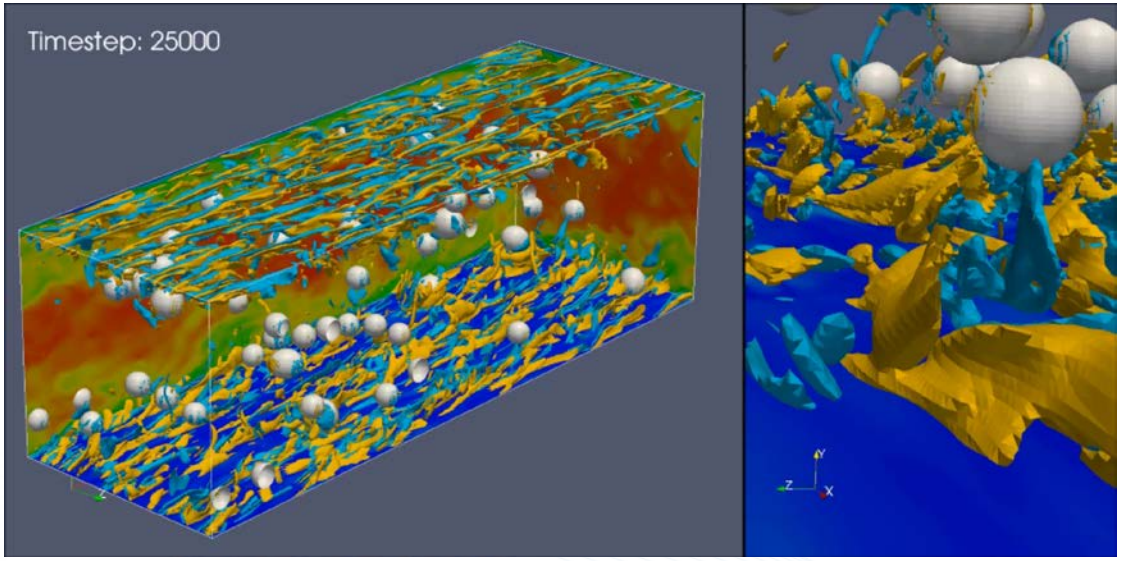
- Concern
  - The review team reinforced the idea that in order to create the desired impact on the U.S. nuclear energy industry, CASL will have to make sure its tools are deployed and used. Specifically, those modeling and simulation tools will have to affect the industry's current designs and engineering practices.

2012 Review Concern

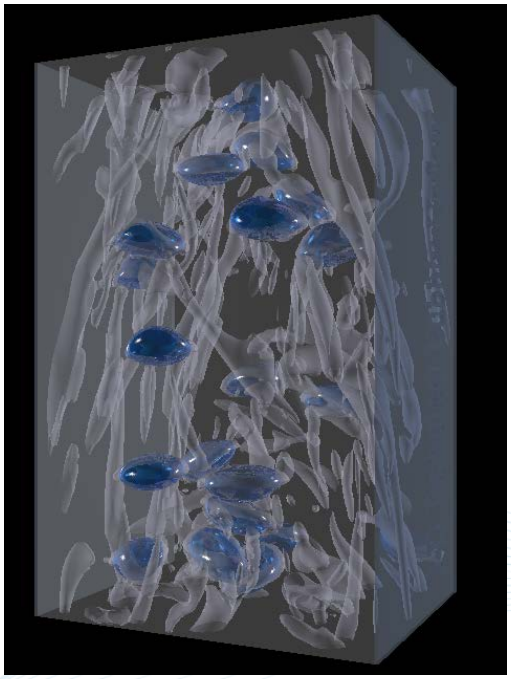
- Concern
  - The review team observes that CASL is still developing its plans for the deployment, use, and support of its software products. The team commends CASL for actively dealing with these issues, but it cautions the importance for CASL to find an appropriate role that does not compete with current Independent Software Vendors (ISV).

ITM/DNS Data Changes Closure Model Development in a Fundamental Way

- Permits direct computation of modeled terms at given points in space/time and to assess their mean and fluctuation components
- Approach in single-phase flows has led to significant advances in understanding and developing closure models
- Provides the foundations for more complete multiphase CFD turbulence modeling

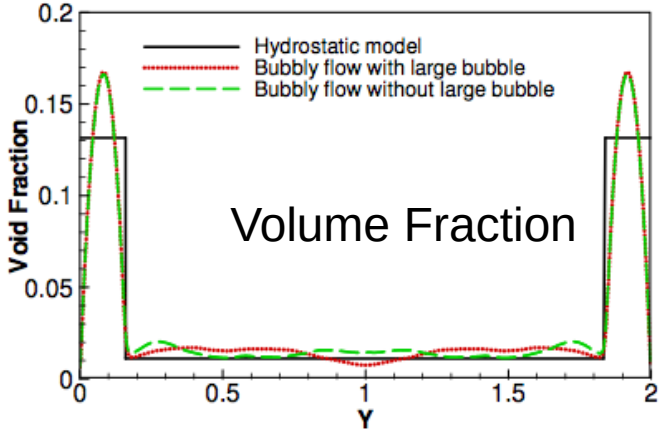


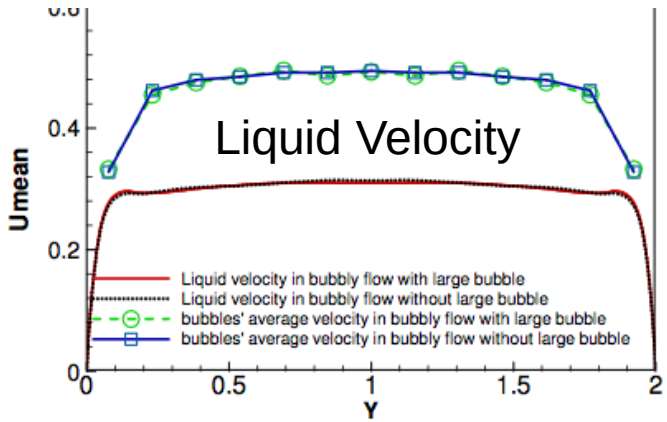
Bolotnov, NCSU

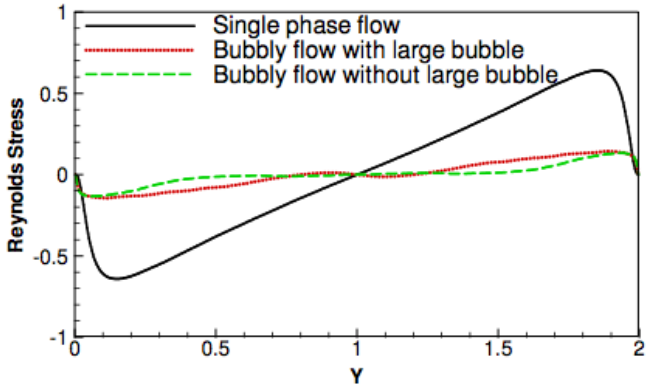


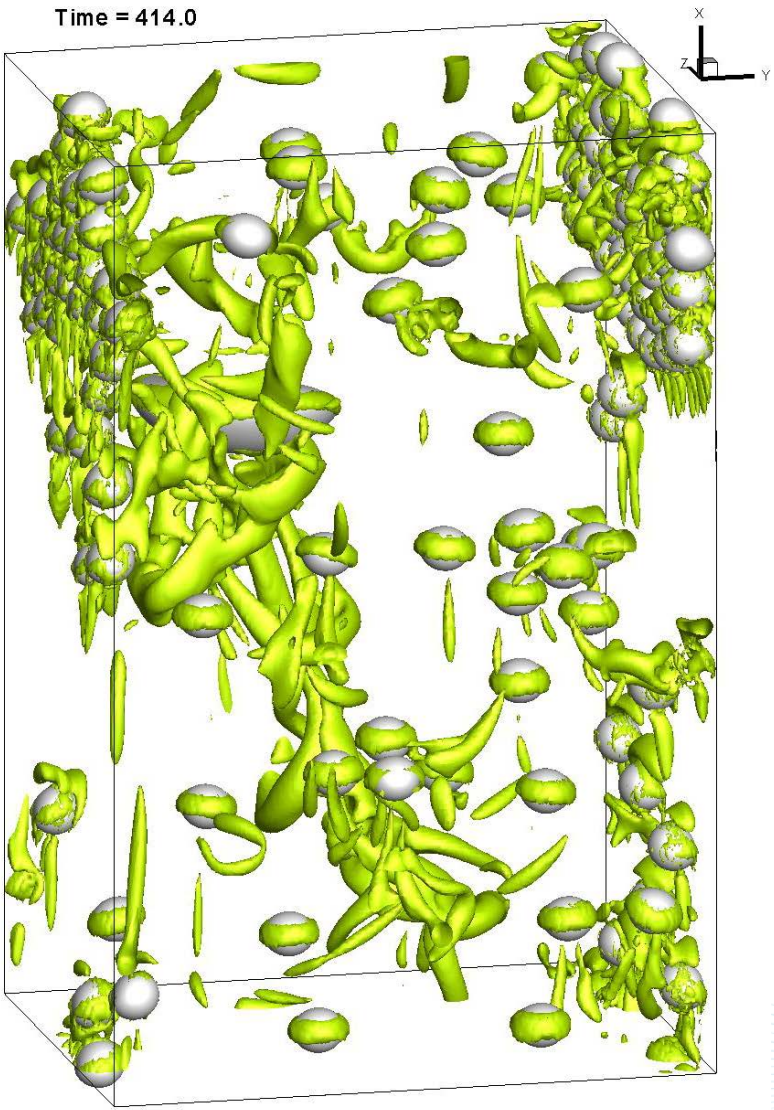
Tryggvason, N. Dame

Developing a DNS Database for Lift/Drag Effects



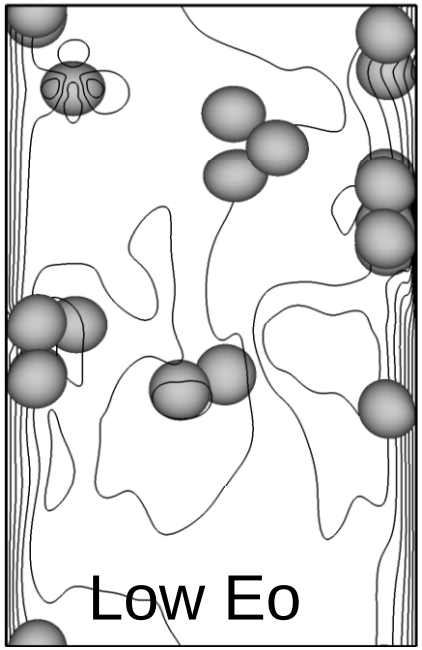


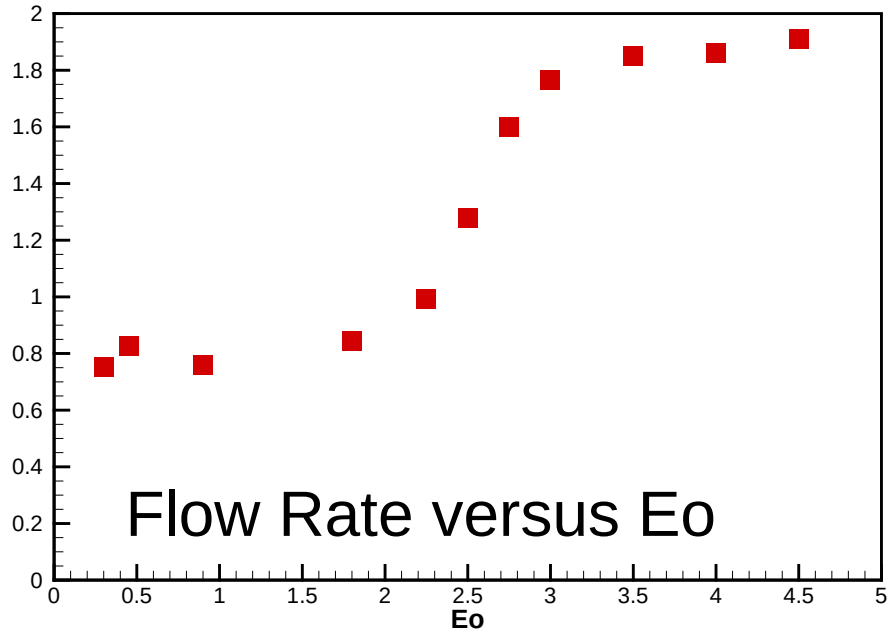


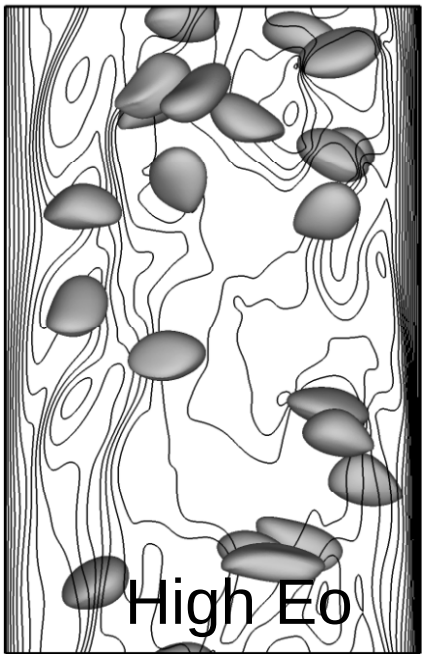


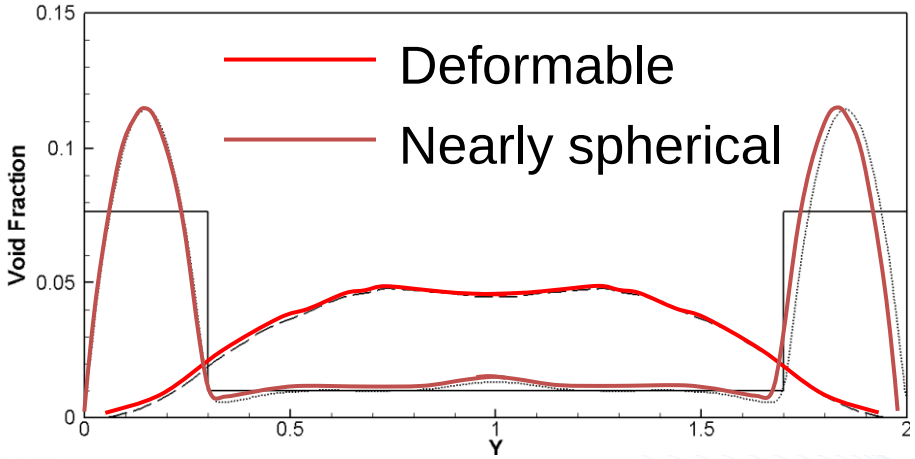
512 x 384 x 256 grids, 192 cores)
Re+ = 250; void faction = 3%

Turublent Upflow -- Bubble Deformability Effects



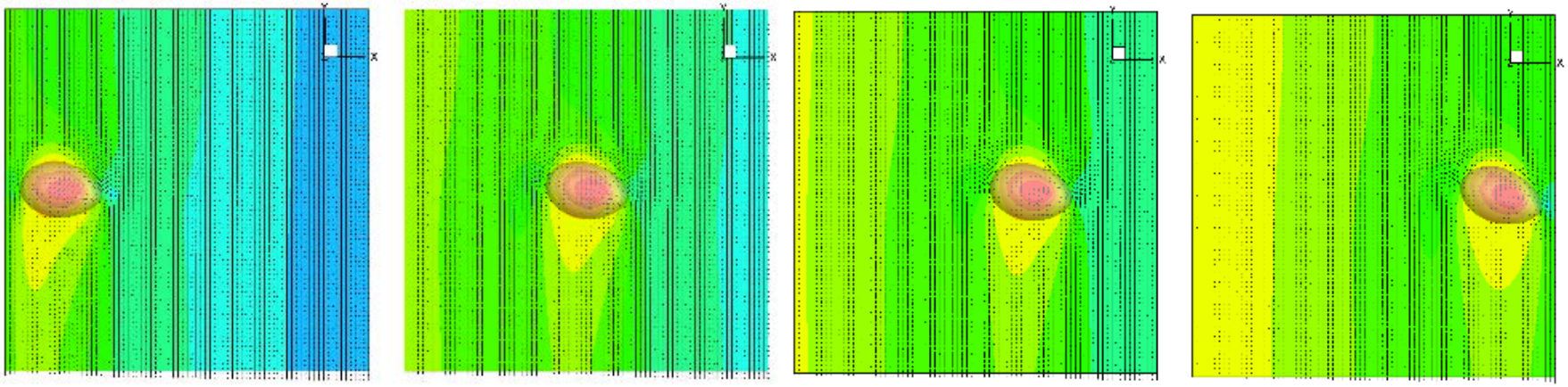


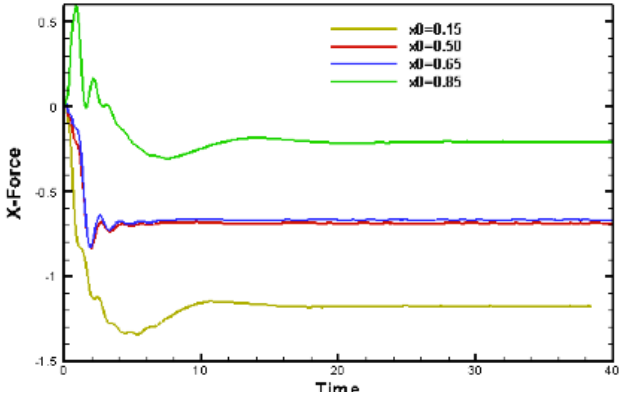


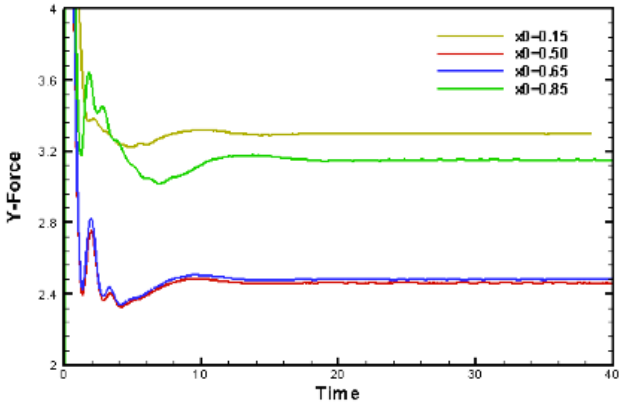


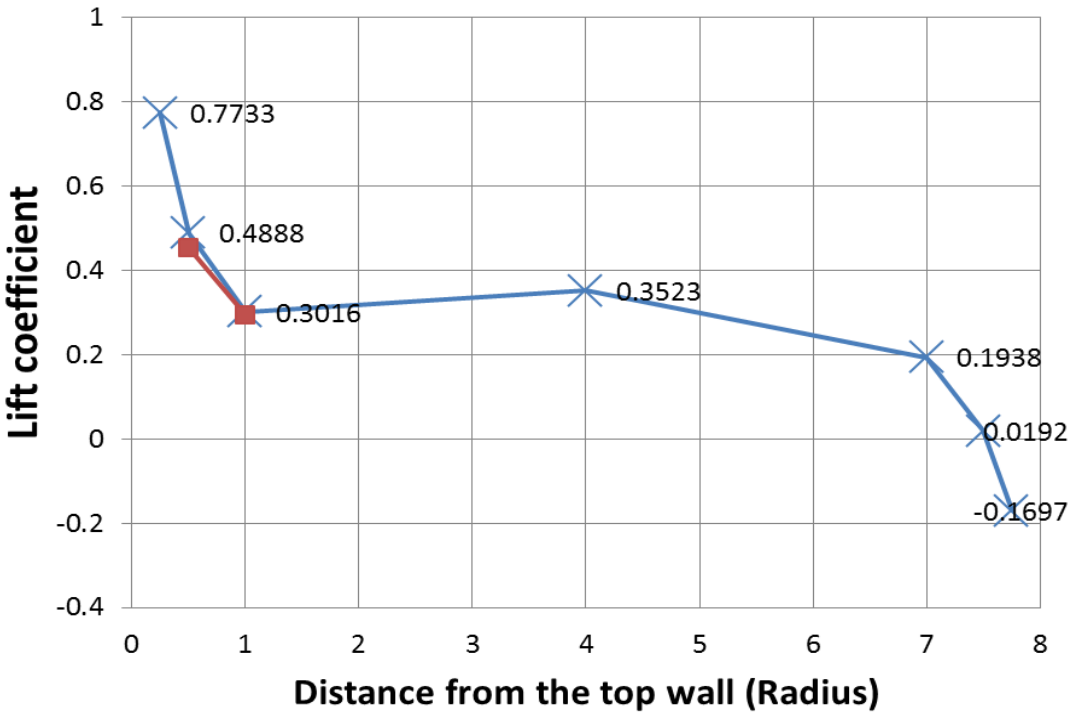
The volume fraction has major influence of the flow behavior. The volume fraction is plotted above and the velocity profiles and the Reynolds stresses to the right. For deformable bubbles, the flow is similar to turbulent flow without bubbles (using rescaled pressure gradient to account for the weight of the mixture).

Lift and Drag on a Single Bubble -- Wall Effects









THM Experiments: From Micro- to Device-Scale

Highly-resolved data are needed for insight, development and validation of closure models

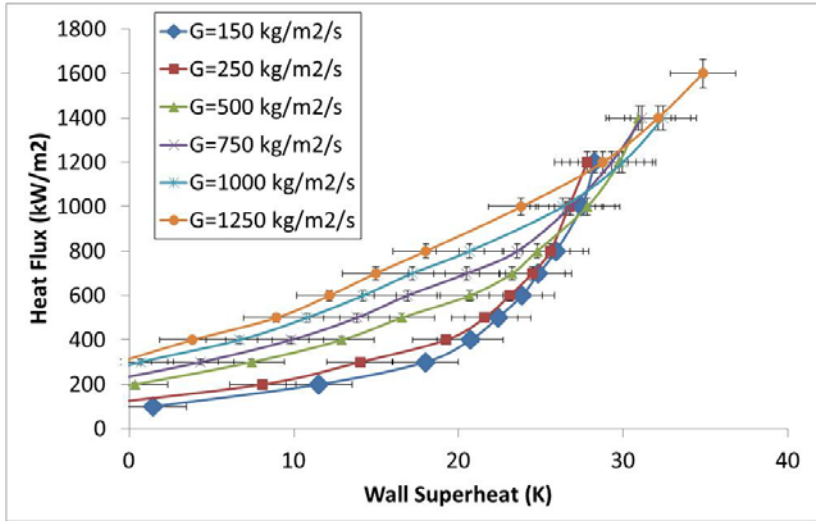
- bubble size vs time
- bubble departure frequency (growth and wait)
- nucleation site density
- areal void fraction
- temperature field (surface-2D and fluid-3D) and velocity field vs time
- microlayer evolution
- All for a meaningful range of conditions, in dimensionless terms: P/P_{cr} (pressure), *Bo* (heat flux), *Re* (flow rate), *Ja* (subcooling), contact angle (wettability), dimensionless roughness (surface finish)

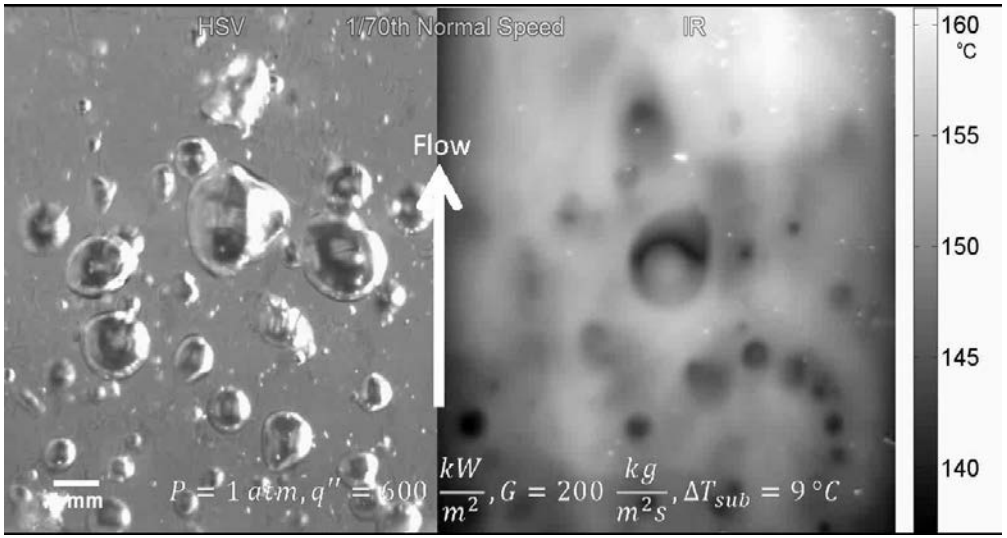
Broad Arsenal of Advanced Diagnostics are Available

- High-speed IR thermography (surface temperature and phase detection, including microlayers)
- High-speed optical video (interface position)
- LIF and PIV (fluid temperature and velocity)
- Micro-heater arrays (surface temperature and heat flux)

Data Archival from Experiments (and ITM/DNS) on VOCC for NE-KAMS

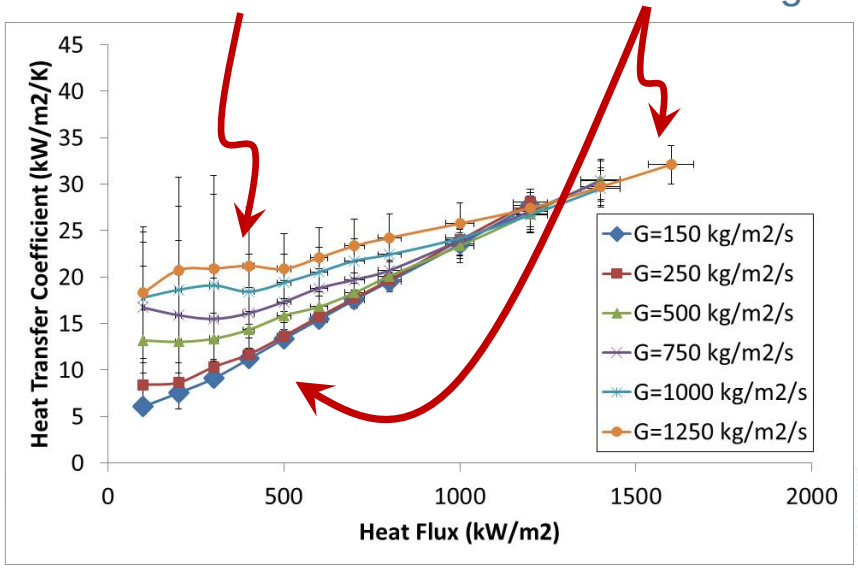
Synchronized High-Speed Video and IR Thermography in Boiling Flows (MIT)

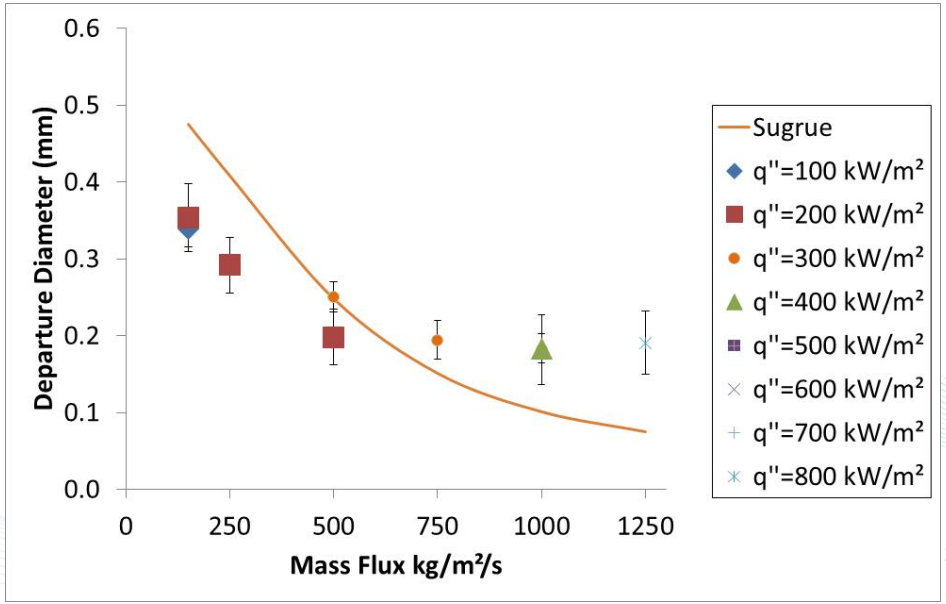




Forced convection

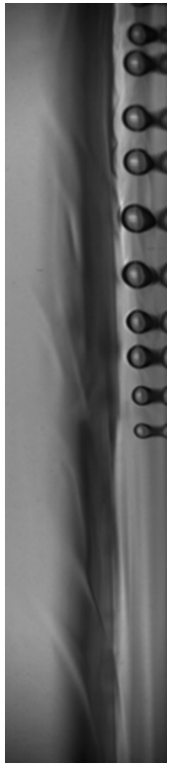
Fully-developed nucleate boiling

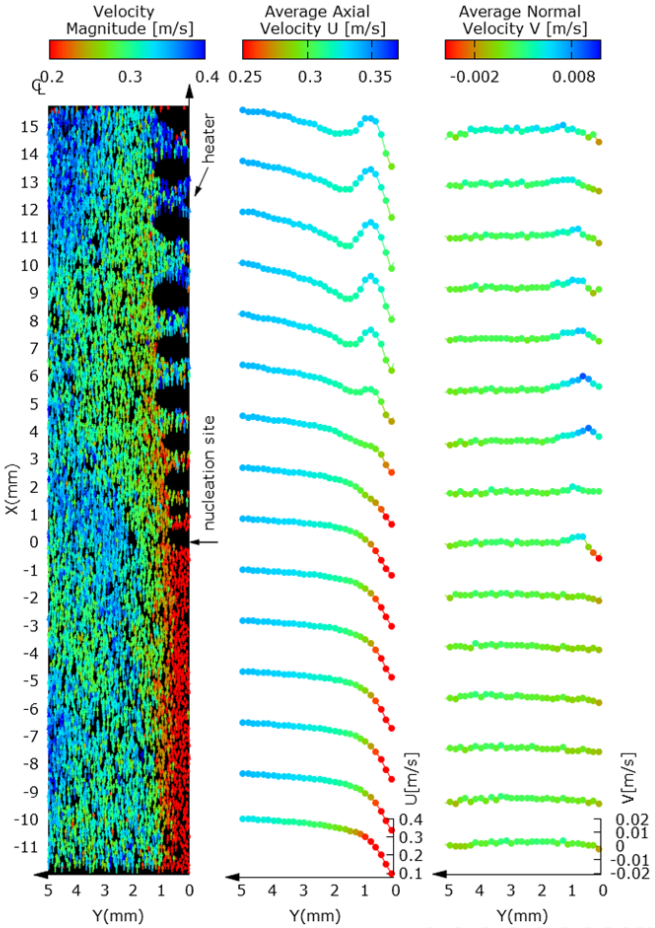


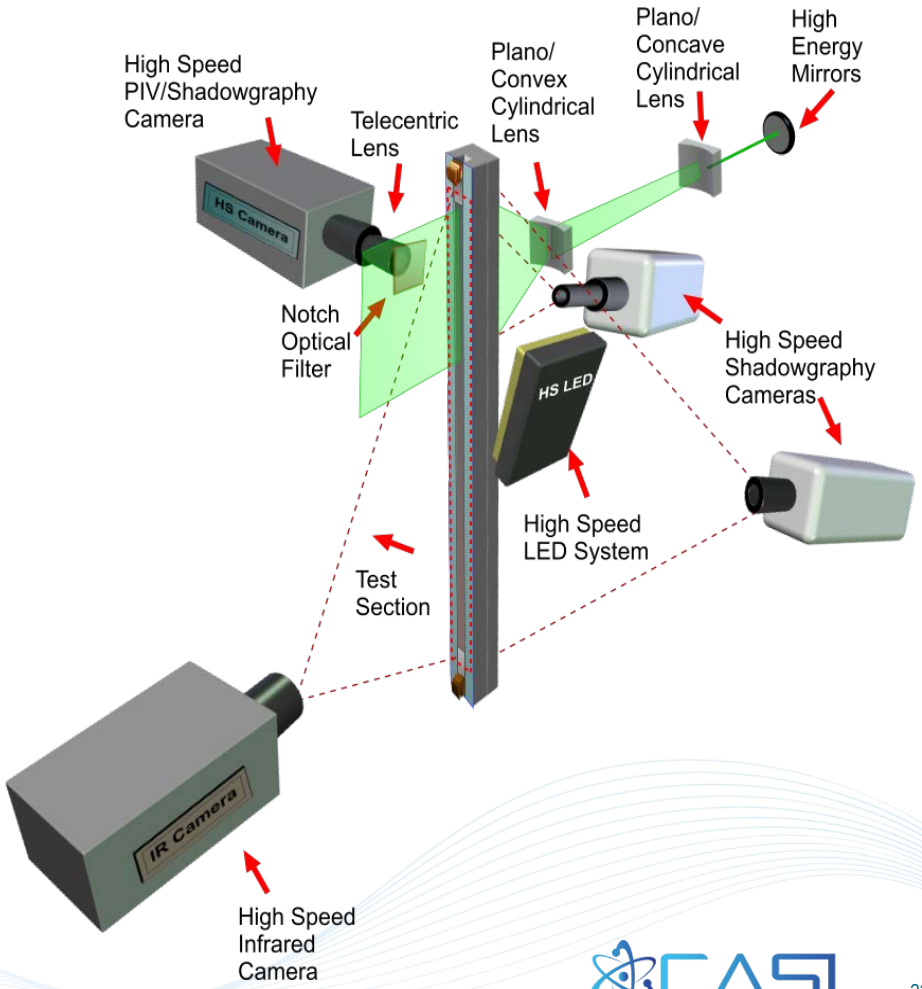


PIV-Shadography and IR Measurements (TAMU)

- Average & instantaneous liquid and bubble velocities
- Advanced derived turbulent statistics (higher-order moments)







Closure Modeling for Multiphase-CFD Applications

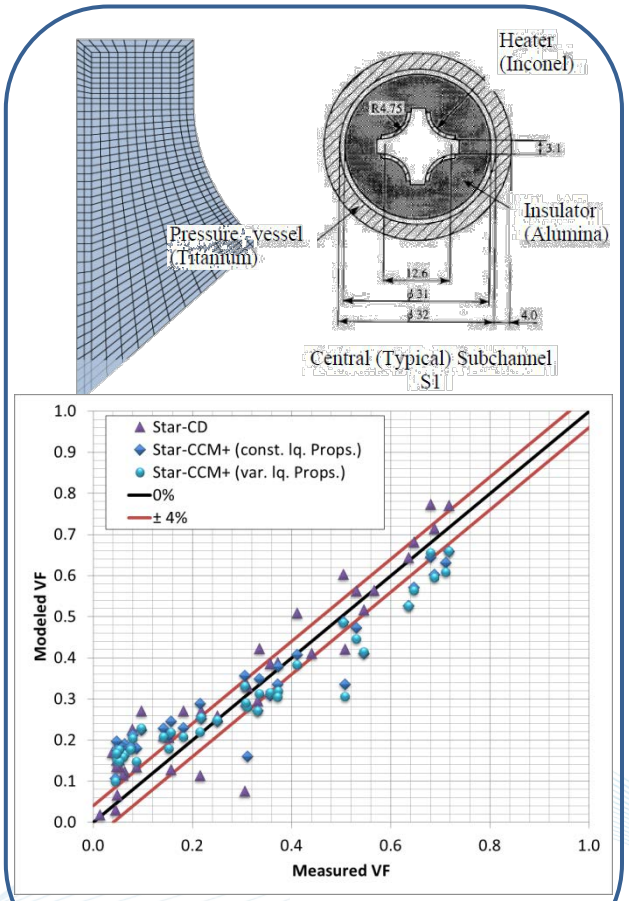
Why New Closures?

- Artisanal subchannel-like calibration produces reasonable results for available well instrumented benchmarks
- It is not possible to extend this calibration with “confidence”
- Defeats purpose of Multiphase-CFD, might as well reduce the complexity of the closure

In order to provide advanced modeling capability for multiphase flow with sub-cooled boiling in VERA:

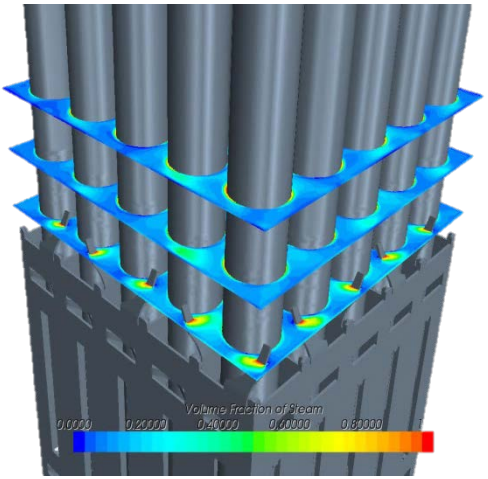
- From Experience
  - Leverage lessons learned in previous attempts (method)
  - State-of-the-art as baseline (reference solution)
  - Focus on hardened simulation capability (industrial relevance)
- New Approach
  - Separation of Framework and Modeling
  - Builds on existing strengths, models and code testing
  - Built-in minimal redundancy
  - Piece-by-piece approach
  - Targeted Work on critical components

PSBT Benchmark - 2010



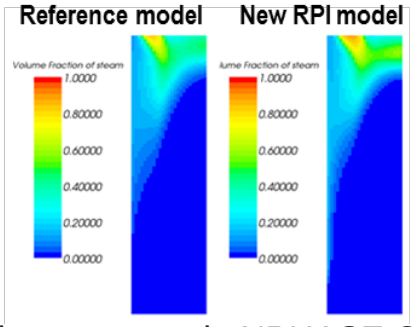
V. Petrov et al.

The approach: physics based, robust, and assessable

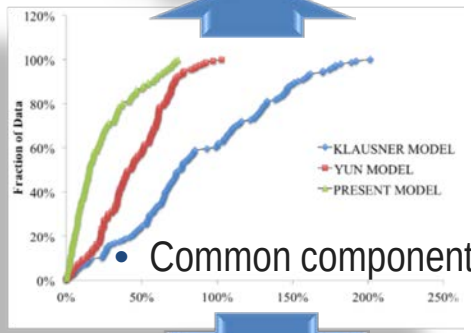


- Baseline Boiling Model Validated vs. PSBT International Benchmark

Step-1

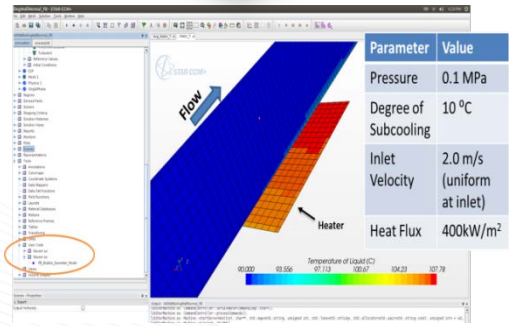


- Advancement via NPHASE Closure

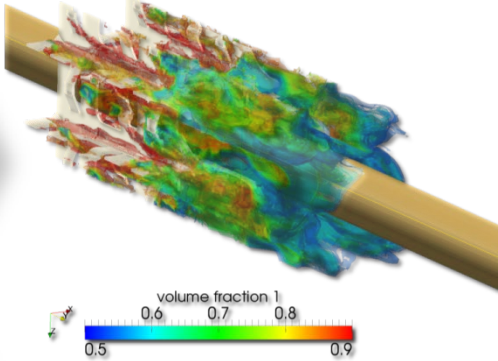


- Common components

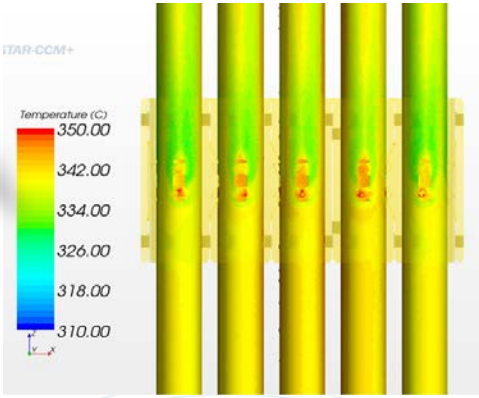
Step-2



- New MIT Closure



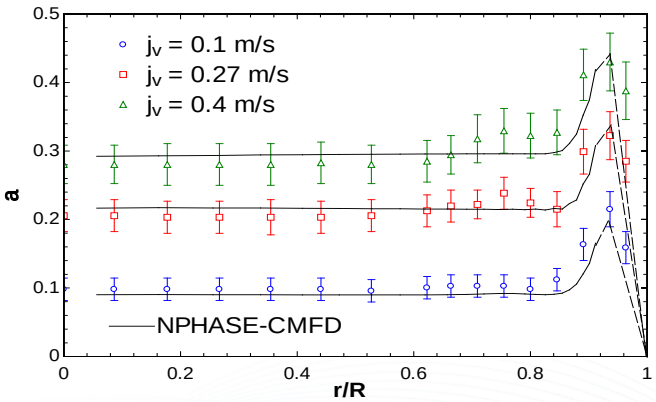
- Pre-validated models available in Hydra-TH

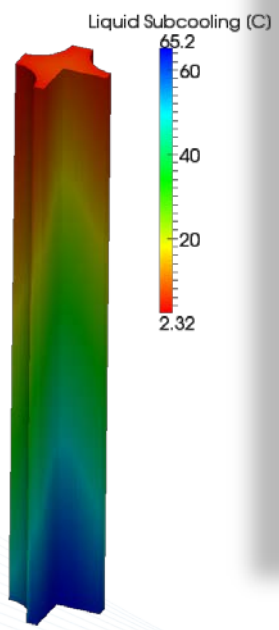


- Immediately available for production use

A Robust Reference Closure for Step-1

- Evaluate a reference closure without code effects
- Leverage extraordinary experience at RPI
- Testing in STAR-CCM+ for immediate accessibility





RPI MODEL

BUBBLE FORCES

Drag force

(1) $\vec{F_D} = -\frac{3}{4}\frac{C_D}{D_b}\alpha\rho_l|\vec{u}_v - \vec{u}_l|(\vec{u}_v - \vec{u}_l)$ — Eq. (1) in Ref. [1]; Eq. (4) in Ref. [2]

(2) $C_D = \frac{24}{Re_b}\left(1 + 0.092Re_b^{0.78}\right)$ — Eq. (2) in Ref. [1]

(3) — Eq. (5) in Ref. [2]

(4) $C_D = \frac{24}{Re_b}(1 + 0.1Re_b)^{0.75}$ — Slide (9) in Ref. [3]

(5) $Re_b = \frac{\rho_l|\vec{u}_v - \vec{u}_l|D_b}{\mu_b}$ — Eq. (3) in Ref. [1]

(6) $F_D = -\frac{3}{4}\frac{C_D}{d_b}\alpha\rho_l u_r^2$ — Slide (4) in Ref. [3]

Lift force

(7) $\vec{F_L} = -C_L\alpha\rho_l|\vec{u}_v - \vec{u}_l| \times (\vec{\nabla} \times \vec{u}_l)$ — Eq. (5) in Ref. [1]

with $C_L = 0.03$ — Ref. [3]

The lift force is acting in the axial direction and takes the form:

(8) $F_L = -C_L\alpha\rho_l u_r\frac{du_r}{dr}$ — Slide (5) in Ref. [3]

Turbulent dispersion force

(9) $\vec{F}_{TD} = -C_{TD}\alpha\rho_l\bar{\bar{k}}_l\nabla\alpha$ — Eq. (6) in Ref. [1]

The turbulent dispersion force is acting in the radial direction. After some manipulations, it becomes:

(10) $F_{TD} = -C_{TD}\alpha\rho_l\frac{d}{dr}[k(1-\alpha)]$ — Slide (5) in Ref. [3]

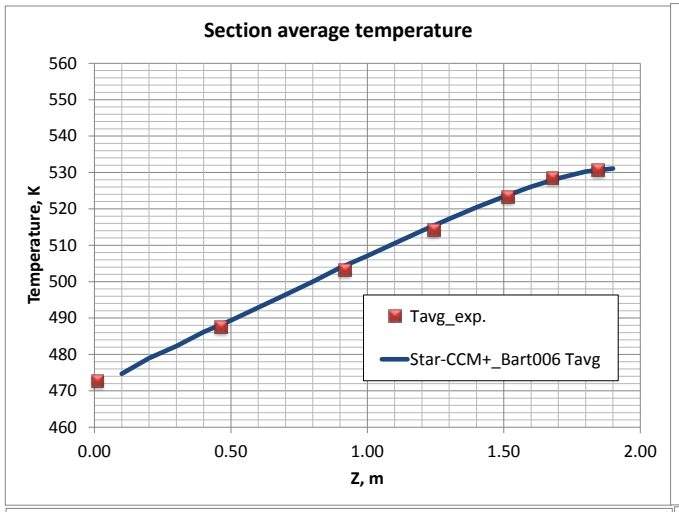
Comparison STAR-CCM+ (reference model) vs Bartolomei experiment and NPHASE

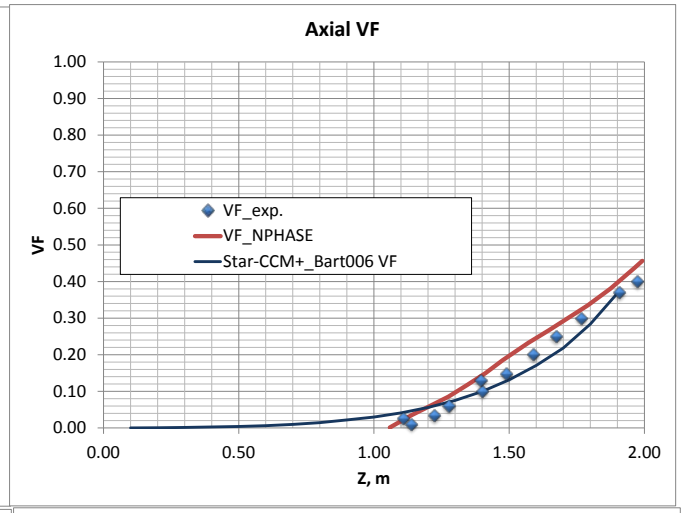
Hydrodynamics:

Lift force (C_L = 0.03), Drag, Virtual Mass, Turbulent Dispersion Forces

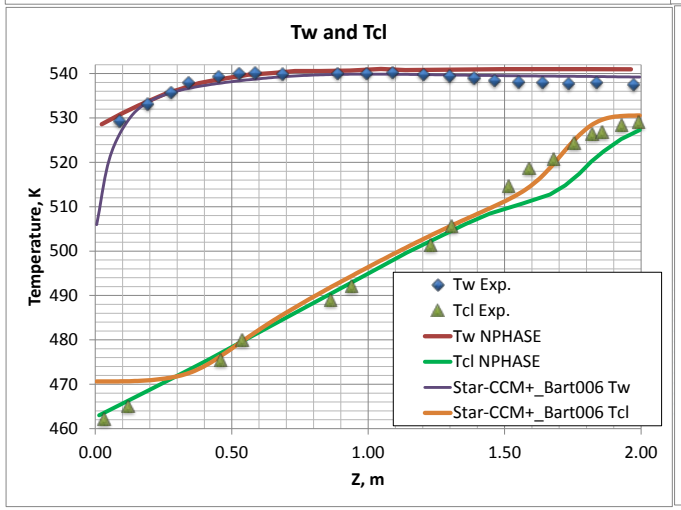
Two-phase flow model:

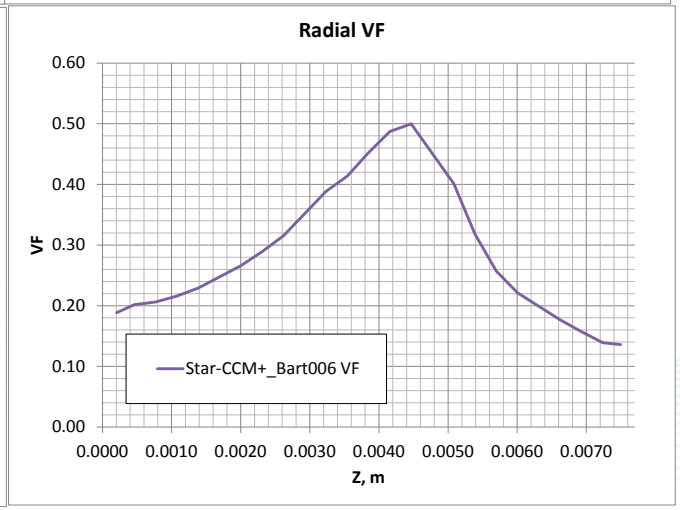
Bubble diameter in the bulk => constant (0.75 mm; interfacial area assuming spherical bubbles)
Heat partitioning => old RPI model (three components of heat flux)
heat transfer from interface to liquid => Ranz-Marshall correlation
Bubble departure diameter => Tolubinski Konstanchuk correlation
Bubble departure frequency => Cole correlation
Nucleation site density => Lemmer-Chawla correlation



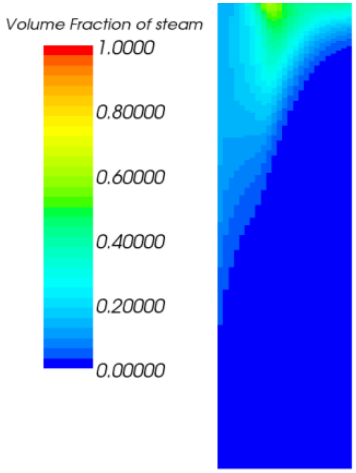


run Bart006 = CCM+ reference model With this combination of models available within STAR-CCM+ the best agreement for the Bartolomei's data could be obtained





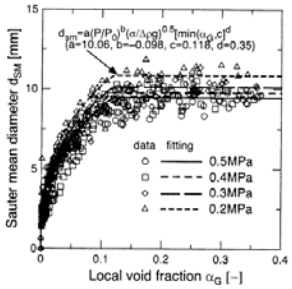
Reference model

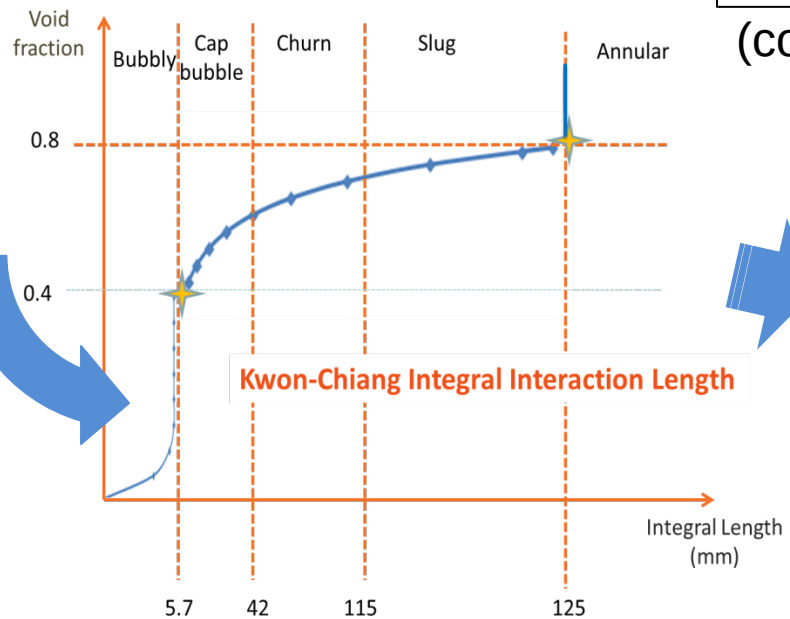


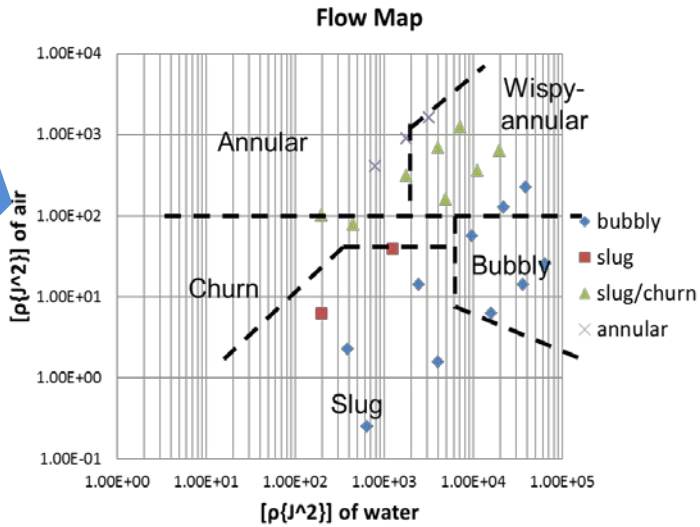
Hardened Hydrodynamics Closure

- A robust closure formulation is required for PWR conditions
- *Robust* requires realistic physics (don't always blame Mark)

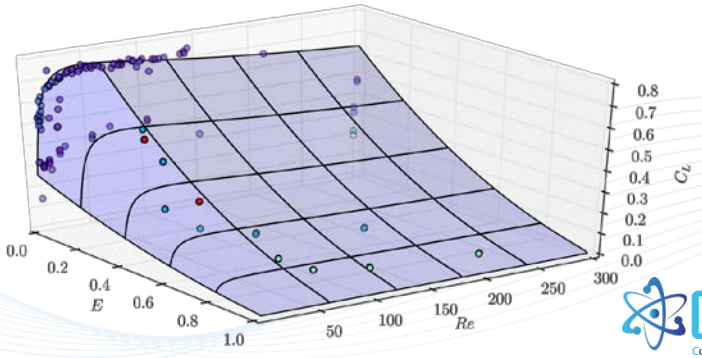
Each region adopts specific Lift and Drag Formulations (continuous)







- A new lift force closure for multiphase CFD
  - Lift force decreases as bubble approaches walls
  - Should eliminate the need for an ad-hoc wall-force

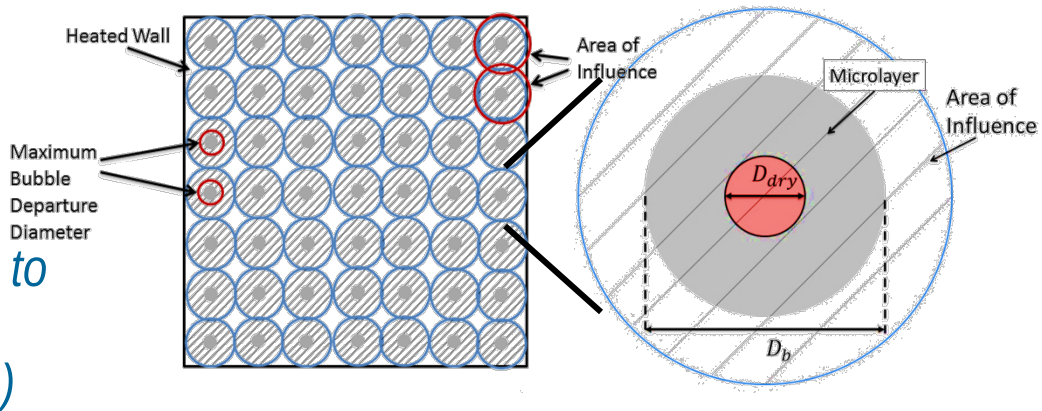


Novel Mechanistic Flow Boiling Model (Step-2)

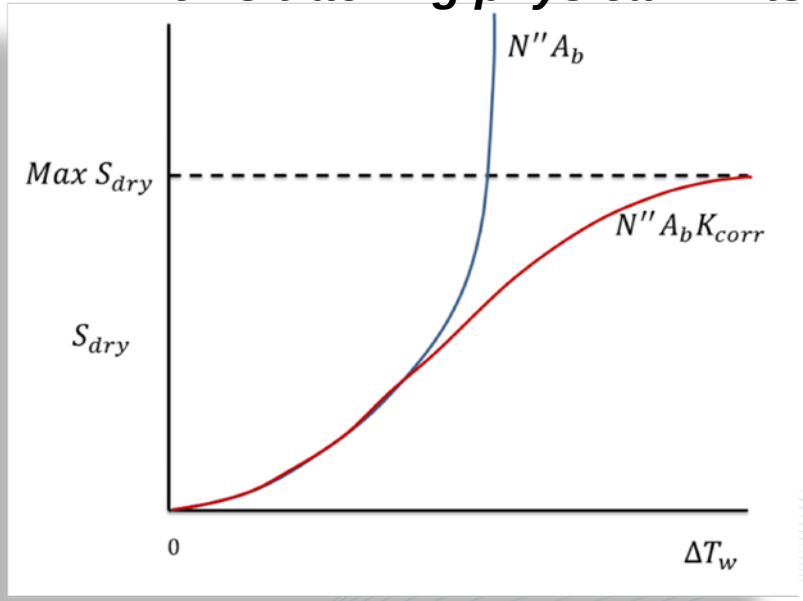
Key Components

Effects of bubble crowding

- *Current models are strongly sensitive to active nucleation site density (require the use of experienced based limiters)*
- *Built in crowding effect eliminates need for limiters*
- *Prediction of dry surface can be directly verified against experimental measurements*
- *DNB can be expressed as the limit of this behavior*
- *Potentially local/scalable model for DNB*



- ***Allows tracking physical limits***



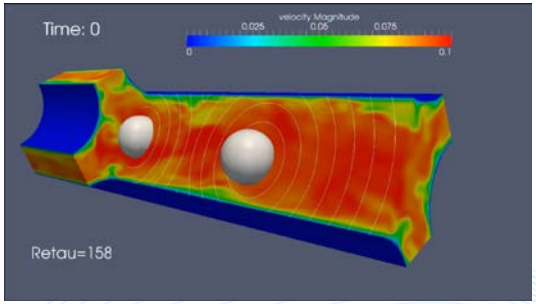
Summary & Future Directions

Summary

- Methods for computing drag/lift using ITM/DNS are providing new insights for momentum closure exchange
- Experiments at MIT, TAMU and CCNY, using combination of IR thermometry, PIV, LIF and HSV, are generating a complete database for development and validation of closure models
- Emergent closure models for momentum exchange, heat flux partitioning for sub-cooled boiling
- Innovative projection-based fully-implicit flow solution algorithms developed for accuracy, stability efficiency for single and multiphase flows

Future Directions

- Demonstration of multiphase boiling flow with Hydra-TH in realistic subchannels with mixing vanes using "vetted" THM closure models
- Continue single-phase V&V, begin multiphase CFD assessment, verification and validation
- Advanced multiphase closures and sub-cooled boiling models
- Advanced turbulence models for single/multiphase flow
- ITM/DNS simulations in support of turbulence closures, model development for momentum/boiling closures
- Coupled physics in VERA with Hydra-TH
- Experimental data used to improve subcooled boiling models
- Extreme-scale computing with Hydra-TH using GPUs on TITAN (time and funding permitting)



Bolotnov, NCSU

THM Roadmap – Towards 2020

- Focus shifts more towards safety, e.g.,
  - Reactivity Initiated Accidents (RIA)
  - Loss-of-coolant accidents (LOCA)
  - Re-flooding events
  - Will require heavy investment in development/testing of multiphase closure models
  - Requirements for documentation, testing, and delivery will increase as the Hydra-TH user base expands

SCOPE OF SIMULATION	LOCA	RIA
Fuel Rod Interaction	• Coolant channel blockage due to ballooning, including co-planar effects	• DNB propagation
Core Including 3D Effects	• Reflood heat transfer • Entrainment • Droplet and grid effects	• Open channel T/H • Boiling and coolant expansion
Vessel Including 3D Effects	• Flow distribution and flashing during blowdown • Downcomer boiling • Boron transport • Dispersed fuel transport and cooling	• Boiling and coolant expansion
Loop Effects	• Steam generator heat transfer • Dispersed fuel transport and cooling • Boron transport	• Steam generator heat transfer

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A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

Validation Data Needs to Support Validation of VERA ModSim Capabilities for Challenge Problems

CASL has an extensive validation activity

- To support development of advanced models and codes
- To assess maturity of predictive capability

  - Benchmark work performed by code team
    - *Each Focus Area: THM, MPO, RTM*
    - *Each VERA Component*

  - Assessment work performed by AMA team
    - *Selected VERA component against a set of SET data*
    - *Coupled VERA component against selected IET data*

  - Yet, the validation scope is deficient relative to domain of Challenge Problems due to a lack of needed data

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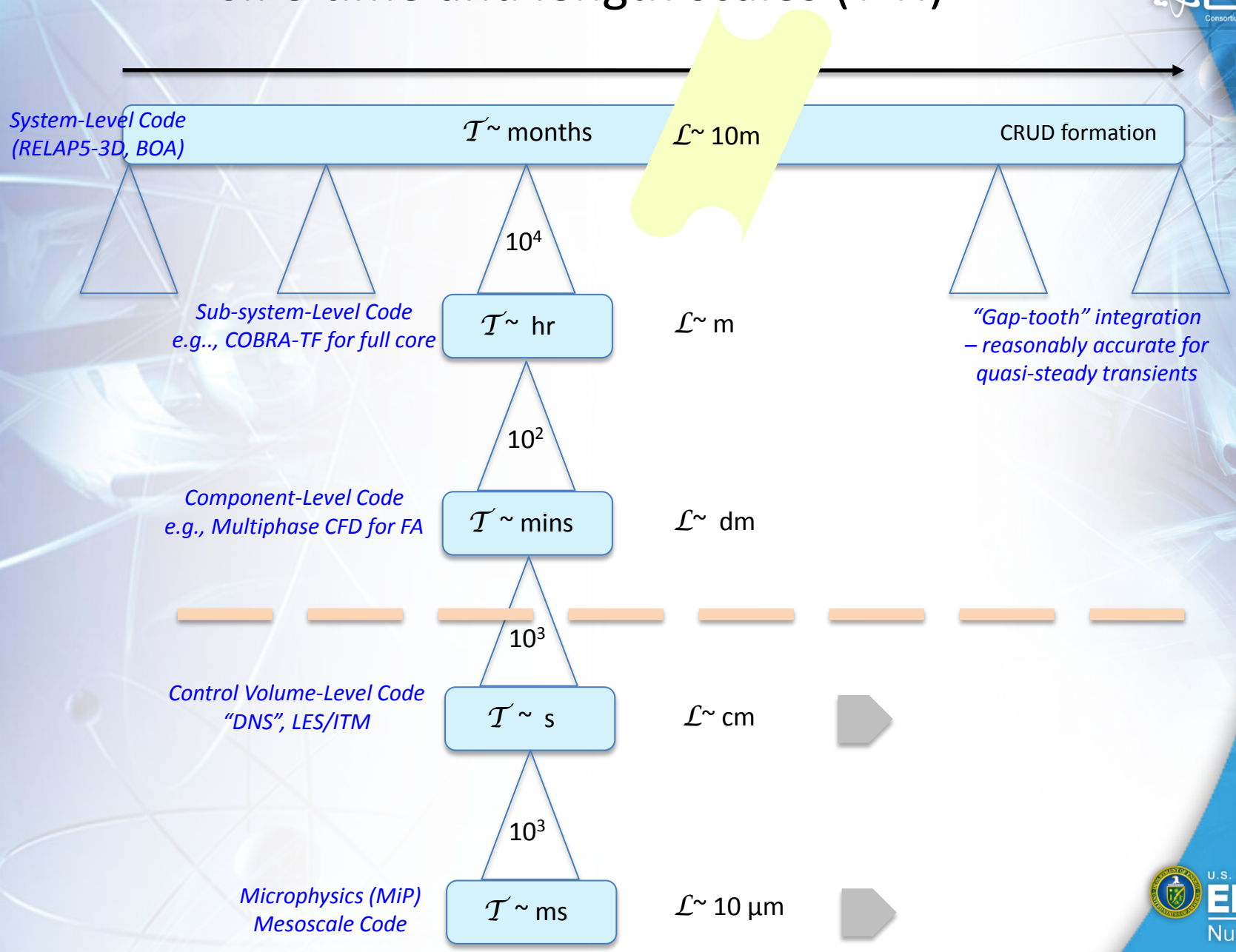
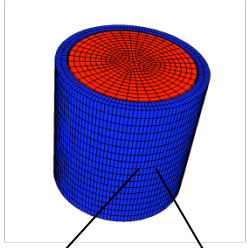
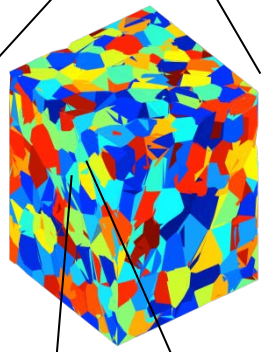
Challenge Problems (CP) & associated solution methods define validation data needs

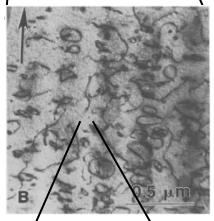
- CRUD (CRUD Induced Power Shift / CRUD Induced Localized Corrosion)
  - Inform PWR core CRUD risk assessment for margin management decisions; reduce uncertainty in CRUD thickness & boron uptake predictions
- GTRF / FAD (Grid-To-Rod Fretting / Fuel Assembly Distortion)
  - Inform fuel assembly structural features, materials, and geometry relationship to fuel system performance; identify core locations and geometric characteristics contributing to flow conditions impacting fuel structural stability
- PCI (Fuel Pellet Clad Interaction)
  - Predict cladding stress and strain, inform margins imposed, and inform fuel pellet-clad geometry relationship to performance during a power maneuver
- DNB (Departure from Nucleate Boiling)
  - Identify sources of conservatism and margin in current practices for typical reload DNB evaluations and on specific DNB correlation calibration experiments
- Cladding Integrity during a LOCA
  - Assess fuel performance during a LOCA and identify sources of conservatism and margin
- Cladding Integrity during a RIA
  - Assess fuel performance during a RIA transient and identify sources of conservatism and margin

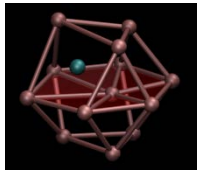
CIPS time and length scales (T-H)











Finite element fuel rod thermal-mechanical code (Peregrine)

MACRO

Constitutive response from
Visco Plastic Self Consistent (VPSC)
polycrystal plasticity model for irradiation growth & creep

POLYCRYSTAL

SINGLE CRYSTAL PHYSICAL LAW

Model for irradiation growth based on nucleation & evolution of dislocation loops

Model for thermal & irradiation creep based on dislocation climb & glide

STATE OF THE ART ATOMISTIC CALCULATIONS

SINGLE CRYSTAL

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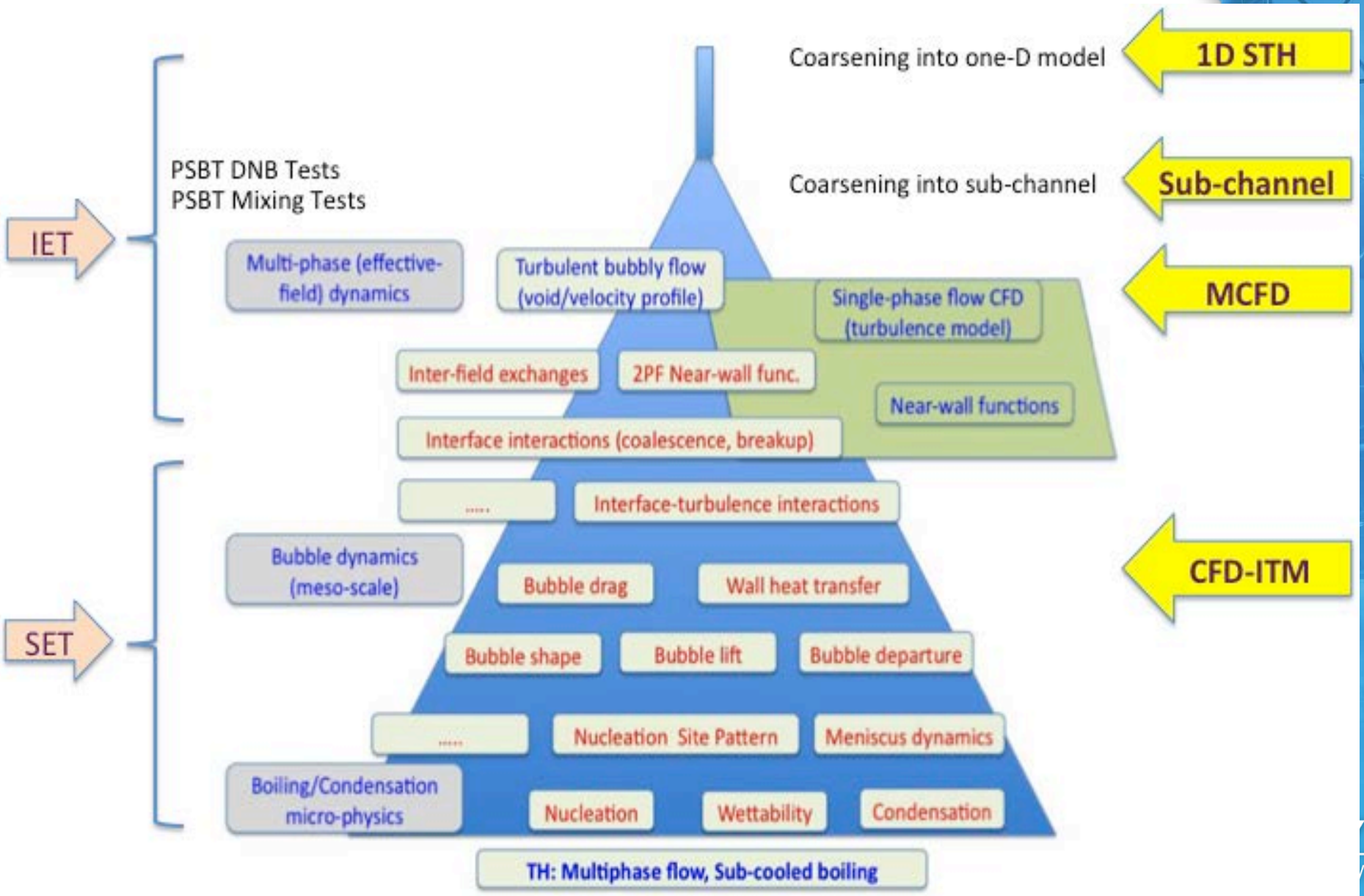
Experiments and Predictive Capability in T-H

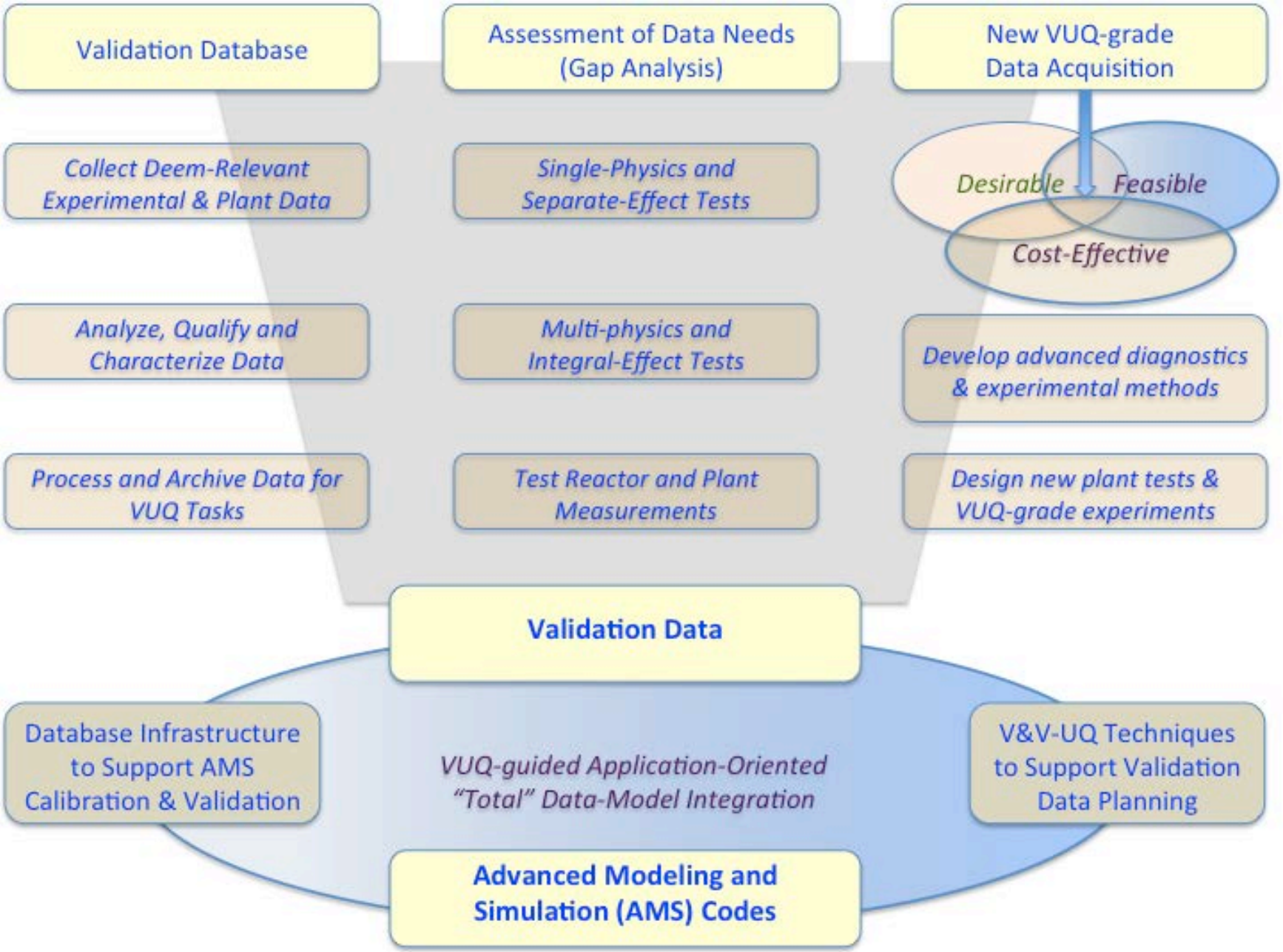


What's different from past validation data?

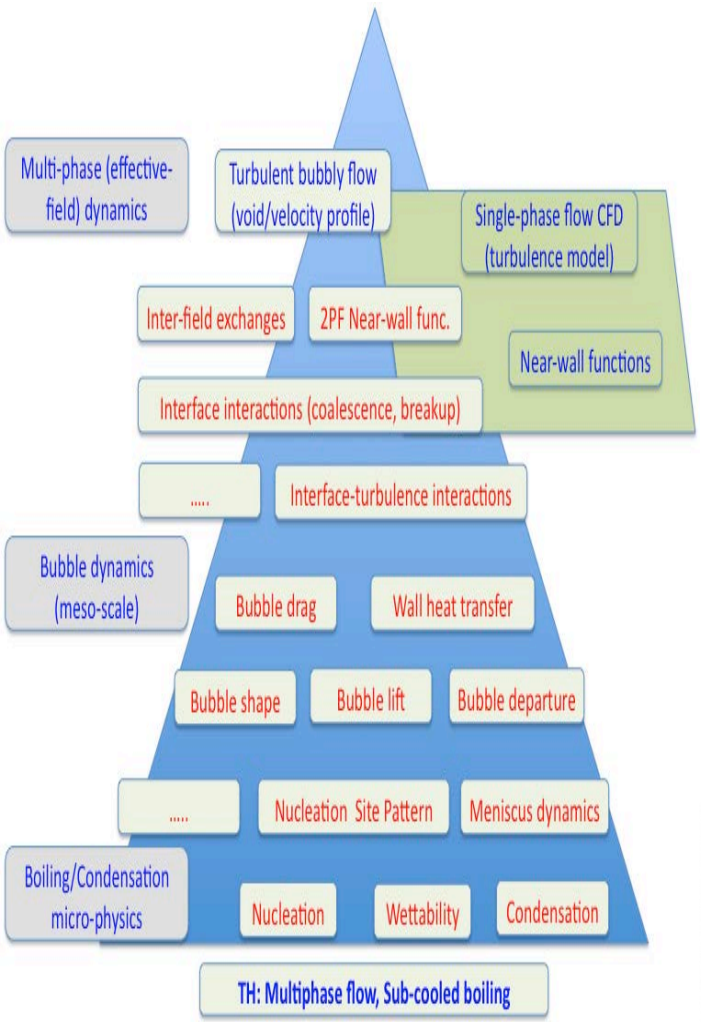
- CASL ModSim involves a wide range of spatial and time scales versus working mainly at the engineering level
  - CASL has identified gaps in data particularly at the lower (micro) scale level, requiring new experiments and development of the associated new instrumentation
  - Multi-physics (effect) modeling and coupling are CASL trademark but also present a VUQ-weaker link

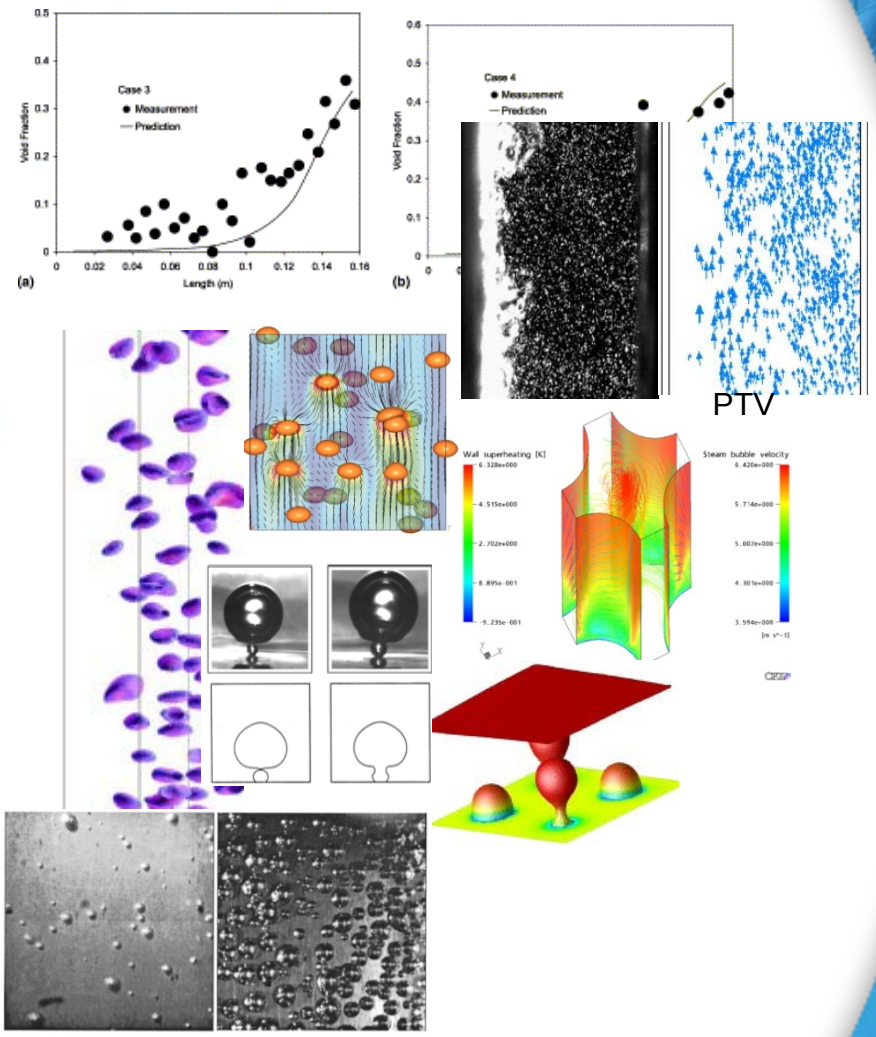
Lower scale experiments sometimes can be accomplished in less costly academic research laboratories

CASL Approach to Validation Data Support



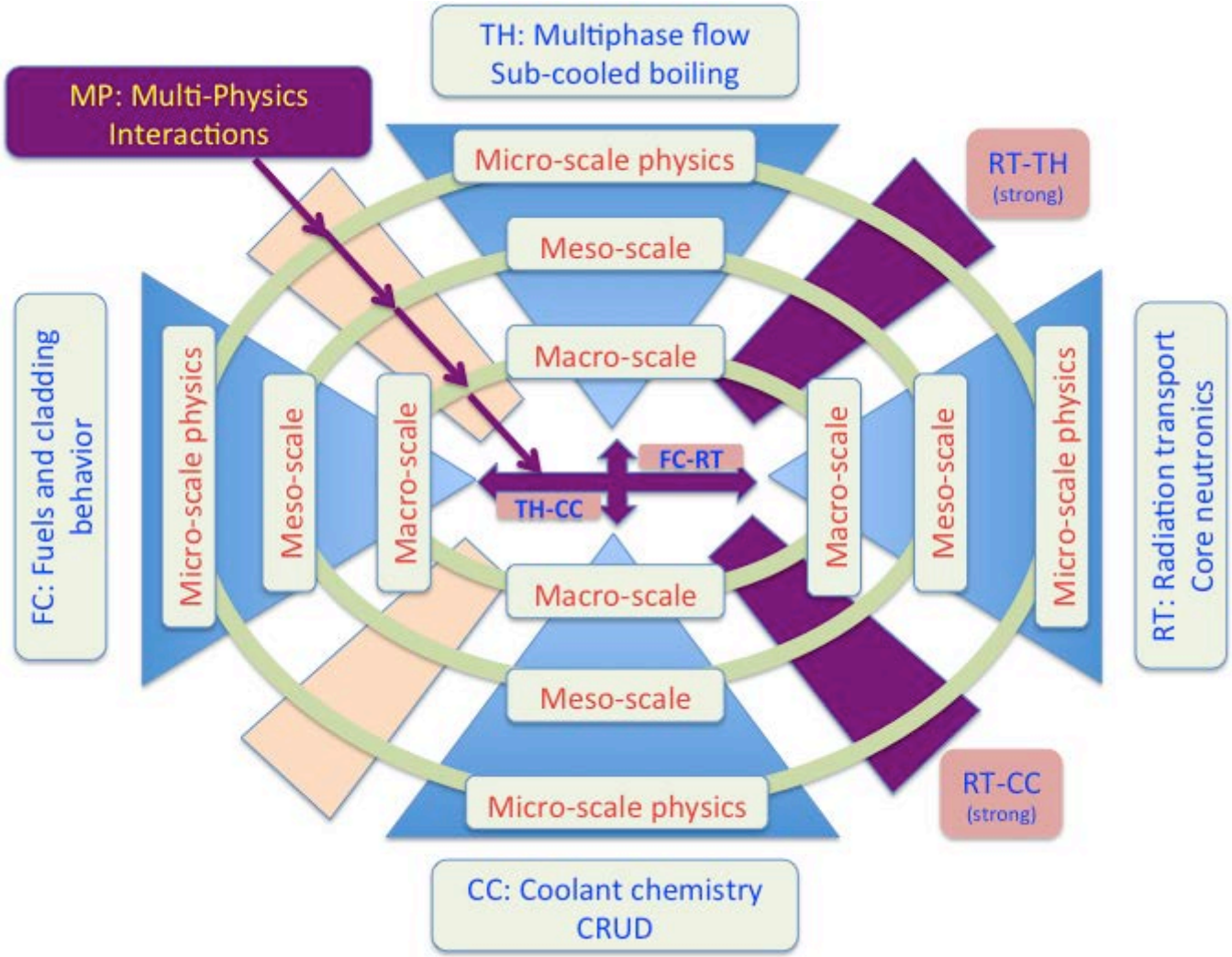
Subcooled Boiling Flows – Data Collection and Characterization





- **Data heterogeneity**: (i) measurement data available at the "system" level – left-most panel – and also at the "sub-model" level – nucleation site density, bubble detachment rate/radius, etc. Missing data at some levels; (ii) differences in data scalability, relevancy and uncertainty.

Example:
CRUD Multi-Physics, Multi-Scale Pyramid



A Survey of CASL SMEs was completed to Capture Validation Data Needs

- Assessment of Overall Status of Validation Data
  - Identify existing Critical Datasets
  - Assessment of Quality of Critical Datasets *currently used for VUQ*
- Identify areas where additional experimental data would make a large impact for CASL to achieve its goal
  - Identify classes of new experiments and experimental data that are most desirable (e.g., having potential to help reduce large uncertainty)
  - Assess technical challenges to deliver desirable datasets

Example: **CRUD Challenge Problem Data Needs Survey**:
- Identified 12 major existing sources of data for validation
- Identified 12 gap areas where data are needed

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Validation Data Gaps

- Gaps between high-fidelity models and data:
  - CRUD physico-chemistry
  - Two-phase thermal-hydraulics
    - Subcooled flow boiling and DNB
  - Fuel and cladding behavior
  - …

- Critical gaps:
  - Data to calibrate multi-physics effect models and to validate coupled multi-physics simulation
    - e.g., TH-CRUD interface

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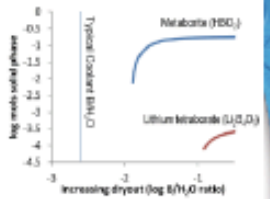
CPIs/SMEs to Identify Needed Validation Experiments

- Challenge Problem defining need
- VERA components to be validated
- What experiment is measuring and conditions of experiment
- Importance of experiment
- Experimental classification
  - Single Effect Test (SET)
  - Integral Effect Test (IET)
  - Reactor Experimental Test (RET)
- Difficulty of performing test
- Approximate cost of test
- Applicability of test to academic research lab

CRUD-1: Crud deposition thermo-dynamics

Description of Experiment

- Measure the composition of deposited crud as the concentration of corrosion products is varied (Ni, Fe, Cr) over a range of temperatures and heat fluxes typical of PWR operating conditions



Plot of increasing dryout resulting in predicted metaborite formation.

Experimental Conditions

- Single heated rod loop at PWR operating conditions and heat fluxes.

ModSim Components Being Validated

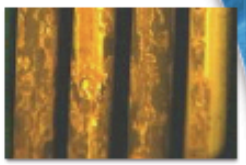
- VERA component MAMBA
- Thermodynamics of crud deposition

- *Importance of Experiment:* High
- *Difficulty of Experiment:* Moderate
- *Type of Experiment:* SET
- *Cost of Experiment:* $0.4M
- *Suitable for Academic Lab:* Yes, although existing industry facilities are already available

CRUD-2: Chemical Reactions in Crud

Description of Experiment

- Measure the material precipitated under elevated concentrations of boric acid and lithium hydroxide in PWR conditions
- Perform autoclave testing to determine what materials precipitate when H3BO3 and LiOH are concentrated to high levels at PWR operating



Experimental Conditions

- PWR conditions – 2250 psi, 650 F, varying concentration of H2BO3 and LiOH

ModSim Components Being Validated

- VERA component MAMBA
- Chemical reactions leading to boron deposition in crud

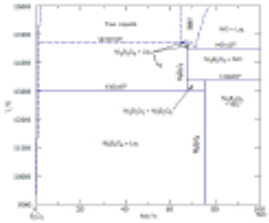
- *Importance of Experiment:* High
- *Difficulty of Experiment:* Moderate
- *Type of Experiment:* SET
- *Cost of Experiment:* $0.2M
- *Suitable for Academic Lab:* Yes*

* Industry also has appropriate testing facilities available

CRUD-3: Composition of Complex Spinel or other oxide phases in CRUD

Description of Experiment

- Phase equilibria studies of model spinel and other phases, such as complex borates, in CRUD. This involves preparation of phase compositions and determination of phase equilibria using x-ray diffraction and microanalysis. Calorimetry and other thermophysical measurements to determine solid solution energies.



Experimental Conditions

- Phase formation can be examined under laboratory conditions that are non-aqueous in order to determine possible phase formation. CRUD simulation can be used to confirm phase formation

ModSim Components Being Validated

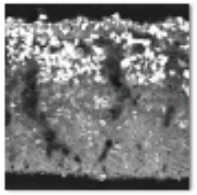
- Data for MAMBA-BDM simulation of CRUD growth and composition

- *Importance of Experiment:* High Understanding composition can guide controlling chemistry
- *Difficulty of Experiment:* Moderate, but will require considerable effort
- *Type of Experiment:* SET Thermophysical/chemical measurements (calorimetry, xrd)
- *Cost of Experiment:* $0.4M
- *Suitable for Academic Lab:* Yes

CRUD-4: Crud deposition efficiency as a function of sub-cooled boiling rate

Description of Experiment

- Measure the efficiency of deposition of particulate and soluble material on heated surfaces undergoing sub-cooled boiling. Vary the liquid concentration of corrosion products and the sub-cooled boiling rate and measure the crud deposition rate.



Experimental Conditions

- Preferably at PWR conditions, however it may be acceptable to do the testing at lower pressures and temperatures.

ModSim Components Being Validated

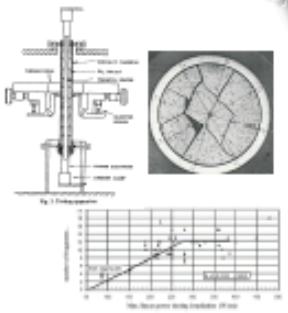
- VERA component MAMBA
- Mass of crud deposited as a function of coolant corrosion product concentration and sub-cooled boiling rate

- *Importance of Experiment:* High
- *Difficulty of Experiment:* Moderate
- *Type of Experiment:* SET
- *Cost of Experiment:* $0.2M
- *Suitable for Academic Lab:* Yes

PCI-1: Fuel Pellet Cracking and Relocation Studies Out-of-Pile SETs

Description of Experiment

- Experiment would evaluate pellet cracking and fragment movement during normal operation. UO_2 fracture behavior and frictional interaction between pieces would be studied under representative thermal and stress conditions.



Experimental Conditions

- Separate effects test using electrically heated pellets to obtain fracture characteristics and crack roughness parameters

ModSim Components Being Validated

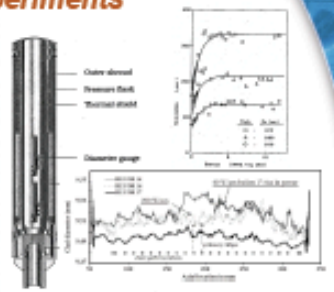
- VERA component Peregrine
- Stress and morphology that leads to cracking
- Dynamic effect of cracked body response in thermal gradient

- *Importance of Experiment:* High
- *Difficulty of Experiment:* Moderate
- *Type of Experiment:* SET
- *Cost of Experiment:* $1-2 M
- *Suitable for Academic Lab:* Yes

PCI-2: Fuel Pellet Cracking and Relocation Studies In-Pile Integral Experiments

Description of Experiment

- Measure pellet-cladding mechanical interaction during in-pile power maneuvers to evaluate gap closure and pellet mechanical compliance. Experiment would evaluate pellet cracking and fragment movement during normal operation.



Experimental Conditions

- Single rod experiments under different burnup, peak power, and power ramp rates
- On-line diameter measurements, thermocouple measurements,

ModSim Components Being Validated

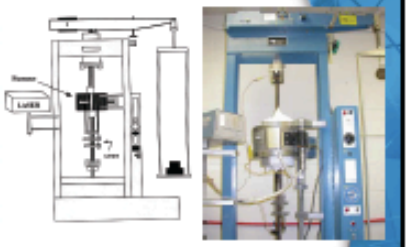
- VERA component Peregrine
- Model parameters describing the fracture and movement of pellet fragments

- *Importance of Experiment:* High
- *Difficulty of Experiment:* High
- *Type of Experiment:* SET/ IET/RET
- *Cost of Experiment:* $5-10 M
- *Suitable for Academic Lab:* No. Integral test in Halden

PCI-3: Zr-Alloy Multi-axial Thermal Creep Tests Out-of-Pile SETs

Description of Experiment

- Multi-axial stress tests to characterize cladding tube thermal creep behavior as function of material constituents, stress ratio, temperature, etc.



Experimental Conditions

- Normal operating temperature, variable microstructure, alloying elements, and stress levels

ModSim Components Being Validated

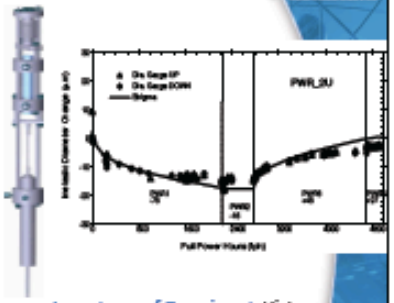
- VERA component Peregrine
- Thermal creep rate model on unirradiated material

- *Importance of Experiment:* High
- *Difficulty of Experiment:* Moderate
- *Type of Experiment:* SET
- *Cost of Experiment:* $1 M
- *Suitable for Academic Lab:* Yes

PCI-4: Zr-Alloy Multi-axial Thermal Creep Tests In-Pile Integral Experiments

Description of Experiment

- Multi-axial stress tests to characterize cladding tube irradiation-induced creep (athermal and thermal) behavior under conditions of fast neutron flux and fluence



Experimental Conditions

- Normal operating temperature, variable microstructure, alloying elements, stress levels, and fast flux/fluence

ModSim Components Being Validated

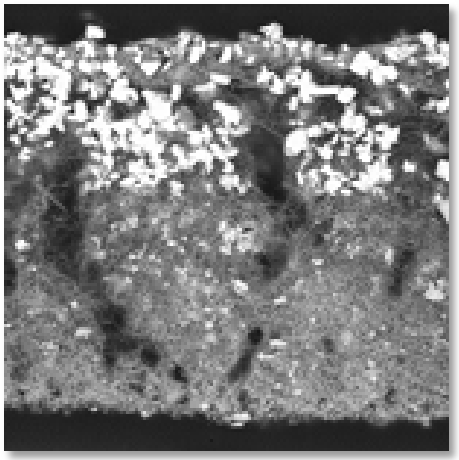
- VERA component Peregrine
- Thermal creep rate model for irradiated material

- *Importance of Experiment:* High
- *Difficulty of Experiment:* High
- *Type of Experiment:* SET and IET
- *Cost of Experiment:* $5 M
- *Suitable for Academic Lab:* No. Requires irradiation environment

CRUD-4: Crud deposition efficiency as a function of sub-cooled boiling rate

Description of Experiment

- Measure the efficiency of deposition of particulate and soluble material on heated surfaces undergoing sub-cooled boiling. Vary the liquid concentration of corrosion products and the sub-cooled boiling rate and measure the crud deposition rate.



Experimental Conditions

- Preferably at PWR conditions, however it may be acceptable to do the testing at lower pressures and temperatures.

ModSim Components Being Validated

- VERA component MAMBA
- Mass of crud deposited as a function of coolant corrosion product concentration and sub-cooled boiling rate

- *Importance of Experiment: High*
- *Difficulty of Experiment: Moderate*
- *Type of Experiment: SET*
- *Cost of Experiment: $0.2M*
- *Suitable for Academic Lab: Yes*

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PCI-2: Fuel Pellet Cracking and Relocation Studies In-Pile Integral Experiments

Description of Experiment

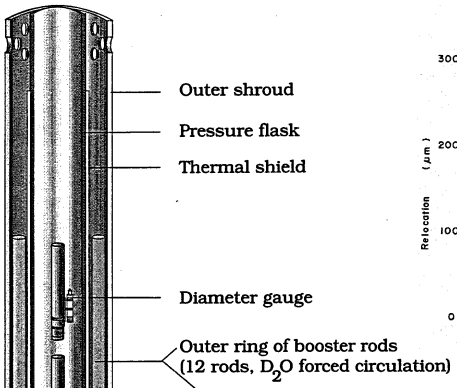
- Measure pellet-cladding mechanical interaction during in-pile power maneuvers to evaluate gap closure and pellet mechanical compliance. Experiment would evaluate pellet cracking and fragment movement during normal operation.

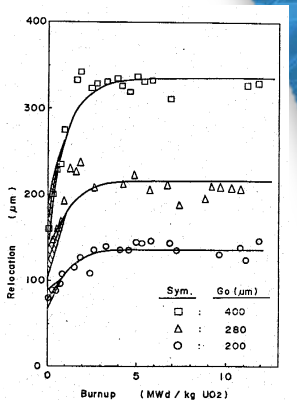
Experimental Conditions

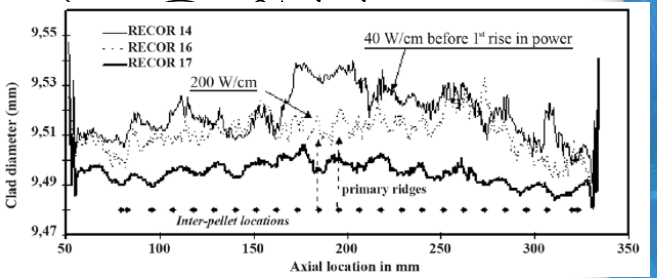
- Single rod experiments under different burnup, peak power, and power ramp rates
- On-line diameter measurements, thermocouple measurements,

ModSim Components Being Validated

- VERA component Peregrine
- Model parameters describing the fracture and movement of pellet fragments







- *Importance of Experiment:* *High*
- *Difficulty of Experiment:* *High*
- *Type of Experiment:* *SET/ IET/RET*
- *Cost of Experiment:* *$5-10 M*
- *Suitable for Academic Lab:* *No. Integral test in Halden*

Summary of CASL's Needed Validation Experiments

Challenge Problem	# of proposed critical exp.	Types of Test	Total Cost	Execution Difficulty
CIPS	7	6 SET, 1 IET	$4 M	Medium
CILC	3	2 SET, 1 IET	$2M	Medium
GTRF	5	3 SET, 1 IET, 1 RET	$3M	Medium
PCI	5	1 SET, 1 RET, 2 IET	$15M	High
DNB	4	3 SET, 1 IET/RET	$5M	Medium
RIA	3	1 SET/RET, 2 IET/RET	$12M	High
LOCA	4	2 SET, 1 IET, 1RET	$4M	Medium

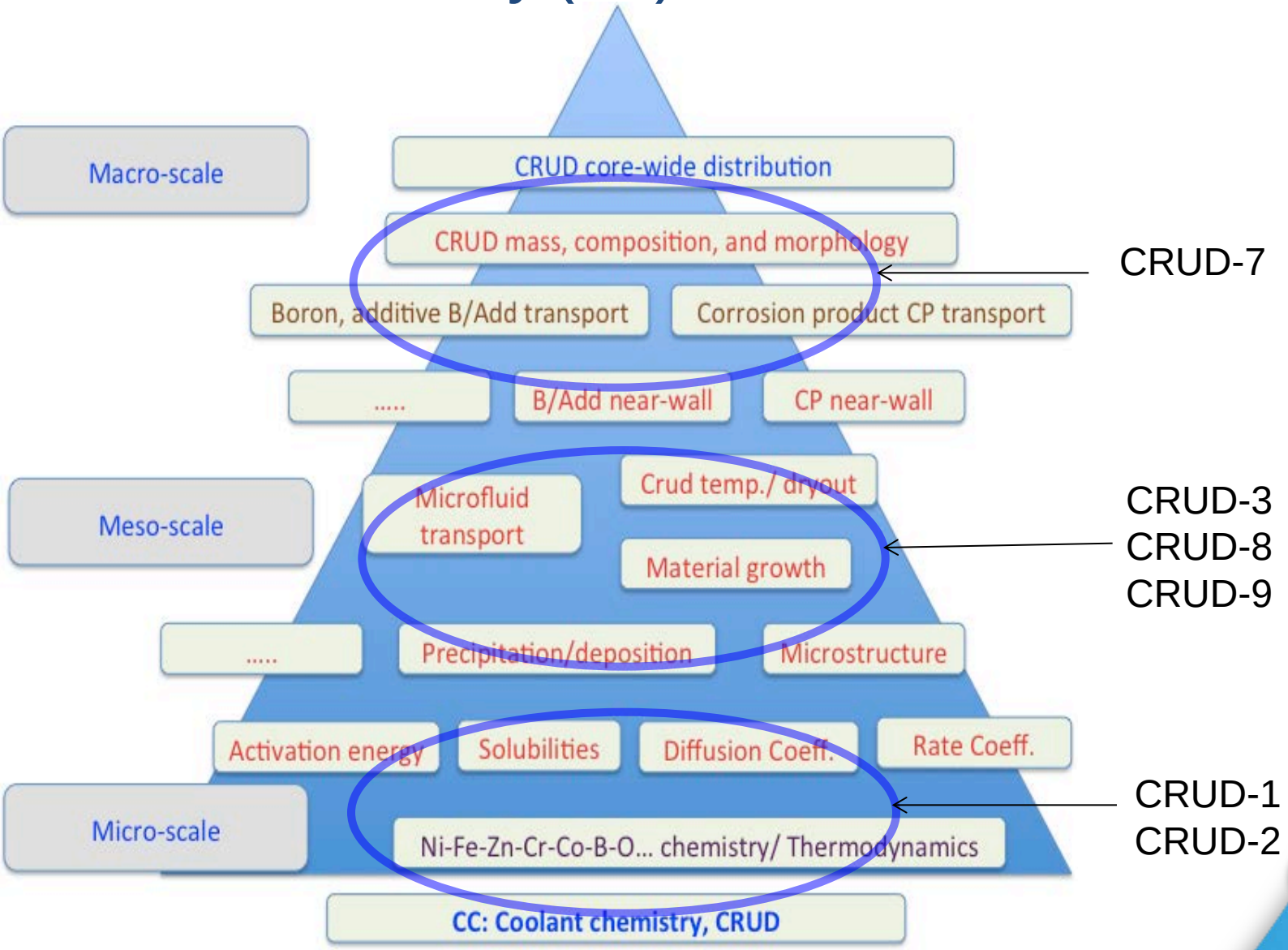
Σ~ $45M

Summary of CASL's Highest Priorities for Validation Experiments

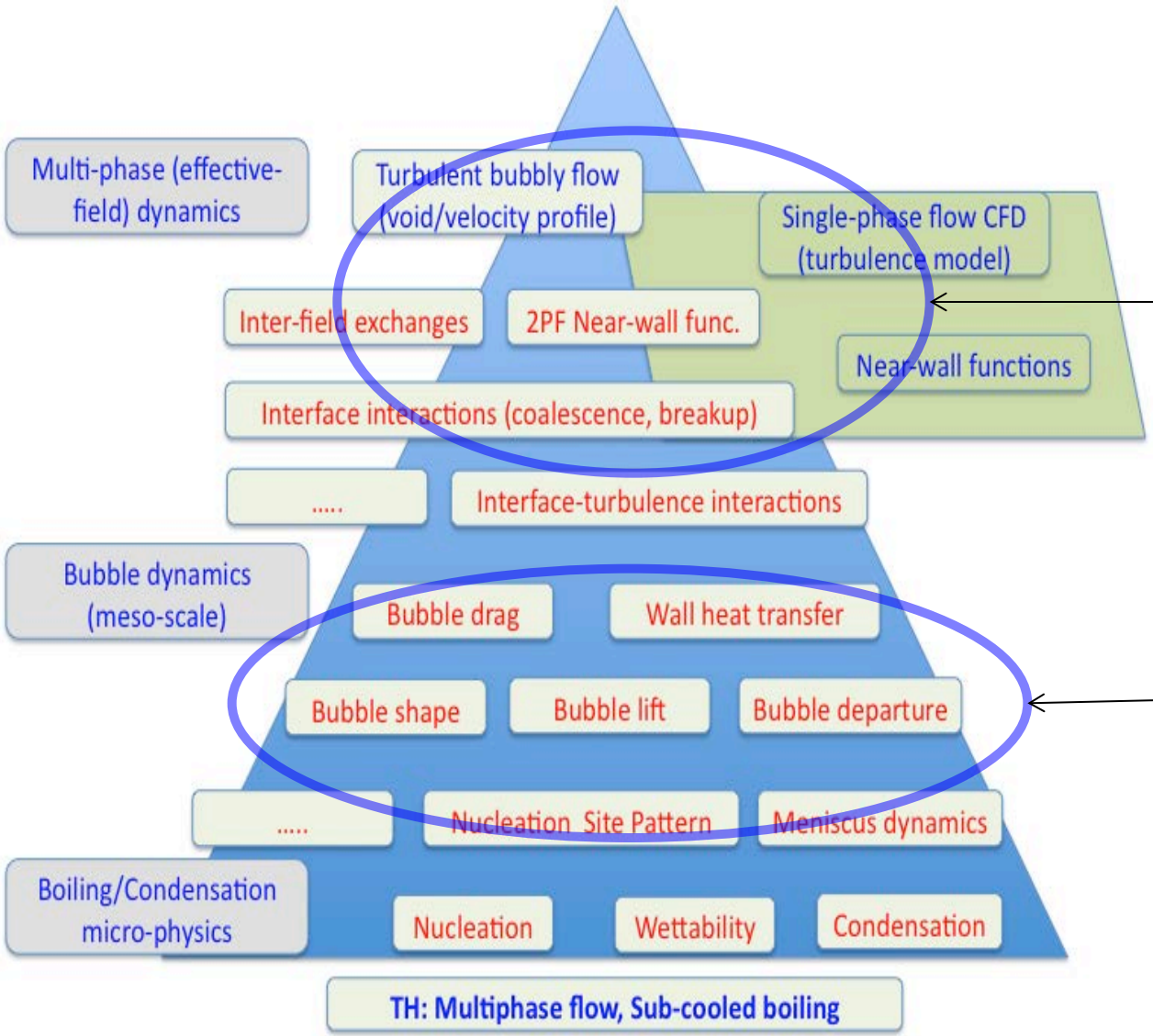
Validation Experiments	Quantities of Interest	Experiment's Conditions	Approximate Cost	Execution Difficulty
CRUD-7	Crud mass	Fuel assembly	$0.8M	Medium
CILC-1	Failure condition	Single rod test	$0.2M	Medium
GTRF-1	Wear rate	High temp	$0.5M	Medium
PCI-1, PCI-2	Pellet cracking	In-pile & out	$5+M	High
DNB-2	DNB location	High P, T, q	$1M	Medium
RIA-1	Fuel Incipient Melting	Power Surge	$3M	High
LOCA-1	Cladding behaviors	Prototypic	$2M	High

One for each Challenge Problem

Validation Experiments Coverage – Coolant Chemistry (CC)



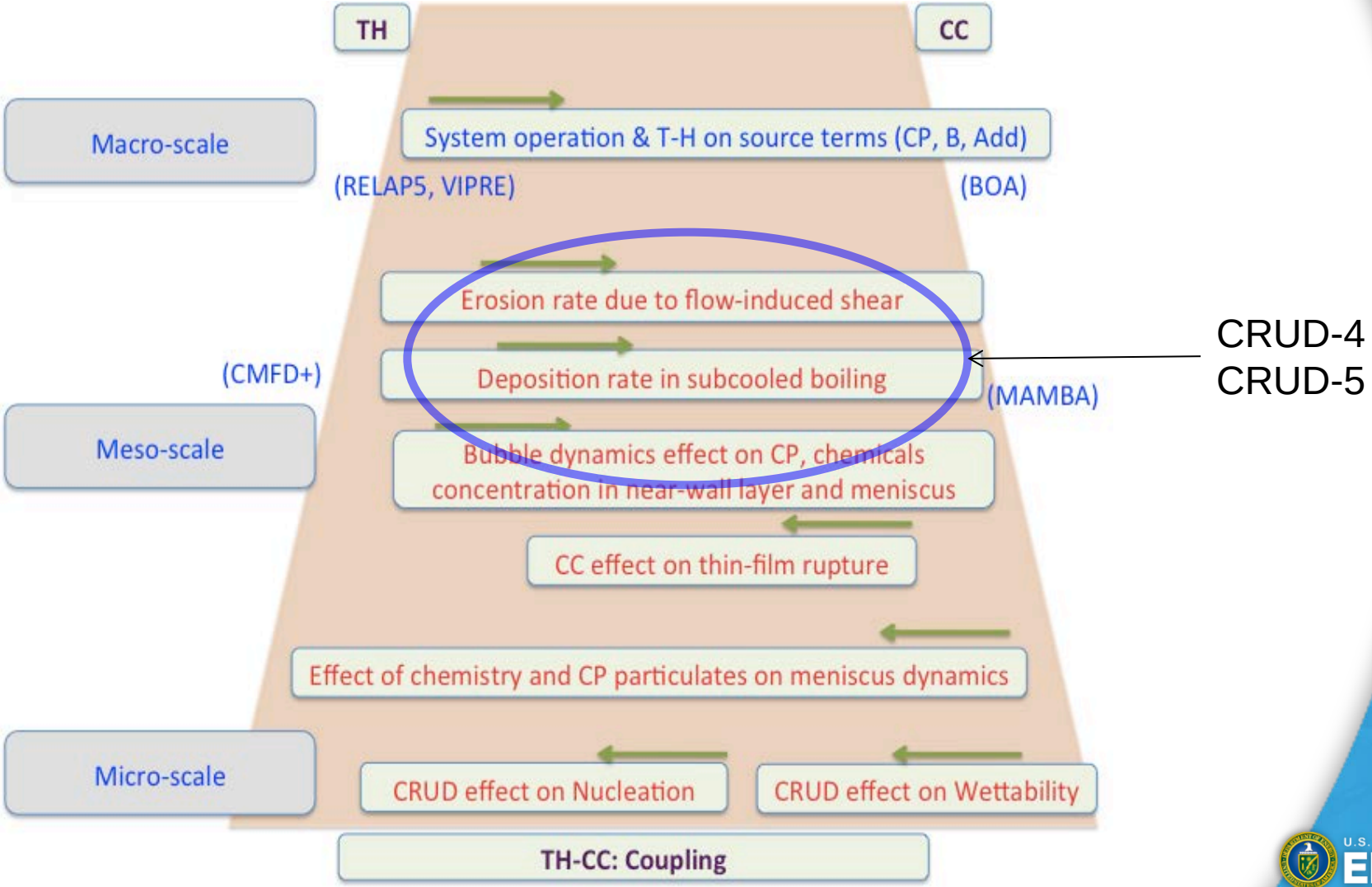
Validation Experiments Coverage – T-H



DNB-1
DNB-2

CRUD-6

Validation Experiments – TH-CC Coupling



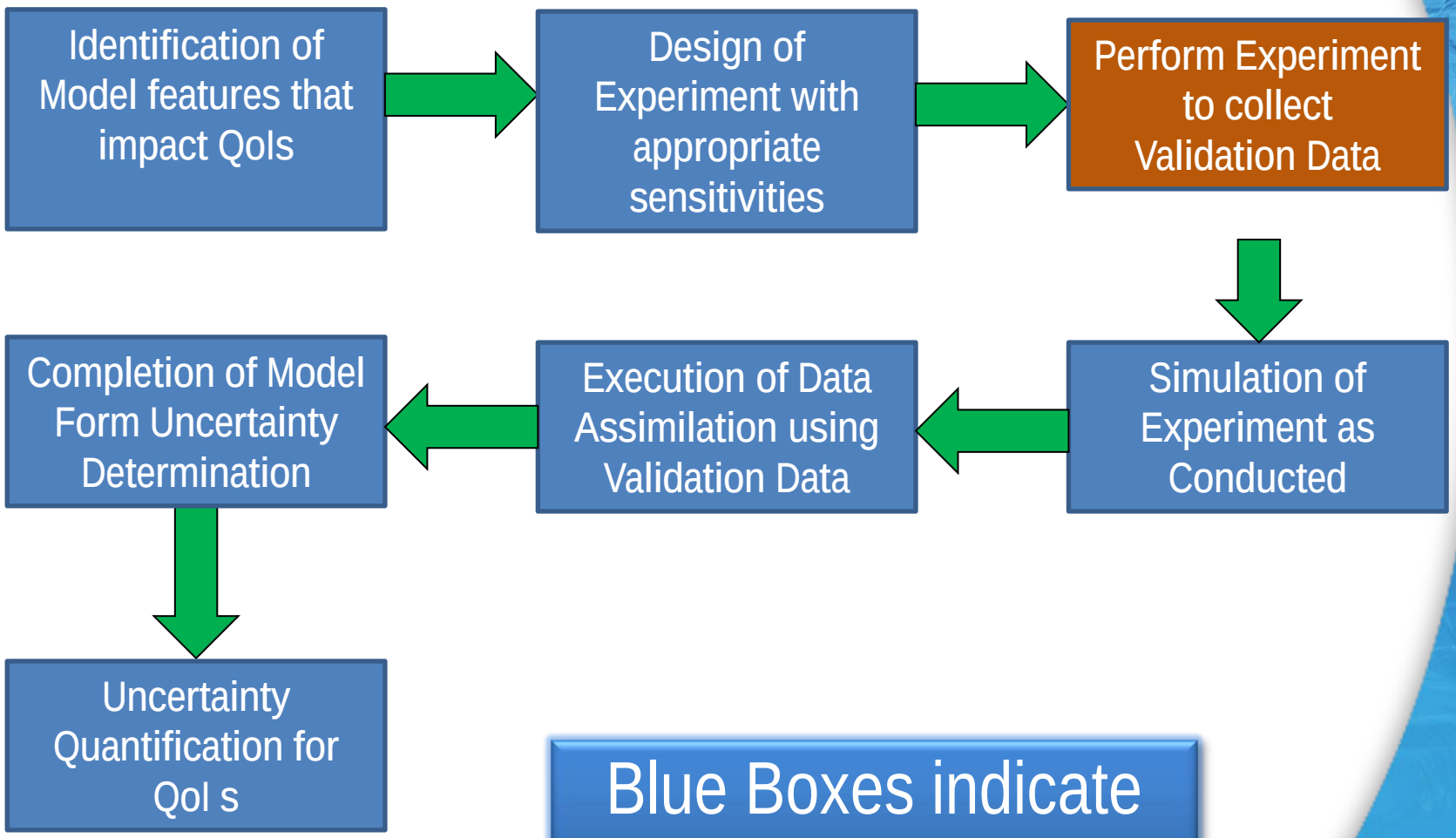
How does experimental design differ from the past?

- ModSim capabilities are used to

1. Define what the **Quantity of Interest** is sensitive to in the model and what model parameters are most contributing to a priori uncertainty
2. Design the validation experiment to reduce posteriori uncertainty by **firstly** simulating proposed experiments to predict instrument readings, **secondly** using this virtual data in data assimilation and **thirdly** determining posteriori uncertainty
3. Redo of above Step 2 now using actual experimental data.

Capabilities to complete data assimilation and uncertainty quantification have greatly advanced

Design & Utilization of Validation Experiments

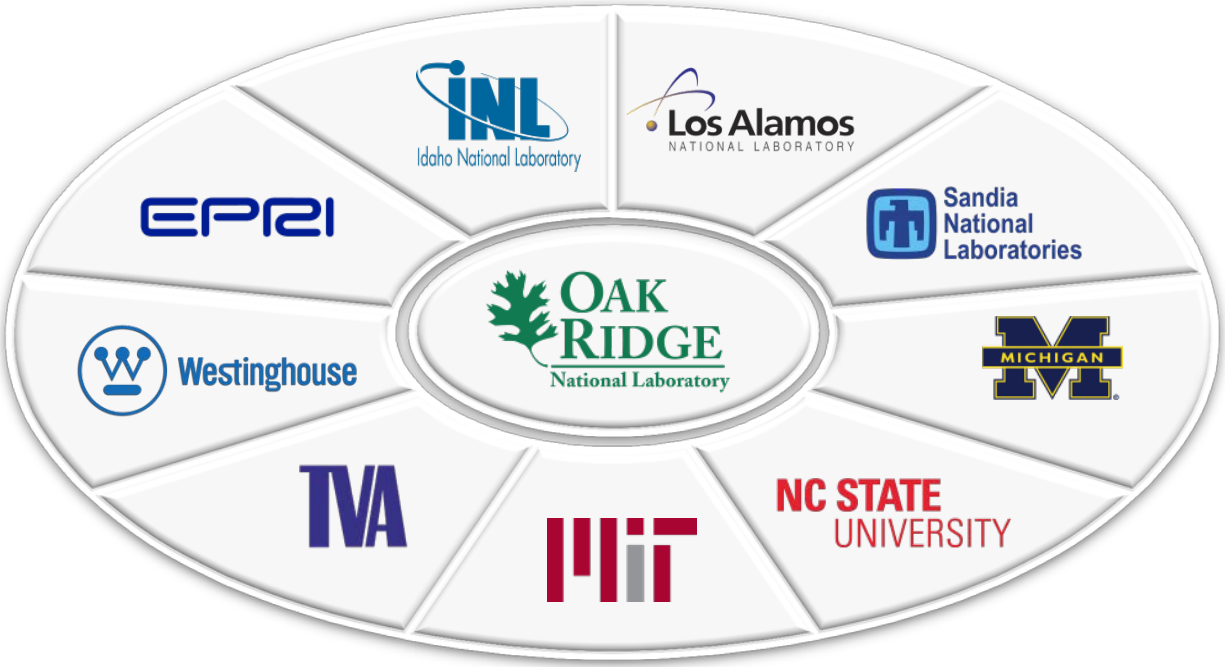


Blue Boxes indicate that ModSim utilized

Concluding Remarks

- Validation data needs survey identified gaps in low-length-scale phenomena and multi-physics interactions
- Needed validation experiments are identified for each Challenge Problem (30 propositions for 7 CPs)
- The proposed experiments include SETs, IETs, RETs
- A majority of proposed experiments is appropriate for university research and university-laboratory collaboration (especially, when a test reactor is needed e.g., NSUF-ATR)
- A validation experimental program should include efforts in
  - development of advanced diagnostics methods to obtain information needed for assessment and calibration of high-fidelity models
  - using advanced simulation capability and modern VUQ methods to design and guide the experiments, and process the data

Questions?



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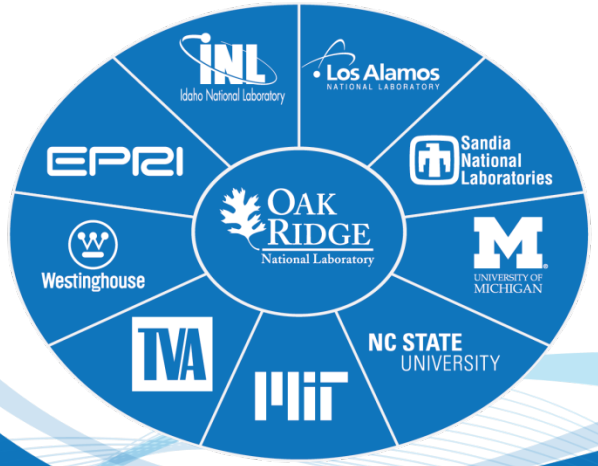
VERA: Description, Status, Plans

Jess Gehin, Scott Palmtag, Andrew Godfrey
Physics Integration Focus Area

Joint Industry and Science Council Meeting
Oak Ridge National Laboratory
September 10, 2013



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Presentation Outline

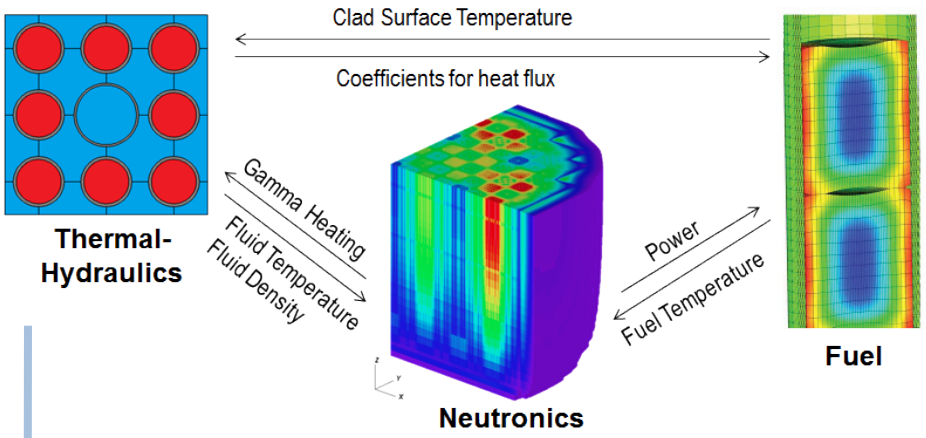
Gehin	Physics Integration Introduction VERA Status Overview
Godfrey	VERA Results – Watts Bar Zero Power Physics Tests • Zero Power Physics Tests • Comparison with measured results
Palmtag	VERA Results – Single Assembly Coupled Physics • Single Assembly Coupled Physics • Initial Challenge Problem Coupling

Physics Integration (PHI)

Integrating the CASL Virtual Reactor

Objectives and Strategies

- Focus on completion of the VERA Core Simulator (VERA-CS) to provide a platform for challenge problem physics integration
- Strong collaboration with other focus areas to integrate advanced M&S capabilities to achieve challenge problem solutions
- Create a useful and usable product for industry applications



Requirements Drivers

- Operational reactor modeling through full power steady-state operation with improved physics
- Challenge Problem analysis capabilities through multi-physics integration of advanced physics capabilities being developed by MPO, THM, RTM
- Enable use of VUQ methodologies for quantification of uncertainties
- Deployment and use of VERA

Outcomes and Impact

- An effective modeling and simulation environment for reactor analysis
- Integrated CASL physics being used to address challenge problems
- VERA deployed through Test Stands and used on Leadership Class computers
- Moving from development to applications

Virtual Environment for Reactor Applications (VERA)

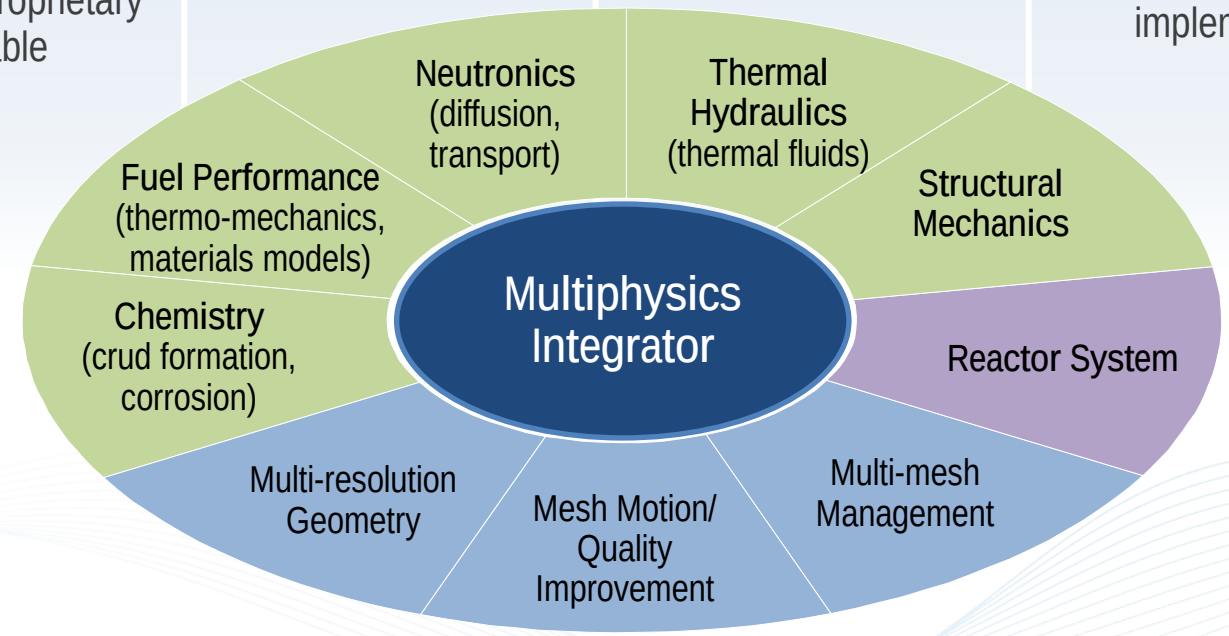
A suite of tools for scalable simulation of nuclear reactor core behavior

- flexible coupling of physics components
- toolkit of components
  - not a single executable
  - both legacy and new capability
  - allows both proprietary and distributable components

- attention to usability
- rigorous software processes
- fundamental focus on V&V and UQ

- development guided by relevant challenge problems
- broad applicability

- scalable from moderate-scale clusters to existing and future HPC platforms
  - diversity of models, approximations, algorithms
  - architecture-aware implementations

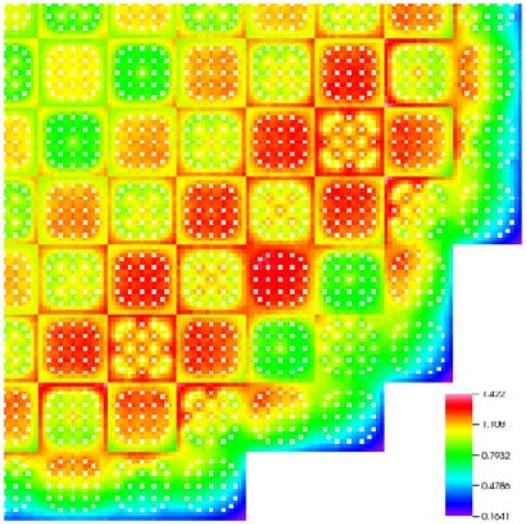


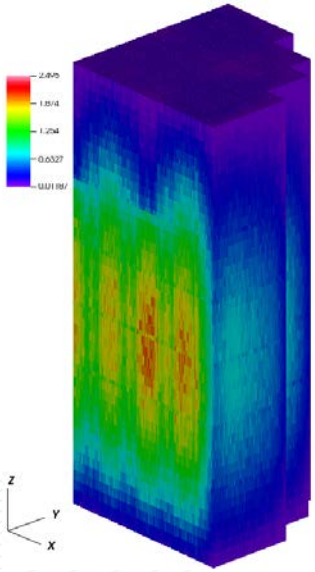
VERA supports a range of PWR core physics and spatial scales

- Neutron transport/Cross Sections
  - Spatial scale: fuel pellet to fuel rod to fuel assembly (assy) to full core
  - Components: Insilico, Shift (ORNL), MPACT (UMich)
- Single-phase and multi-phase thermal hydraulics
  - Subchannel spatial scale: fuel assy to full core
  - CFD Spatial scale: fuel sub-assy (3x3 rods) to fuel assy (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 Development Approach

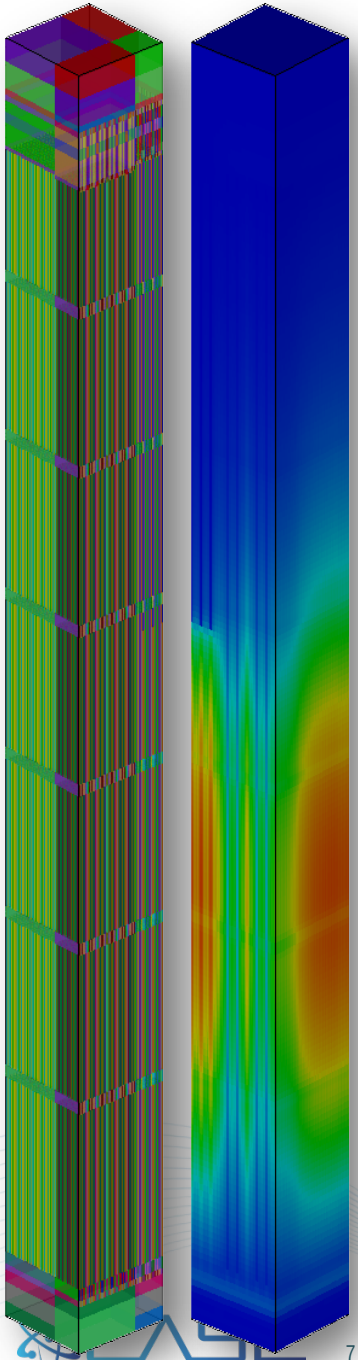
- VERA consists of a “Core Simulator” capability
  - Develop “base” capability with core simulator (neutronics – thermal-hydraulics – fuel performance)
  - Will provide capability to model multi-cycle full power operation
  - Progression benchmarks to drive development and verification in a systematic fashion
- VERA Challenge Problem Capability
  - After obtaining initial “base” capability with coupled neutronics/subchannel for a single assembly
  - Integrate physics capabilities being developed by other FAs to provide challenge problem modeling
    - Coupling Peregrine and MAMBA Challenge Problem Physics
- Emphasis on usability
  - While we use leadership class computing (e.g. Jaguar, Titan) the software must be functional on industry computing resources
  - Input and output must be easily learned and used by engineerins and analysts to allow large-scale calculations to be set up with minimal effort





VERA-CS vs. Industry Core Simulators

Physics Model	Industry Practice	VERA-CS
Neutron Transport	3-D diffusion (core) 2 energy groups (core) 2-D transport on single assy	Transport-based 23+ energy groups
Power Distribution	nodal average with pin-power reconstruction methods	explicit pin-by-pin(*)
Thermal-Hydraulics	1-D assembly-averaged	subchannel (w/crossflow)
Fuel Temperatures	nodal average	pin-by-pin(*) 2-D or 3-D
Xenon/Samarium	nodal average w/correction	pin-by-pin(*)
Depletion	infinite-medium cross sections quadratic burnup correction history corrections spectral corrections reconstructed pin exposures	pin-by-pin(*) with actual core conditions
Reflector Models	1-D cross section models	actual 3-D geometry
Target Platforms	workstation (single-core)	1,000 – 300,000 cores



(*) pin-homogenized or pin-resolved depending on application

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 w/ Xenon

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**

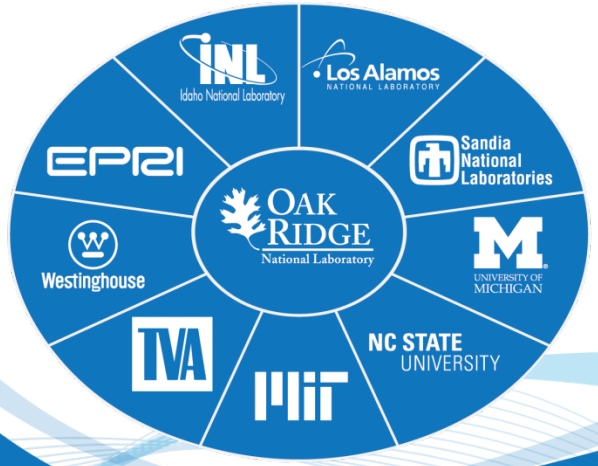
VERA Status Summary and FY14 plans

- Accomplishments and Status
  - Build/test infrastructure in place
  - Individual code components integrated
  - Common input defined and implemented for neutronics and subchannel thermal-hydraulics
  - Initial physics coupling (focus on core simulator)
  - Benchmark progression problems 1 – 6 capabilities
  - Initial comparisons with operational plant data
  - VERA components deployed to WEC for 1st Test Stand
- FY14 Plans
  - Continue core simulator development including depletion (complete through problem 10)
  - Continue component integration and coupling (VERA-CS with Peregrine, MAMBA)
  - VUQ Integration (expose parameters)
  - Development of common output
  - Support Test Stand releases and installation

```
[ASSEMBLY]
 title "Westinghouse 17x17"
 npin 17
 ppitch 1.260
 uo2 U31 10.257 / 3.1
 cell 1     0.4096 0.418 0.475 / U31 he zirc
 cell 100           0.561 0.602 / mod   zirc      ! guide tube
 lattice FUEL1
    100
      1 1
      1 1 1
    100 1 1 100
      1 1 1   1 1
      1 1 1   1 1 100
    100 1 1 100 1   1 1
      1 1 1   1 1   1 1 1
      1 1 1   1 1   1 1 1 1
 axial A1   11.951
    FUEL1 377.711
 grid END inc  1017 3.866
 grid MID zirc 875  3.810
 grid_axial
    END  13.884
    MID  75.2
    [...]
    MID 336.2
    END 388.2

 lower_nozzle  ss 6.05  6250.0  ! mat, height, mass (g)
 upper_nozzle  ss 8.827 6250.0  ! mat, height, mass (g)

 lower_nozzle_gap_height  4.231
 lower_pincap_height      1.67

 upper_nozzle_gap_height  2.12
 upper_pincap_height      1.67
 upper_plenum_height      16
                                ! assembly_dancoff_map

 !! dancoff
 !!   0.000
 !!   0.287 0.315
 !!   0.287 0.315 0.315
 !!   0.000 0.287 0.286 0.000
 !!   0.287 0.316 0.316 0.284 0.299
 !!   0.288 0.317 0.316 0.287 0.267 0.000
 !!   0.000 0.286 0.286 0.000 0.270 0.286 0.321
 !!   0.287 0.319 0.319 0.286 0.315 0.335 0.333 0.337
 !!   0.323 0.322 0.321 0.322 0.320 0.322 0.323 0.322 0.310
```

VERA Benchmarking using Watts Bar 1 Cycle 1 Zero Power Physics Test Data

Andrew Godfrey



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Problem 5 – Zero Power Physics Tests

- CASL Level 1 milestone report completed on June 7, 2013
  - Revision 1 contains updated results
- Report CASL-U-2013-0105-001 publicly available
  - Measured plant data released by TVA
  - Predicted results from current licensed methodology released by Westinghouse
  - Model based solely on publicly available specifications
- Description of Physical Reactor and startup physics test data
- Description of VERA components utilized
- Description of reference solutions
- Analysis demonstrates good agreement with measured plant data by all codes

Successful Application of VERA to Actual Power Plant Conditions

Primary Contributors

- Oak Ridge National Laboratory
  - Reactor physics, analysis, and testing
  - SCALE – Cross sections and KENO-VI Team
  - Radiation Transport (Denovo)
  - Software and Infrastructure
- Tennessee Valley Authority
  - Nuclear power plant operations and data
- University of Michigan
  - Reactor physics methods (MPACT)
- Westinghouse Electric Company
  - Industry methods and software
  - Physics testing methods and benchmarking

Exceptional Partnership

Core Physics Progression Problems

- Benchmark problems to guide development and demonstrate capability to solve real-world problems (prioritized requirements)
- Has significantly improved communication and understanding of needed reactor analysis capabilities

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

- Specifications designed and executed by AMA based on WBN1
- Checkpoints built-in for comparisons to measured data
- Problem 5 – Physical Reactor ZPPT – represents the Level 1 Milestone
- Problem specs available at: http://www.casl.gov/docs/VERA_Benchmarks_1-5_r2_disclaimer.pdf

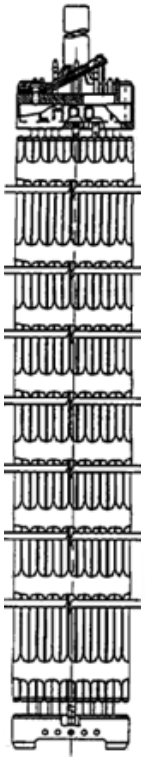
Capability-driven Development and Testing

Bold items represent comparisons to measured data

CASL Physical Reactor – Watts Bar Nuclear 1

Description

- Owned and operated by TVA in TN (near ORNL)
- Cycle 1 startup January 1996
- Typical Westinghouse 4-loop PWR
- 3411 MW_{th}; HZP = 557 ºF
- Unit 2 under construction – startup ~2015



Cycle 1 Core Loading Properties

- 193 17x17 fuel assemblies
- ~50,952 fuel rods
- ~7000 Pyrex discrete burnable absorber rods
- 1368 hybrid B_4C/AIC control rods
- Eight spacer grids per assembly
- Soluble boron as chemical shim

Three Assembly Types

	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

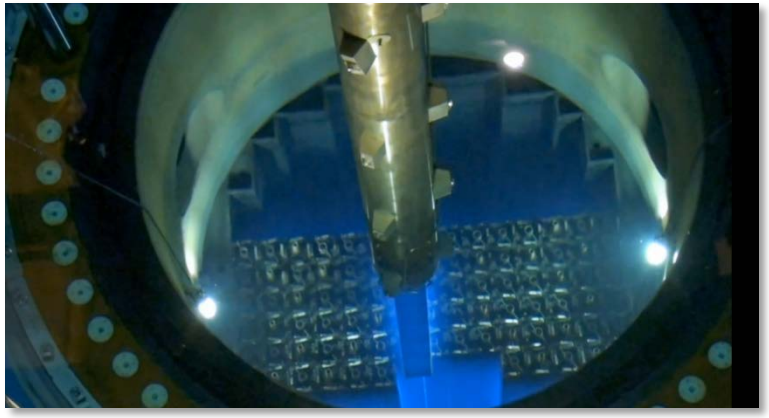
Eight Control Rod Banks

	H	G	F	E	D	C	B	A
8	D		A		D		C	
9						SB		
10	A		C				B	
11				A		SC		
12	D				D		SA	
13		SB		SD				
14	C		B		SA			
15								

¼ of radial core geometry shown

WBN1 Cycle 1 Zero Power Physics Tests

- Plant testing for each fuel cycle prior to initial power escalation
- Confirms reactor core is loaded as designed
- Ensures the operating reactor meets regulatory specifications



- Validates reactivity parameters assumed in accident analyses
- Common source of measured data for methods and software validation
- Tests include:
  1. Initial Criticality
  2. Control Rod Bank Reactivity Worths
  3. Differential Soluble Boron Reactivity Worth (DBW)
  4. Isothermal Temperature Reactivity Coefficient (ITC)

Analysis Components

VERA Development

1. Common ASCII input*
2. Improved multi-group cross sections (L3:RTM.SUP.P6.01)*
3. Metadata and meshing
4. Improved neutron transport*
5. Common HDF5 output and post-processing*

Reactor Analysis

1. Startup testing data collection and transmittal (L3:AMA.APP.P6.02)
2. Development of model specs*
3. Obtained Rod Swap bank worth methodology
4. Application of VERA*
5. CE Monte Carlo reference results (L3:AMA.VDT.P6.04)*
6. Industry methods results*
7. Analysis and Documentation* (L1:CASL.P7.01)

Contributions from VRI, RTM, and AMA

*Subsequent Slide on this Item

VERA Common ASCII Input

- Simple, intuitive interface for engineers to build complex models
- One input for multiple physics codes (xsecs, transport, T/H, fuel)
- Free format, minimum characters, and credit for symmetry

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

  fuel U21 10.257 94.5 / 2.110
  fuel U26 10.257 94.5 / 2.619
  fuel U31 10.257 94.5 / 3.100

  cell 1      0.4096 0.418 0.475 / U21 he zirc
  cell 2      0.4096 0.418 0.475 / U26 he zirc
  cell 3      0.4096 0.418 0.475 / U31 he zirc
  cell 4                 0.561 0.602 / mod   zirc
  cell 5                 0.418 0.475 /     he zirc

  lattice LAT21
        4
        1 1
        1 1 1
        4 1 1 4
        1 1 1 1 1
        1 1 1 1 1 4
        4 1 1 4 1 1 1
        1 1 1 1 1 1 1 1
        1 1 1 1 1 1 1 1 1
```

```
[CORE]
  size 15
  rated 3411 131.68
  apitch 21.5
  height 406.337

  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

  crd_bank
    D  -  A  -  D  -  C  -
    -  -  -  -  - SB  -  -
    A  -  C  -  -  -  B  -
    -  -  -  A  - SC  -  -
    D  -  -  -  D  - SA
    - SB  - SD  -  -  -
    C  -  B  - SA  -
    -  -  -  -
```

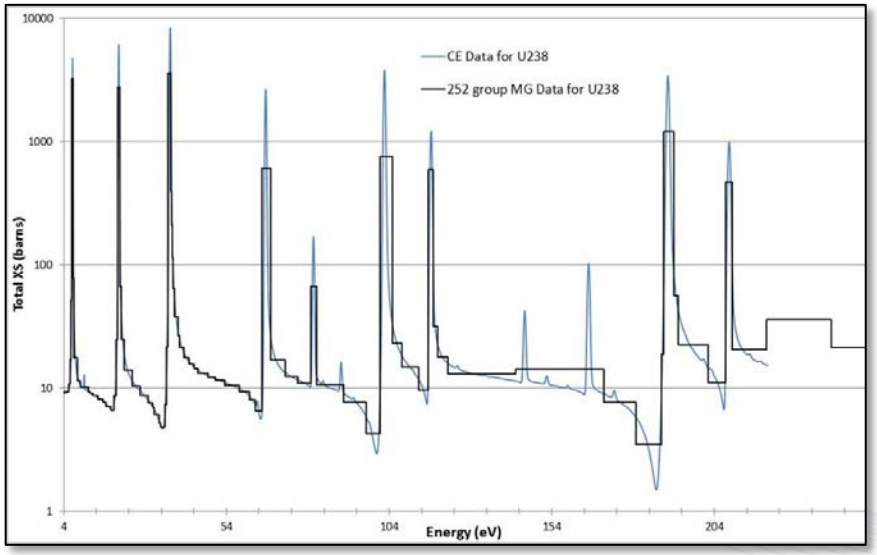
```
[CASEID]
  title 'WBN1 Cycle 1'

[STATE]
  power   0.0     ! %
  tinlet  557.33  ! F - 565K
  tfuel   565.0   ! K
  boron   1285    ! ppmB
  modden  0.743   ! g/cc
  feedback off
  sym qtr

  rodbank SA 230
          SB 230
          SC 230
          SD 230
           A 230
           B 230
           C 230
           D 167
```

Multi-Group Cross Sections

- New 252 group ENDF/B-VII.0 library (SCALE 6.2 Beta)
  - Includes 'IR' factors for Bondarenko self-shielding method
- New 60 group ENDF/B-VII.0 'subgroup' library (56g being tested)
- Generated with enhanced SCALE AMPX codes
- Pointwise spectrum for PWRs used for processing
- Significant testing and development with Continuous Energy Monte Carlo

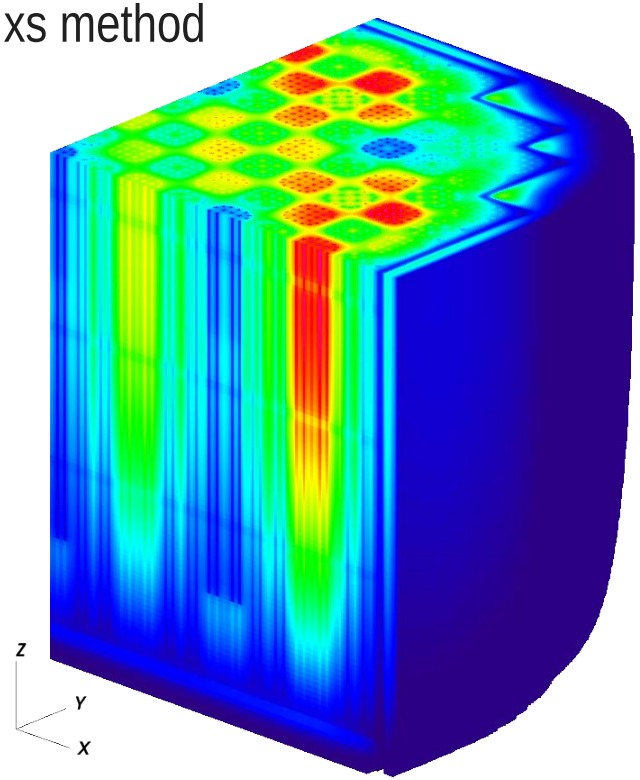


CE and MG structures for Total U-238 Cross Section

New Multi-Group Libraries and Methods Capable of Continuous Energy Performance

3D Neutron Transport

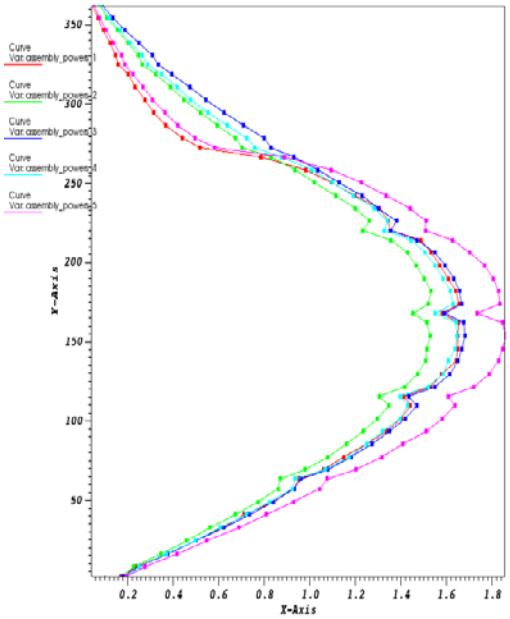
- Two deterministic methods being developed:
  - MPACT 2D/1D "pin-resolved" approach using sub-group xs method
  - Insilico approach currently using 1D cross sections from SCALE with S_N and SP_N transport
- Milestone used Insilico 3D SP_N methods
  - Pin-homogenized cross sections
  - 2x2 mesh per fuel rod
  - ≈1" maximum axial mesh size
  - 23 energy groups (collapsed from 252g)
  - 3D S_N method too large for TITAN
- Cross section processing and transport calculations performed in parallel on 676 cores and ~ 5.3 TB of memory
- Runtime = 33 minutes on TITAN for quarter-core eigenvalue calculation without T/H feedback

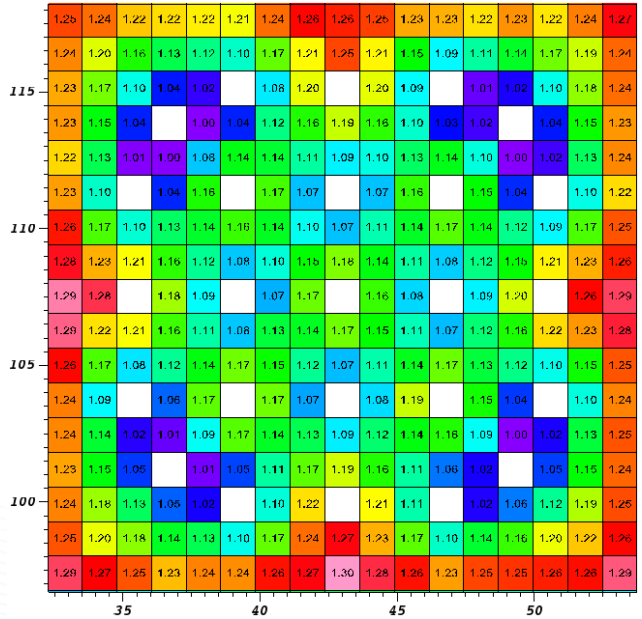


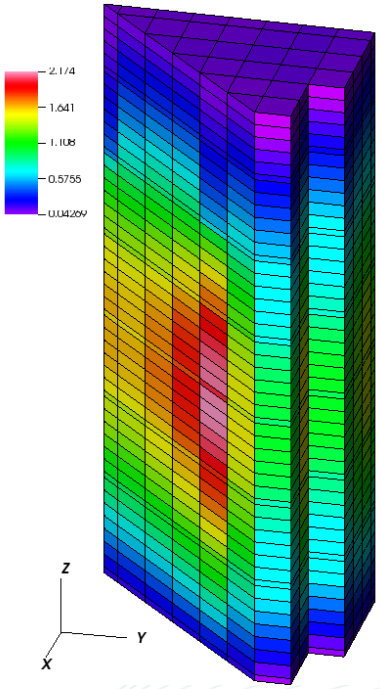
Insilico Watts Bar 1 3D Thermal Flux Distribution

VERA Common HDF5 Input

- Public standardized hierarchical binary format chosen for output
- Accessible by many languages such as FORTRAN, C/C+, Java, etc.
- Free utilities available for data viewing and manipulation
- Post-processors developed for code comparisons, sensitivity studies, and visualization



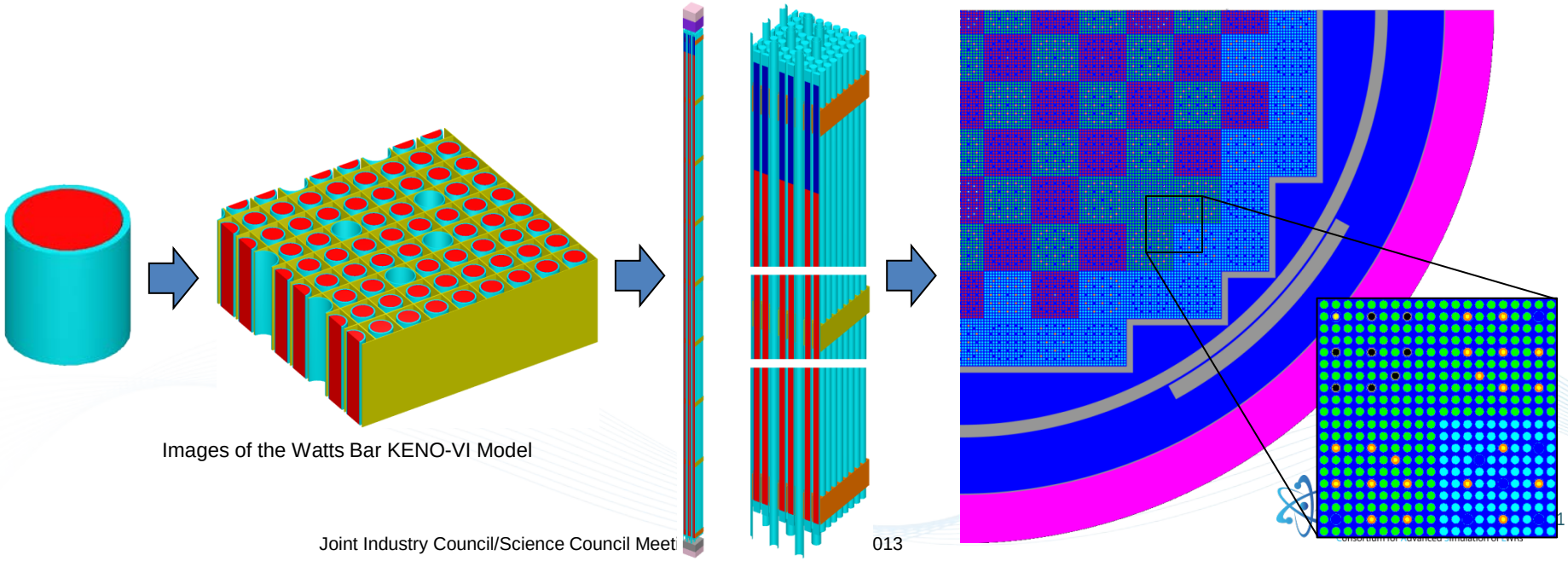




Images from VisIt of VERA Output Data

Numerical Reference Solution – KENO-VI

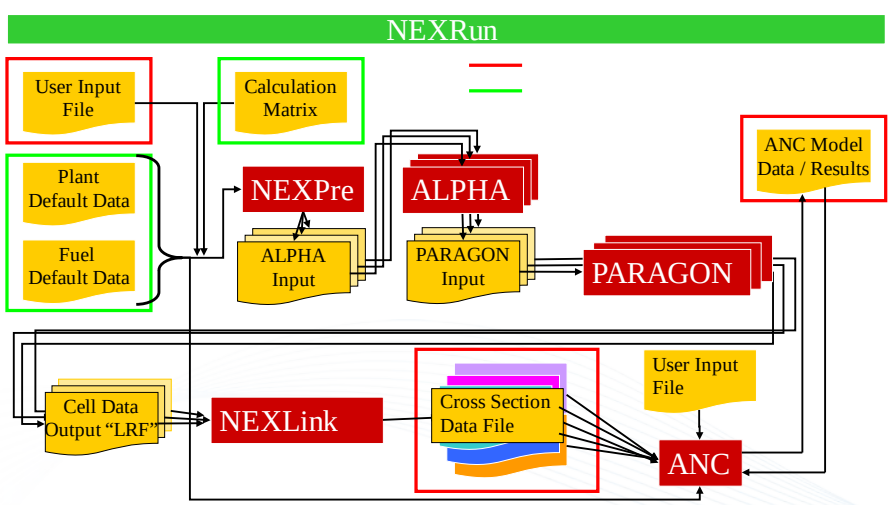
- SCALE 6.2 criticality code KENO-VI used for high fidelity, neutronics-only reference
- Continuous energy Monte Carlo method of particle transport is most rigorous with fewest approximations but requires significant computational resources
- KENO-VI generalized geometry supports models for fuel, annular poisons, rod plenums, semi-explicit spacer grids, and a simplified core structure
- Parallel version permits very large numbers of particles for reduced statistical uncertainties.
- Power distributions obtained for Core Physics Problems 1-4

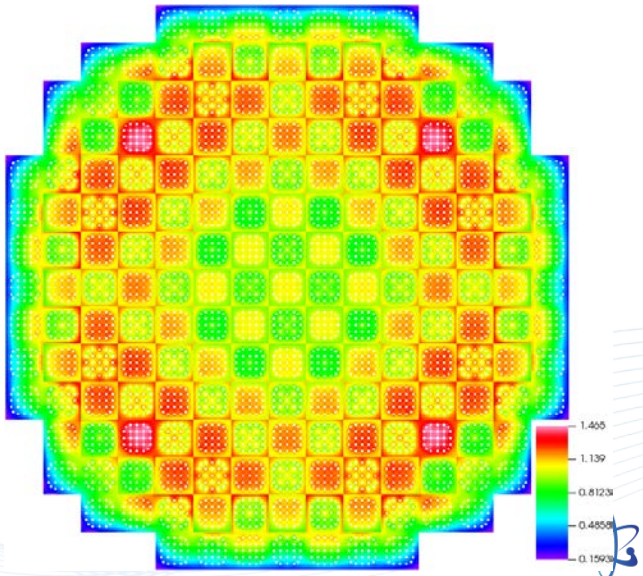


Images of the Watts Bar KENO-VI Model

Current Industrial Solution - NEXUS

- Westinghouse's NEXUS core simulator methodology applied for comparison to VERA
- State-of-the-art nodal methods consistent with US industry licensing and analyses
  - PARAGON lattice physics for detailed analysis of 2D fuel assembly segments with reflective boundaries
  - ANC9 two group 3D nodal diffusion method
  - Flux and power solved on nodal basis from parameterized macroscopic cross sections based on 3D thermal/hydraulic conditions (moderator density, fuel temperature, etc)
  - Pin level detail is reconstructed from form factors calculated by the 2D infinite lattice calculations
- NEXUS has been licensed by the US NRC for analysis of PWRs since Feb. 2007
- V&V and licensing activities demonstrate high pedigree for reactor analyses





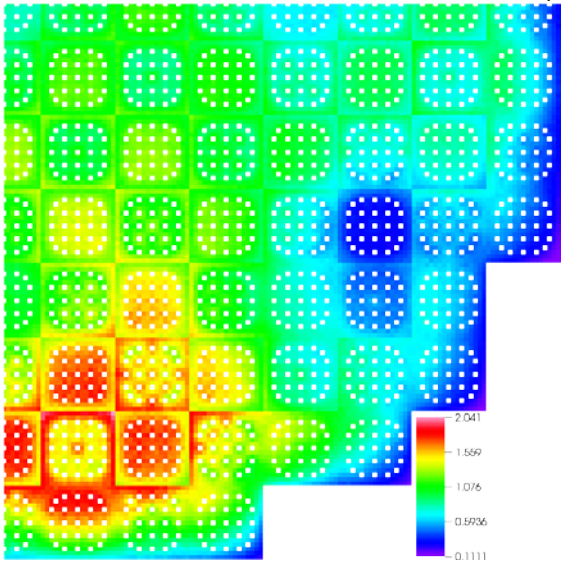
NEXUS Methodology and Reconstructed Pin Powers for Watts Bar 1

WBN1 Zero Power Physics Testing Analysis

Description

- Initial criticality achieved by withdrawing Bank D to 167 steps withdrawn (≈3/4) with soluble boron concentration of 1293 ppmB
- Bank D worth measured by reactimeter during system dilution and bank insertion ("boron swap")
- Other bank worths inferred by "rod swap" with Bank D – criticality always maintained
- Boron worth (DBW) calculated from Bank D measurement dilution
- Temperature coefficient (ITC) measured by reactimeter while reducing reactor coolant system temperature by 4°F

KENO Radial Fission Distribution for Bank SC Swap



Calculations

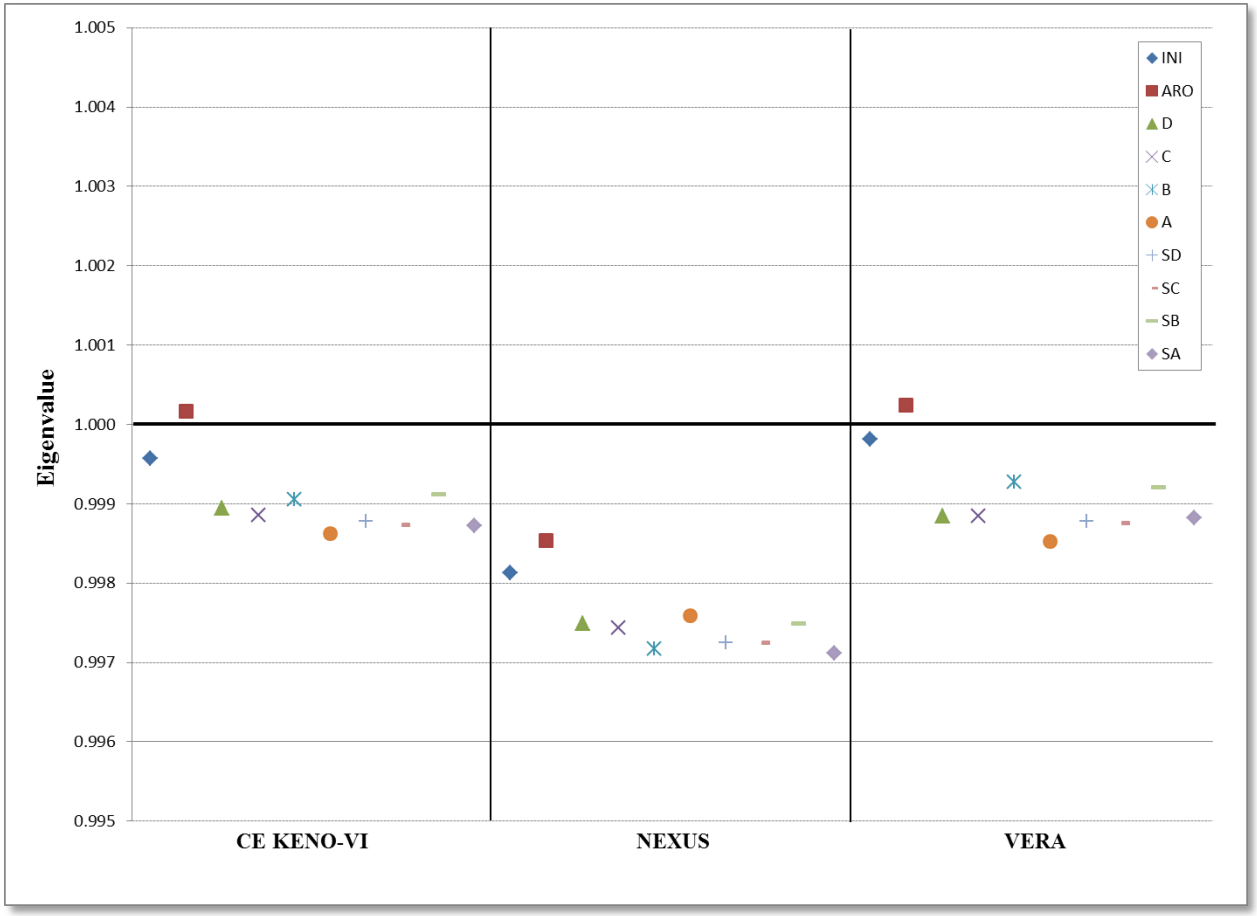
- Ten critical conditions simulated
- Recalculated rod swap "shadow factors" and inferred Bank worth measurements
- Calculated reactivity worth of each bank (ARO)
- Calculated DBW and ITC directly

Approximations and Adjustments

- +78 pcm boron-10 isotopic abundance correction
- -53 pcm rotational symmetry correction for Banks SC and SD
- Small thermal expansion correction

Criticality Results

Critical	Reactivity Difference (pcm)		
	KENO	NEXUS	VERA
Initial	-43 +/- 5	-187	-19
ARO	16 +/- 5	-147	24
D	-106 +/- 6	-251	-116
C	-114 +/- 5	-257	-116
B	-94 +/- 6	-284	-73
A	-138 +/- 5	-242	-147
SD	-122 +/- 5	-276	-122
SC	-127 +/- 5	-276	-124
SB	-89 +/- 5	-252	-79
SA	-128 +/- 6	-289	-117
Avg.	-94 +/- 5	-246	-89
St. Dev.	48	45	54



- ✓ All results agree well with measured conditions
- ✓ VERA results very close to CE KENO-VI

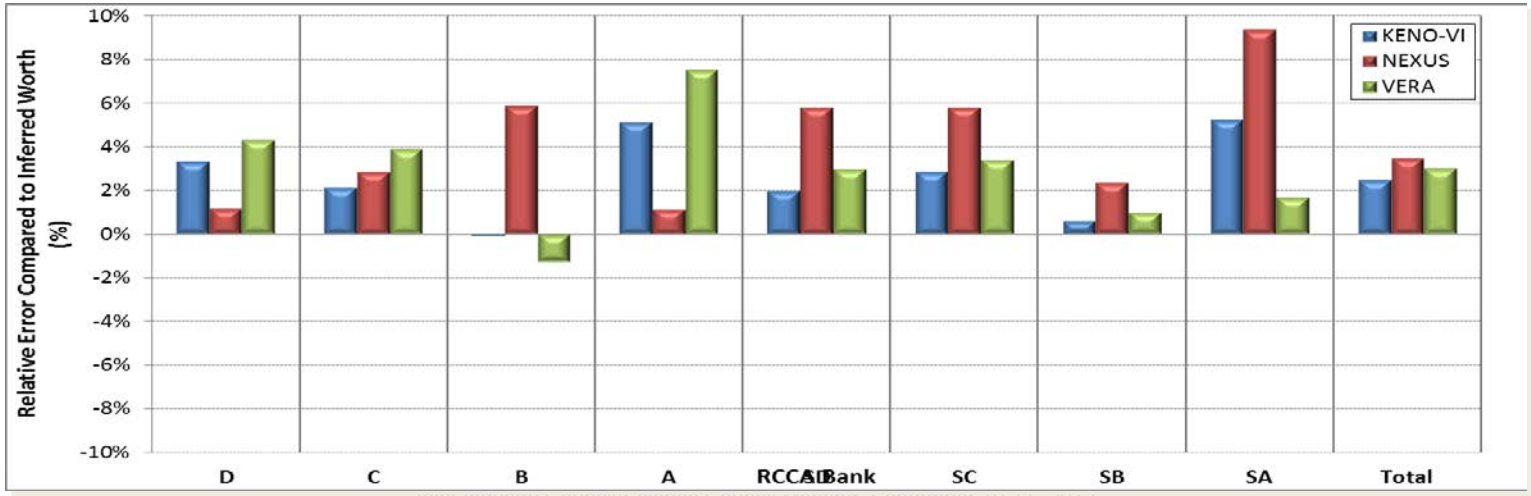
†Typical acceptance criteria for reactivity agreement is 0.005 or 500 pcm

Control Bank Worth Results

Bank	Original Measured Worth (pcm)	Worth Difference (pcm)			Relative Worth Error (%)		
	WBN1	KENO	NEXUS	VERA	KENO	NEXUS	VERA
D	1342	45	16	58	3.3%	1.2%	4.3%
C	940	20	27	37	2.1%	2.9%	3.9%
B	871	-1	51	-11	-0.1%	5.9%	-1.3%
A	830	44	10	64	5.1%	1.1%	7.5%
SD	495	9	28	14	2.0%	5.8%	3.0%
SC	494	14	28	16	2.9%	5.8%	3.4%
SB	1048	7	25	10	0.6%	2.3%	1.0%
SA	431	22	40	7	5.2%	9.3%	1.7%
Total	6451	160	224	196	2.5%	3.5%	3.0%

✓ Very Good Agreement

†Typical acceptance criteria = 10-15%



Differential Boron Worth and Isothermal Temperature Coefficient Results

	DBW (pcm/ppmB)	Difference (pcm/ppmB)
Measured	10.8	--
CE KENO-VI	10.1	-0.7
NEXUS	10.1	-0.7
VERA	10.1	-0.7

	ITC (pcm/°F)	Difference (pcm/°F)
Measured	-2.2	--
CE KENO-VI	--	--
NEXUS	-2.2	-0.1
VERA	-3.9	-1.7

- All DBW's agree and are less than 1 pcm/ppmB from measurement
- CE KENO-VI cannot produce an accurate ITC for a 4ºF perturbation
- The VERA ITC is too negative and requires additional investigation

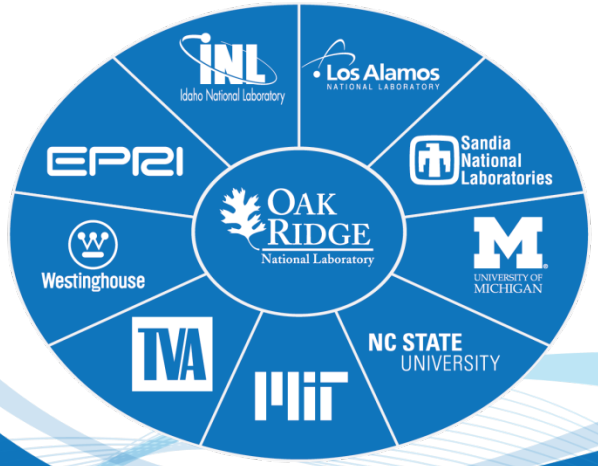
†Typical acceptance criteria is ≈10% (1 pcm/ppm) for DBW and 1 pcm/F for ITC

Summary

- VERA used to perform start-to-finish neutronics analysis of Watts Bar 1 Cycle 1 startup physics testing
- CASL partner collaboration very effective (Industry-Lab-University)
- VERA results agree well with measured data, CE Monte Carlo, and industrial licensed methods results
- VERA ITC needs more investigation
- L1 milestone completed successfully
- Capability supported deployment of Westinghouse Test Stand

Benchmark Problem #6 Multi-Physics Coupling for a Single Assembly

Scott Palmtag



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Consortium for Advanced Simulation of LWRs

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 w/ Xenon

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 6 – PWR Single Assembly

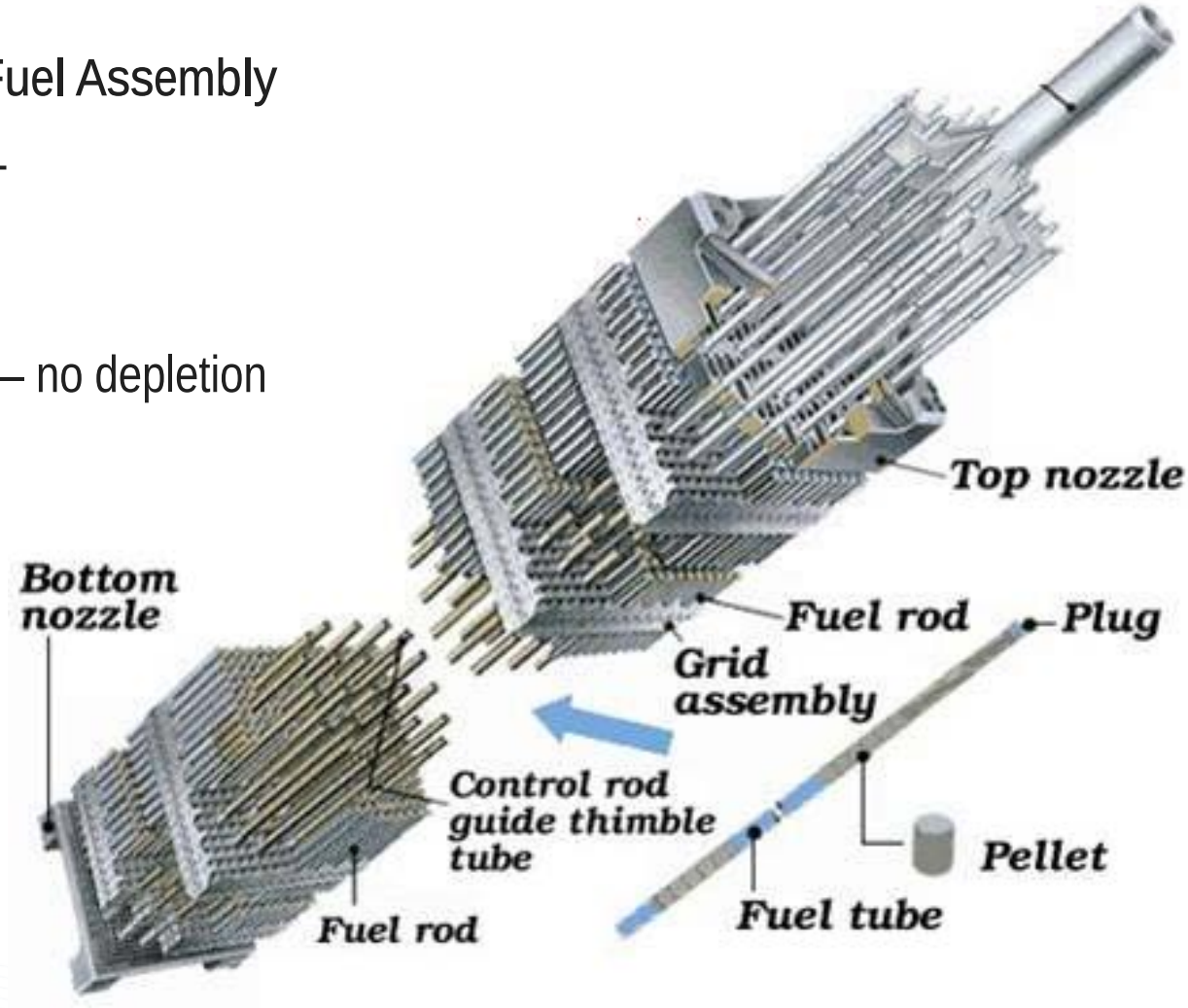
17x17 Westinghouse Fuel Assembly

Watts Bar Unit 1 Cycle 1

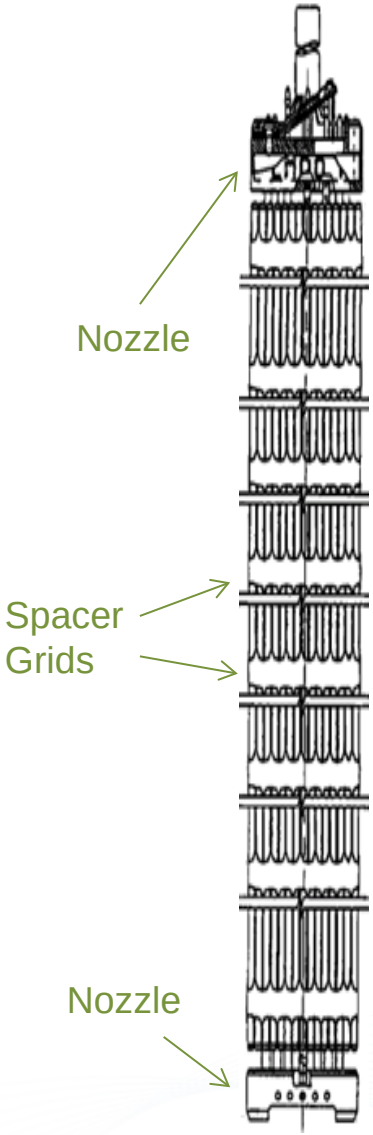
Hot Full Power (HFP)

Beginning of Life (BOL) – no depletion

- Fuel Pins
- Plenum
- End Plugs
- Cladding
- Guide Tubes
- Spacer Grids
- Nozzles
- No Control Rods



Common Input – VERAin



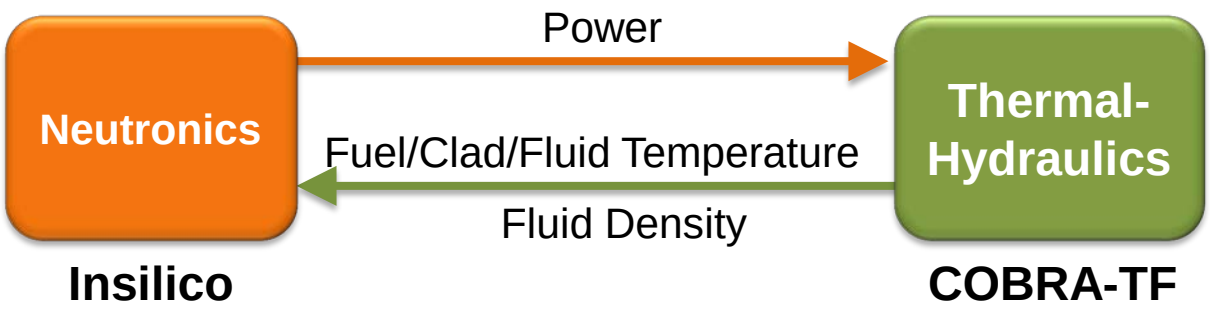

```
[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260

  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
```

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

```
 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
```

Coupling of neutronics and thermal-hydraulics components for hot full-power beginning of life assy.

- AMA progression problem 6
  - neutronics (cross sections + neutron transport)
  - thermal-hydraulics (fluid flow and fuel/clad temperatures)

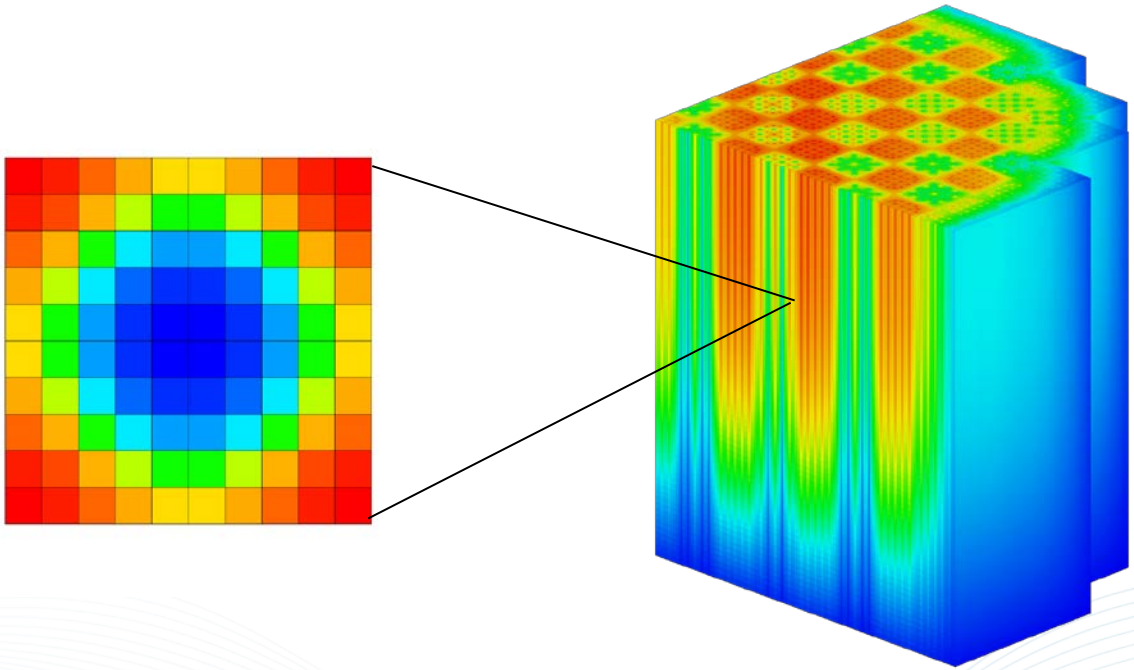


- Coupling becomes more complicated with more codes, but we've done it.
- Challenges are related more to data transfer than "framework".

Neutronics – Insilico

- Part of the Exnihilo environment
- Transport solver is S_N (pin-resolved) or SP_N (pin-homogenized)
- Built in cross section processing with XSProc
- S_N uses the KBA implementation which solves the problem on a Cartesian grid and can scale efficiently to over 100,000 processors

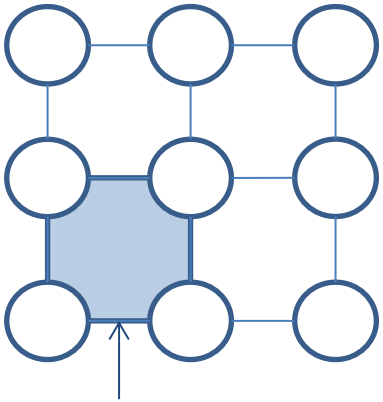
S_N Pin Resolved



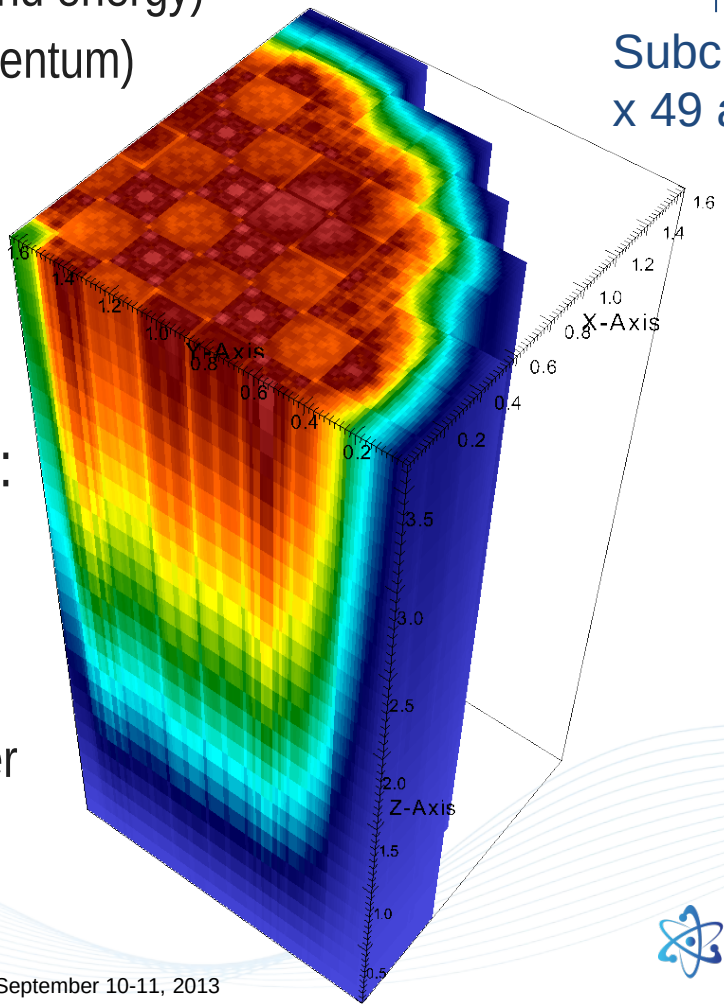
Efficient Scaling to Large 3D Problems

Thermal Hydraulics – COBRA-TF

- COBRA-TF (CTF) subchannel code from Penn. State Univ.
- 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
- Pin conduction model
- Built-in material properties
- Since bringing in for CASL / VERA:
  - dramatically reduced memory usage
  - dramatically increased performance
  - dramatically expanded test coverage
  - implementing parallel version for further reduction in run-times

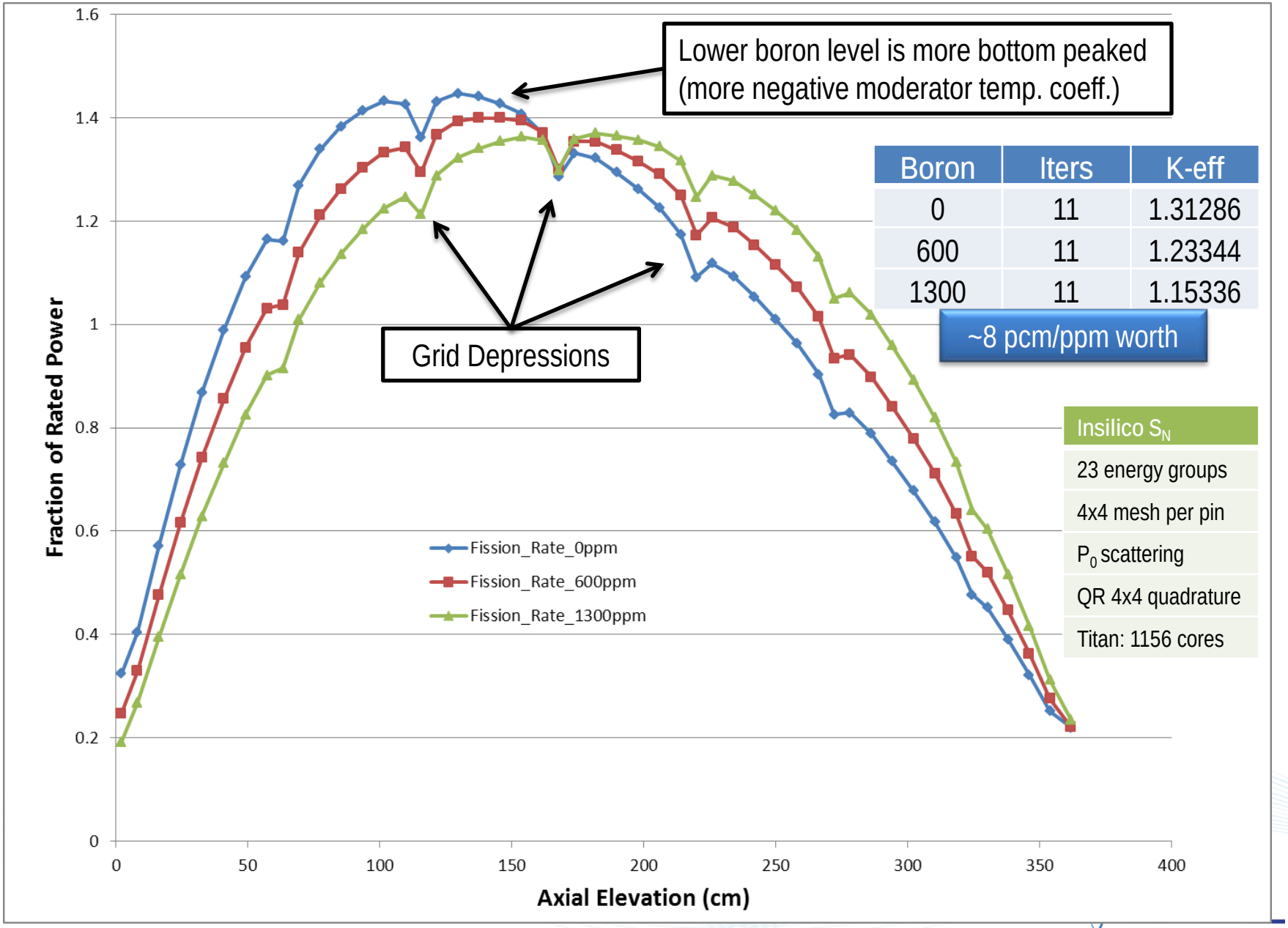


Subchannel area
x 49 axial levels



Coupled Results – Boron Concentration

Prob. #6



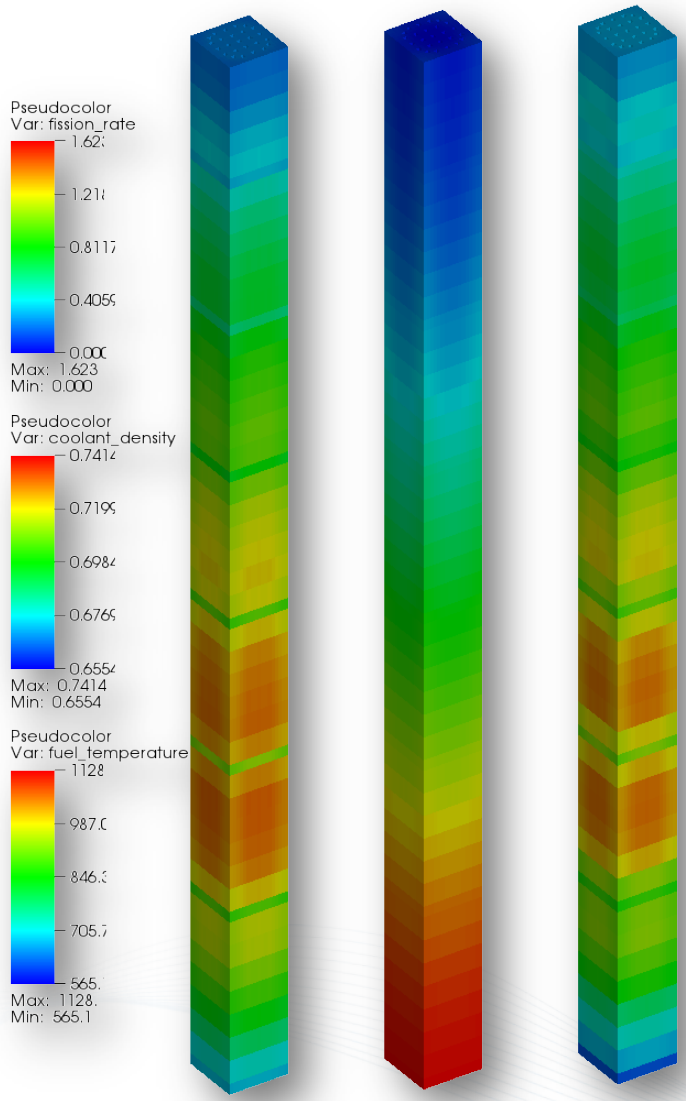
Boron	Iters	K-eff
0	11	1.31286
600	11	1.23344
1300	11	1.15336

~8 pcm/ppm worth

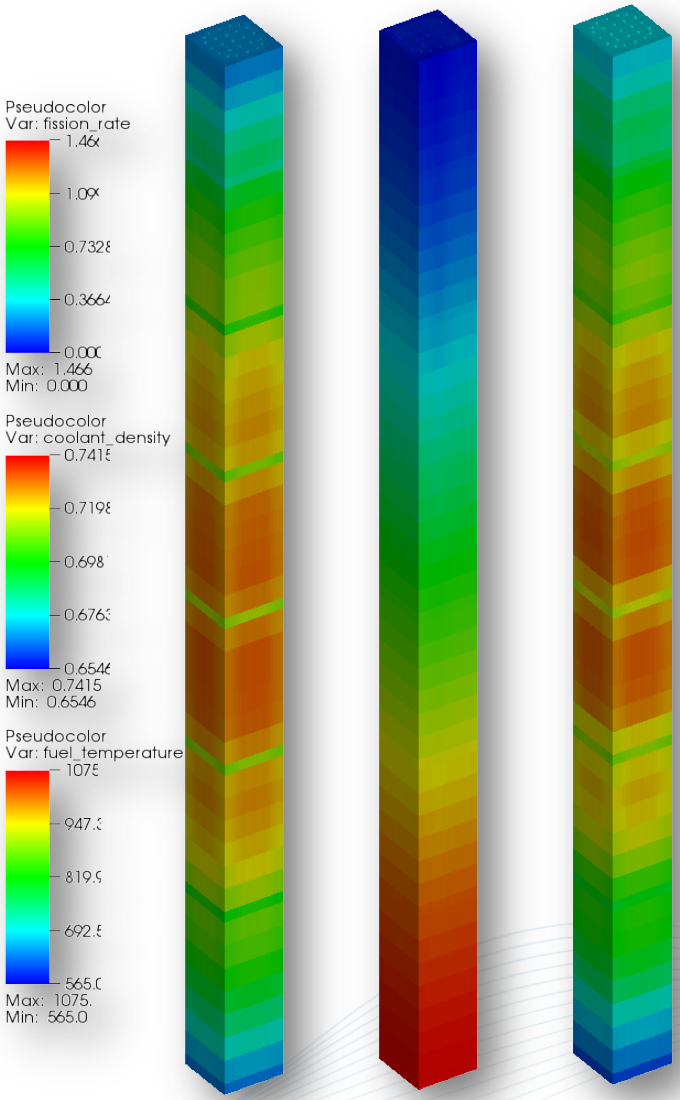
Insilico S_N
23 energy groups
4x4 mesh per pin
P_0 scattering
QR 4x4 quadrature
Titan: 1156 cores

Prob. #6

VERA Simulation of Hot Full Power Assembly
(neutronics with fluid / moderator temp. feedback)



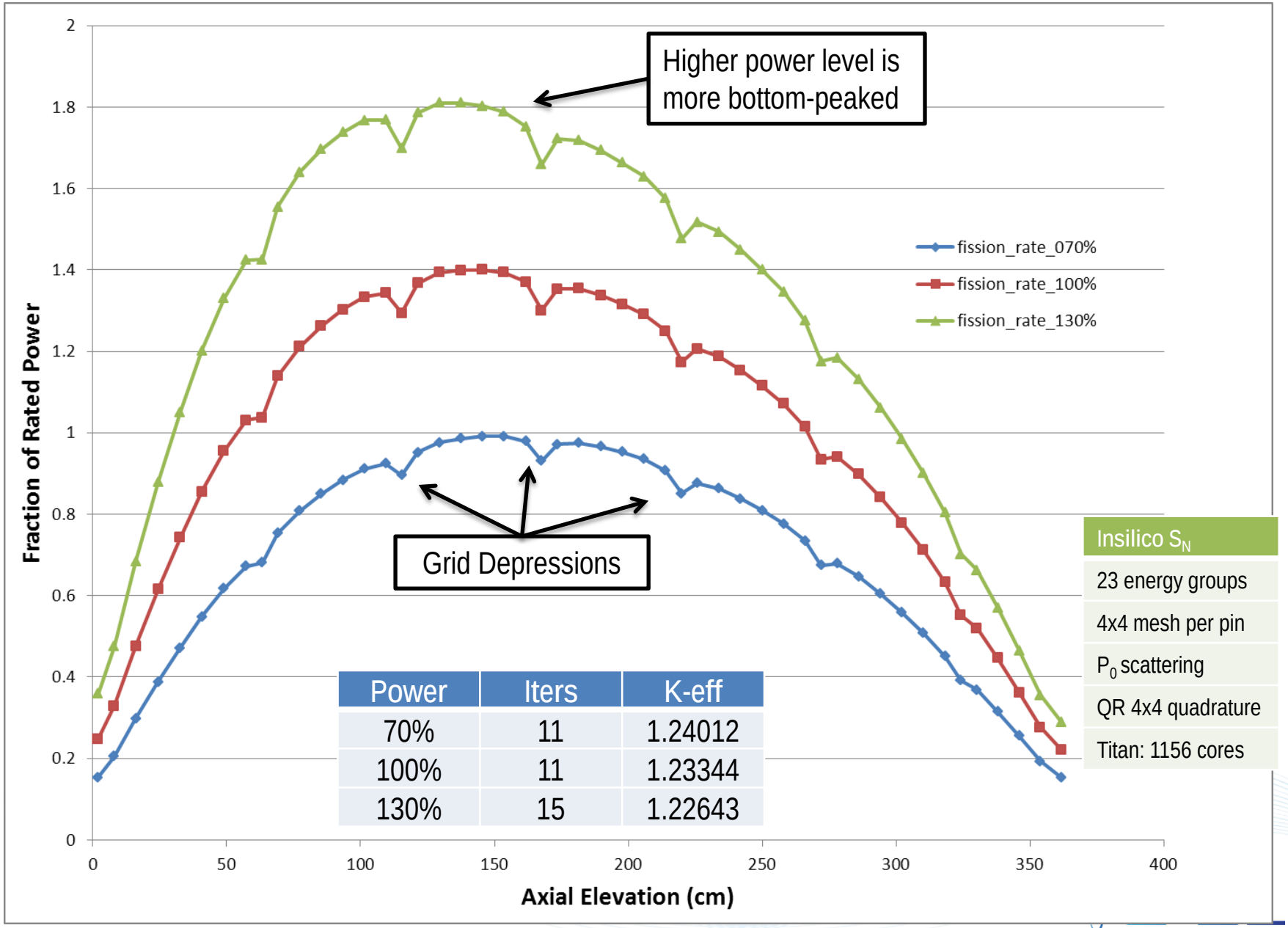
0 ppmB



1300 ppmB

Coupled Results – Power Level

Prob. #6



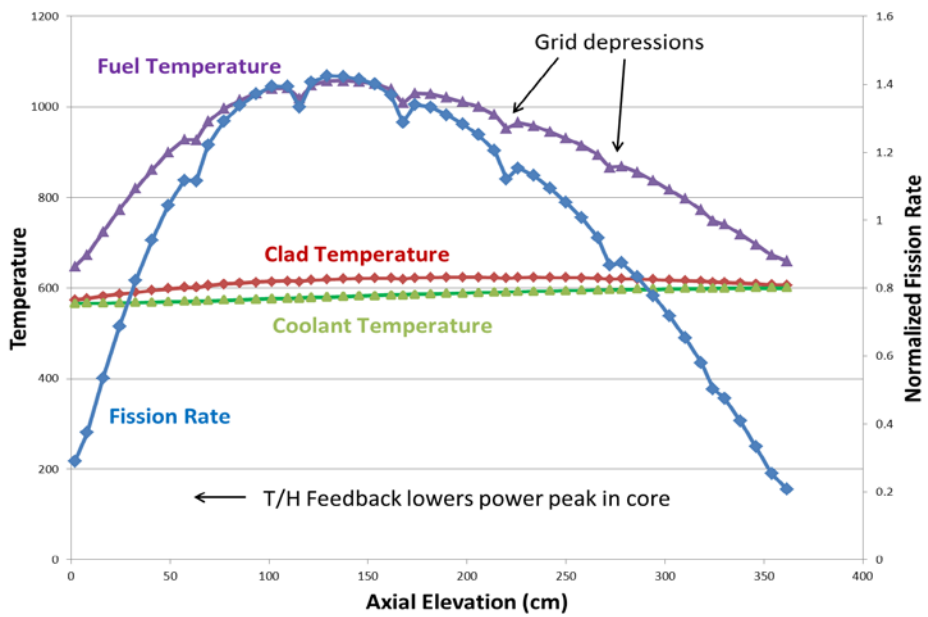
Power	Iters	K-eff
70%	11	1.24012
100%	11	1.23344
130%	15	1.22643

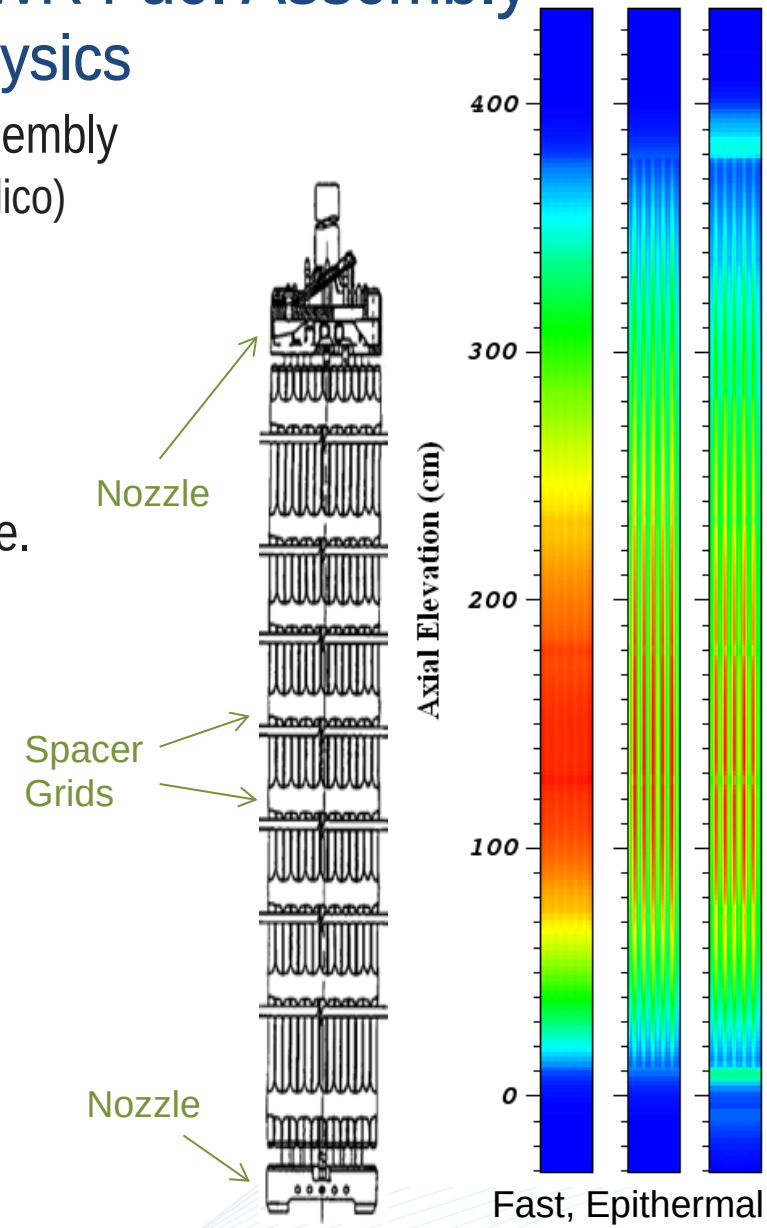
Insilico S_N
23 energy groups
4x4 mesh per pin
P_0 scattering
QR 4x4 quadrature
Titan: 1156 cores

Prob. #6

VERA Multiphysics Simulation of PWR Fuel Assembly
- Base for adding Challenge Problems Physics

- Coupled multiphysics model of WEC PWR fuel assembly
  - Neutron transport to calculate power distribution (Insilico)
  - Thermal-Hydraulics in coolant (COBRA-TF)
  - Heat conduction in fuel rods (COBRA-TF)
  - Neutron cross sections as function of temperature and density (XSProc)
- Next step is scaling up to a 1/4 reactor core simulation in support of a DOE reportable milestone.



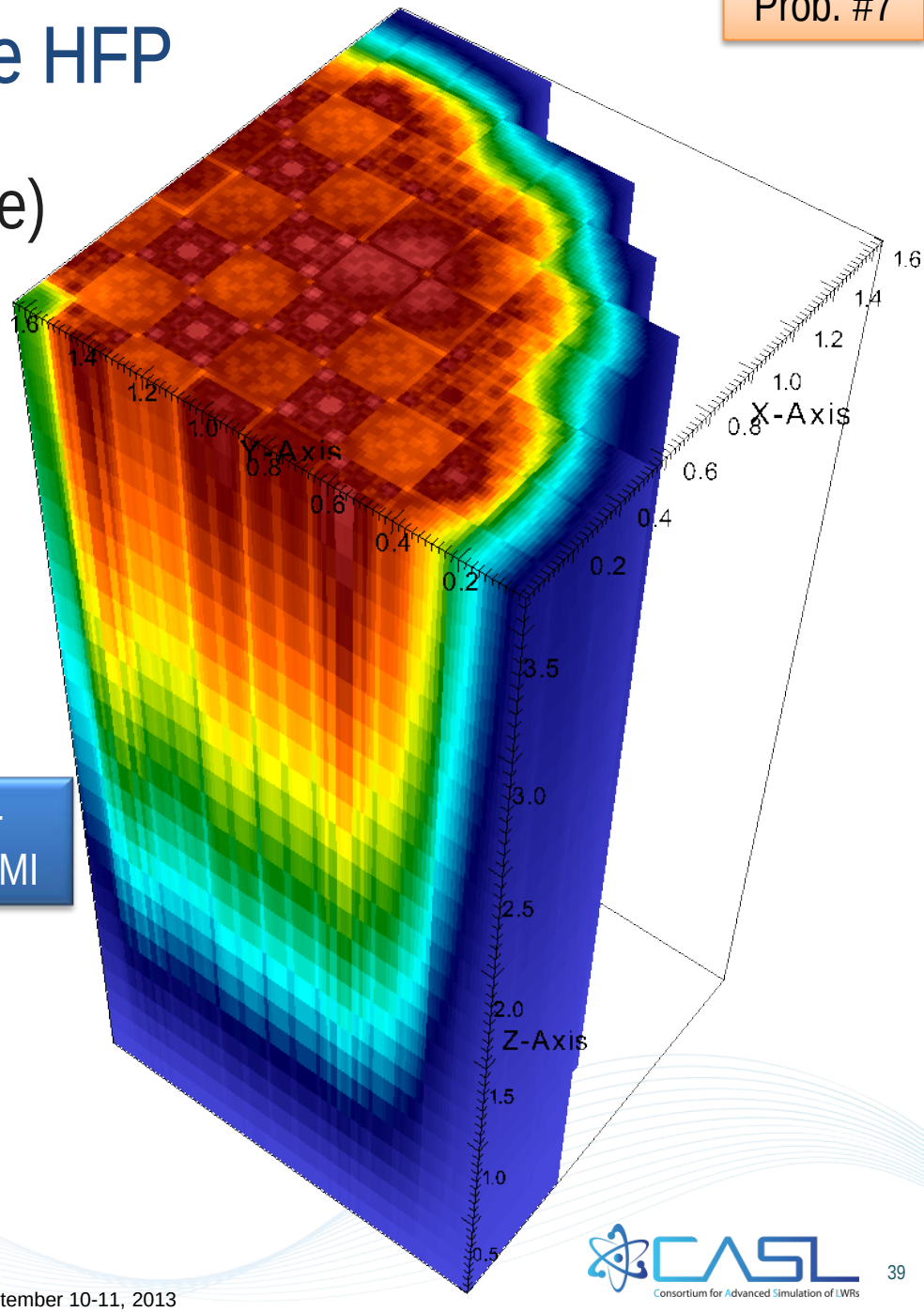


Fast, Epithermal, and Thermal Flux Profiles

Prob. #7

Next: Problem 7 – Full Core HFP

- Combine Problems 5 (Full-Core) and 6 (coupled T/H)
- Full-Core COBRA-TF
- Full-Core Insilico/MPACT
- Boron search
- Equilibrium Xenon



COBRA-TF Full-Core Model of TMI

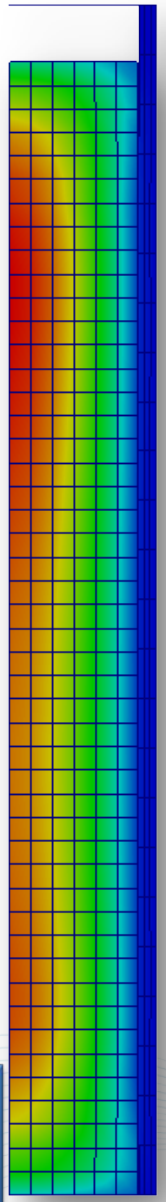
Coupling results to be used in DOE-Reportable Milestone L2:AMA.P7.02 due 9/30/2013

Challenge Problem Coupling – PCI

PCI CP

- Starting with existing Problem 6 capability and adding advanced MOOSE-based PEREGRINE fuel performance capability
- 2D R-Z PEREGRINE model for every rod
- PEREGRINE/Insilico/CTF compiled in one executable using Tribits build system
- Using MOOSE DTK capability

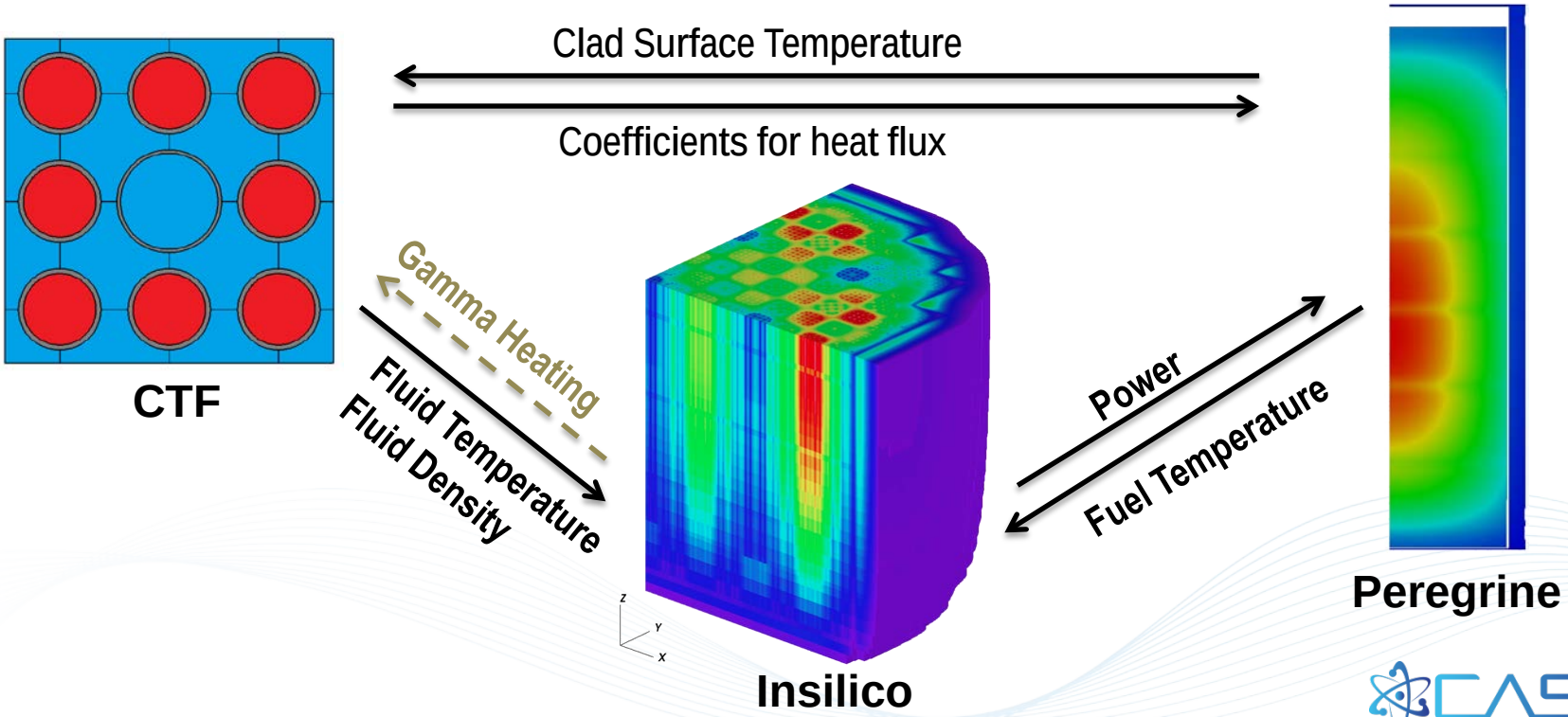
Results documented in DOE-Reportable Milestone L2:VRI.P7.02 (7/31/2013)



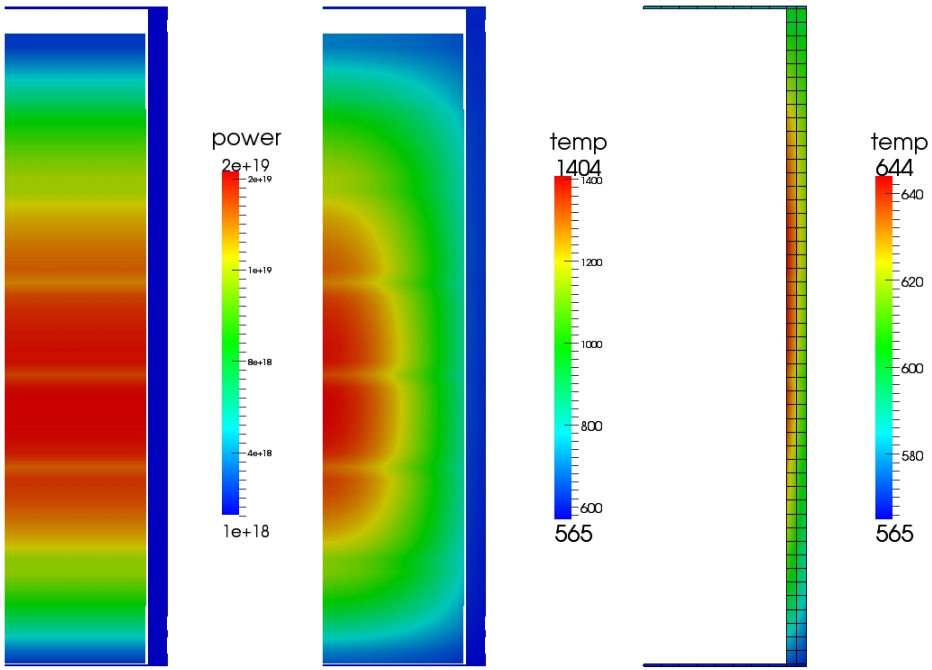
PEREGRINE r-z mesh for a single fuel rod

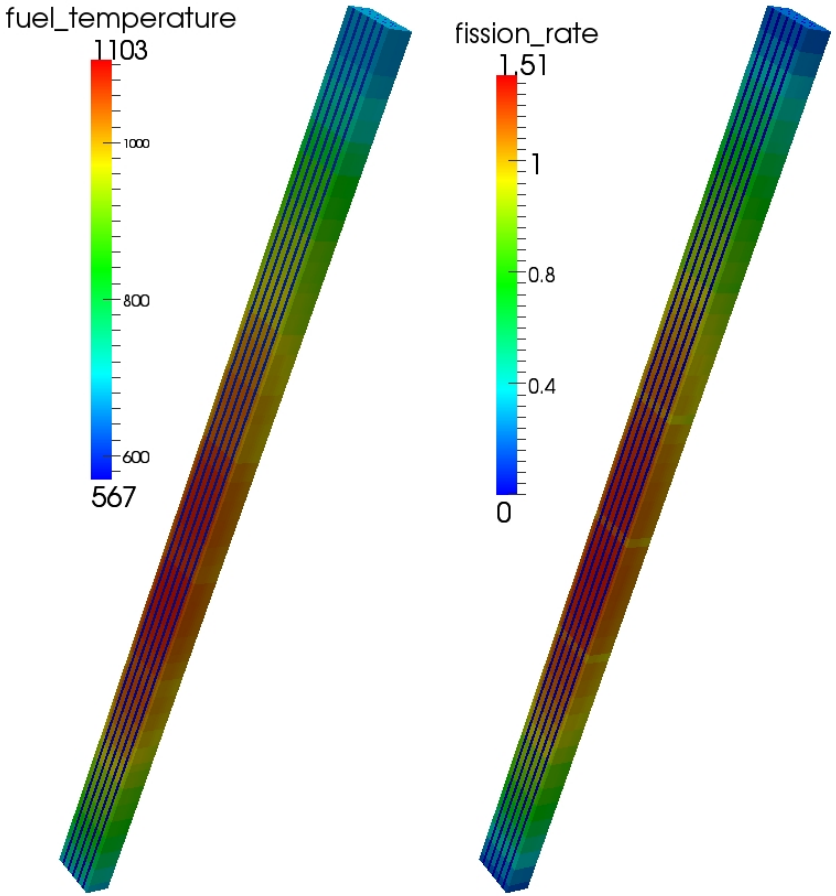
CTF / Insilico / Peregrine Coupled Driver

- Applications are run in their own MPI process space
  - can overlap if desired
  - reduce collisions and improved algorithms performance
- Data Transfers are handled through DTK with MPI sub-communicators



Peregrine Coupling results for 17x17 WEC Assembly
(AMA progression problem 6)





Fission rate (from Insilico) and temperature in Peregrine for a selected rod. The plot on the right is scaled to show clad temps.

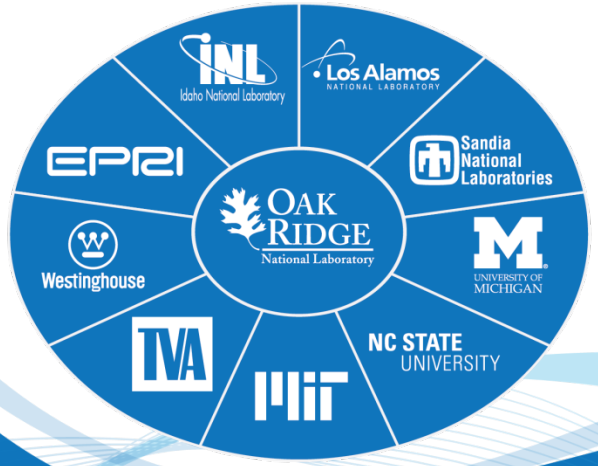
Insilico averaged fuel temp. and fission rate

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

VOCC Laboratory Demonstrations - Selected VERA Applications

CASL Joint Industry and Science Council
Oak Ridge National Laboratory
September 10, 2013



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CASL
Consortium for Advanced Simulation of LWRs

Virtual Office, Community and Computing

April Lewis, CASL CIO

And VOCC Lab Director

Creating Today's Collaborative Tomorrow in Energy Science Modeling and Simulation

* Developing an effective paradigm for sharing high performance computing, visualization and information resources for communities of geographically distributed energy scientists.

VOCC One-Roof Core Components

Central

physical lab space(s) with virtual extensivity to people and technology resources

Shared modeling and simulation (compute, meshing, render, and visualization resources).

Integrated with a single custom collaborative Communication Environment

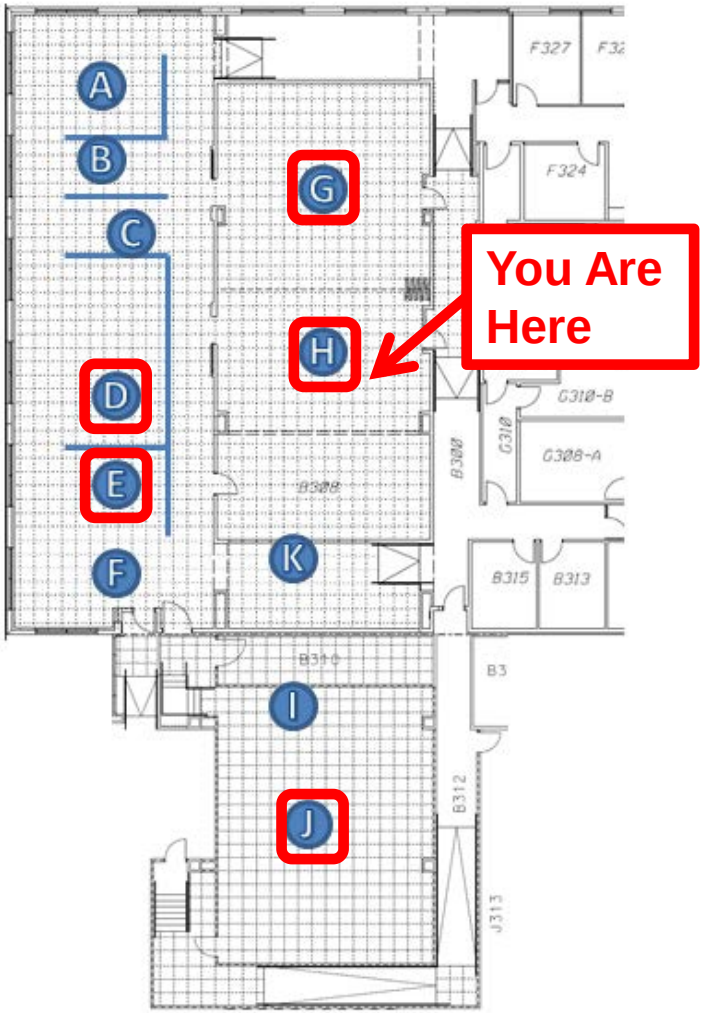
People and expertise

"Work Social – Insightful Innovation"

** Users of Terascale/Petascale computing, drivers of Exascale development

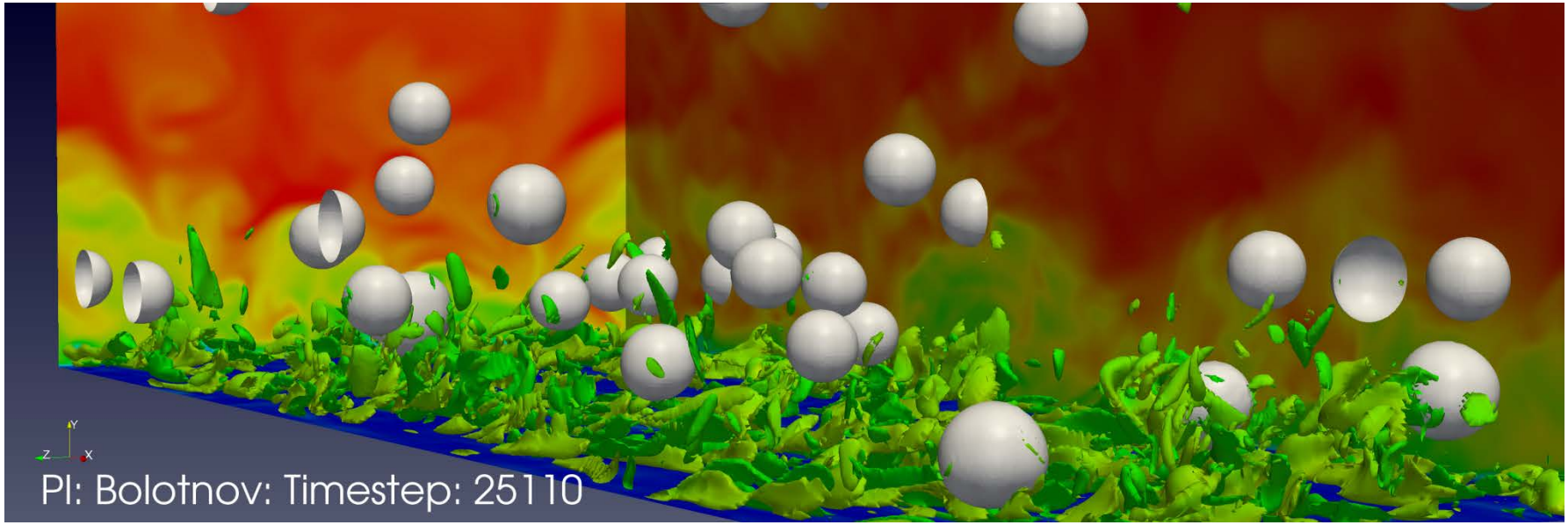
Demonstrations - Selected VERA Applications

1. (G) Immersion Room (THM) – Bubble Model
2. (J) F-5 (AMA) – Fibrous Debris Project
3. (H) Waldo (MPO) – Crud build up and fuel performance
4. (D) I-DEATE Stations 4&5 (PHI) – NiCE demo – VERA usability/workflow
5. (E) I-DEATE Station 6 (PHI) - Exploration of VERA Results, VERA input / demo, COBRA-TF activities



1. Immersion Room (THM): Turbulent bubbly channel flow

- Fully resolved turbulent with 60 bubbles simulated using 21 million computational elements on 11,200 cores (Titan supercomputer)
- Wall is on the bottom and top (not seen), periodic boundary conditions on other faces
- Half-channel is shown, the bubbles concentrate near the wall due to lift force effect
- Hair-pin turbulent vorticities (yellow/green structures) show the turbulence production process originating near the high—mean-shear region at the wall.
- Level-set method is used for bubble tracking, which allows for bubble coalescence and deformation
- Used to develop new bubbly flow turbulent models to be applied for realistic reactor coolant flow conditions

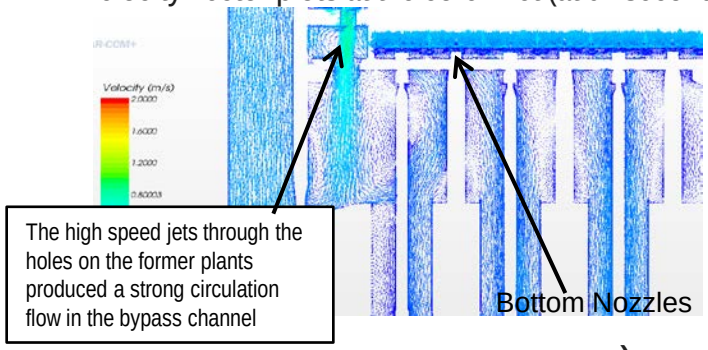


Report Provided to Committee

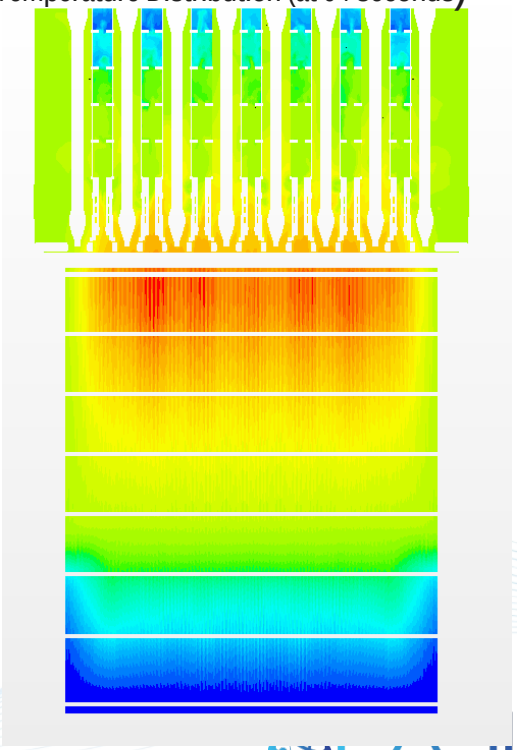
2. F-5 (AMA): CFD Applications: Demonstration of Large-Scale CFD Application - Fibrous Debris Flow Blockage

- Used vessel model of WBN1 previously developed with Star-CCM+
- Demonstration to a time-dependent, multi-phase simulation to determine viability
  - Industry Council supported application to Fibrous Debris blockage
  - Pressure drop variation for simulating fibrous debris accumulation was applied in Bottom Nozzle region through Porous Medium model.
  - The pressure loss increase from the normal condition to the maximum debris build up is applied to Bottom Nozzle region in 30 second
- Provided demonstration of difficulties encountered in applying computationally intensive large-scale simulations – Lessons carry over to use of Hydra-TH
- Provides a demonstration to industry of the value of being able to perform large-scale reactor simulations (presented to Industry Council in March)

Velocity vector plots at the core inlet (at 94 seconds)

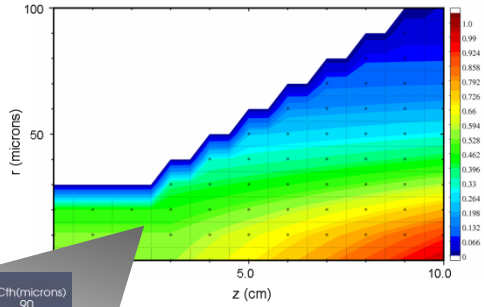


Temperature Distribution (at 94 seconds)



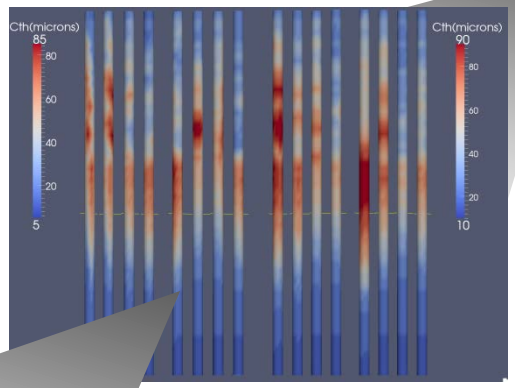
3. Waldo (MPO): MPO Approach to CRUD

Pragmatic approach, complementary to BOA, to address the mechanistic process of CRUD formation and growth, and subsequent impact on CIPS and CILC.



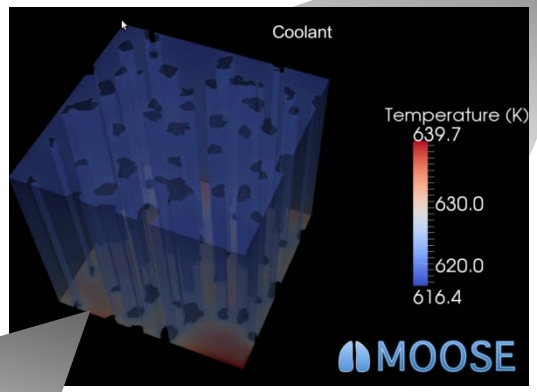
2D MAMBA

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



3D MAMBA

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

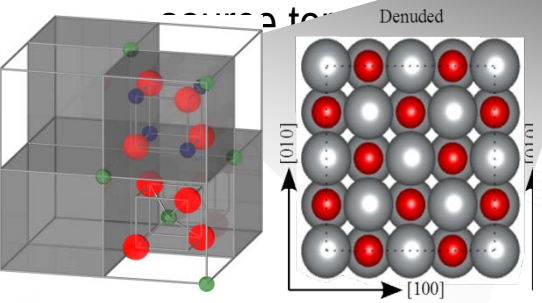


MAMBA-BDM

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

Thermodynamics

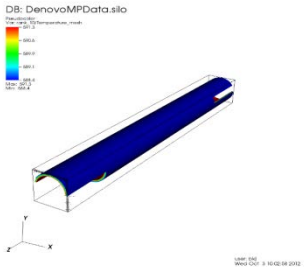
Mostly atomistic scale calculations that address CRUD phase stability, nonstoichiometry, solvation and potentially



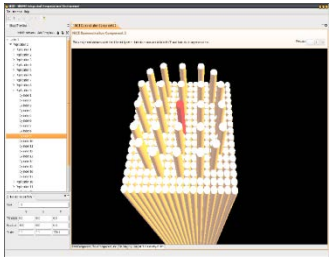
4. I-DEATE Stations 4&5 (PHI)

billingsjj@ornl.gov

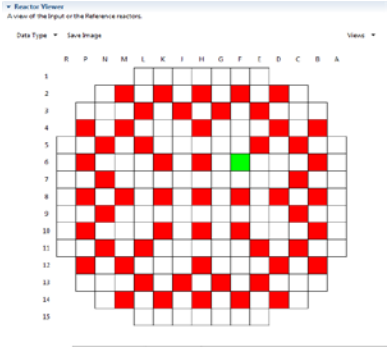
Jay Jay Billings
Research Staff
Oak Ridge National Laboratory
billingsjj@ornl.gov
@jayjaybillings
+jayjaybillings



Jordan Deyton
Research Associate
Oak Ridge National Laboratory
deytonjh@ornl.gov



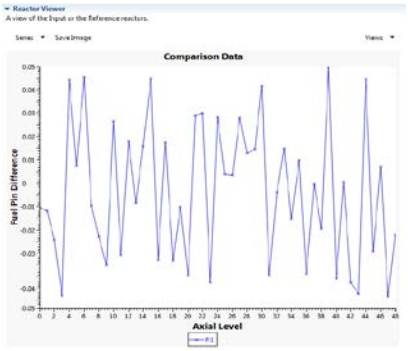
Project Web Page
http://niceproject.sourceforge.net

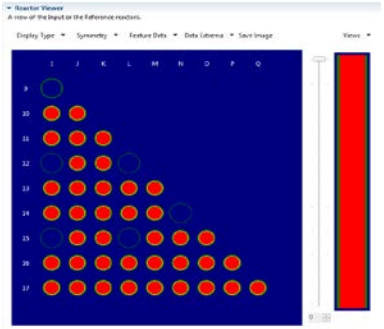


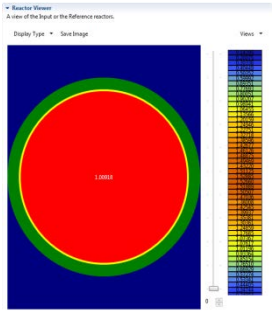
Modeling and simulation made NiCE!

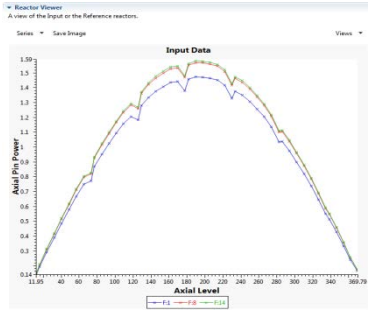
A 100% open source project for workflow and data management developed at Oak Ridge National Laboratory for DOE-NE, DOE-EERE and LDRD/WFO. Available cross-platform (Win32, Linux, Mac) and soon via rich web clients.

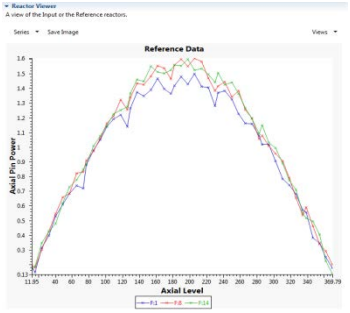
In addition to analysis, NiCE supports input generation, local and remote job launch and other common tasks. Everything is made easy for users and developers.





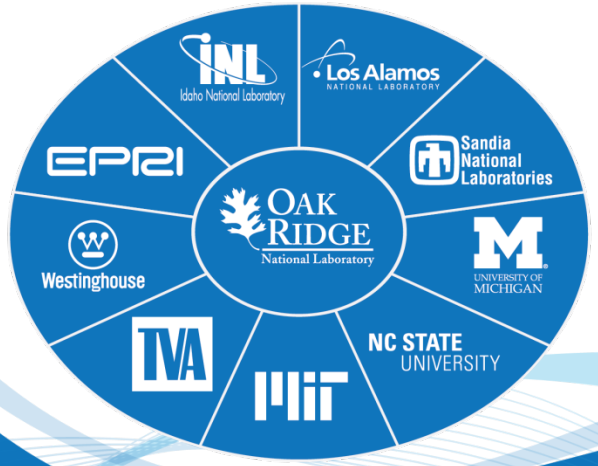






5. I-DEATE Station 6 (PHI) Exploration of VERA Results (VERA Input, Full-core neutronics, Coupled single-assembly)

Joint Industry Council / Science Council Meeting
Oak Ridge National Laboratory
Sept 10-11, 2013



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

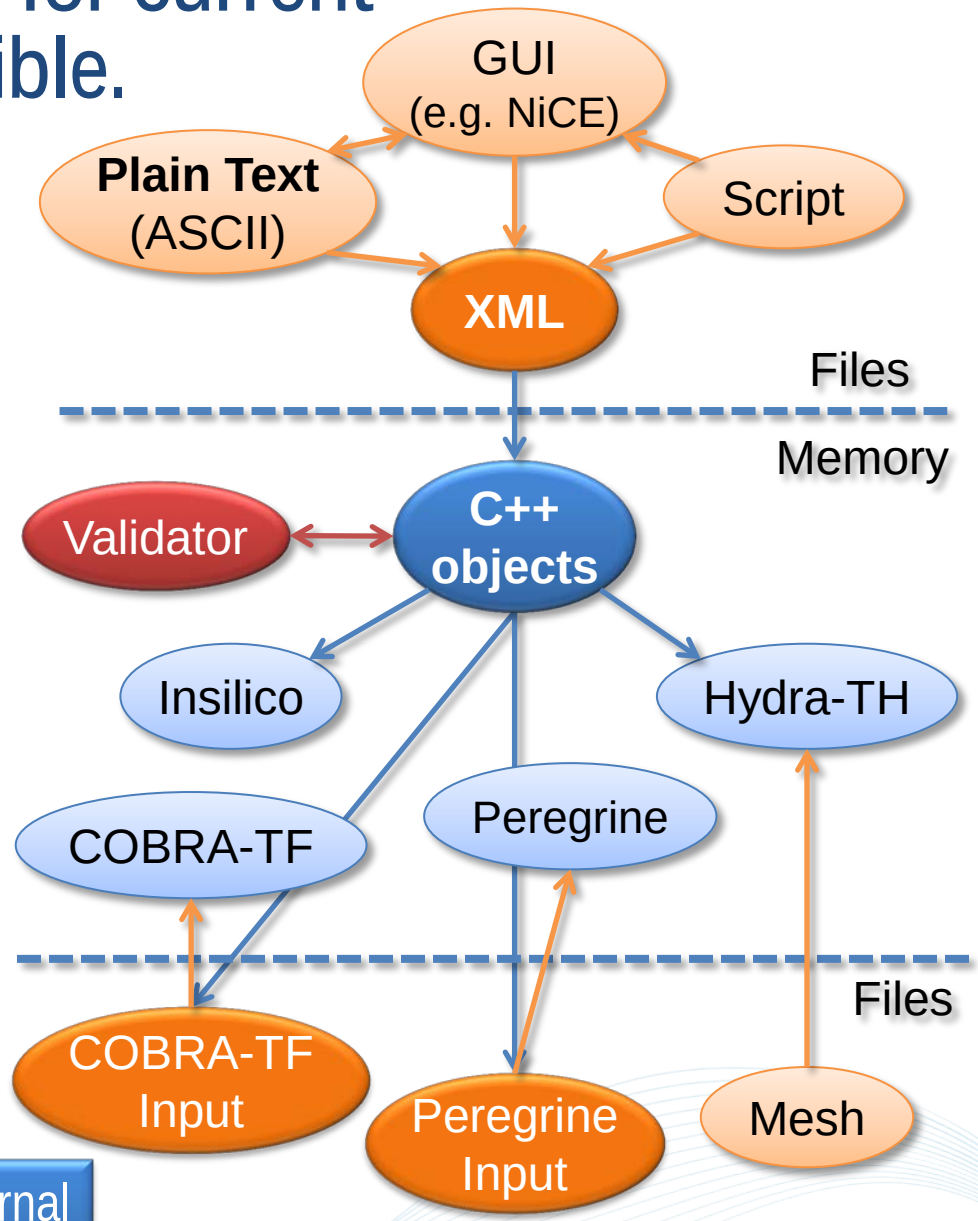
CASL
Consortium for Advanced Simulation of LWRs

Overview

- VERA Input
- Zero Power Physics Tests (ZPPT)
  - full-core neutronics
    - Insilico (S_N and SP_N)
    - MPACT (MOC)
- Hot Full-Power Beginning of Life Assembly
  - coupled neutronics (Insilico SP_N) + thermal-hydraulics (COBRA-TF)
    - Coupled vs. non-coupled
    - Convergence behavior
    - Void fraction / vapor generation vs. power
  - coupled neutronics + T-H + fuel performance (Peregrine2D)
    - Convergence behavior

VERA input is comfortable for current industry users and extensible.

- ability to create, archive, compare, and modify input similar to current industry workflows
- attributes of real reactors
  - assemblies, poisons, control rods, non-fuel structures, baffle, power, flow, depletion, boron search, detectors, etc.
- eliminate inconsistencies between physics components through use of a common geometry description
- will evolve as needed
- currently using VERA input
  - Insilico (S_N, SP_N, Monte Carlo)
  - COBRA-TF
  - MPACT
  - Peregrine



Discussing with VUQ how best to expose internal component model parameters for SA/UQ.

AMA Progression Problem 3: Hot Zero Power Assy.

```
[CASEID]
  title 'CASL Problem 3'
!=====================================================================
!  Sample input for Problem 3 (Single-assembly)
!  Draft 1 - 6/28/2012 - based on XML on parameter list Wiki page
!  Draft 2 - 6/28/2012 - minor changes (Andrew), Wiki PL also updated
!=====================================================================

[STATE]
  power  1.0e-7        ! %
  tinlet 620.33        ! F - 600K
  tfuel  600.0         ! K - 600K
  boron  1300          ! ppmB
  modden 0.743         ! g/cc
  feedback off

[CORE]
  size 1                ! 1x1 single-assembly
  rated 17.67   0.5     ! MW, Mlbs/hr
  apitch 21.5
  height 406.328
  core_shape
    1
  assm_map
    A1
  lower_plate ss 5.0 0.5   ! mat, thickness, vol frac
  upper_plate ss 7.6 0.5   ! mat, thickness, vol frac
  bc_rad reflecting
  he he 0.000176
  inc inc 8.19
  ss ss 8.0
  zirc zirc 6.56
```

```
[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260
  uo2 U31 10.257 / 3.1
  cell 1     0.4096 0.418 0.475 / U31 he zirc
  cell 100          0.561 0.602 / mod    zirc       ! guide tube
  lattice FUEL1
     100
       1 1
       1 1 1
     100 1 1 100
       1 1 1   1 1
       1 1 1   1 1 100
     100 1 1 100 1   1 1
       1 1 1   1 1   1 1 1
       1 1 1   1 1   1 1 1 1
  axial A1   11.951
     FUEL1 377.711
  grid END inc  1017 3.866
  grid MID zirc 875  3.810
  grid_axial
     END  13.884
     MID  75.2
     [...]
     MID 336.2
     END 388.2

  lower_nozzle  ss 6.05  6250.0  ! mat, height, mass (g)
  upper_nozzle  ss 8.827 6250.0  ! mat, height, mass (g)

  lower_nozzle_gap_height  4.231
  lower_pincap_height      1.67

  upper_nozzle_gap_height  2.12
  upper_pincap_height      1.67
  upper_plenum_height      16

 !! dancoff                   ! assembly_dancoff_map
 !!   0.000
 !!   0.287 0.315
 !!   0.287 0.315 0.315
 !!   0.000 0.287 0.286 0.000
 !!   0.287 0.316 0.316 0.284 0.299
 !!   0.288 0.317 0.316 0.287 0.267 0.000
 !!   0.000 0.286 0.286 0.000 0.270 0.286 0.321
 !!   0.287 0.319 0.319 0.286 0.315 0.335 0.333 0.337
 !!   0.323 0.322 0.321 0.322 0.320 0.322 0.323 0.322 0.310
```

```
[EDITS]
!  3in intervals in active fuel
  axial_edit_bounds
          11.951
          15.817
          [...]
          369.7898
          377.711

[DENOVO]
    eq_set        ld
    eigen_solver  arnoldi
    tolerance     1e-06
    Pn_order      1
    dimension     3
    mesh          4
!    eigenvalue_db:
        k_tolerance  0.0001
        L2_tolerance 0.001
        energy_dep_ev  false
    mat_library   test_comp.sh5
    max_delta_z   2.54
    num_blocks_i  40
    num_blocks_j  40
    num_z_blocks  64
    num_groups    23
    num_sets      6
!    quadrature_db:
        azimuthals_octant  4
        polars_octant      4
        quad_type          qr
!    silo_db:
        silo_output  vera
!    upscatter_db:
        upscatter_tolerance  1e-05
    xs_library     "v7-238ir"
   new_grp_bounds
       8.2085e+05
       [...]
```

Core Simulator Progression Problems Drive VERA Development

FY11

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

FY12

- #1 2D Hot Zero Power (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 w/Xenon

FY14

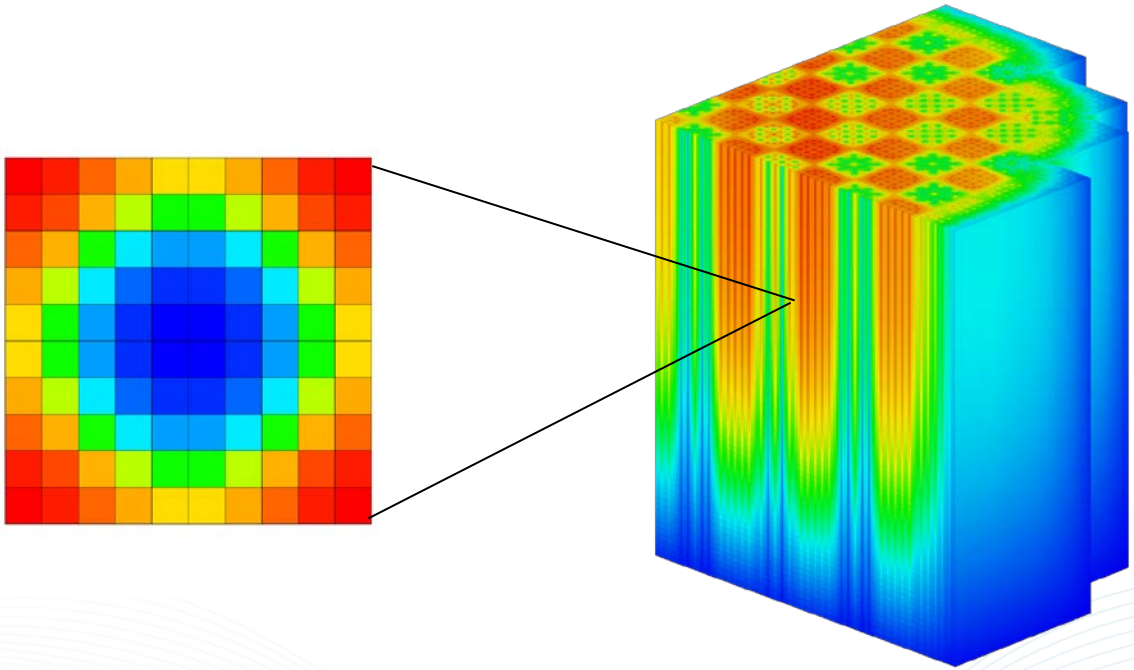
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

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

Neutronics – Insilico

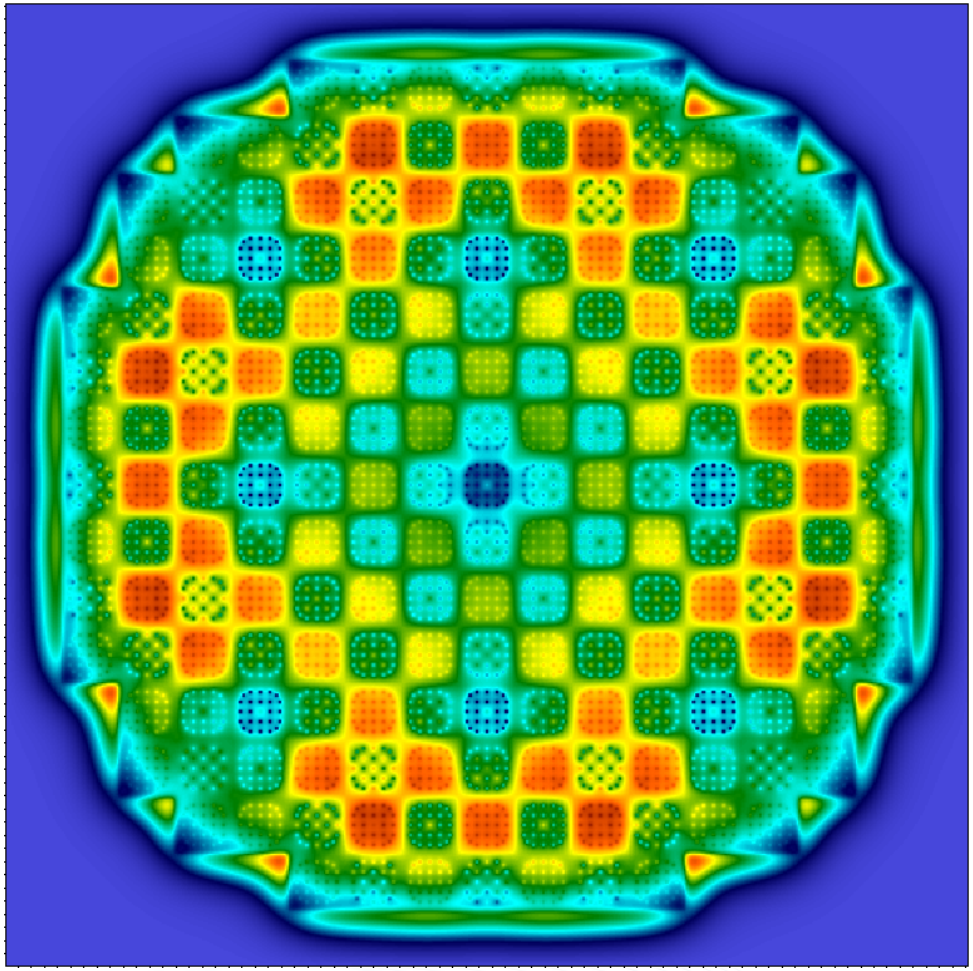
- Part of the Exnihilo environment
- Transport solver is S_N (pin-resolved) or SP_N (pin-homogenized)
- Built in cross section processing with XSProc
- S_N uses the KBA implementation which solves the problem on a Cartesian grid and can scale efficiently to over 100,000 processors

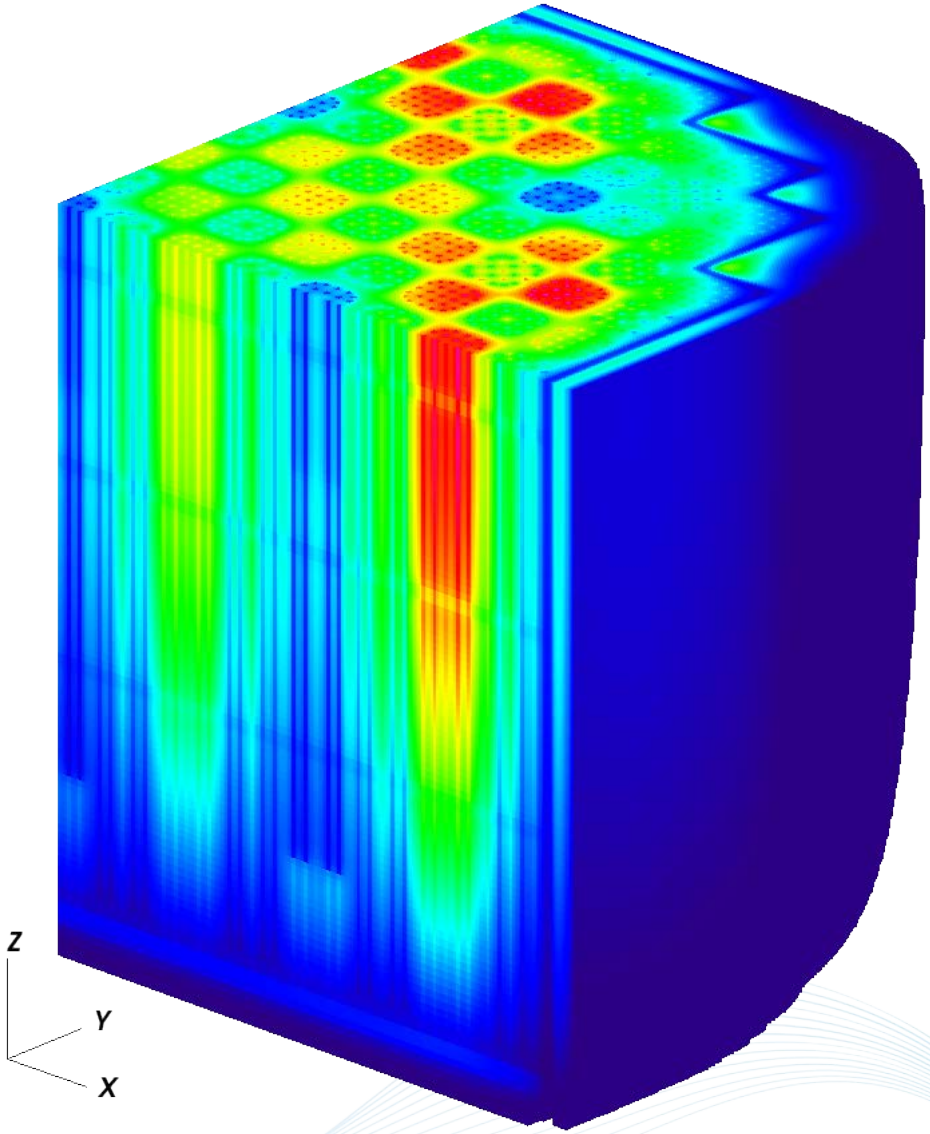
S_N Pin Resolved



Efficient Scaling to Large 3D Problems

Insilico thermal flux for AMA problem 5 using SP_N, generated from VERA ASCII input.





Core Simulator Progression Problems Drive VERA Development

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FY14

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- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

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

Problem 6 – PWR Single Assembly

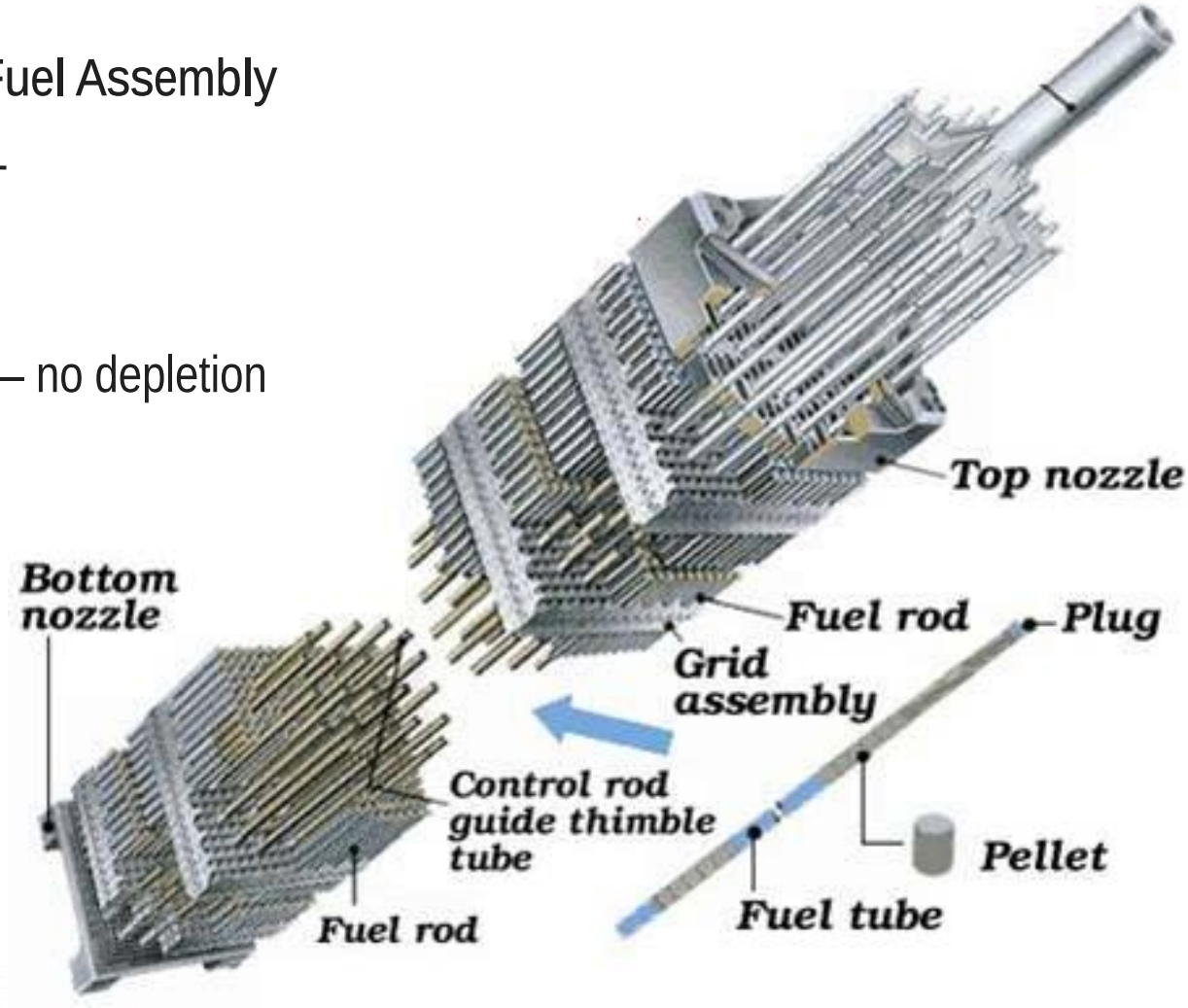
17x17 Westinghouse Fuel Assembly

Watts Bar Unit 1 Cycle 1

Hot Full Power (HFP)

Beginning of Life (BOL) – no depletion

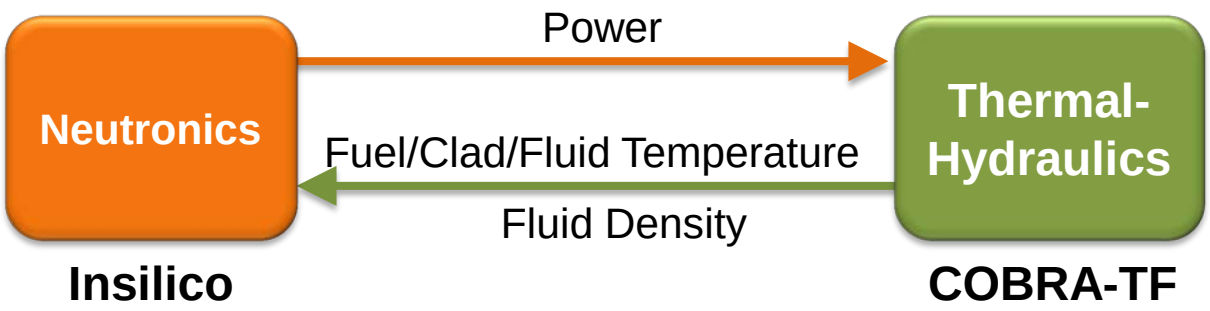
- Fuel Pins
- Plenum
- End Plugs
- Cladding
- Guide Tubes
- Spacer Grids
- Nozzles
- No Control Rods



Coupling of neutronics and thermal-hydraulics components for hot full-power beginning of life assy.

Prob. #6

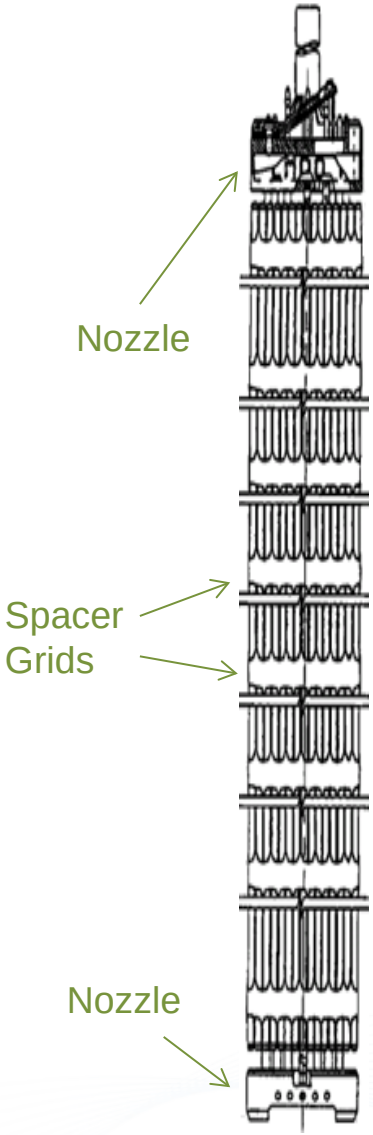
- AMA progression problem 6
  - neutronics (cross sections + neutron transport)
  - thermal-hydraulics (fluid flow and fuel/clad temperatures)



- Coupling becomes more complicated with more codes, but we've done it.
- Challenges are related more to data transfer than "framework".

Data Transfer Kit (DTK) will be discussed later.

Common Input – VERAin



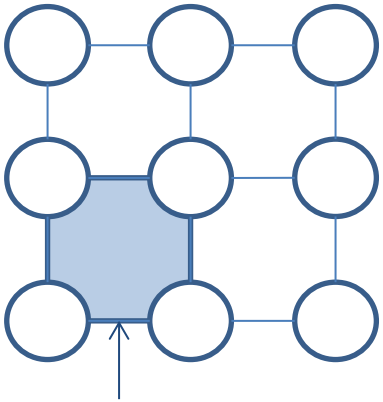

```
[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260

  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
```

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

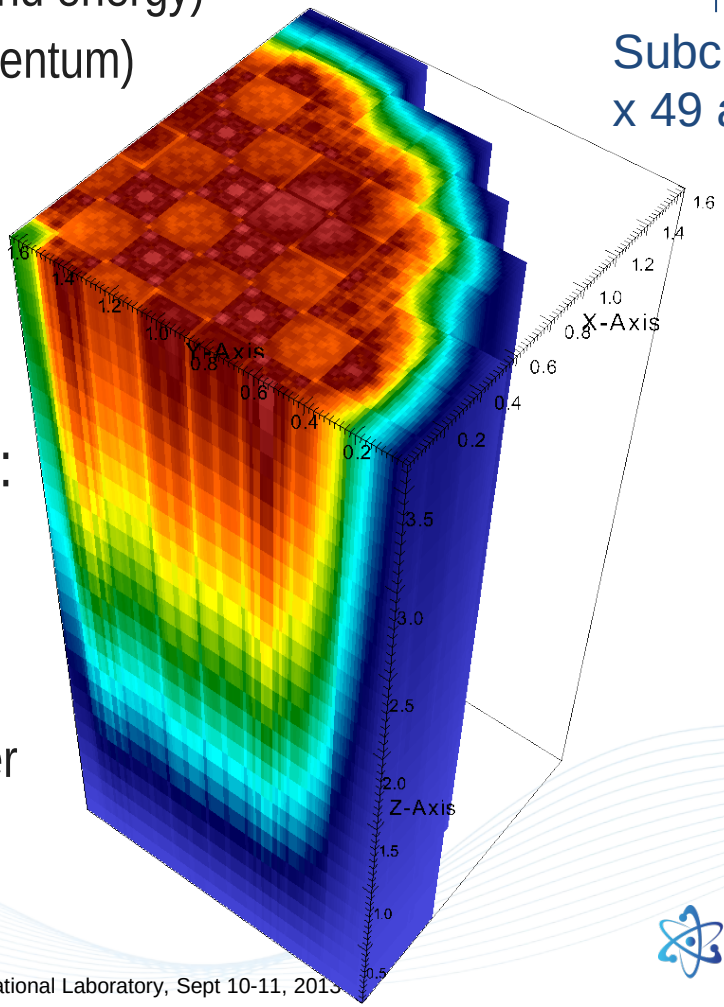
```
axial A1    6.050
    LGAP1  10.281
    PCAP1  11.951
    FUEL1 377.711
    PLEN1 393.711
    PCAP1 395.381
    LGAP1 397.501

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
```

Thermal Hydraulics – COBRA-TF

- COBRA-TF (CTF) subchannel code from Penn. State Univ.
- 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
- Pin conduction model
- Built-in material properties
- Since bringing in for CASL / VERA:
  - dramatically reduced memory usage
  - dramatically increased performance
  - dramatically expanded test coverage
  - implementing parallel version for further reduction in run-times

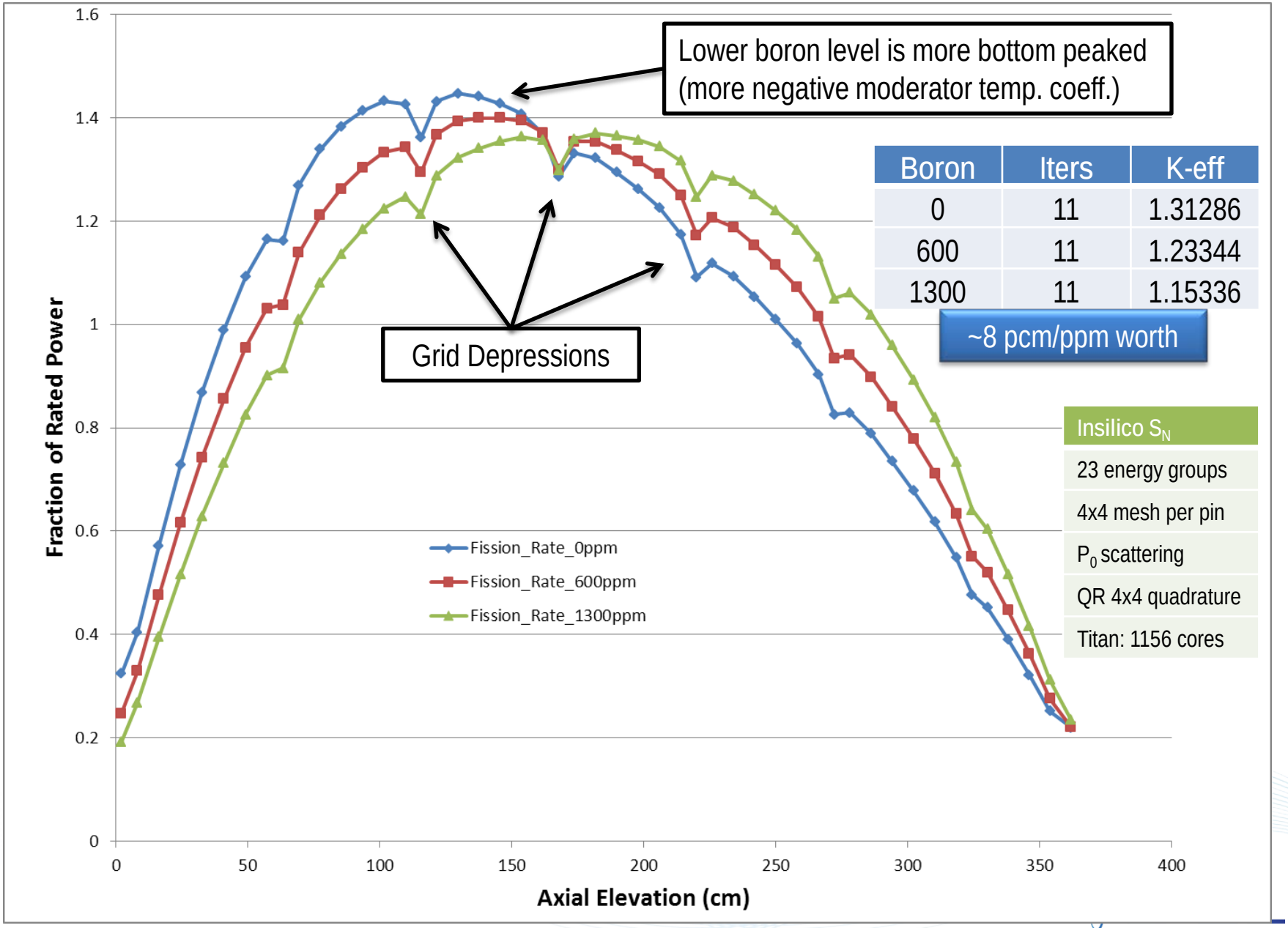


Subchannel area x 49 axial levels



Coupled Results – Boron Concentration

Prob. #6



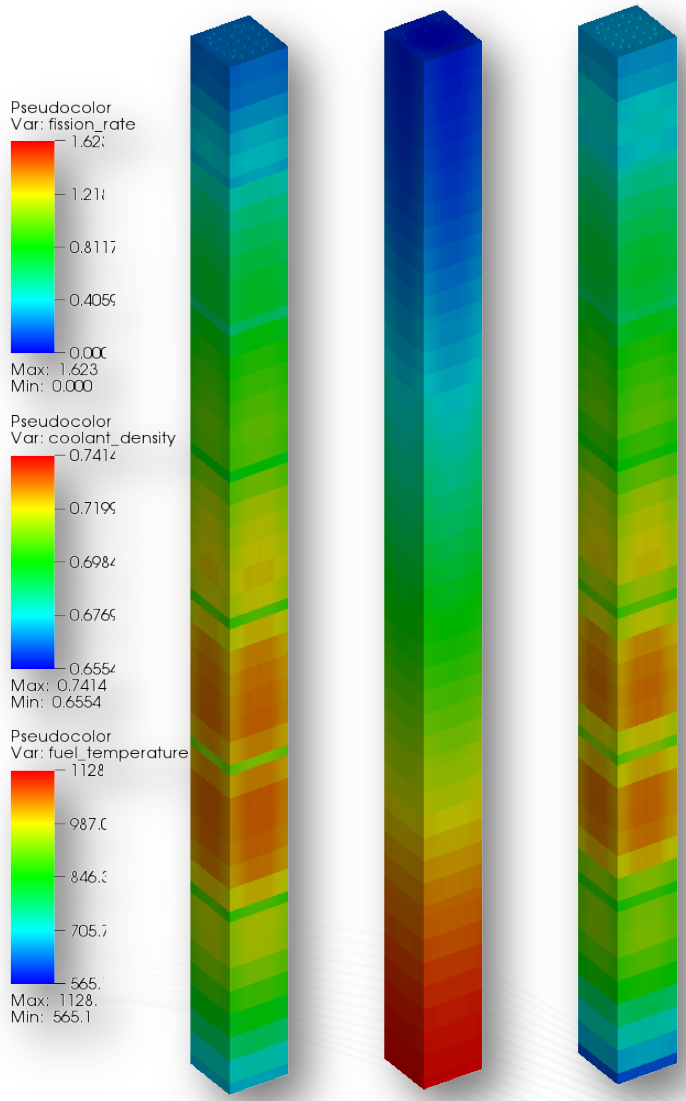
Boron	Iters	K-eff
0	11	1.31286
600	11	1.23344
1300	11	1.15336

~8 pcm/ppm worth

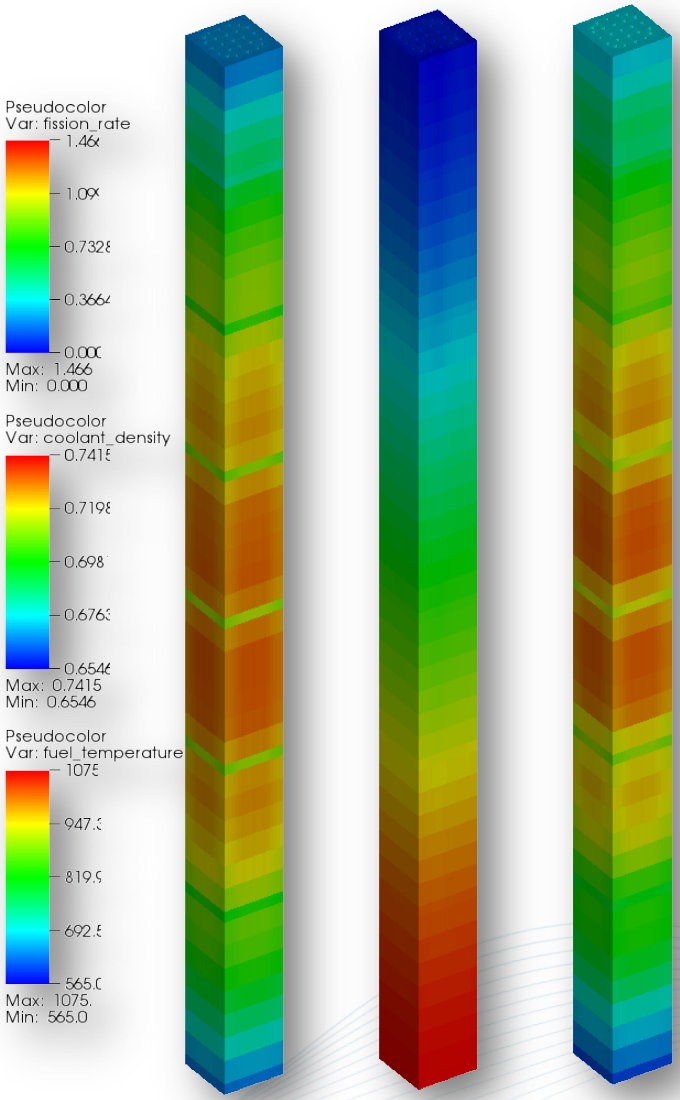
Insilico S_N
23 energy groups
4x4 mesh per pin
P_0 scattering
QR 4x4 quadrature
Titan: 1156 cores

Prob. #6

VERA Simulation of Hot Full Power Assembly
(neutronics with fluid / moderator temp. feedback)



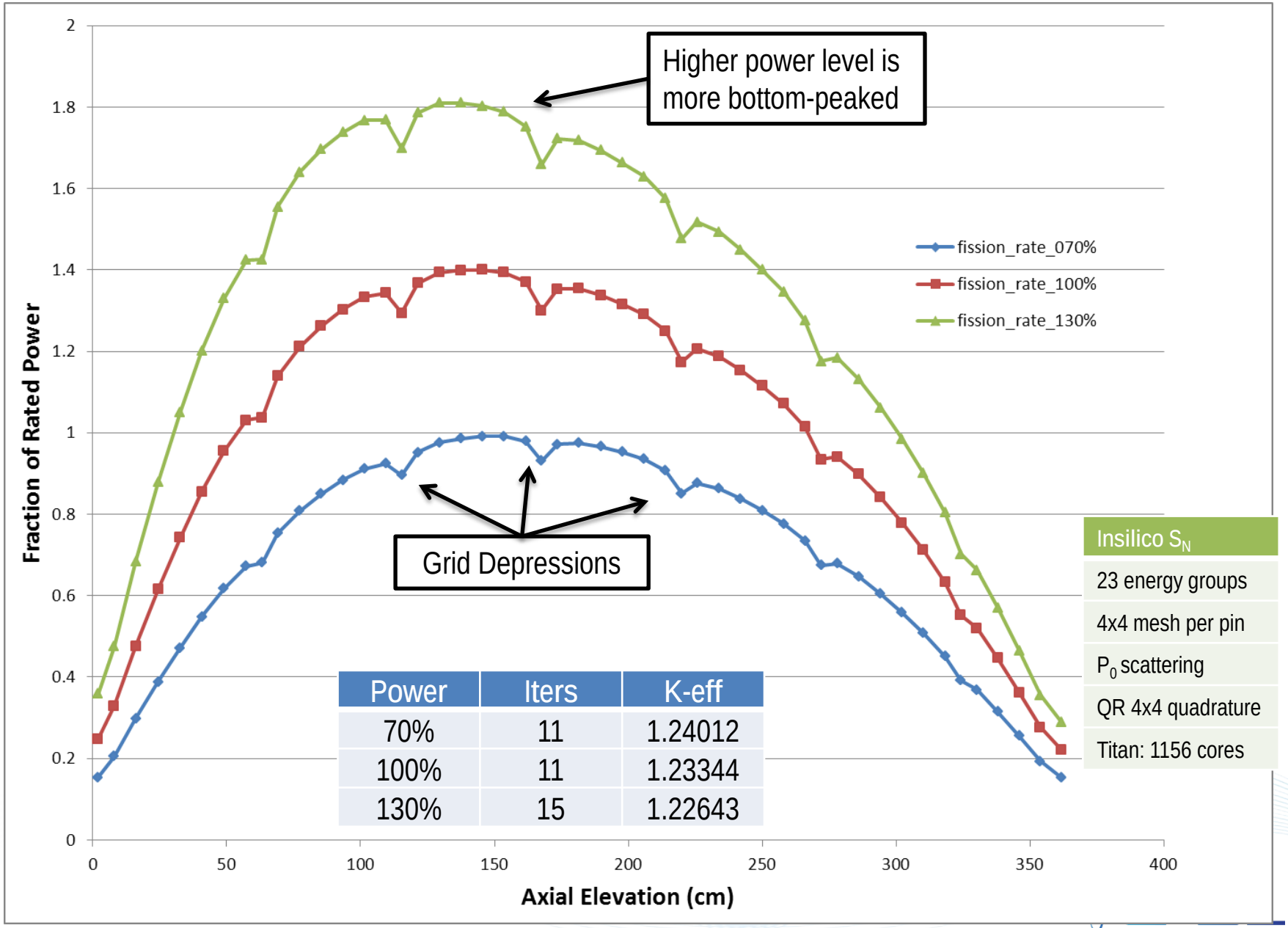
0 ppmB



1300 ppmB

Coupled Results – Power Level

Prob. #6

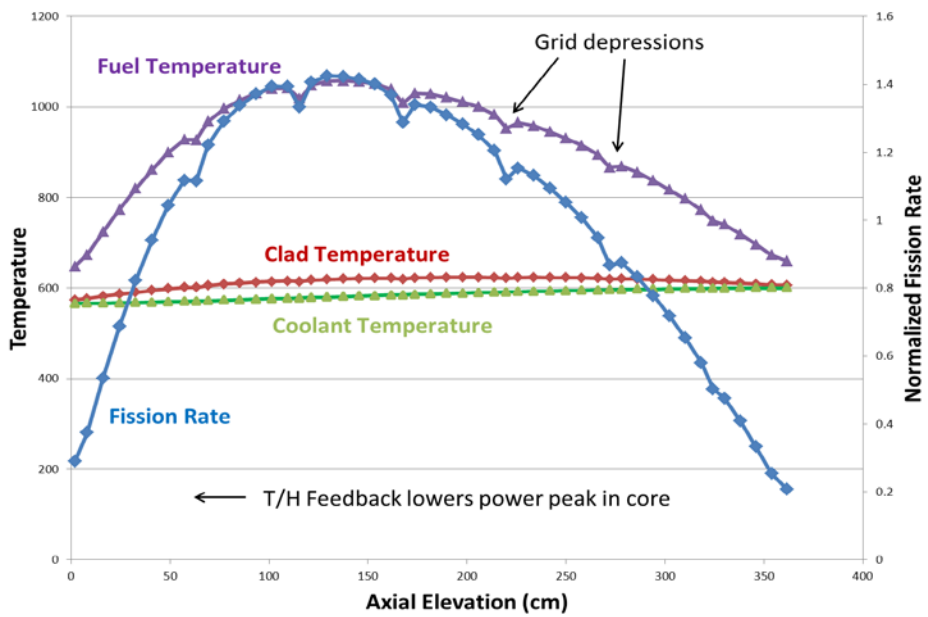


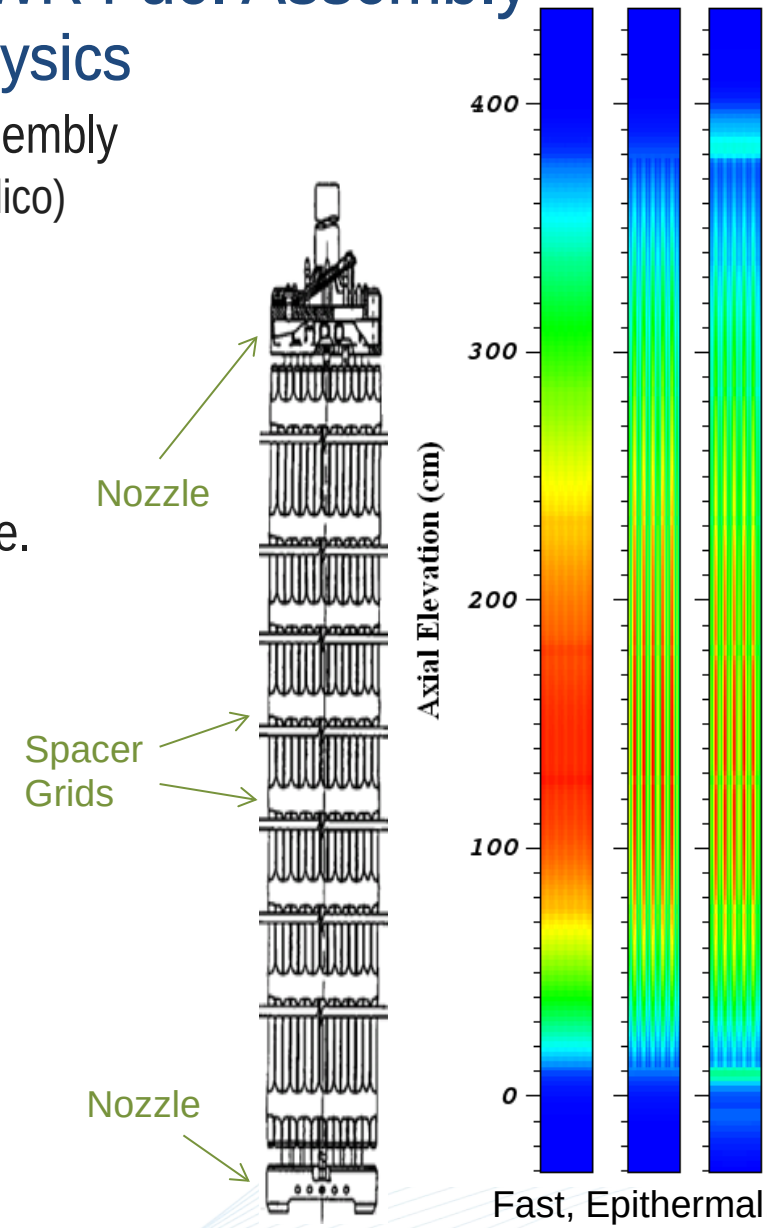
Power	Iters	K-eff
70%	11	1.24012
100%	11	1.23344
130%	15	1.22643

Insilico S_N
23 energy groups
4x4 mesh per pin
P_0 scattering
QR 4x4 quadrature
Titan: 1156 cores

VERA Multiphysics Simulation of PWR Fuel Assembly
- Base for adding Challenge Problems Physics

- Coupled multiphysics model of WEC PWR fuel assembly
  - Neutron transport to calculate power distribution (Insilico)
  - Thermal-Hydraulics in coolant (COBRA-TF)
  - Heat conduction in fuel rods (COBRA-TF)
  - Neutron cross sections as function of temperature and density (XSProc)
- Next step is scaling up to a 1/4 reactor core simulation in support of a DOE reportable milestone.

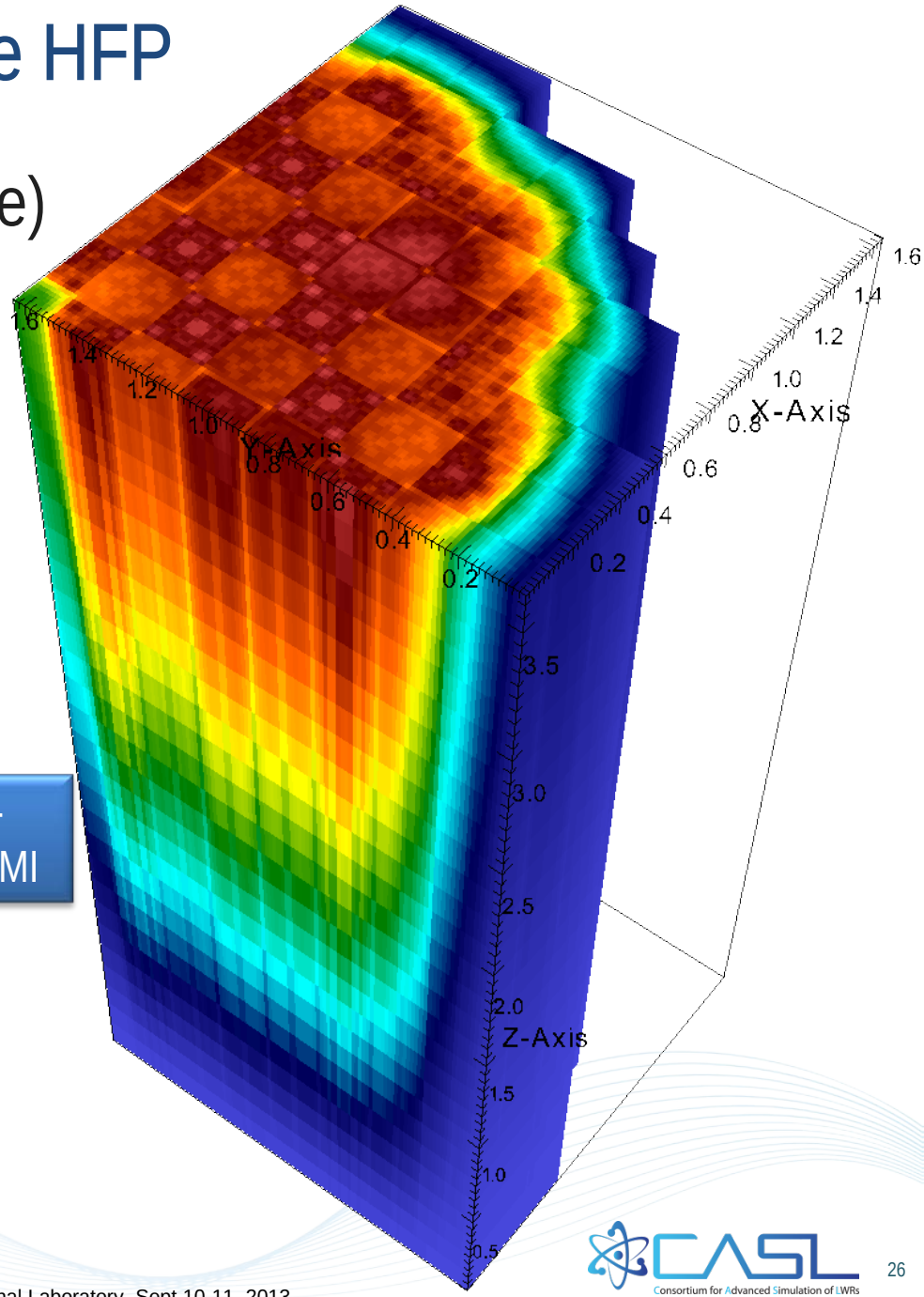




Fast, Epithermal, and Thermal Flux Profiles

Next: Problem 7 – Full Core HFP

- Combine Problems 5 (Full-Core) and 6 (coupled T/H)
- Full-Core COBRA-TF
- Full-Core Insilico/MPACT
- Boron search
- Equilibrium Xenon



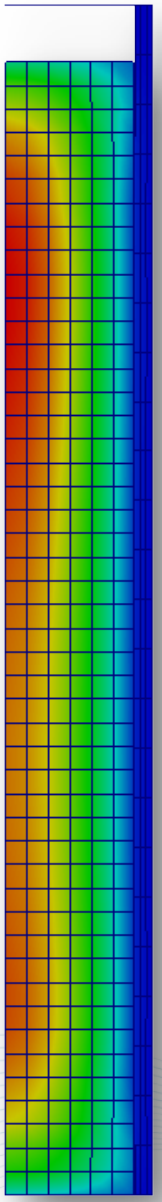
COBRA-TF Full-Core Model of TMI

- *Coupling results to be used in DOE-Reportable Milestone L2:AMA.P7.02 due 9/30/2013*

Coupled VERA-CS Capability for Pellet-Clad Interaction (PCI) Challenge Problem

- Extend basic Problem 6 capability
  - replace COBRA-TF fuel rod model with MOOSE-based Peregrine fuel performance capability
- 2D R-Z Peregrine model for every rod

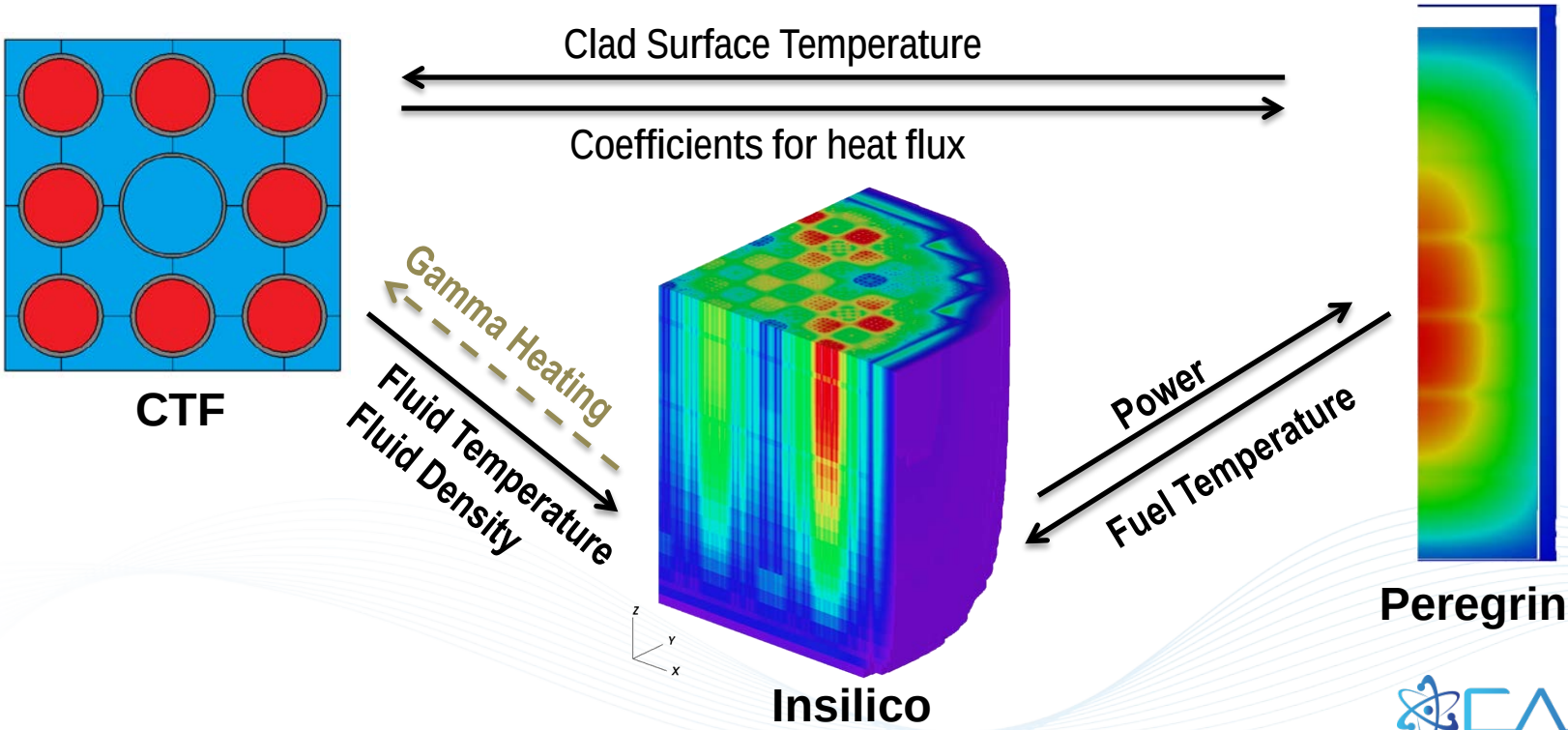
Results documented in DOE-Reportable Milestone L2:VRI.P7.02 (7/31/2013).



PEREGRINE r-z mesh for a single fuel rod

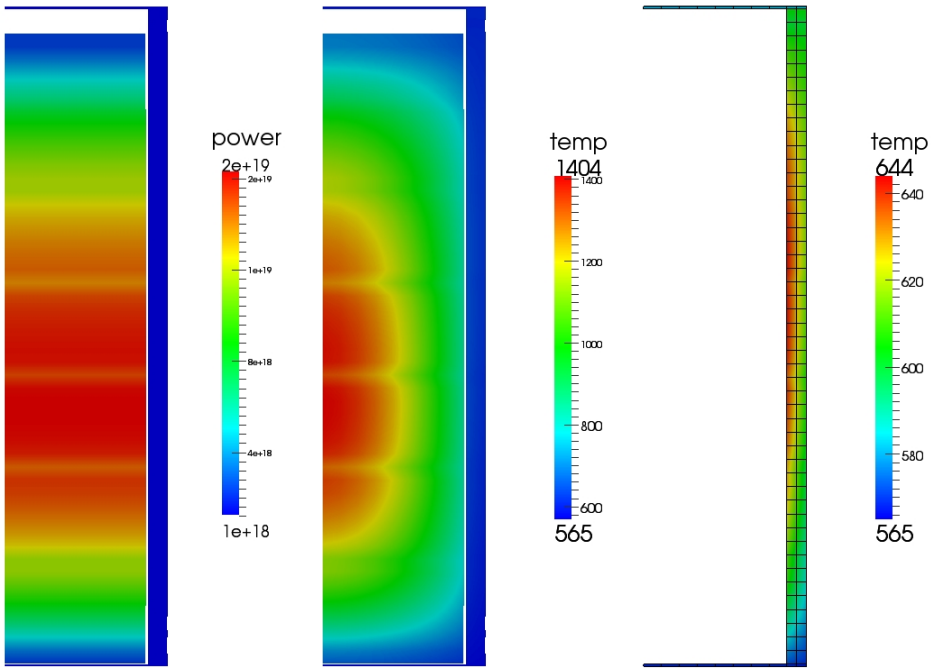
CTF / Insilico / Peregrine Coupled Driver

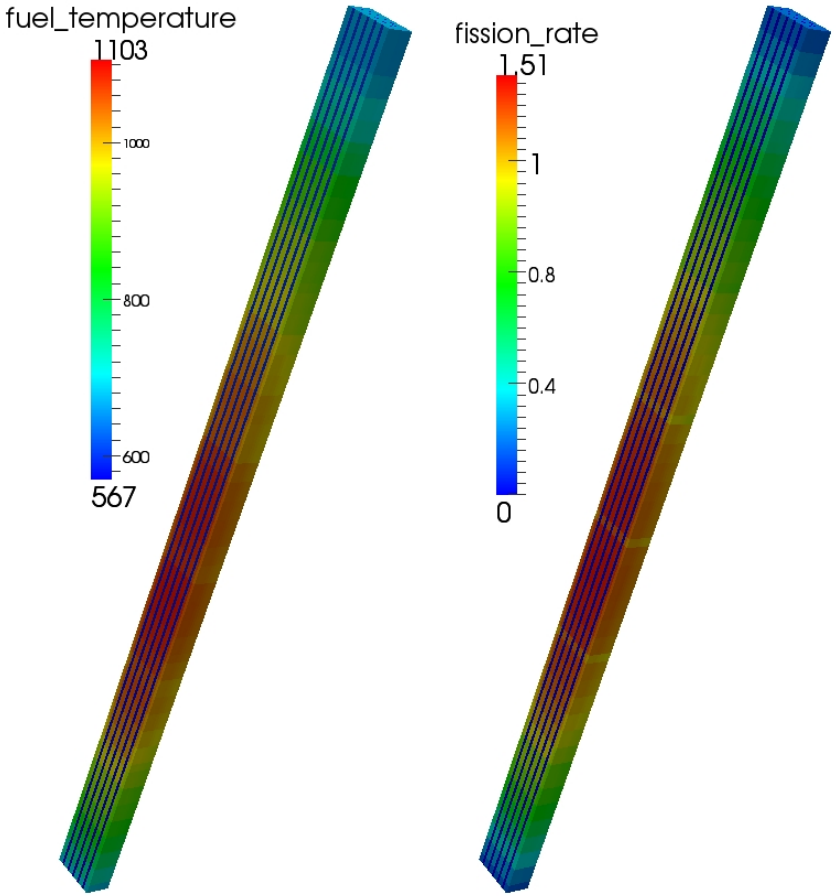
- Named **Tiamat**, multi-headed dragon (Babylonian mythos)
  - easy to add new "heads" provided the apps meet integration criteria
- All applications are run in their own MPI process space
  - can overlap if desired
  - reduce collisions and improved algorithms performance
- Data Transfers are handled through DTK with MPI sub-communicators



Coupled results for 17x17 WEC Assembly
(AMA progression problem 6)

Prob. #6



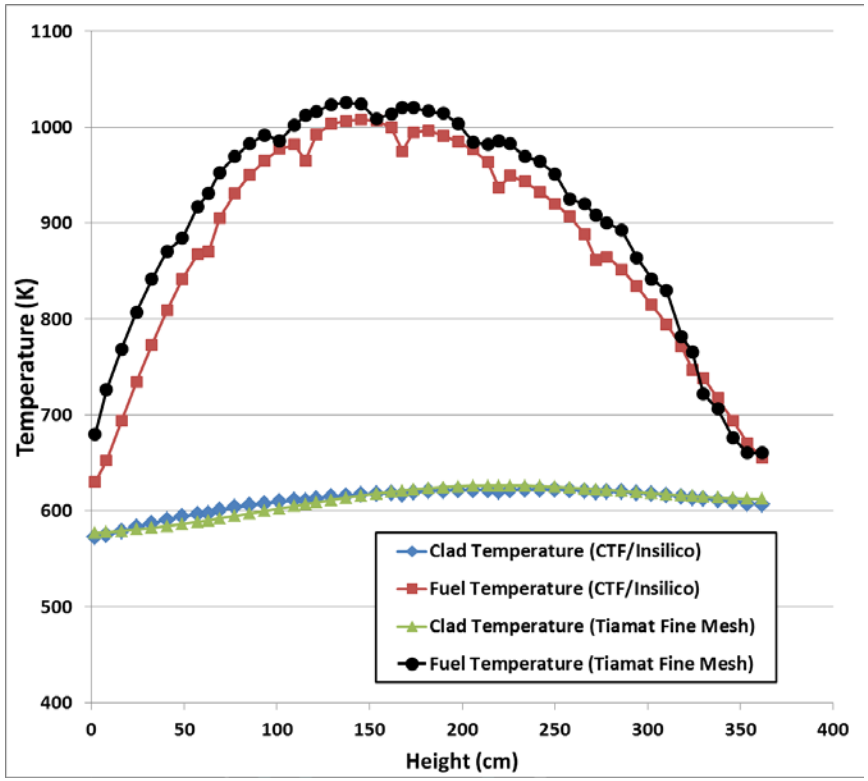


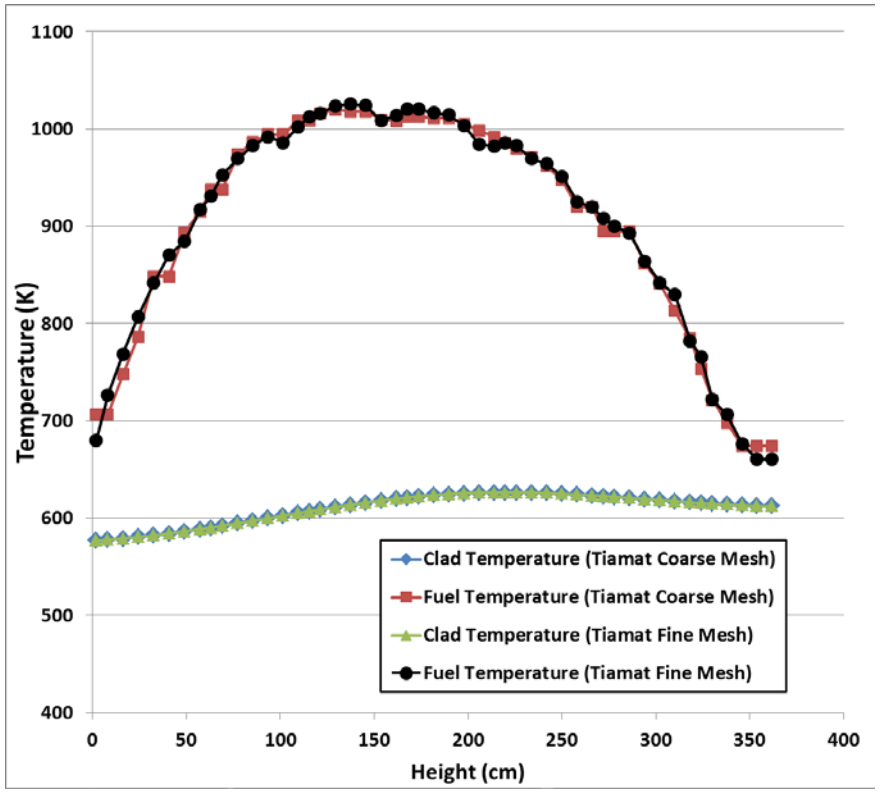
Fission rate (from Insilico) and temperature in Peregrine for a selected rod. The plot on the right is scaled to show clad temps.

Insilico averaged fuel temp. and fission rate

Coupled results for 17x17 WEC Assembly
(AMA progression problem 6)

Prob. #6





Tiamat vs. CTF+Insilico coupled capability

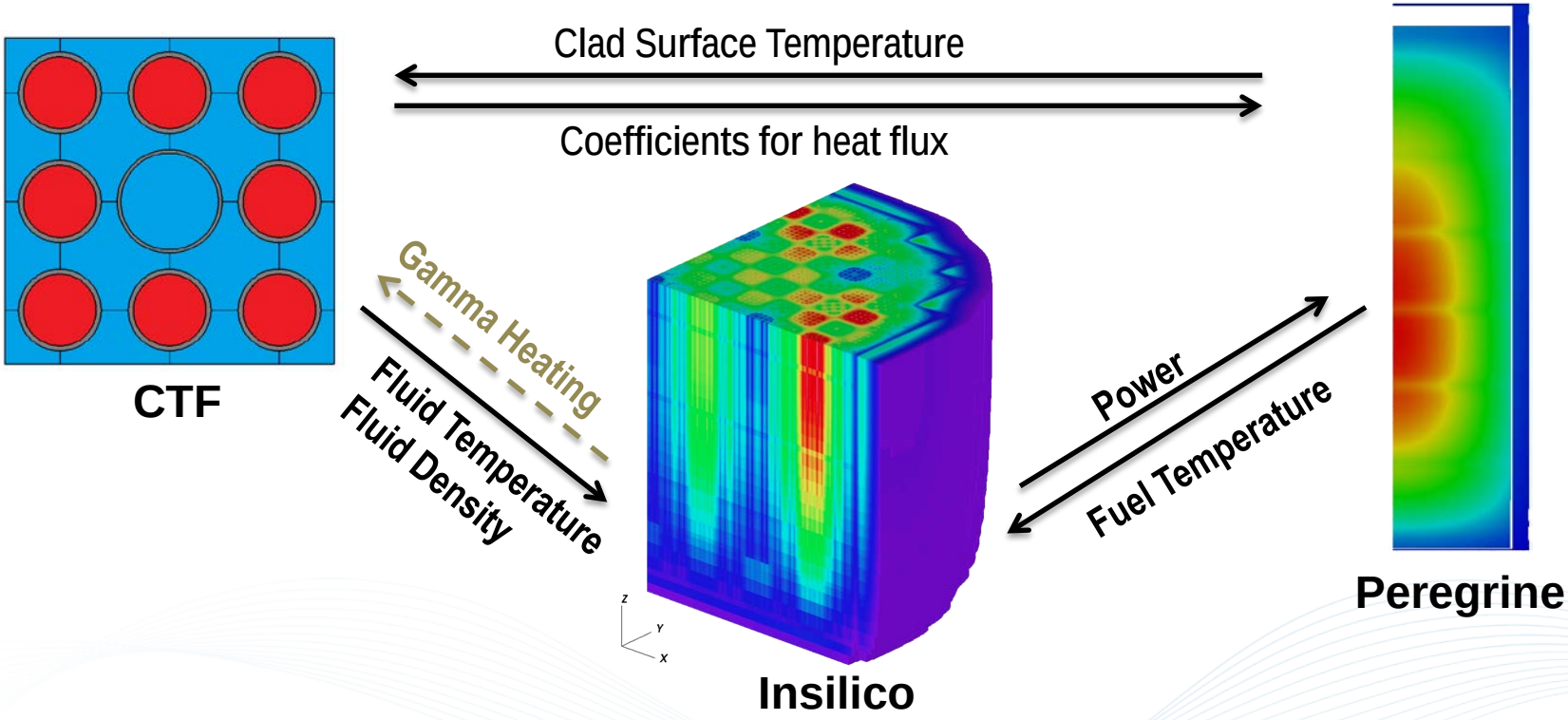
- need to investigate consistently higher Tiamat / Peregrine temperatures and apparent offset
  - substantial differences between CTF and Peregrine rod models
  - boundary condition treatments

Coarse mesh vs. "fine" mesh

- more smearing with coarse mesh (as expected)
- further refinement studies needed

Tiamat represents a significant new VERA capability.

- Successfully integrated MOOSE/Peregrine into VERA
- Successfully coupled MOOSE/Peregrine with COBRA-TF and Insilico
- Developed new multiphysics driver ("LIME2")
  - evolution of LIME first formally described in PoR-3 milestone L3:VRI.PSS.P3.01, "LIME 2.0 Design Report"
- Developed new data transfer mechanisms for specific applications

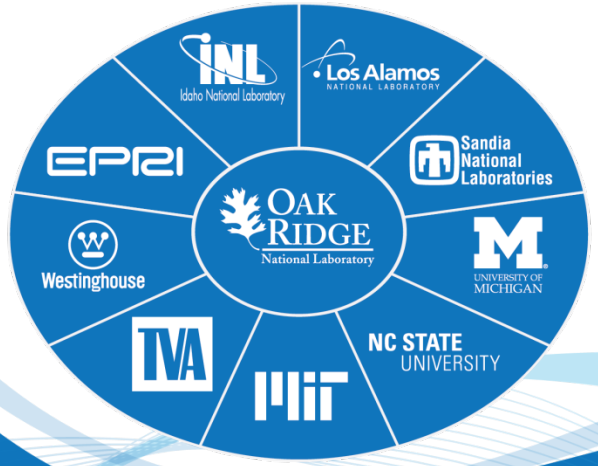


Currently testing – Report details further development needs.

Welcome to the Seventh Industry Council Meeting!

Industry Council Chairman: Heather Feldman (EPRI)

CASL Industry Council
Oak Ridge National Laboratory
September 11, 2013



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

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 or Service Providers	Independent Software Vendor	Computer Technology Companies	Ex-Officio
Dominion	AREVA	Battelle	ANSYS	Cray	BOD
Duke Energy	GNF	Bettis /NNPP	CD-adapco	IBM	DOE
EDF	mPower	EPRI	GSE Systems	NVIDIA	
Exelon	NuScale	Rolls Royce			
TVA	WEC	Studsvik Scandpower			

Technology Transfer Vehicle

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

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Consortium for Advanced Simulation of LWRs

rss feed follow us on

Search go

HOME ABOUT CASL PARTNERS R&D ORGANIZATION RESOURCES CONTACT US

Industry Council

Chairman: Heather Feldman, EPRI

LINK TO RESOURCES

Industry Council Resources

LINK TO UPDATES

Upcoming Webcast and Meeting

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.

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

Action Items (1 of 2)

Action	Due Date	Status
Determine if CASL Proposal Summary Document is on the IC website and add it if it is not there. Add the Product Description Document to the IC website.	30-Apr-13	Complete
Deliver a progress report to the Industry Council identifying future IC pilot studies that benchmark VERA capabilities against 1) current methods, and 2) industry data.	13-Jun-13	13-June-13 Presentation IC Webcast
Industry Council to provide Rose Montgomery with feedback on the Product Description Document. Due by next webcast.	30-Jun-13	Complete
Develop a survey on how IC members plan to use VERA in-house and on in-house requirements for safety and non-safety software codes. Send out the survey by the next webcast (June timeframe) with the intent to review the results at the September Industry Council meeting.	30-Jun-13	Complete 11-Sept-13 Presentation
Provide a prioritized list of validation data needs. Ask the Industry Council to review prioritization of the list. The list will be distributed to the IC prior to the next webcast (June timeframe).	30-Jun-13	10-Sept-13 Lunch Talk
Tech Notes is the quarterly newsletter. Distribute the latest issue to the IC by the next webcast.	30-Jun-13	Complete

Action Items (2 of 2)

Action	Due Date	Status
Heather Feldman to provide access to full list of published works/solution technologies (via link to CASL website) on the IC website.	**30-Jun-13**	**In-Progress**
Provide Program Plan to Industry Council in June/July for review and comment with the intent for comments to to be due by the September Industry Council Meeting.	**31-Jul-13**	**Program Plan in CASL Internal Review**
Heather Feldman to obtain NiCE traning announcement from Jay Jay Billings and sent it out to the IC.	**15-Aug-13**	**In-Progress**
Deliver a presentation to the Industry Council regarding modularity of VERA to couple with industry codes. Consider proprietary codes of fuel vendors, engineeering service vendors, and plant owners with propriety algorithms and data that are business-essential.	10-Sep-13	11-Sept-13 Presentation
Lead the Industry Council subcommittee on the development of the Value Proposition to identify an example and provide the results at the September Industry Council Meeting.	30-Sep-13	11-Sept-13 Presentation
Coordinate an effort to explore workflow software and VERA Modularity. Results of the effort will be reported at the September Industry Council meeting.	30-Sep-13	11-Sept-13 Presentation
Contact Heather Feldman if interested in obtaining a test stand (external test stands) and to provide proposals.		

Agenda for Joint Industry and Science Council Meeting on September 10, 2013

- CASL technical accomplishments past 12 months (PoR6 and PoR7)
- Challenge Problems – Charters, Implementation Plans, Results
- Progress Made in THM Focus Area
- Working Lunch – Validation Data Needs Assessment
- VERA: Description, Status, Plans
- VOCC Laboratory and Demonstrations of selected applications of VERA

Agenda for Industry Council on September 11, 2013

8:30	Welcome and Introductions	Heather Feldman
9:00	Test Stands – Overview – Westinghouse Perspective Presentation	 Doug Burns Fausto Franceschini
10:30	*Break*	
10:45	Survey - VERA End User Uses and In-House Requirements	Matt Sieger
11:15	IC Project – VERA Value Proposition	Heather Feldman
11:45	*Working Lunch* – Thoughts on Phase 2 (2015-2020) Scope	Doug Kothe
12:45	VERA Interoperability – Overview – CD-adapco Perspective Presentation	 John Turner Eric Volpenhein
1:30	*Break*	
1:45	Industry Council Round Robin	All
2:45	Industry Council Action Items	Heather Feldman
3:00	Science Council Out Briefing of Major Findings	Bill Weber (Acting Chair)
3:45	Adjourn	

Science Council joins Industry Council

Industry Council Review of CASL Documents

- Since March
  - Product Description, Revision 1
    - Sent out after March IC; available on the website
- Coming Soon
  - Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Tests, Revision 1
  - CASL Program Plan
  - Industry Workflows and Use Cases

CASL values IC feedback

March 2014 Meeting

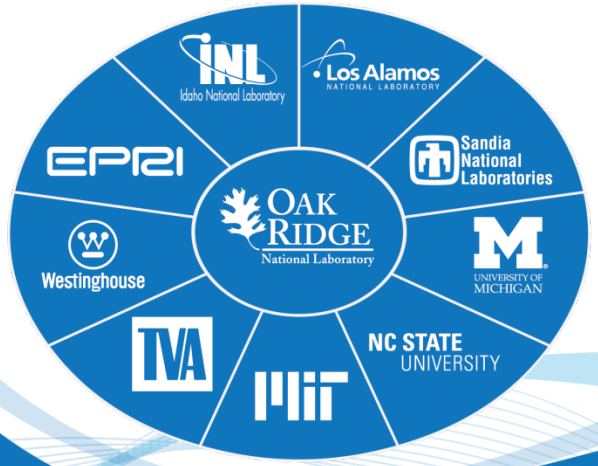
- Potential Dates
  - Tuesday-Wednesday, March 11-12, 2014
  - Tuesday-Wednesday, March 25-26, 2014
- Potential Hosts
  - EPRI
  - Interested in hosting?
- Potential Topics
  - Deployment
  - Other topics?

Finalize dates and host

Test Stand Status

Doug Burns (INL)
Rose Montgomery (TVA)
Heather Feldman (EPRI)
Fausto Franceschini (WEC)

CASL Industry Council Meeting
Oak Ridge National Laboratory
September 11, 2013



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CASL
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CASL Test Stands: Becoming a Reality

- Technology deployment is a high priority CASL objective and Test Stands are a key component of the deployment process
  - Early deployment into industrial environment for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
  - The deployment supports testing how well VERA can be built on different machines, and it allows users to work with the tools using their systems
  - CASL provides support for loading the tools and training
  - The user is responsible for developing a test report detailing identified issues; CASL is responsible for incorporating necessary upgrades
  - Host organizations self-fund a portion of the Test Stand effort

Test Stand Release Process

- A disciplined process is followed to minimize costs and maximize benefits to the Test Stand host and CASL
- Steps include:
  - Prospective host develops and submits a Test Stand simulation proposal
  - CASL evaluates the proposed simulation scope against the establish criteria
    - *Relative importance of the problem to the proposing organization*
    - *Ability for VERA (at the time of test stand deployment) to support the simulation objectives*
    - *CASL's return on investment: rigor of use, support for validation, external staff funding (cost share)*
  - Prior to release, the VERA snapshot is reviewed and tested to verify capabilities, and ensure intellectual property, export control, and license requirements are satisfied
    - *CASL performs a readiness review prior to deployment and issues a Test Stand release approval that identifies known software limitations and upgrade plans*
  - Host executes Test Stand scope, identifies lessons learned, and develops a review report
  - CASL develops a Test Stand completion report using host input and implements necessary action plans

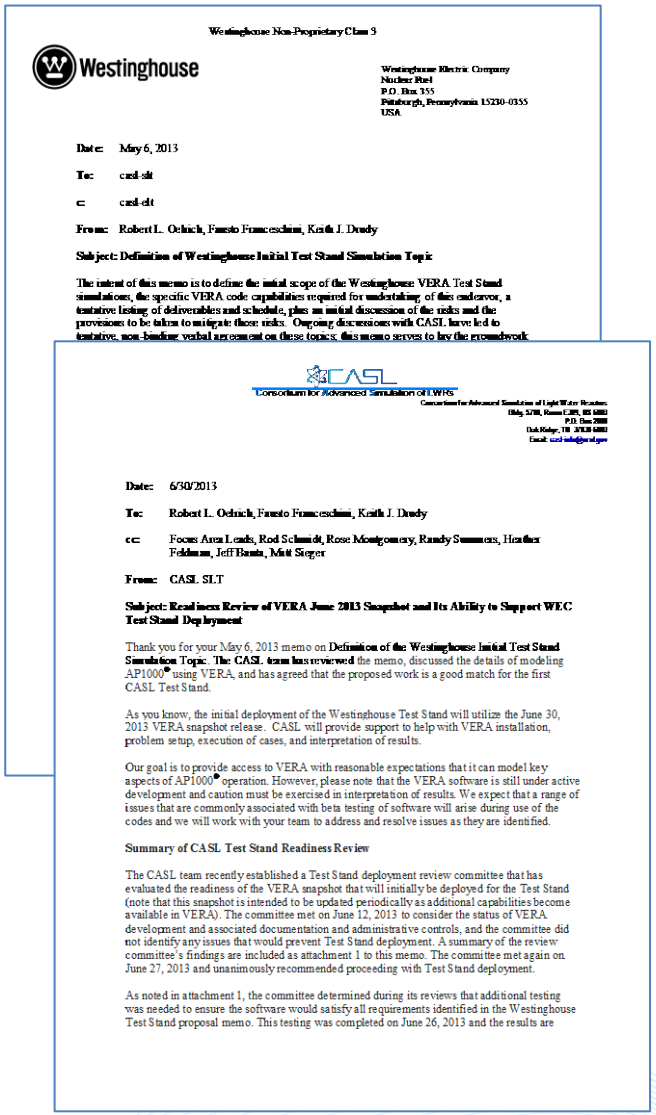
Current Test Stand Schedule

	Deployment Target Date	Initial Simulation Completion Target
Westinghouse Test Stand	June 28, 2013	November 30, 2013
EPRI Test Stand	December 31, 2013	June 30, 2014
TVA Test Stand	April 30, 2014	October 31, 2014
Non-Partner Test Stand	October 31, 2014	March 31, 2015

- Pre-deployment steps include
  - Simulation topic selection: ~ 10 weeks before deployment
  - Pre-installation testing complete: ~ 6 weeks before deployment
  - Readiness review complete: ~ 2 weeks before deployment

Westinghouse (WEC) Test Stand

- Initial focus of the WEC Test Stand is on neutronics
  - Comparison with industry codes to understand benefits of a high fidelity solution for commercial core simulations
- AP1000® PWR selected for the initial VERA application
  - Challenging core design and operational features (MSHIM™)
  - First core with fresh fuel enables cleaner code comparison
  - Plant measurements available soon from units under construction
- WEC SMR being considered as a follow up
- Other WEC cores will follow
  - Range of cores, fuel types and measurements available
  - Expand VERA validation basis
  - Troubleshooting current reloads



Westinghouse Non-Proprietary Class 3

Westinghouse

Westinghouse Electric Company
Nuclear Fuel
P.O. Box 355
Pittsburgh, Pennsylvania 15230-0355
USA

Date: May 6, 2013

To: casl-slt

cc: casl-slt

From: Robert L. Oelrich, Fausto Franceschini, Keith J. Drudy

Subject: Definition of Westinghouse Initial Test Stand Simulation Topic

The intent of this memo is to define the initial scope of the Westinghouse VERA Test Stand simulations, the specific VERA code capabilities required for undertaking, of this endeavor, a tentative listing of deliverables and schedule, plus an initial discussion of the risks and the provisions to be taken to mitigate those risks. Ongoing discussions with CASL have led to tentative, non-binding verbal agreement on these topics; this memo serves to lay the groundwork

CASL
Consortium for Advanced Simulation of LWRs

Consortium for Advanced Simulation of Light Water Reactors
Bldg. 5700, Room E-105, MS 6001
P.O. Box 2008
Oak Ridge, TN 37831-6001
Email: casl-info@ornl.gov

Date: 6/30/2013

To: Robert L. Oelrich, Fausto Franceschini, Keith J. Drudy

cc: Focus Area Leads, Rod Schmidt, Rose Montgomery, Randy Summers, Heather Feldman, Jeff Banta, Matt Steger

From: CASL SLT

Subject: Readiness Review of VERA June 2013 Snapshot and Its Ability to Support WEC Test Stand Deployment

Thank you for your May 6, 2013 memo on **Definition of the Westinghouse Initial Test Stand Simulation Topic**. **The CASL team has reviewed** the memo, discussed the details of modeling AP1000® using VERA, and has agreed that the proposed work is a good match for the first CASL Test Stand.

As you know, the initial deployment of the Westinghouse Test Stand will utilize the June 30, 2013 VERA snapshot release. CASL will provide support to help with VERA installation, problem setup, execution of cases, and interpretation of results.

Our goal is to provide access to VERA with reasonable expectations that it can model key aspects of AP1000® operation. However, please note that the VERA software is still under active development and caution must be exercised in interpretation of results. We expect that a range of issues that are commonly associated with beta testing of software will arise during use of the codes and we will work with your team to address and resolve issues as they are identified.

Summary of CASL Test Stand Readiness Review

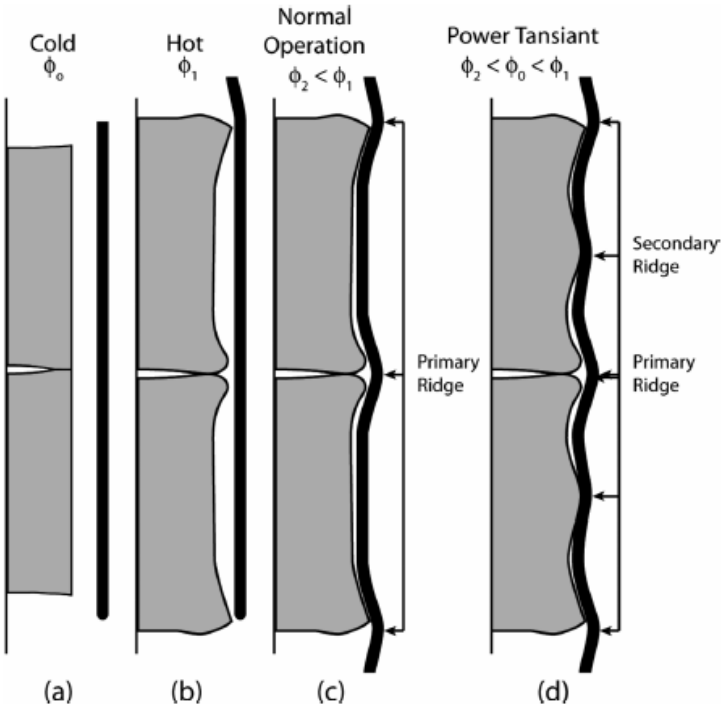
The CASL team recently established a Test Stand deployment review committee that has evaluated the readiness of the VERA snapshot that will initially be deployed for the Test Stand (note that this snapshot is intended to be updated periodically as additional capabilities become available in VERA). The committee met on June 12, 2013 to consider the status of VERA development and associated documentation and administrative controls, and the committee did not identify any issues that would prevent Test Stand deployment. A summary of the review committee's findings are included as attachment 1 to this memo. The committee met again on June 27, 2013 and unanimously recommended proceeding with Test Stand deployment.

As noted in attachment 1, the committee determined during its reviews that additional testing was needed to ensure the software would satisfy all requirements identified in the Westinghouse Test Stand proposal memo. This testing was completed on June 26, 2013 and the results are

EPRI Test Stand

- Proposed Topic
  - Fuel rod performance simulation (coupled Peregrine/Cobra-TF)
  - EPRI proposal memo has been received
- Pending:
  - CASL response to EPRI proposal
  - Implementation of code modifications determined to be needed
  - Pre-installation testing and Test Stand deployment
- The CASL Test Stand will be one of the first applications on the new EPRI machine

Illustration showing PCMI stresses with operation



Source, Fuel Reliability Guidelines: Pellet-Cladding Interaction (EPRI Product 1015453)

ELECTRIC POWER RESEARCH INSTITUTE

Consortium for Advanced Simulation of LWRs

TVA Test Stand

- TVA's vision of VERA as a multipurpose tool is captured in TVA's list of potential Test Stand scope and application:
  - (List shows options that are being considered by TVA; problem selection will be completed early next calendar year)

  - Watts Bar 1 lower plenum flow anomaly investigation
  - Vulnerability to CRUD/CILC due to fuel design changes and a new steam generator at Sequoyah
  - Fuel Assembly distortion at Sequoyah
  - Sequoyah fuel design vulnerability to GTRF due to transition core
  - Bellefonte baffle wall hole/slot effects
  - PWR CRUD/AOA modeling
  - Reactor grid wear observations in B&W-type plants
  - Watts Bar 2 startup predictions

Current External Test Stands Options

- On-going Test Stand discussions with Industry Council members:
  - AREVA
    - CASL visited AREVA in Lynchburg, VA on May 21
    - Follow Up Calls on June 27 and August 29
      - AREVA has proposed specific test stand simulation topics
  - GSE Systems
    - CASL visited GSE Systems in Sykesville, MD on June 26
    - Follow up is being planned
- Other interested Industry Council members:
  - ANSYS
  - mPower
  - Rolls Royce

Will need to establish license process and self-funding agreement

Test Stand Preparation Lessons Learned

- To avoid conflict with CASL's VERA development path while supporting Test Stand activities, three points of contact within CASL should be established
  - Test Stand manager
    - *Identify target VERA snapshot to be used and any updates*
    - *Understand VERA capabilities needed and work with VRI to ensure timely availability*
    - *Manage release reviews for Test Stand*
  - Installation manager
    - *Work with host IT representatives to ensure successful installation of VERA*
    - *Test with virtual machine*
  - Technical support manager
    - *Assist with technical questions as they arise*
- Create and test VERA installation on a virtual machine representative of the host to be used for the Test Stand
- Establish, as early as possible, any minor modifications of VERA needed to support Test Stand objectives and establish milestones for development and testing

VERA Test Stand at Westinghouse
Genesis

- Westinghouse is actively engaged in developing, applying and validating VERA
  - Advice on industrial requirements for VERA capabilities development
  - Support to AMA for VERA progression problems
  - Validation with Westinghouse in-house core physics package
- Full core reactor analysis capabilities are maturing in VERA
  - CASL.003 Milestone on Operational Reactor Model Demonstration
- VERA test stand at Westinghouse is the logical next step
  - Opportunity to deploy VERA in an industrial setting
  - Scope and plan defined (memo issued by Westinghouse)
  - VERA capabilities evaluated (memo issued by CASL)
  - VERA built and released on June 28 2013 on the Westinghouse clusters
  - *VERA simulations at Westinghouse ongoing*

VERA Test Stand at Westinghouse – Rationale

- Deploy a practical high-fidelity tool at the industry's site to analyze current and future commercial LWRs
  - Operating plants
  - Advanced plants (AP1000® PWR, SMR)
  - New operational features (MSHIM™)
  - Advanced fuels
  - Support products and method development
- Assess feasibility of VERA industrial implementation
  - To obtain reference solutions (short-term)
  - As next generation industry tool (long-term)

AP1000® and MSHIM™ are trademarks or registered trademarks of Westinghouse Electric Company LLC in the United States and may be registered in other countries throughout the world. All rights reserved. Unauthorized use is strictly prohibited.

VERA Test Stand at Westinghouse
Creating Synergies

- Between VERA and Westinghouse Core Designers:
  - Quantify benefits of high fidelity solution
  - Evaluate usability of VERA from an industry user's perspective
  - Understand range of applicability of VERA on typical industrial clusters
  - Expand VERA capabilities with latest trends in industrial core design and operational features
- Between VERA and Westinghouse Method Developers:
  - Provide feedback to CASL on methods to alleviate VERA computational burden
  - Inform Westinghouse on effectiveness of advanced nuclear method developments
- Between VERA and Westinghouse Software and IT Personnel:
  - Understand hardware and software environments for VERA industrial deployment
  - Develop process to streamline future VERA deployments
- Between VERA and Westinghouse R&T:
  - Apply VERA to the design and evaluation of new plants and new fuels

VERA Test Stand at Westinghouse
Personnel

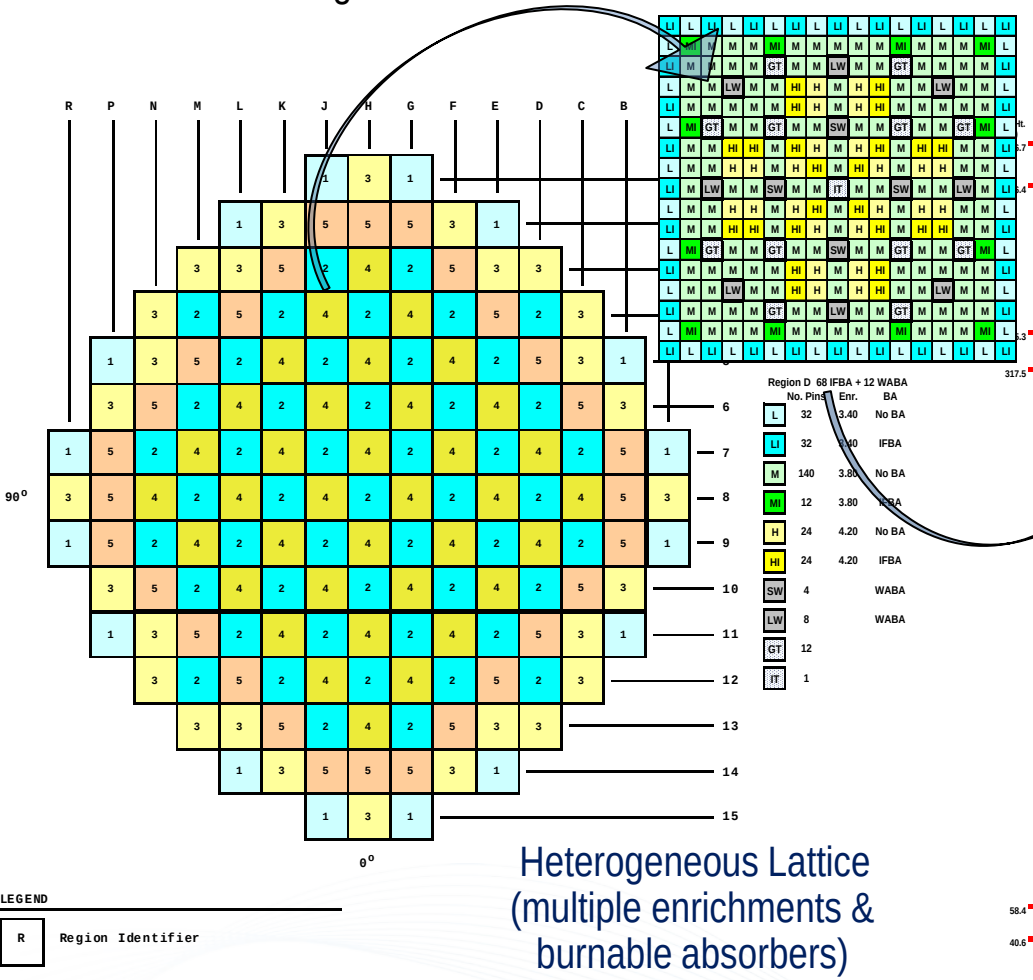
- Westinghouse:
  - R. Oelrich, Manager, PWR Core Methods
  - K. Drudy, Manager, New Reactor Technology
  - F. Franceschini, core physicist - Technical Lead
  - J. Kulesza & G. Fischer, VERA build
  - J. Secker (AMA) and D. Salazar (AP1000®)
  - A. Graham, Intern, University of Michigan, VERA simulations
  - Westinghouse nuclear methods personnel
- CASL:
  - J. Gehin ORNL - Physics Integration Focus Area Lead
  - R. Schmidt, SANDIA National Lab - Test Stand Manager:
  - R. Bartlett, ORNL - Installation and VERA code updates:
  - A. Godfrey ORNL - Analysis Support

VERA Test Stand at Westinghouse
Computational Resources

- Selected VERA components built and operational at Westinghouse
  - Insilico and MPACT for neutronics, COBRA-TF for coupling
  - Built on schedule at the end of June, updated in August 2013
  - Development versions available from VERA repository
  - Installation process and lessons learned available for future test stands
- Westinghouse cluster for VERA in the 500-1,000 cores range
  - Dedicated VERA cluster at Westinghouse being assembled
  - Most of the calculations performed on the Westinghouse clusters
  - Supercomputers utilized as backup computational resources

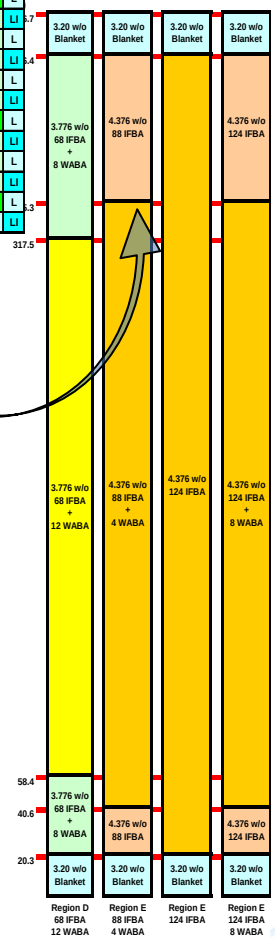
VERA Test Stand at Westinghouse
Scope: AP1000 Advanced First Core Analysis

5-Region Very Low Leakage
Core Loading Pattern

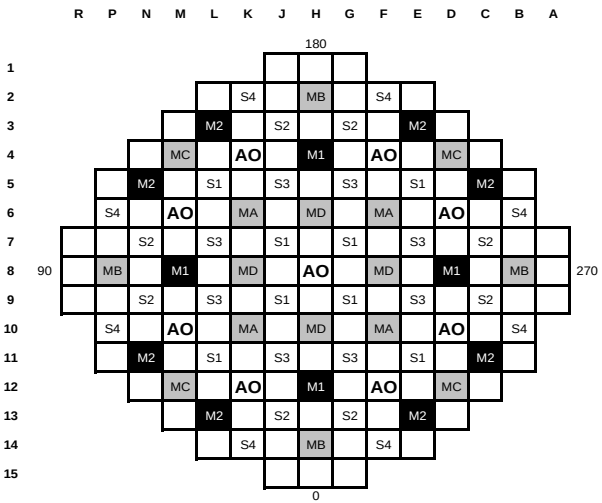


Heterogeneous Lattice
(multiple enrichments & burnable absorbers)

Heterogeneous
Axial Stack



MSHIM Banks
(Rodded Operation w/ Bank Swap)



Bank ID	Group Association	Cluster Design Type	# of Clusters
MA	MSHIM Control	Gray	4
MB	MSHIM Control	Gray	4
MC	MSHIM Control	Gray	4
MD	MSHIM Control	Gray	4
M1	MSHIM Control	Black	4
M2	MSHIM Control	Black	8
AO	Axial Offset Control	Black	9
S1	Shutdown	Black	8
S2	Shutdown	Black	8
S3	Shutdown	Black	8
S4	Shutdown	Black	8
	Total		69

LEGEND

R Region Identifier

VERA Test Stand at Westinghouse – Simulations

- AP1000 Start-up Physics Tests – simulations ongoing
  - Hot Zero Power Simulations
  - 2D single and multi-lattice
  - 3D assembly and multi-assembly
  - HZP 3D core calculations with Rod Worth, ITC, Boron Worth
- AP1000 Hot Full Power – as VERA capabilities developed/deployed
  - Coupling and feedbacks
  - Depletion, shuffling and next cycle(s)
- Comparisons
  - KENO Monte Carlo-based solution
  - Westinghouse in-house NEXUS core physics package
  - Measurements as available from AP1000 startups

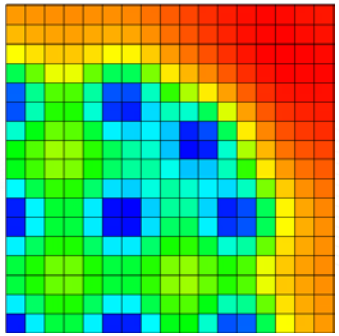
VERA Neutronics Codes

Insilico

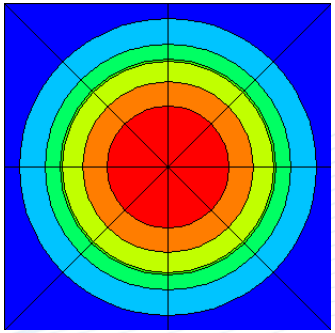
- 252g 1D XSProc
- 3D Denovo
  - 23g 3D Transport
  - Cartesian mesh
- SPN with Pin-Homogenized XS
- Moderate compute requirements
  - 1 Lattice with IFBA in <1 min on 16 Intel cores t 3.0 GHz

MPACT

- ORNL 56-64g libraries
- 2D/1D method
  - Planar MOC
  - 1D Nodal method
- Sub-pin resolution
- Larger compute requirements
  - 1 Lattice with IFBA in ~20 min on 16 Intel cores t 3.0 GHz



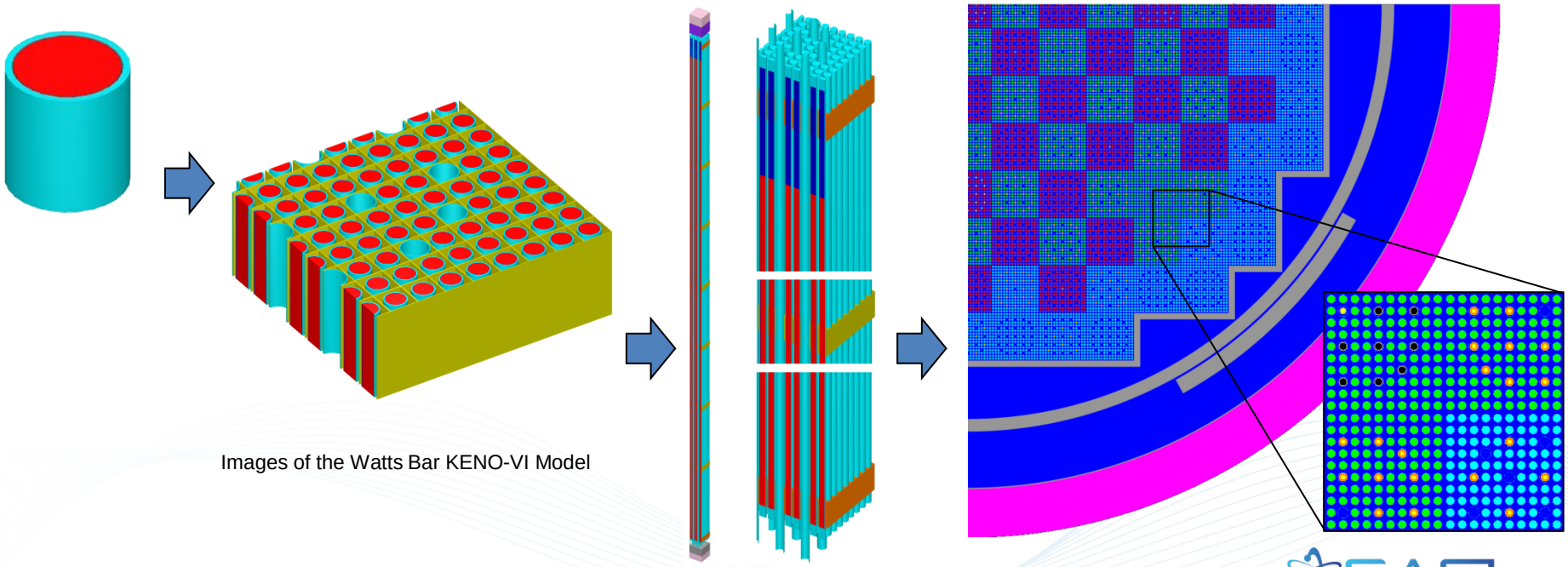
SPN 2x2 Pin Cell



MPACT MOC

Numerical Reference Solution – KENO-VI

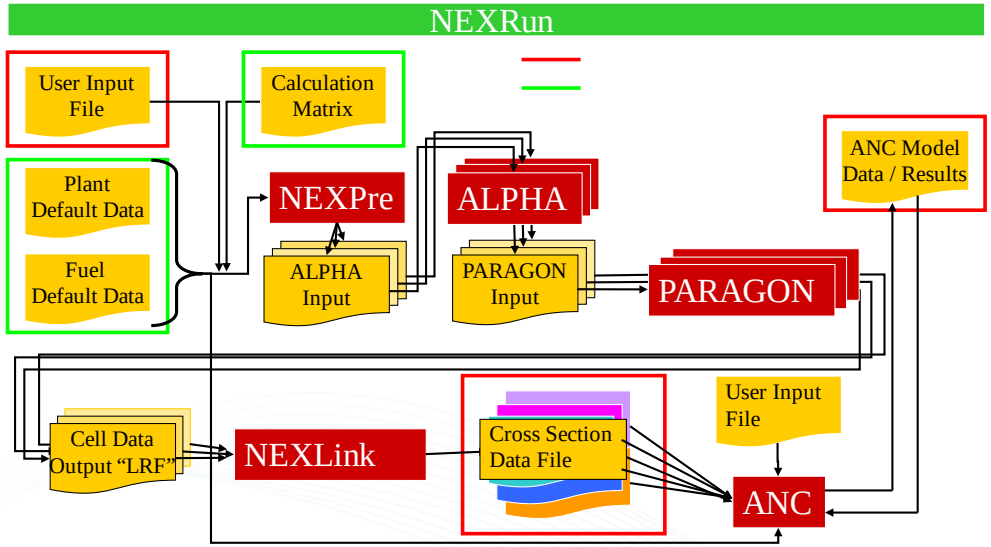
- SCALE 6.2 KENO-VI used for high fidelity, neutronics-only reference
  - Continuous energy (CE) Monte Carlo (MC) method of particle transport
  - Rigorous geometry, neutron transport and cross-sections
  - Requires significant computational resources but parallelism allows high numbers of particles for reduced statistical uncertainties.
  - Provide power distributions for 2D core and 3D assembly numerical comparisons

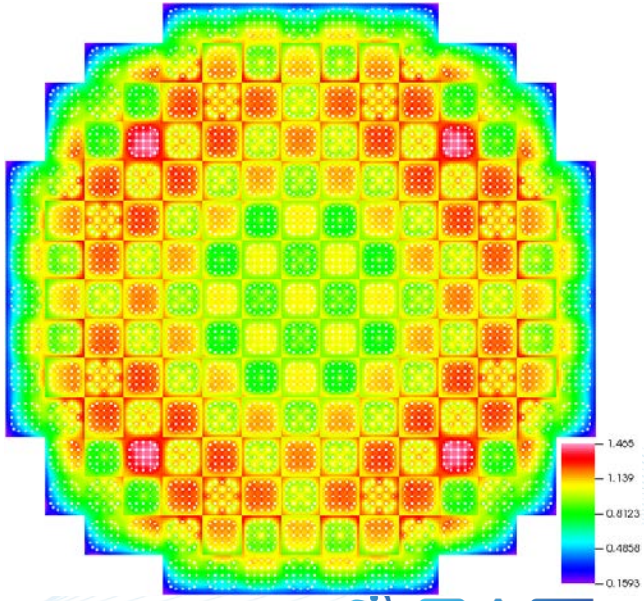


Images of the Watts Bar KENO-VI Model

Industrial Solution – Westinghouse NEXUS

- Westinghouse's state-of-the-art core physics package NEXUS
- NRC-licensed nodal method with specific AP1000-related developments
  - PARAGON lattice physics with ENDF B7 based library
  - ANC9 two group 3D nodal diffusion for core calculations
  - Flux and power solved on nodal basis from parameterized macroscopic cross sections with feedbacks
  - New Pin Power Reconstruction ("Pseudo Pin by Pin") copes with rodded operation
  - MSHIM Maneuver Simulation Capabilities





NEXUS Methodology and Reconstructed Pin Powers for Watts Bar 1

VERA Test Stand at Westinghouse
Initial Feedback is a Positive One

- VERA build process has been automated with very limited user's intervention
  - A lengthy and painful process if not tackled properly and systematically
  - Now streamlined and documented in the "VERA installation guide"
  - Can be used for future deployments and for updates of the Westinghouse build
- AP1000 HZP simulations are in progress and on-track to reach objectives
  - Some issues and development delays in MPACT currently limit its use
  - Insilico SPN relies on less-robust methods but lower computational requirements and can be used more effectively on the Westinghouse clusters
  - Significant validation effort of VERA is entailed and is underway (KENO)
- Preliminary results confirm VERA's prediction capabilities
  - Excellent reactivity prediction compared to KENO. Pin power distribution needs more vetting
  - Valuable information to expand VERA validation basis is being generated
- Hot Full Power coupled core analysis with depletion is required for a comprehensive assessment of VERA
  - Computational requirements vs. potential improvements over current industry tools

VERA Test Stand at Westinghouse – Anticipated Path Forward

- Complete and document AP1000 simulations
  - Pending resolution of current issues with the codes
- Expand VERA to other Westinghouse cores
  - Evaluate transport effects for smaller cores (SMR)
  - Troubleshoot operating core anomalies
- Assess feasibility of VERA industrial implementation
  - to generate reference solutions (short-term)
  - as next generation industry tools (long-term)
- Share knowledge gained with and from other CASL partners

Compatibly with VERA capabilities development and schedule

VERA Test Stand at Westinghouse
Considerations for Future Test Stands

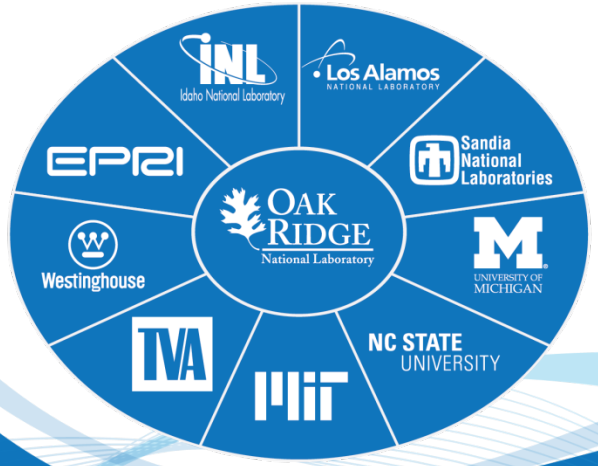
- Leverage Westinghouse's experience to facilitate future VERA deployments
  - Flexibility and commitment on the user's and CASL's site to cope with inevitable issues of tools in development and early deployment is warranted
  - Provide dedicated cluster with ~500-1,000 cores at the customer's site
  - Building VERA is not for the faint of heart: though the process has now been greatly smoothened and automated, plan some time and provide expert personnel for the build
  - Consider making provisions for updating VERA as new capabilities are being developed. Still, updates should be properly tested before being deployed/accepted.
  - Ensure that the capabilities available in VERA match the scope of the intended simulation: set the expectations right.
  - Allow proper time and resources for specific VERA validation on the simulations being performed
  - Documentation ("Manuals") can be sparse and user needs to learn by examples and communication with CASL experienced personnel
  - VERA common input is a big plus: very intuitive, properly structured and effective

VERA Test Stand at Westinghouse – Summary

- Westinghouse is fully committed to the success of VERA
  - Supports VERA validation with AMA work and Westinghouse tools
  - First-of-a-kind VERA deployment in the Westinghouse test stand
- Westinghouse's test stand scope selected is in synergy with VERA capability development planning and goals
  - AP1000 advanced core as the bridge from current to future PWRs
- Challenges in build process, simulation execution and compute resources exist but can be overcome
  - Lessons learned will help future VERA deployments
- VERA test stands are landmark opportunities for advancing simulation capabilities of commercial LWRs
  - Availability of a high-fidelity tool for industrial reactor physics analysis

Survey - VERA End User Uses and In-House Requirements

Matt Sieger, ORNL
CASL QA Manager



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Purpose

- Last March CASL presented an overview of our QA program.
- The survey was intended to gather detailed input from IC members regarding near-term and long-term VERA QA needs and institutional acquisition requirements for safety and non-safety software codes.
- The questions are intended to be starting points for discussion; respondents were encouraged to elaborate and/or extend the scope if desired.
- CASL distributed 7 questions to IC members in June 2013 and received 11 responses.
- This presentation summarizes “What we heard.”

1. What are your potential safety- and non-safety-related applications of VERA?

- Primarily non-safety applications:
  - Benchmarking of production tools
  - Investigation and general information
  - Modeling of operational events with no impact to public safety (CIPS, CILC)
- Safety-related investigations (DNB, RIA, LOCA) for general information only.
- Cost/Benefit ratio for obtaining NRC approval for safety-related applications is not yet clear

2. What expectations do you have for “out of the box” quality?

- Easy to install
  - Assume target computer may be air-gapped from the internet
  - Pre-packaged installer with minimal external dependencies
  - Clear instructions and test cases
  - Ideally, compiled executables would be delivered with cksum or md5sum numbers.
- Some initial instability/lack of robustness is OK, but going forward expect a very stable product (annual releases).
- Robustness will be expected and evaluated based on availability of feature list specification for each delivered component. At least one verification case should be provided for each listed feature.
- Training on installation, execution, maintenance, and upgrades.

3. What documentation do you require?

- Installation guide and User manual are must-haves
  - Including installation verification guide/test cases
- Functional requirements specification (features list), with verification test results
- Detailed theory/methods manual
- Technical design documentation is needed for SR applications
- Application methodology and examples
- V&V plan and results with references to base analyses
- Programmer's manual is desired for future development
- Software QA plan

4. What are your QA Requirements?

- All software would be expected to be generated to an appropriate QA plan, the rigor forming part of the analysis risk assessment process.
- Appropriate planning and documented evidence of project planning, requirements, design, implementation, testing, installation checkout, usability testing, release, distribution, support, maintenance, and retirement.
- Error reporting and resolution protocols, maintain a log of issues

5. How can CASL best support this construction of a V&V pedigree?

- Support a number of test stands and accumulate practical experience of usage
- CASL to draft a comprehensive V&V plan, keep a central repository of test cases, possibly create a Validation Users Group to share information
- Maintain an official test suite and strong configuration control
- The qualification of each subroutine or module should be documented in a periodically updated Verification and Validation Report
- Focus on generic V&V and make available to all
- Explicit statement of capabilities and supporting V&V documentation for each
- Provide UQ methodology examples

6. How do you prefer to submit issues, suggestions, and support requests?

- An established error reporting protocol with impact categorization, tracking, and timely followup
- A monitored user forum
- A web-based support interface is desirable
- Email
- Searchable database of all submitted issues & resolution status
- PoCs for more detailed support
- Annual user group meeting or teleconference

7. Are there any specific QA needs not covered above?

- Consideration needs to be given to maintenance and upkeep of the product, including the QA aspects of the system used to track and resolve issues, and feedback of changes to users.
- Rigorous validation of VERA's underlying models is more important than organizational QA requirements.
- CASL QA needs should be considered in 2 steps:
  - 1) QA needs for R&D of VERA software, and
  - 2) QA needs for industrial deployment and applications.
- Tracking all users of VERA for updates to software components, documentation, trouble reports, and error reports

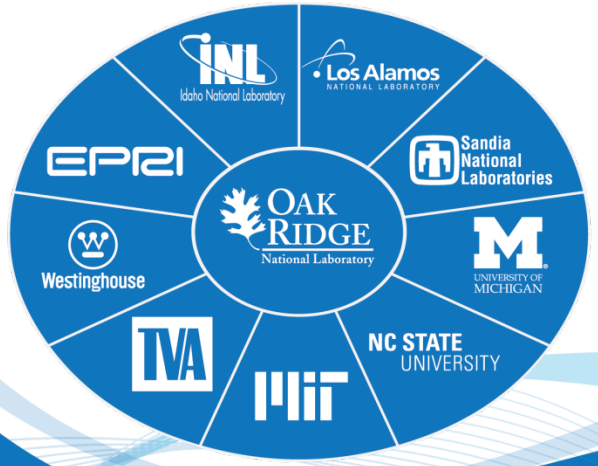
Next Steps

- Next Steps
  - CASL will present a follow-up presentation at the March IC meeting to give an update on QA deliverables and expectations
- Comments?

IC Project - VERA Value Proposition

Heather Feldman (EPRI)

CASL Industry Council Meeting
Oak Ridge National Laboratory
September 10-11, 2013



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Background

- Proposed during September 11, 2012 Industry Council
- Action Item
  - *Consider new IC project: To help prioritize and guide future work, evaluate "value proposition" of CASL products relative to key industry drivers.*
- Project recommended at CASL BOD Meeting January 31, 2013
- Subsequent meetings within CASL and with IC members identified options with differing methods and measures
- Decision-makers increasingly ask for value assessment of new projects and for alternative approaches
- Strawman presented at March 26-27, 2013 Industry Council

Problem Statement

- CASL has an objective to **deliver technology and products** that are **used and useful by industry** to effectively provide safe and cost-effective electricity from nuclear power for **benefit of the U.S. public.**
- CASL technology and products are sufficiently developed and planned in order to assess their value with respect to this objective.
- Such a value assessments would
  1) verify projected value,
  2) inform decisions for tasks and resource allocation,
  3) provide justification for future CASL funding,
  4) prioritize future work scope.

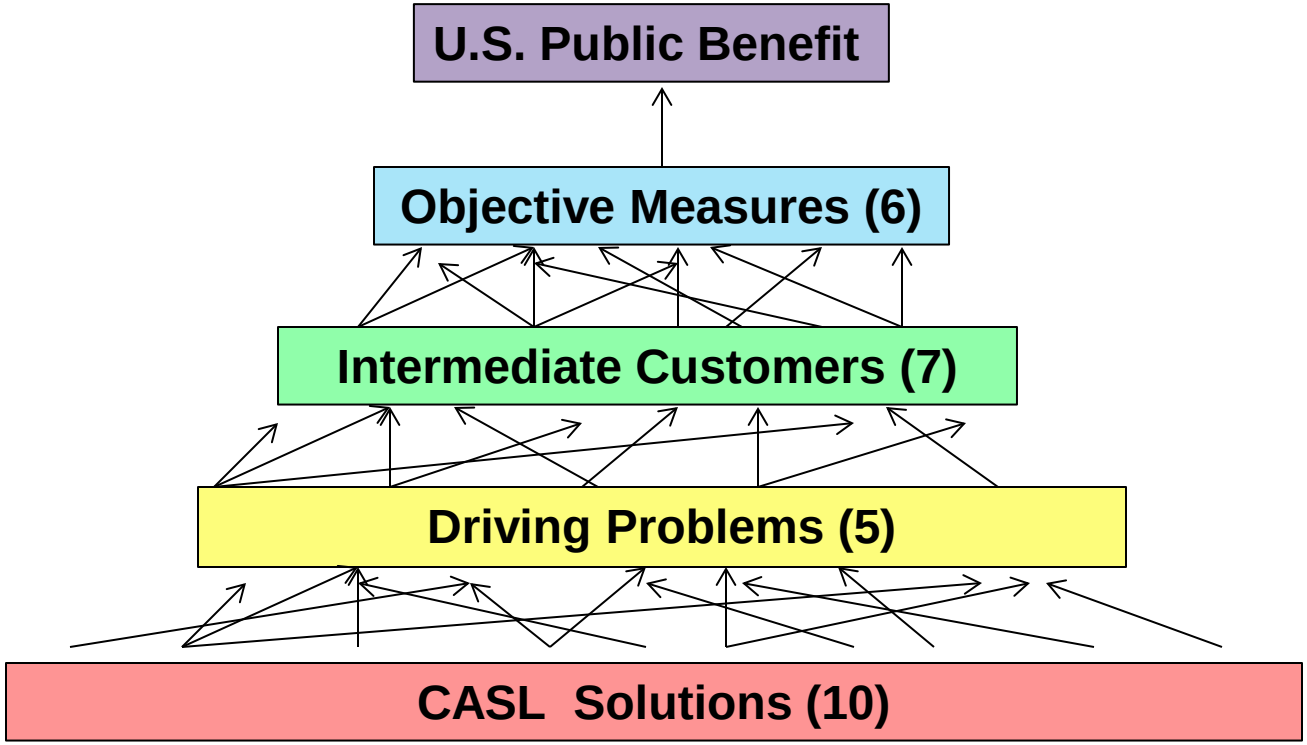
Elements of a Value Assessment

- The value assessment is a commitment of value to be delivered. It states the reason to support continued development and to use the product. It must clearly identify:
  - Customer: who receives the value?
  - Problem: what problem is solved for the customer?
  - Solution: what is your solution for the problem?

- The value assessment can focus on customers, problems, or solutions
  - For a customer, what is the aggregate value from solutions to problems?
  - For a problem, what is the aggregate value of solutions to customers?
  - For a solution, what is the aggregate value of solutions to customers?

CASL Value Assessment Strawman

Proposed March 2013



Value Proposition Subcommittee

Members

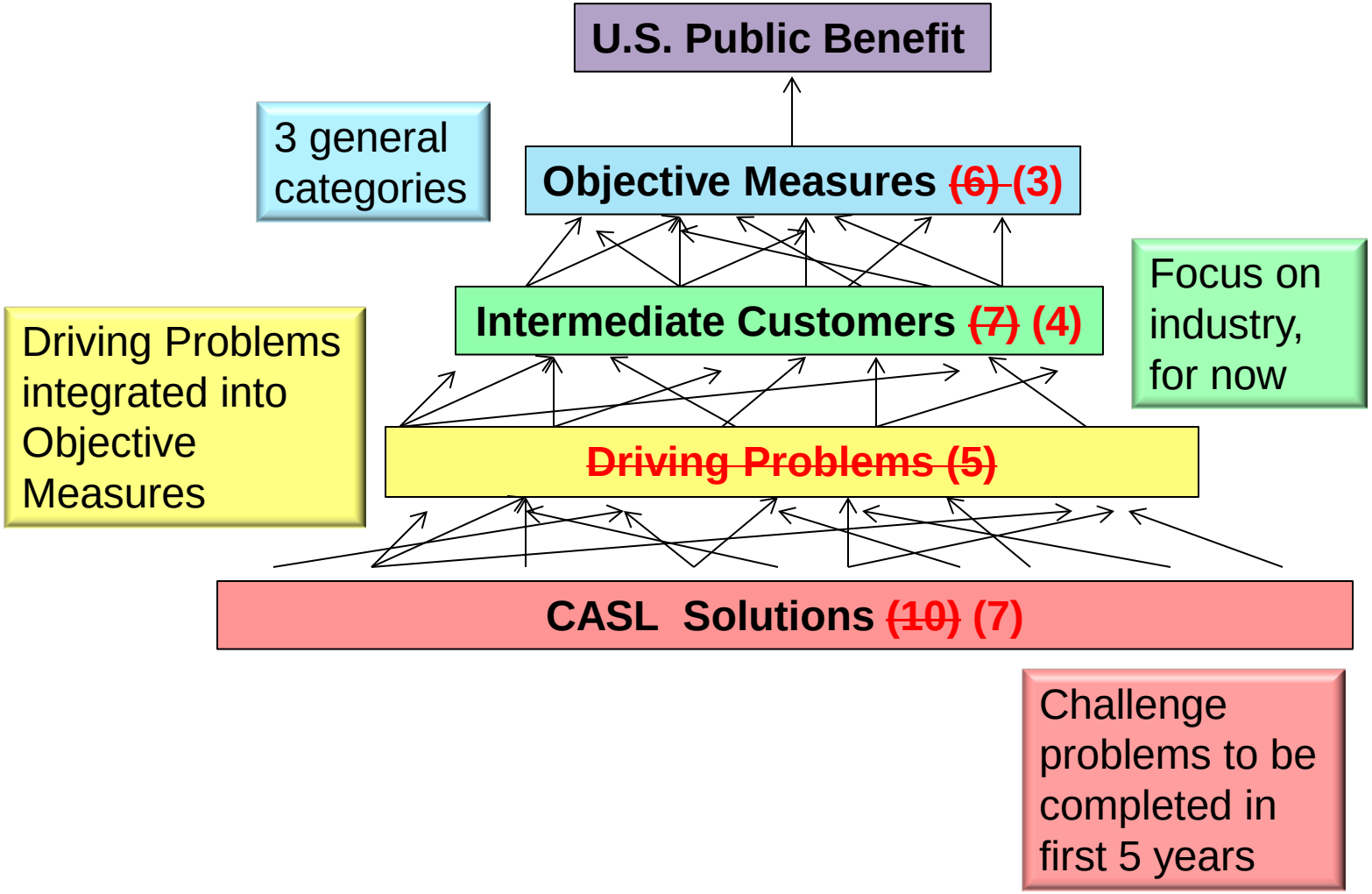
- Bill Arnold (mPower)
- Heather Feldman (EPRI)
- Steve Hess (EPRI)
- Rose Montgomery (TVA)
- Bob Oelrich (Westinghouse)
- Jeff Secker (Westinghouse)
- Scott Thomas (Duke Energy)

Contact Heather if interested in joining subcommittee

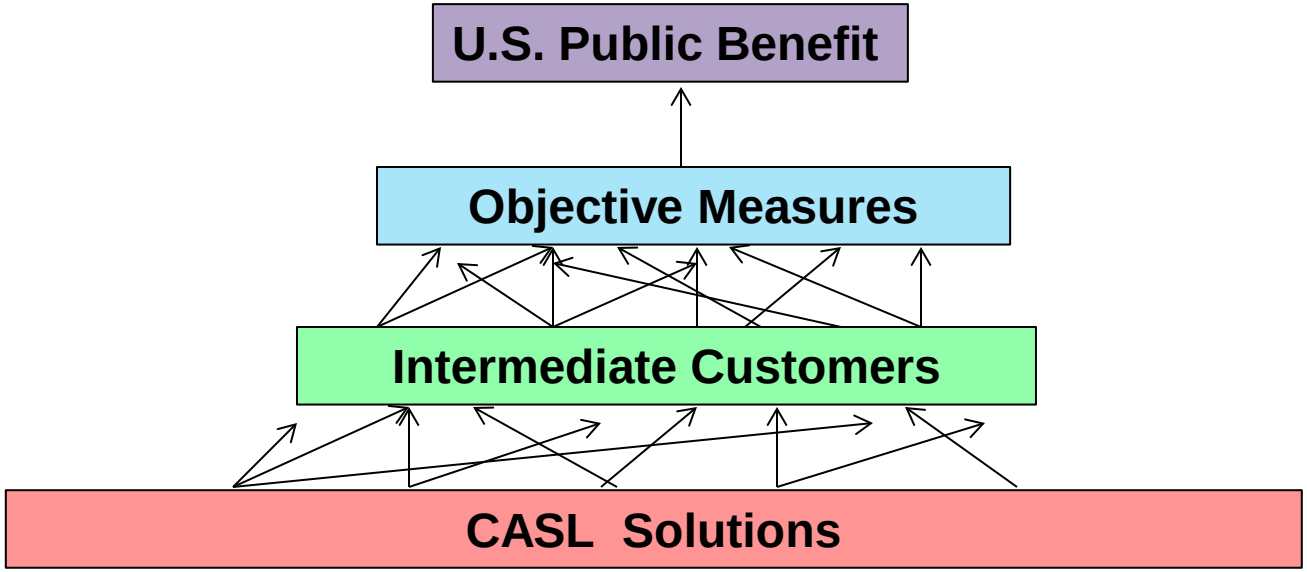
Discussions

1. May 15 – Kick Off Call
2. May 29 – CRUD Challenge Problems
3. August 9 – Process Refinement
4. August 23 – Review Value
5. Next meeting – September TBD

CASL Value Assessment Process



CASL Value Assessment Process



CASL Solutions

Challenge Problem	Description and Impact	Simulations Gaps and Drivers
Crud-induced power shift; crud-induced localized corrosion	High uncertainties in crud source, thickness, boiling surface area, and margin to fuel leakage affect fuel management and thermal margin in many plants, limiting power uprates	More accurate, higher resolution models for boiling surface area, crud deposition, boron uptake and cladding oxidation rate for each rod in core, with boron feedback in neutronics
Grid-to-rod fretting	Rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation affect wear, especially for fuel near the core shroud	Reliable predictions of grid to rod gap, turbulent flow excitation, and resulting rod vibration and wear at any location in core
Pellet-clad interaction	Cladding creep-down onto pellets, followed by pellet expansion, creates local cladding stresses at pellet imperfections, resulting in clad failure sometimes assisted by SCC	Sufficient 3D geometric detail of fuel rod material property changes; pellet growth, cracking and fission product release; cladding stresses, creep, fracture and SCC attach; fuel-cladding binding; and coupling to neutronics and T-H
Departure from nucleate boiling	Local clad surface dryout, affected by detailed flow patterns and mixing, cause dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures	3D subchannel and CFD tools to model detailed flow patterns downstream of mixing grids for single and two-phase flow, coupled to detailed pin-resolved radiation transport and fuel performance models for application to DNB transients (e.g., RIA, Loss of Flow)
Cladding integrity during a reactivity insertion accident and loss of coolant accident	Physical changes during transient (e.g., swelling and burst, oxidation mechanics), leading to clad failure followed by fuel dispersal	Enhanced fuel rod models, with improved predictive capability for normal operations to obtain fuel initial conditions at initiation of accident simulation, and transient fuel rod behavior

Immediate Customers

1. Existing PWR/BWR Owner/ Operators
2. NSSS and fuel vendors (Gen II, III, SMRs)
3. Engineering service companies and suppliers
4. Industry R&D organizations (e.g. EPRI)

Objective Measures

1. Low-cost and availability of electric power
   - Capacity factor
   - Fuel cycle cost
   - Capital cost per unit energy (operational flexibility, load-following)
   - O&M Cost (e.g. eliminate mitigating actions)
   - Utilization of natural resources (e.g. higher burn-up fuel)
   - Enhanced reliability
2. Safety
   - Nuclear safety
   - Personnel dose
   - Minimization of nuclear waste (higher burn-up fuel)
3. Global competitiveness in nuclear technology
   - Advancement of Modeling and Simulation
   - Competitive US knowledge base (e.g. workforce, training)
   - Attracting new talent
   - Enhancing innovation of new technologies

Example Matrix Input from Subcommittee

CASL Solution	Intermediate Customers	Objective Measures	US Public Benefit	US Public Benefit	US Public Benefit	US Public Benefit	US Public Benefit
CIPS	Existing PWR/BWR Owner/ Operators	Low-cost and availability electric power	L	H	M	L	H
CIPS	Existing PWR/BWR Owner/ Operators	Safety	L	H	H	L	M
CIPS	Existing PWR/BWR Owner/ Operators	Global competitiveness in nuclear technology	M	M	H	L+	L

More Work is Needed

Starting Place for CIPS History and Impact

- 49 known fuel cycles in at least eighteen PWRs in the United States, most recently in 2010
- Examples consequences
  1. One plant - reduce power to approximately 75% for the final third of the operating cycle
  2. Purchase additional fuel assemblies when designing new cores to reduce peaking factors and steaming rates to reduce the susceptibility of CIPS
  3. Burden on plant engineering and operations resources and can distract management attention from other important issues
  4. Significant corrosion product releases at shutdown for refueling outages
     - Higher plant dose rates due to large particulate releases
     - Additional filter changes during the cycle and at shutdown
  5. In some cases, load follow was not recommended due to CIPS

Sources: "PWR Axial Offset Anomaly (AOA) Guidelines, Revision 1" (EPRI Product 1008120) and FRED (EPRI Database)

Starting Place for CILC History and Impact

- Four PWR corrosion-related fuel failure events between 1990 and 2008 in the United States
- Core design seems to have the greatest influence on the failures
- Prediction of sub-cooled nucleate boiling and the associated surface area is important
- Example consequence
  - Fuel leaker

Source: "Fuel Reliability Guidelines: PWR Fuel Cladding Corrosion and Crud" (EPRI Product 105449)

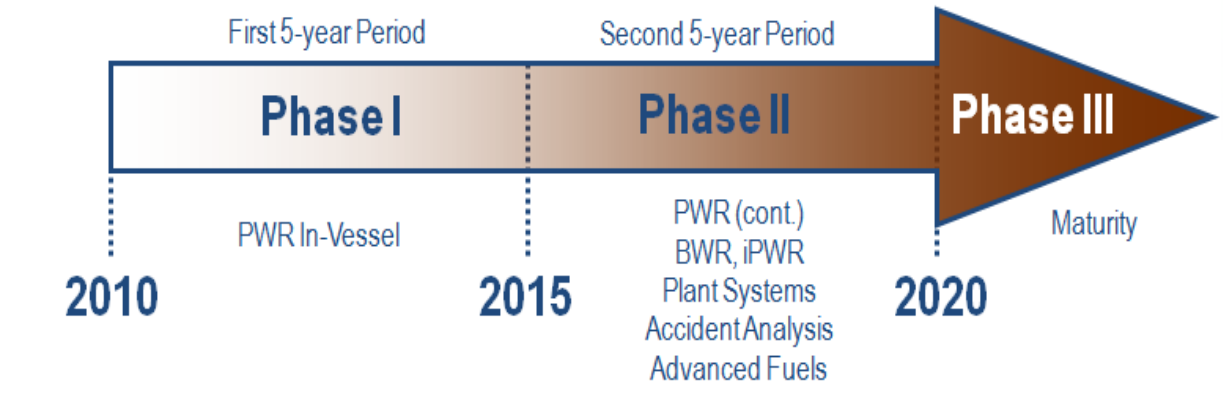
Next Steps

- Complete the history and impact for CIPS and CILC
- Assess value of VERA for CIPS and CILC for the intermediate customers and objective measures
- Evaluate process
- Assess other challenge problems

Thoughts on Phase II (second 5 years)

Doug Kothe, CASL Director

Industry Council Meeting
September 12, 2013



Time Table for Phase II Major Activities

- Phase I (first 5 years) ends July 2015

1) Define process for decision making regarding technical scope and partners (proposal already made to BOD - to be discussed now)
2) Receive instructions from DOE-NE on renewal process (when???)
3) Discuss and finalize technical scope and partners (Oct-Dec 2013)
4) Prepare and submit renewal proposal (Jan-March 2014)
5) Review and decision on renewal by DOE-NE (April-July 2014)

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High Level Scope Options

- Reactor types other than currently operating PWRs;
- Beyond the reactor vessel and contents to the nuclear power plant;
- The lifecycle of current and advanced nuclear fuel; and
- Support for severe accident analysis.

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Questions CASL Board of Directors Asked?

1) *Who are our customers, and what are their needs?*

2) *What is the value proposition for CASL moving forward?*

3) *Should there be any change in the CASL vision or mission from Phase 1?*

4) *What should be the scope, emphasis, and balance of the next five-year plan for Phase 2?*

5) *What should CASL stress in competency development in Phase 2?*

6) *What process should be used to develop the detailed proposal?*

7) *What support does CASL need to develop a successful proposal for Phase 2?*

8) *What effort should be devoted to sunset planning?*

Draft answers contained in CASL Program Plan

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Draft Steps Towards Scope Definition

1. Discuss with current industry partners;
2. Discuss with potential new industry partners;
3. Summarize discussions mentioned above;
4. Present to current partners their summary;
5. Refine the summary and present to the current and prospective IC members (perhaps restricted to nuclear power industry affiliated members);
6. Refine the summary and present to full BOD (Board to decide whether first screened by a subcommittee);
7. Finalize the summary; and
8. Assign writing assignments for the technical portion of the proposal.

- DOE or NRC will not have direct involvement in defining the technical scope.
- Engaging current and prospective IC members allows for deeper engagement of nuclear utilities.

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Possible Challenge Problems

Table D3: Challenge Problems limiting LWR performance

Challenge Problem (CP)	Operational CP	Safety CP	Power Uprate	Higher Burnup	Life Extenssion	PWR	i PWR	BWR
CIPS / CILC	✓		✓	✓		✓	✓	
GTRF	✓			✓		✓	✓	
PCI / PCMI	✓		✓	✓		✓	✓	✓
FAD	✓		✓	✓		✓	✓	
DNB / Dryout		✓	✓			✓	✓	
Clad Integrity during LOCA		✓	✓	✓		✓	✓	✓
Clad Integrity during RIA		✓	✓	✓		✓	✓	✓
Reactor Vessel Integrity		✓	✓		✓	✓		✓
Reactor Internals Integrity		✓	✓		✓	✓	✓	✓
Channel Bow	✓		✓	✓				✓
Shadow Corrosion	✓		✓	✓				✓
Debris Fretting	✓			✓				✓
Core Instability		✓	✓					✓
Natural Circulation Behavior	✓						✓	
Steam Generator Structural Analysis	✓						✓	
Vessel Components Fluence and Material Performance		✓					✓	
Safety Systems Performance		✓					✓	
Source Term Evaluation		✓		✓		✓	✓	✓
Core Uncovering Tolerance		✓	✓	✓		✓	✓	✓
Advanced Fuels Forms	✓	✓	✓	✓		✓	✓	✓
Spent Fuel Storage Behavior		✓		✓		✓	✓	✓

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Possible Phase II Challenge Problems

1. Fuel Distortion
   - PWR: Fuel Assembly Distortion (FAD)
   - BWR: Channel Box Distortion
2. Departure from Critical Heat Flux (CHF) & Post-CHF
   - PWR: Departure from Nuclear Boiling (e.g. RIA, LOCA, locked rotor)
   - BWR: Dryout (e.g. RIA, LOCA)
3. LOCA
   - PWR & BWR: Fuel performance (e.g. ballooning, burst, oxidation)
   - PWR & BWR: 3D in-vessel thermal-hydraulics (e.g. quenching, steam binding)
4. Fluid-Structure Interactions
   - PWR: Steam generator tubes secondary side
   - PWR & BWR: Steam separator-dryer
5. NSSS Corrosion
   - PWR & BWR: Piping and vessel liners (Iron based alloys)
   - PWR: Steam generator tubes (Nickel based alloys)
   - BWR: Hidden corrosion
6. Natural Circulation & Flow Stability
   - PWR, BWR, iPWR: Passive Safety Systems
   - BWR & NuScale: RCS Normal Operations

Leveraging common underlying physics across PWR & BWR Challenge Problems

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Draft High Level Scope Priority Guidance

- First Priority: **Completion of capabilities and solution insights development for seven CPs being worked upon**, along with completion of steps required for **deployment to industry**, e.g. V&V, UQ and documentation, followed by the appropriate support for deployed capabilities. For certain CPs, expansion of scope to outside the vessel will be necessary.
- Second Priority: Enhancement of existing capabilities to address **several CPs associated with BWRs**. CPs that broaden capabilities beneficial to both BWRs and PWRs would be favored; that is, share a **common *Challenge Phenomena***.
- Third Priority: **Completion of three CPs that were planned** for completion in Phase 1 but not initiated, i.e. fuel assembly distortion (FAD) and two lifetime extension CPs. They **would be in competition for selection with new PWR CPs** for pursing in Phase 2.

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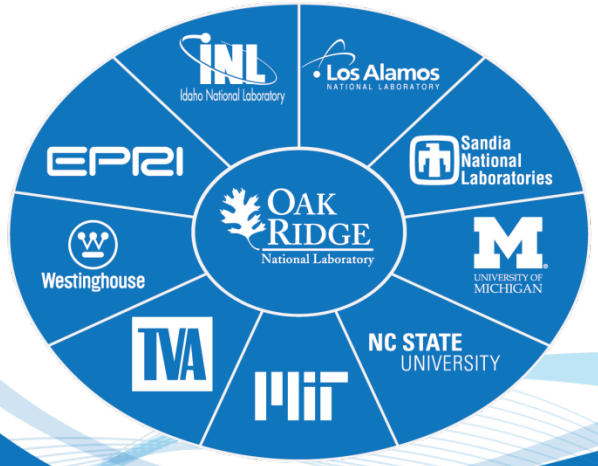
VERA Interoperability and Standardization

Joint Industry Council / Science Council Meeting
Oak Ridge National Laboratory
Sept 10-11, 2013



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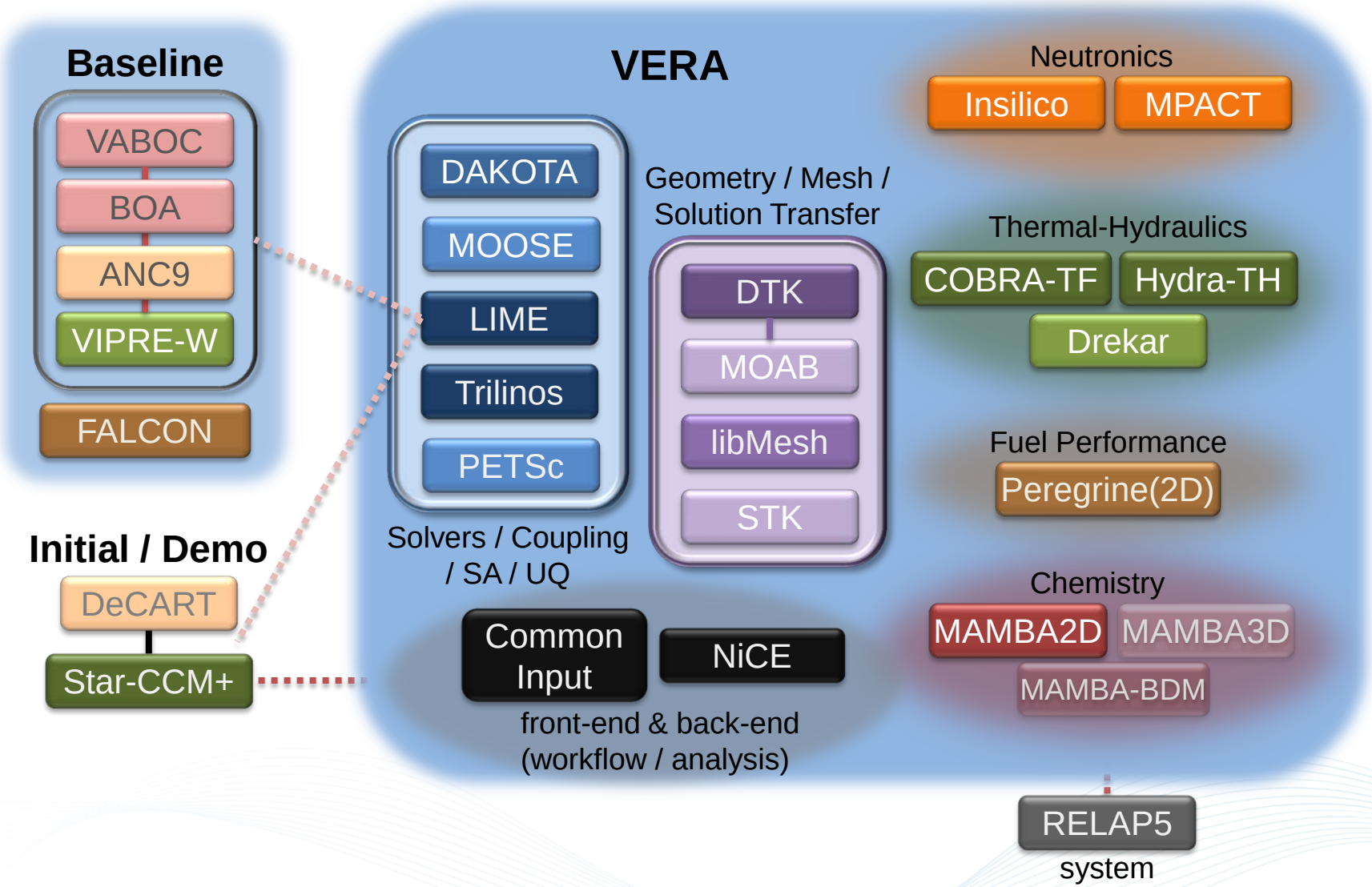
Virtual Environment for Reactor Applications (VERA): Interoperability and standardization

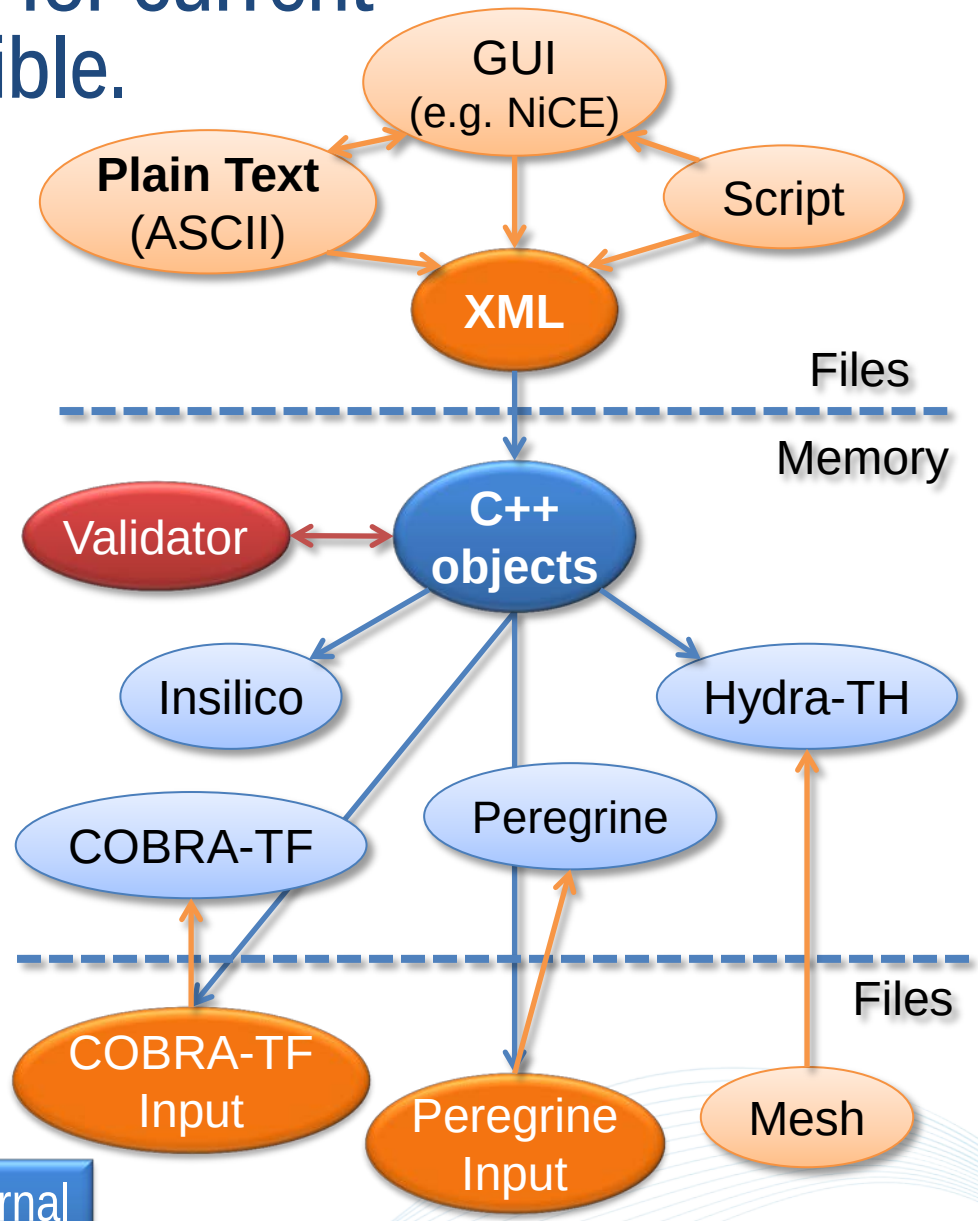
- the "E" in VERA is significant
  - VERA is a toolkit of components within a coherent environment
- three primary scenarios for interaction with external codes / components
  1. share input / output file formats
  2. replace VERA components with different (potentially proprietary) components to produce new applications
     - difficulty depends in part on granularity (models/correlations or entire physics components)
  3. use VERA components (or applications) in another environment
- which is of more interest to IC members?
- both 2 & 3 require collaboration on interfaces (APIs)

VERA 3.1 snapshot (07/2013)



VERA input is comfortable for current industry users and extensible.

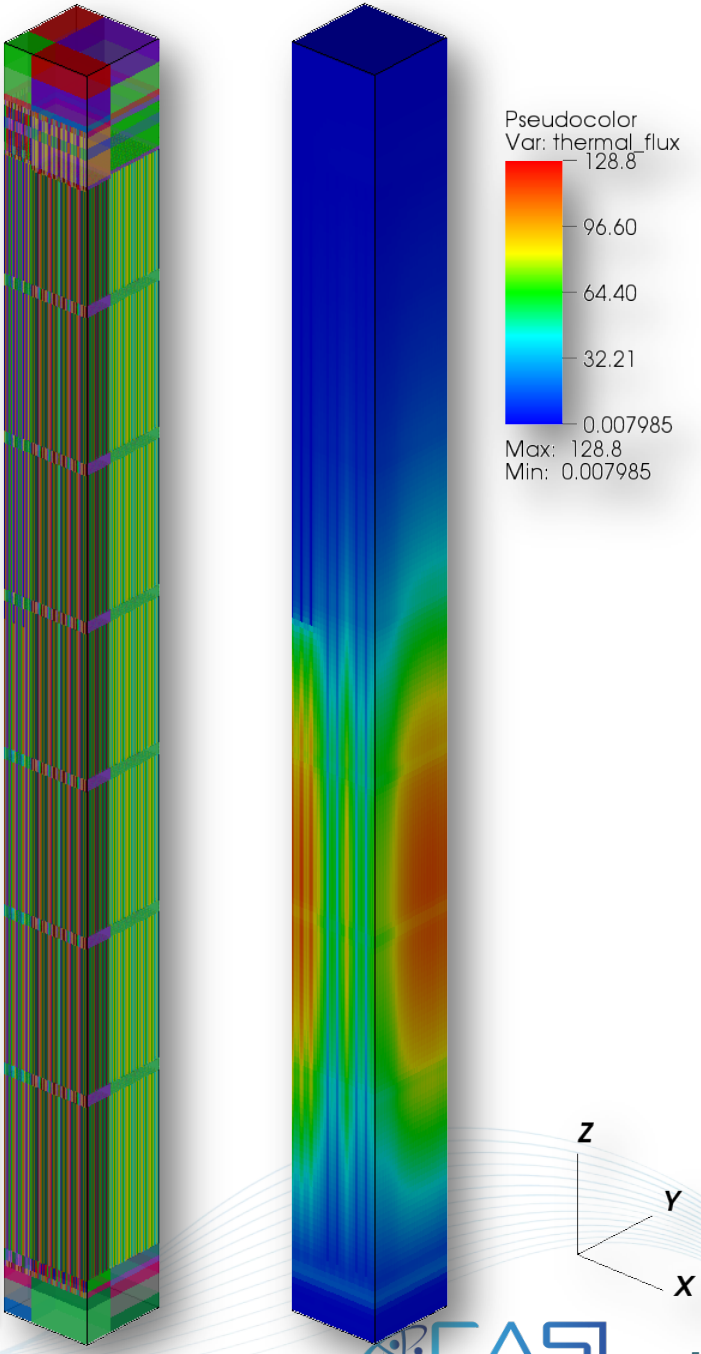
- ability to create, archive, compare, and modify input similar to current industry workflows
- attributes of real reactors
  - assemblies, poisons, control rods, non-fuel structures, baffle, power, flow, depletion, boron search, detectors, etc.
- eliminate inconsistencies between physics components through use of a common geometry description
- will evolve as needed
- currently using VERA input
  - Insilico (S_N, SP_N, Monte Carlo)
  - COBRA-TF
  - MPACT
  - Peregrine



Discussing with VUQ how best to expose internal component model parameters for SA/UQ.

VERA Common Output

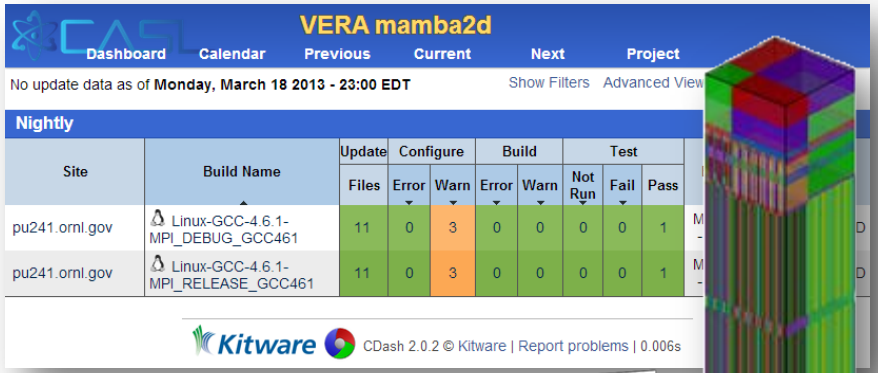
- fine-mesh results written to **SILO** files for visualization in tools such as VisIt / ParaView
- pin-by-pin distributions (from multiple codes) written to a common **HDF5** format that can be post-processed to create user edits
  - 2D/3D pin distributions
  - 2D/3D assembly distributions
  - peaking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

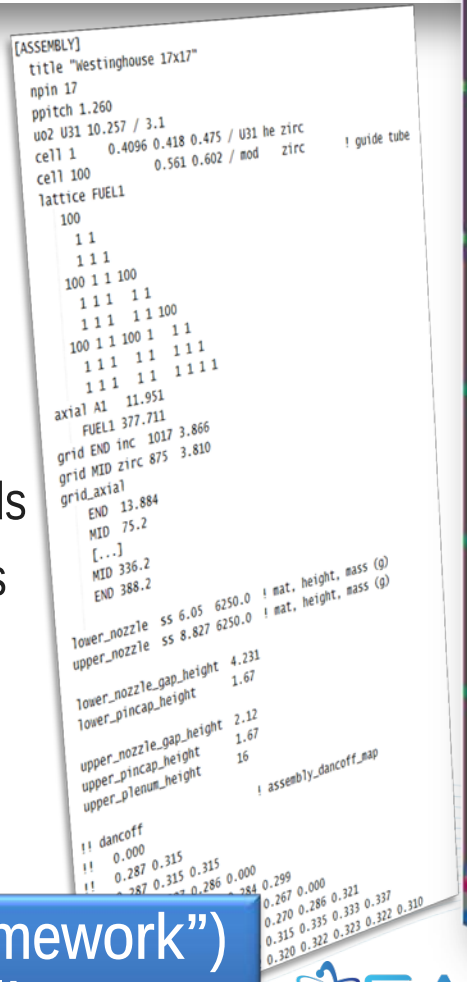


Insilico fission rate for full assembly, generated SILO file and VisIt

Coupling Challenges and Solutions

- Challenges
  - Many codes assume they are the “master”
  - Conflicting dependencies and build systems
  - Existing codes that have a life of their own outside CASL
  - Multiple languages (primarily Fortran and C++)
  - Disparate input and output formats and conventions
  - Different meshes and discretizations
- Solutions
  - Common build system that extends widely-used standards
  - Philosophy of continuous integration (catch and fix issues and conflicts as early as possible)
  - Standardize input / output (and restart)
  - Develop infrastructure components as necessary (e.g. DTK for solution transfer)

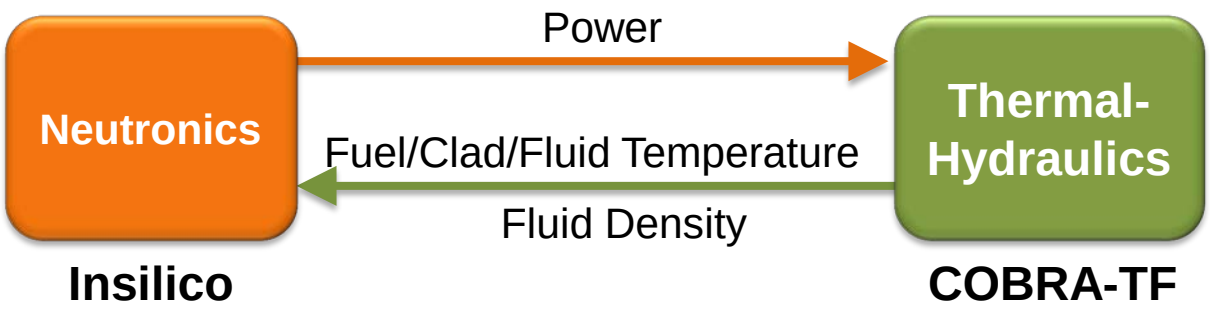




The “mechanics” of nonlinear iteration (the “framework”) is not the most challenging aspect of coupling.

Coupling of neutronics and thermal-hydraulics components for hot full-power beginning of life assy.

- AMA progression problem 6
  - neutronics (cross sections + neutron transport)
  - thermal-hydraulics (fluid flow and fuel/clad temperatures)

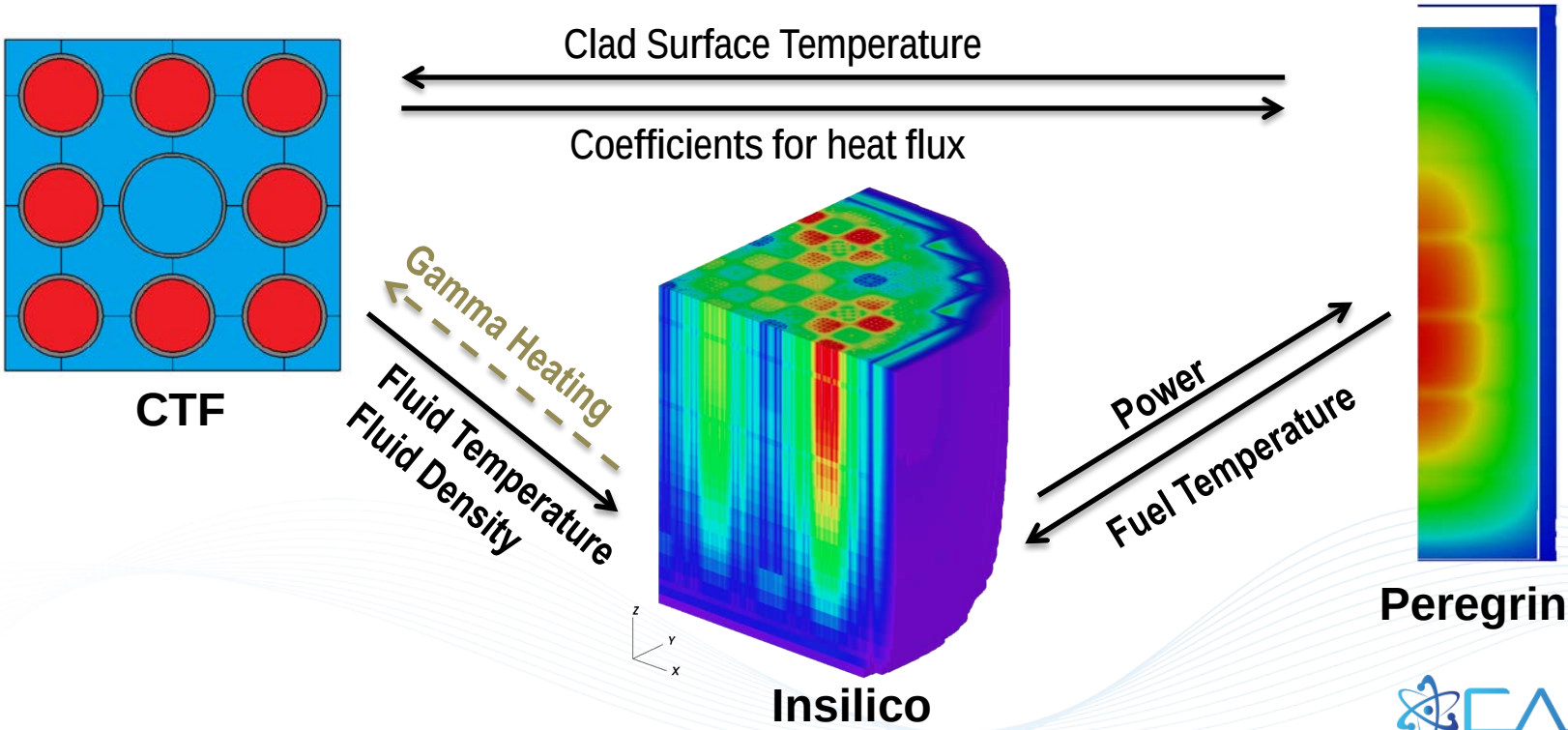


- Coupling becomes more complicated with more codes, but we've done it.
- Challenges are related more to data transfer than "framework".

Data Transfer Kit (DTK) will be discussed later.

CTF / Insilico / Peregrine Coupled Driver

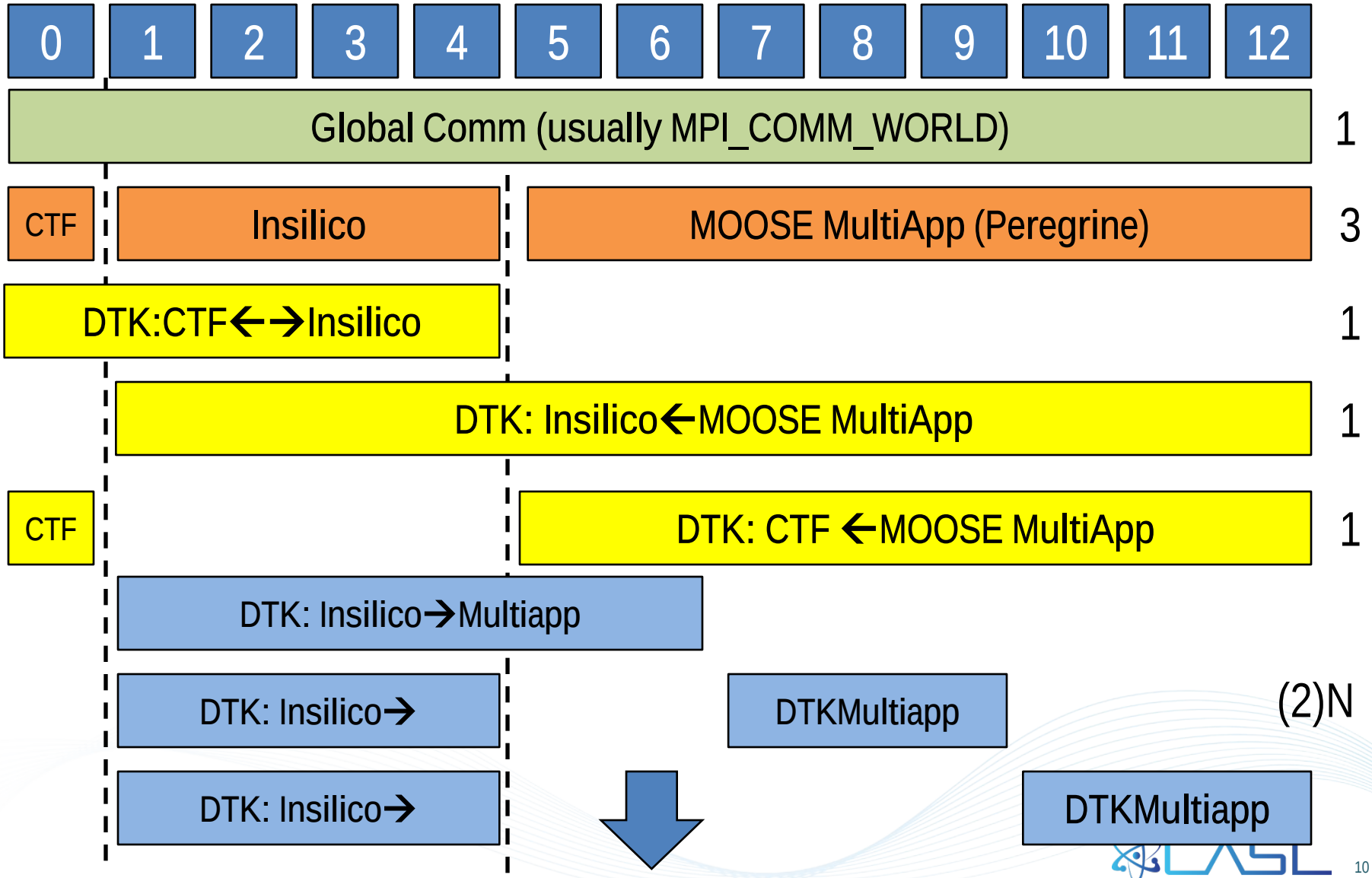
- Named **Tiamat**, multi-headed dragon (Babylonian mythos)
  - easy to add new "heads" provided the apps meet integration criteria
- All applications are run in their own MPI process space
  - can overlap if desired
  - reduce collisions and improved algorithms performance
- Data Transfers are handled through DTK with MPI sub-communicators



Modifying a code for integration can be challenging, but not necessarily in obvious ways.

- Exposing input parameters and output responses is one of the most challenging aspects
  - Parallel distribution, data structures, units and coordinates, …
- Codes are no longer top of the software food chain (main()):
  - No global variables, using namespace declarations in headers
  - “Solve” can be called multiple times
  - Must be able to reset if any physics fails a “step”
  - Can not control/manipulate the parse of input
  - Can not redirect output streams, must allow ostreams to be set
  - Can not assume MPI_COMM_WORLD anywhere in your code (must accept an MPI communicator)
  - In-source builds are dangerous
- Memory management strategies are critical (RCPs)
- Robust error handling

A Multiphysics Distributor
(Four levels of MPI Communicators)

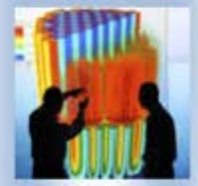


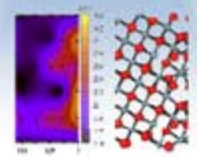
Relationship of VERA to Commercial Software
(Independent Software Vendors – ISVs)

- CASL is using commercial software tools wherever appropriate
  - meshing (HEXPRESS/Hybrid), visualization (Ensight), CFD (CD-adapco)
- CASL is collaborating with ISVs as well as appropriate
  - discussions with ANSYS on workflow tools
  - initial discussions with GSE – potential Test Stand candidate
  - initial coupling efforts with Star-CCM+ have now evolved into a deeper discussion of application programming interfaces (APIs) to facilitate closer coupling (see quote below)

"CD-adapco is in the business of CAE software because we are constantly reminded of the unique insights and value that it offers. Working with the remarkable talent and resources of the CASL development team is an extraordinary opportunity to extend the range and scope of capability well beyond current off-the-shelf technology. Our success is assured by helping to make the very best technology accessible, reliable, and cost-effective for our customers. A seamless union of CASL VERA and STAR-CCM+ is a clear opportunity to serve that mission and we are committed for our common good to incorporate an efficient and versatile API for this purpose."

- Eric Volpenhein, Nuclear Energy and National Labs Sales Lead, CD-adapco





STAR-CCM+ / VERA Interoperability

CASL Industry Council Meeting
Oak Ridge National Lab
September 11, 2013

Eric Volpenhein, CD-adapco
Nuclear Energy and National Lab Sales Lead

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

What is it?

- **Capability to use STAR-CCM+ representations and solutions in a coordinate, efficient, and straight-forward manner with select VERA tools**
  - Neutronics
  - Mamba
  - Hydra-TH
  - FSI (explicit)
  - Fuel performance
  - Subchannel thermal / hydraulics

Why?

- **STAR-CCM+ provides a complete environment for high fidelity CFD and select multi-physics modeling supporting a very broad range of industries and institutions, including the nuclear power industry.**

- **VERA offers an accelerated and, in many cases, unique pathway to advanced capabilities, technologies, and resources that can benefit our clients in nuclear power:**
  - specific phyiscal models, e. g., neutronics, crud, fuel performance
  - advanced closure and subscale models, e. g., CHF, multi-phase flow
  - more robust and scalable solution methods, particularly for tightly coupled multi-physics
  - Additional validation
  - integrated uncertainty quantification
  - Ultra high performance compute resources and experience
  - others

Why? (cont)

- **Serves the interests of our clients to provide an efficient pathway from STAR-CCM+ to VERA for enhanced modeling & analyses**
- **Serves the interests of CASL to help focus limited resources on advancing technology**
- **Serves the interests of CD-adapco to leverage experience in working with CASL / VERA to the STAR-CCM+ community**

CASL: Virtual Environment for Reactor Analysis (VERA)

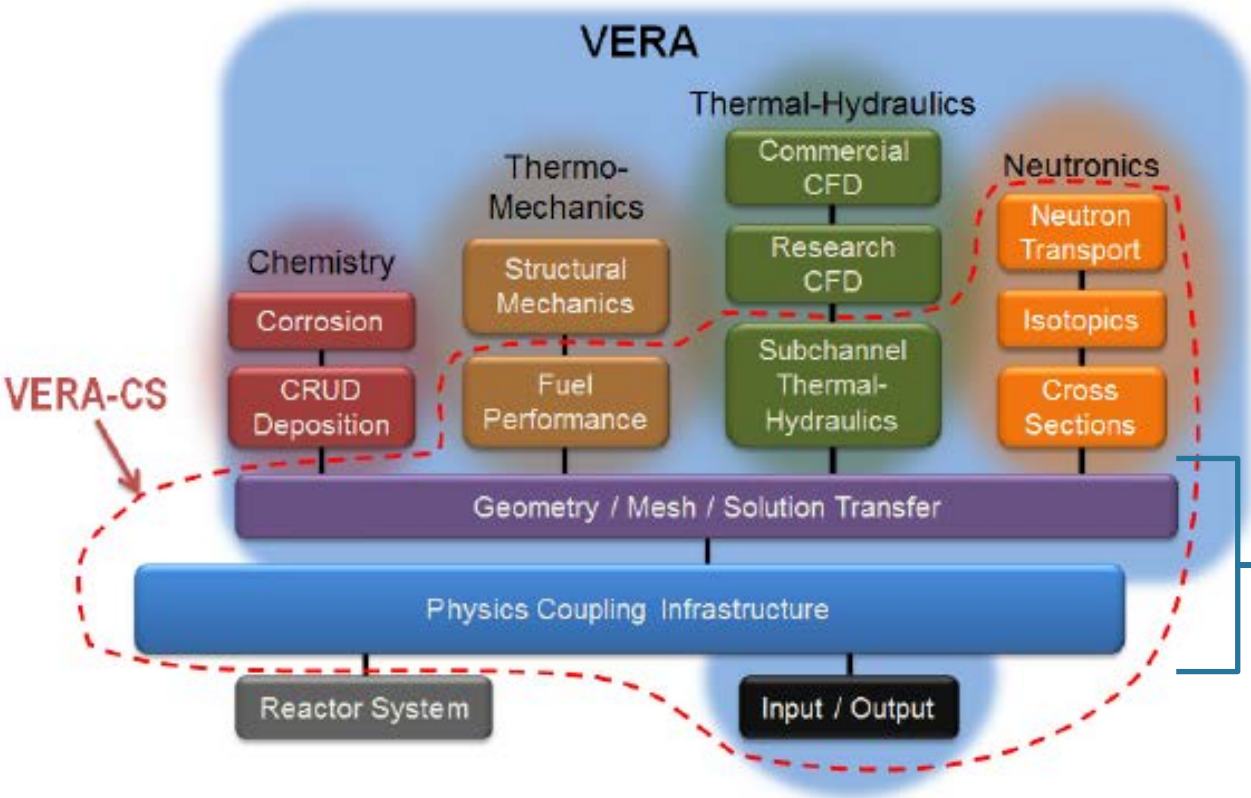
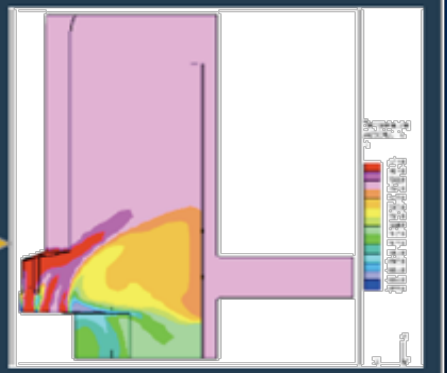


Fig. 3. VERA components that comprise VERA-CS

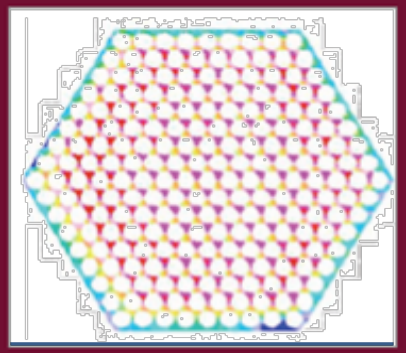
Requires efficient and scalable data exchange in spatially and time accurate manner

Nuclear Energy Advanced Modeling & Simulation (NEAMS)

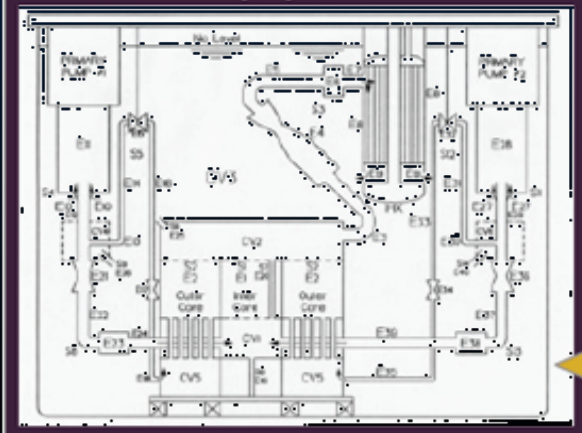
RANS CFD
STAR-CCM+
Detailed Cold Pool



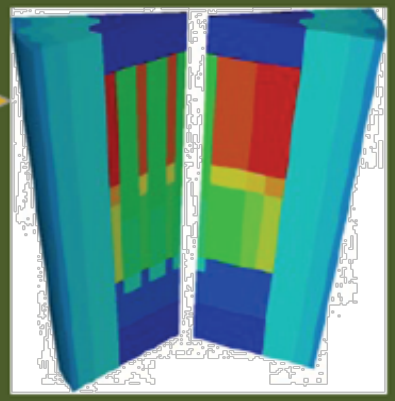
RANS CFD
Star-CCM+ or Nek5000
7 (Simplified) Full Assemblies



System Model
SHARP Driver
+ SAS4A/SASSYS components
Full SFR Primary System



Neutronics
Diff3D/Variant + MC^2-3
Full Core



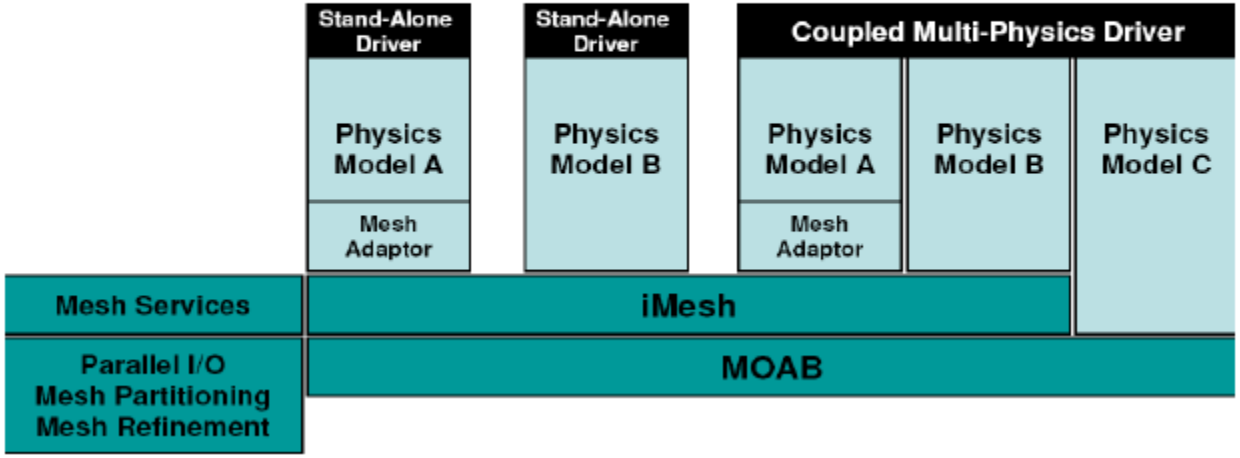
LES CFD
Nek5000
Single Full Detail Sub-Channel

Structural Mechanics
Diablo
Full Assembly Stress and Deformation

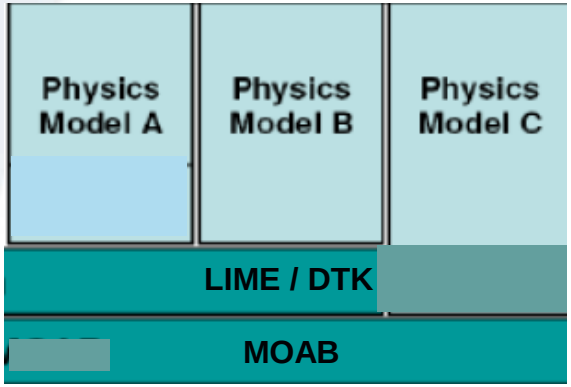
Argonne NATIONAL

MOAB / DTK

NEAMS (SHARP)



CASL



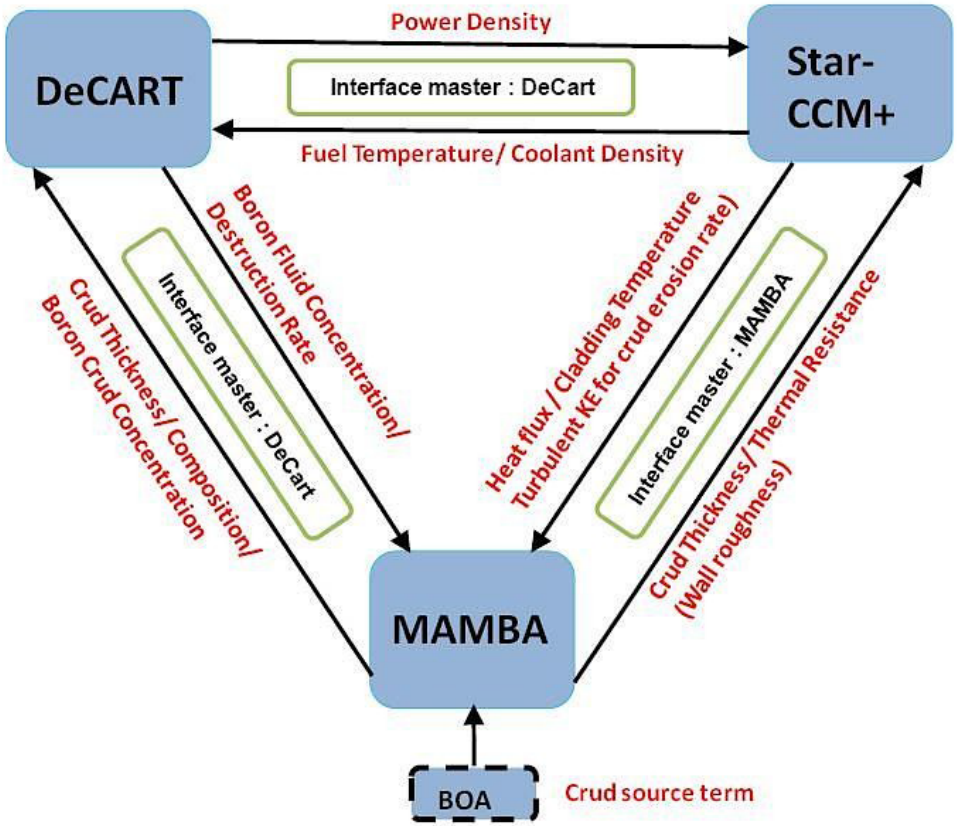
STAR-CCM+ Data Exchange

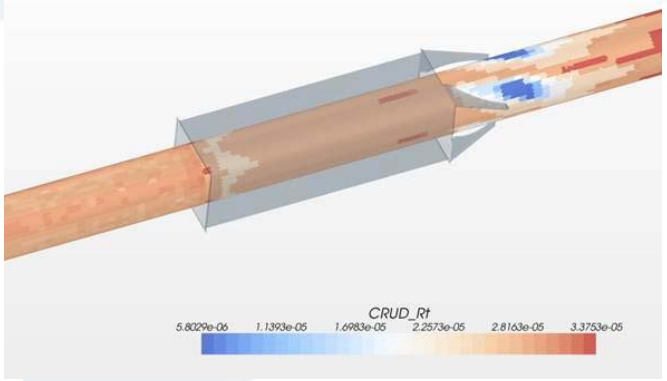
Current Methods for Data Exchange

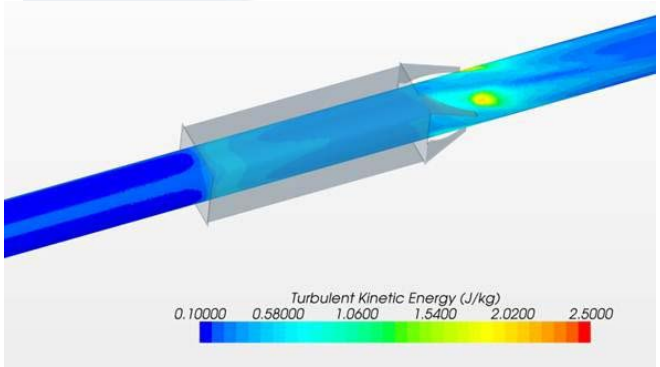
- **File Based Transfer: Import/Map/Export**
  - Data exchange via files on a hard-disk
  - CAE code need not be resident in memory
  - Often called “Loose Coupling”
  - User responsible for exchange synchronization (Java programming)

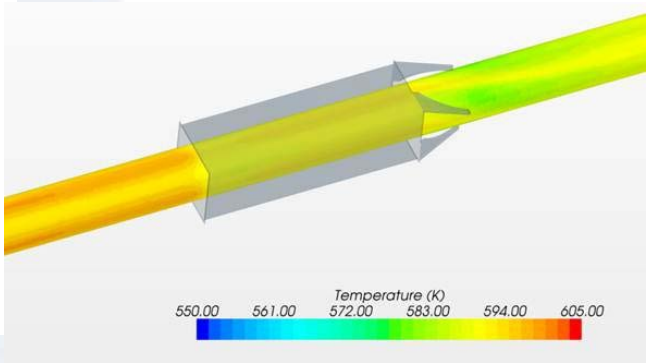
- **Socket Based Transfer: Co-Simulation API**
  - API controls exchange synchronization
  - Data exchanged via sockets
  - CAE code and STAR-CCM+ both executing in memory
    - STAR-CCM+ to STAR-CCM+ Co-simulation
    - STAR-CCM+ to 1D external Codes
      - GT Power, Wave, Olga, AMESim, Relap5
    - STAR-CCM+ to Abaqus Co-Simulation using Abaqus API

CASL: Current Method with Iterative File Exchange



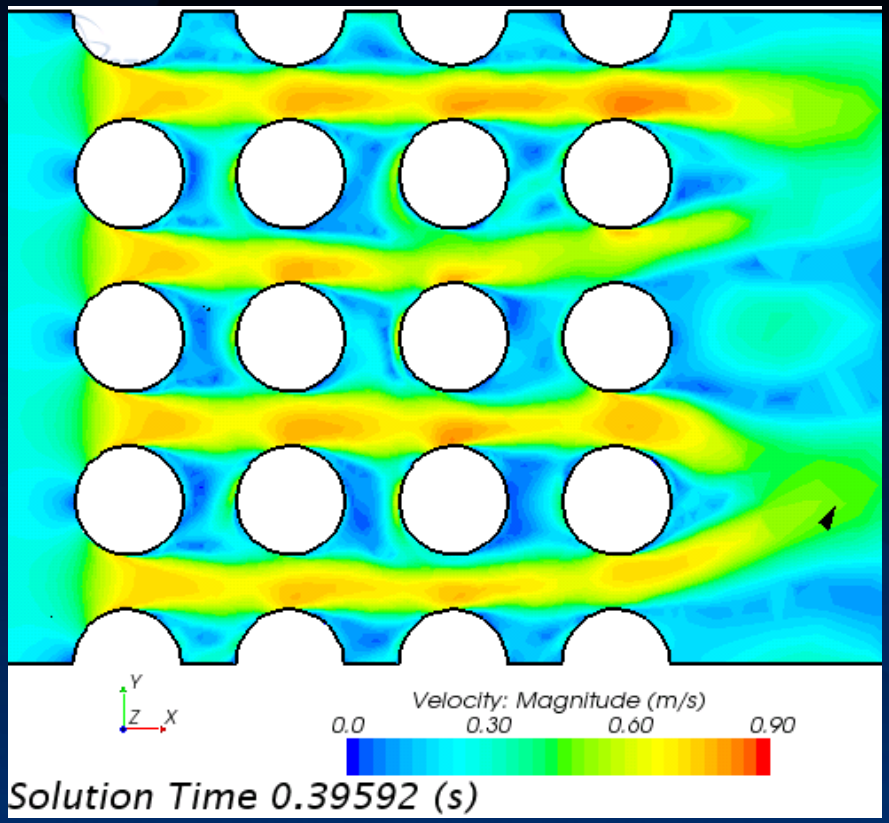


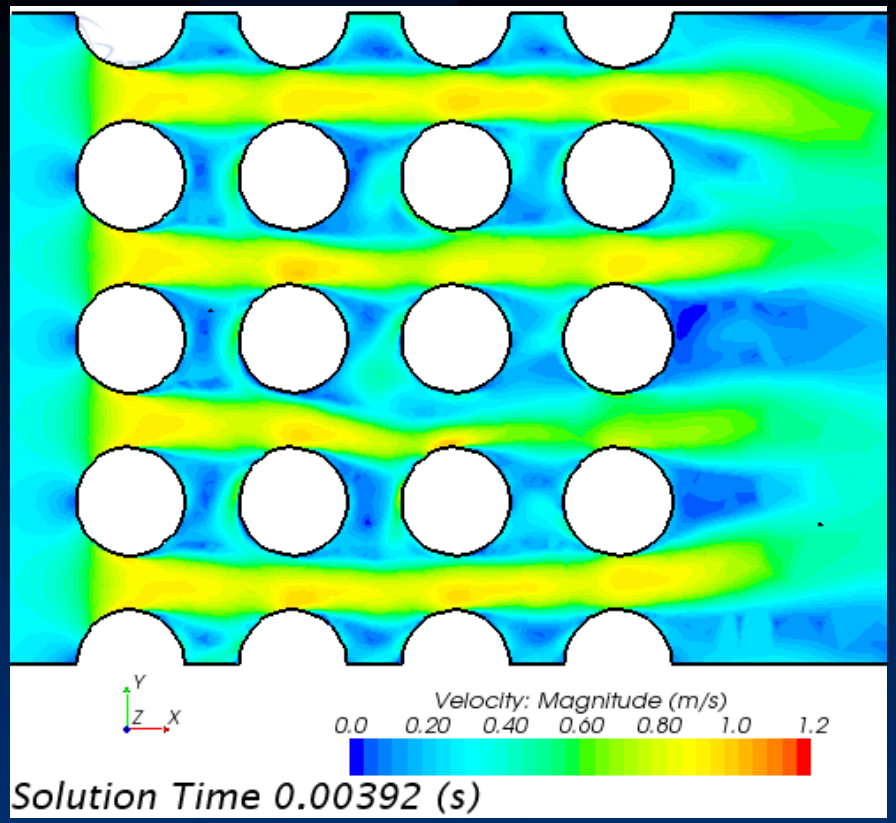




STAR-CCM+/Abaqus: Implicit FSI via socket exchange

Fluid velocity





Vu=0.25m/s **Velocity Mag** **Vu=0.31m/s**

STAR-CCM+ exchange via MOAB / DTK

- **Information needed by MOAB / DTK to coordinate generalized, in memory, core-2-core data exchange is not presently distributed locally by STAR-CCM+**

- **Data must be re-assembled via the head node before exchange**

CASL / NEAMS API

Innovation Forum May 20, 2013

Idea: CASL / NEAMS API

- **API for MOAB (Mesh-Oriented Database) / DTK, an open-source, national lab developed utility shared between CASL, NEAMS, and others**
  - Mesh-2-Mesh mapping on multi-processors
  - Any location, not just boundaries
  - Concurrent and in memory
  - MOAB / DTK does the mapping (to / from), need local (per core) access to STAR-CCM+ mesh information and solution variables

- **Future:**
  - interface with COUPE / LIME for solution control of coupled codes
  - Interface between Validation and Uncertainty Quatification (VUQ) modules and adjoint solver
  - IBM Blue Gene Q port

APPROVED