Consortium for Advanced Simulation of LWRs

CASL Industry Council Meeting
March 17-18, 2015 – Charlotte, NC
Minutes

The tenth meeting of the Industry Council (IC) for the Consortium for Advanced Simulation of Light Water Reactors (CASL) was held on March 17-18th at the EPRI offices in Charlotte, North Carolina. The Industry Council was chaired by Scott Thomas of Duke Energy.

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

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

Day 1 – March 17, 2015

Welcome and Introductions (Scott Thomas)
Scott Thomas opened the meeting with a welcome and review of the agenda and everyone introduced themselves.

CASL Phase 2 Review (Alex Larzelere)

Alex Larzelere began the Industry Council meeting with a welcome and extended his appreciation to the Industry Council for their active participation in CASL. He highlighted the approval of Phase 2 for CASL. Key points supporting the Renewal Panel's approval were that the CASL team regularly completed technical milestones in a timely manner and the annual review panel questions from the DOE-HQ were answered satisfactorily. Phase 2 goals will include broadening the scope of VERA to include BWR modeling challenges as well as increased depth of PWR challenge problems. In addition, a working group will be established and a framework for the requirements of a post-CASL entity will be developed.

CASL Status and Phase 2 Plans (Doug Kothe, Jess Gehin, Paul Turinksy)
Doug Kothe, CASL Director, Paul Turinsky, Chief Scientist, and Jess Gehin, incoming Director of CASL, provided an overview of the CASL project technical accomplishments. Doug noted how the CASL IC role became greatly appreciated by the DOE NE, and how the Industry Council guidance will be needed as VERA is distributed among users. Doug noted that Dr. Jess Gehin will take over as CASL Director starting April 1st, 2015. The current technical capabilities of VERA were described in overview, and the FY15 milestones were listed. The HPC Innovation Excellence award received by NCSU for their work in Innovative Thermal Hydraulic methods. Phase 2 plans were covered, it was noted that there is a $121.5M USD renewal that extends CASL to FY20. VERA capabilities will be extended for PWRs and iPWRs, and BWR work will be added to the scope.

VERA-CS Development and Benchmarking (Ben Collins)
Ben Collins presented an overview of VERA-CS benchmarking. Highlights of the discussion included:

- Several key additions were made to VERA including direct coupling to CTF, depletions, and integration with MAMBA and BISON-CASL are in progress.
- Watts Bar Cycle 1 and the cycle 1 of the BEAVRS benchmark have been completed.
- Shuffling allows multi-cycle depletions to be calculated.
- Benchmarks to B&W 1484 and 1810 critical experiments were reviewed.

BEAVRS benchmark comparison were discussed thoroughly. During Cycle 1, VERA underpredicted cycle boron by an average of 27 ppm, and the average RMS flux map comparisons were 3.03% for 2D predictions and 4.8% for 3D. Watts Bar Cycle 1 and the AP1000 with WABA poisons were modeled. Future work will include CIPS analysis, completion of the BEAVRS benchmark, BWR geometry, and AP1000 depletion.

Validation and Modeling Applications Update (Yixing Sung, Vince Mousseau)
Yixing Sung and Vince Mousseau presented an Update on Validation and Modeling Applications (VMA) The CASL VMA focus area provided an update on VMA Phase I accomplishments, application examples and phase 2 development strategy and data challenges. VMA combines Validation and Uncertainty Quantification (VUQ) with Advanced Method Applications (AMA) to provide tighter coupling between assessment and application of VERA with its Verification, Validation, and Uncertainty Quantification (VVUQ). Phase I accomplishments included releases of DAKOTA and its user guideline for optimization, UQ, parameter estimation and sensitivity/variance analyses, initial VVUQ assessments of CASL tools, VERA-CS component study, and data collection. VUQ application examples included VERA Progression Problem 6 UQ study and turbulent mixing parameter calibration. The planned work in Phase II will move from capability development to application-drive production deployment, including code VVUQ and Challenge Problem VUQ focusing on CIPS, PCI and DNB. VMA will continue to rely on support from the industry partners on data identification and collection for CASL use.

EDF Advances in Thermal Hydraulics Simulation (Didier Banner)
Didier Banner (EDF) presented EDF's activities in the field of thermal-hydraulics. The major motivations are related to safety issues, performance, long-term operation of NPPS, fuel issues and innovative reactors. His presentation was focused on CFD dealing with complex flows and geometries. EDF has developed a suite of thermal-hydraulic codes for single-phase flow (Code_Saturne, which is open source) and two-phase flow (Code_Neptune/ co-developed with French partners). His presentation dealt with interoperability issues, HPC capabilities and validation. Applications were also shown such as pressurized thermal shock, complex flows downstream of a mixing grid or boron dilution. It was agreed that EDF will propose a test case in T/H that could be also studied with CASL tools (i.e Hydra-TH).

Thermal Hydraulics (THM) Update (Doug Kothe)
Doug Kothe and Emilio Baglietto presented an overview of the CFD progress with Hydra-TH. Currently the targets are generic N-field multiphase capabilities that is applicable to PWR and BWRs. There has been progress on several fronts:

- There are key goals in the next year regarding implementation of multiphase flow and development of next generation boiling models

- Single phase predictions are relatively mature, there have been reasonable differences between STAR-CCM and Hydra-TH wear work rates.
- The impact of CRUD on sub-cooled boiling is being investigated by creating surfaces with synthesized CRUD and performing sub-cooled boiling measurements.

Gen II heat partitioning is under development; a new physically based wall-boiling model for CFD has been proposed. The results so far show improved wall temperature predictions with both low and high pressures. Momentum closure is in progress, the implementation of drag forces showed lift inconsistencies. Work is on-going to compare to Tomiyama experimental results. There is also on-going work to compare TAMU two-phase data to Hydra-TH.

DNB Challenge Problem Update (Yixing Sung)
Yixing Sung, the DNB Challenge Problem Integrator, provided an update on CASL DNB modeling and simulation. DNB is a safety-related challenge problem being addressed by CASL for both fuel hardware design improvement through high-fidelity M&S and margin quantification in accident analysis through multi-scale and multi-physics M&S. Phase 1 accomplishments included applications of the CTF subchannel code to rod bundle test data analyses, RIA transient simulation, and reactor core modeling under DNB limit conditions of loss of flow, steamline break and Reactivity Insertion Accident (RIA). Current work in progress includes application of coupled neutronic and T/H code system VERA-CS for evaluating reactor core responses with respect to DNB during HZP SLB event with or without offsite power, application of CFD code for evaluating fuel bundle DNB-related response

VERA Use Case Discussion (Dennis Hussey)
Dennis Hussey presented the status of the VERA deployment plan. A table of industry use cases was presented and their expected resource requirements and value were discussed. It was noted that the use cases will vary from operational (how to assist plants with risk assessments) and design (when fuel assembly designs can be rated prior to experimentation).

Discussion of TVA Test Stand: Lower Plenum Flow Anomaly (Rose Montgomery, Bill Byrd)
Bill Bird and Rose Montgomery presented the on-going results from the TVA test stand. Meshes have been generated for the vessel, and several trial simulations have been performed. A convergence study was performed to see the difference in results from changing the convergence criteria from 1e-2 to 1e-5. It was noted that there was minimal difference between 1e-4 and 1e-5, which will help with reducing run time.

The meeting was adjourned for the day.

Day 2 – March 18, 2015

VERA Working Group Discussion (Rose Montgomery)
The next morning the Industry Council began with a discussion of the VERA Working Group. Rose led the discussion and several options about how the working group will interact with the post-CASL entity. Dennis Hussey went through several potential models for the post-CASL entity.

Assymetric RCS Flow/Temperature Insights needed for Safety Analysis (Scott Thomas, Jeff Abbott)

Jeff Abbott was unable to attend, so this presentation was not made, but the materials are included in the minutes. Scott Thomas provided some discussion of the needs as well as the value of the work presented on the DNB challenge problem.

Fuel Materials and Chemistry Update (Chris Stanek)

Chris Stanek from Fuel Materials and Chemistry presented an update to the CRUD challenge problem and discussed in detail the three-dimensional modeling of a PCI failure using BISON-CASL and compared the results to the EPRI FALCON model. The VPSC model was described and plans to apply the model to RIA and LOCA scenarios are shown.Future steps include improving the material properties and fuel performance behavior (fission gas release, thermal expansion and creep), and including clad corrosion and hydriding.

Round Robin Feedback

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

John Hannah (GNF):

> John noted that BWR core simulator not in phase 2 scope, and there will be limited BWR geometry capability. It would assist GNF to know what scope is planned for BWR modeling. It was noted that specifications for the BWR geometry for VERA-CS development are available. The discussions about BWR PCI, RIA, LOCA encouraging to hear. DAKOTA was interesting, and he thought it useful to quantify the variability of the manufacturing tolerances. For example, do they exceed modeling tendencies? Make VERA available to people in the future. It's hard to jump in, can modules be developed to be run separated for individual runs. There will be a parallel track as it's not licensed.

John Harrold (Dominion Resources, Inc.):

> Equipment reliability, design challenges are an industry problem and there should be some consideration of how CASL can be applied to future needs to address unknowns, not as much on current applications. Significant progress has made in Crud modeling, especially the feedback mechanisms. This should be focused on supporting better risk analysis. Uncertainty quantification discussions are encouraging. Distinguishing the different types of uncertainty (design, model). This should be used to identify where resources should be provided and what CASL should focus on. Get the tool to be used to do probabilistic estimates, and how uncertainties of sub-models apply or not to an overall estimate. Workshops are a great idea, great for education and sustained use. Get VERA into the educational system, there will be downstream applications. When taking advantage of an operating plant, looking for public interest, goals are increased output. Unlikely in the immediate term unless involved in licensed applications (crud may be an exception). It looks like CASL is unique in scope. Align with industry workflow (licensing), incorporate uncertainty into analyses.

Zeses Karoutas (Westinghouse):

> There appears to be a viable multi-tool product in development. Crud has done well (looking at the entire core), combining with crud source, boron deposition, followed up for CIPS/CILC. Risk

assessment without NRC licensing example is there. Regarding the PCI RIA and LOCA with steam line break, if these tools prove out, fuel vendors may consider submitting to NRC for licensing. New engineers need to be trained, less siloing of disciplines is needed, instead a multi-physics background is needed for the code results interpretation.

Rose Montgomery (TVA):

Optimistic about the set of tools, there will be broader application of several disciplines, getting the tools into the users hands is important. Tech transfer and commercialization is a key challenge.

Chris Stanek (CASL):

Involvement of industry has been key to getting FMC problems solved.

Ian Stevenson (Dassault Systemes Simulia Corp.):

DS/Simulia interoperability is a key feature. Don't underestimate the need for multi-physics training as not all practicing users will be familiar with all of the model complexity.

Walt Schwartz (Ansys):

More utility involvement is a strong indicator of progress, encourage them to contribute. Model examination is a strength, not accepting status quo is important. Take advantage of the 5 years to get deployment.

Brad Black (Duke Energy):

Using VERA after 5 years needs CASL to demonstrate actual value that can justify membership dues (as well as the human and compute resources). It's an easier sell. Do the best to estimate value, even if a relative estimate, starting from the use cases.

Tyrone Stevens (Exelon):

Excited about increased collaboration and data sharing. Interested in the LPFA modeling of Watts Bar, it's also noted in Byron (which may be impeller related). Exelon has several failures where data should be available. For example, the Braidwood PCI failure data should prove useful for benchmarking. Ginna had a flow induced failure, TMI corner failures. There are also in-core tilt problems at Braidwood and TMI. Exelon is willing to share the data to work with the team and help build a success story.

Chris Lewis (Areva)

Benchmarking results and actual comparisons are encouraged (crud comparison in particular). Consider using that as an example of real world success. Like accident tolerant fuel, plants are heading to the end of their lifetime, they are less likely to implement changes. Therefore there is a need to get these tools to market, in particular elements that can be implemented quickly. Then develop tools that address Gen 3 and beyond. Licensing: a lot of work to be done to introduce to the NRC. Use VERA to advise reduced order methods used by the utilities. Users group/working

group should consider the licensing effort in the long term. Atomistic models are not necessarily recognized by NRC but they could inform them. It's clear the codes need high performance computers, may put limits on the user base. Perhaps the models can be used to inform the engineering tools.

Bob Wall (Bechtel Marine Propulsion Corp):

Uncertainty quantification is insightful, and glad to see it early in the Phase 2 process. Multi-phase CFD is going well.

Alan Copestake (Rolls Royce):

Pleased for Phase 2 approval. Good plans and milestones in place. Benchmarking runs and work in the area are going well. Continue to seek more industry involvement. VUQ is doing well, but don't forget the manufacturing tolerances. Consider looking at the uncertainties to determine what the tolerances should be. EDF work is doing great. T-H is doing well, but still a challenge. Use cases shouldn't push too far into the value, but they are useful to show what the models may be capable of. Working group discussion is good to have now and start improving them. Materials performance has done well, and it's clear that the models are working. The need for the changing engineer applying an integrated toolset. VERA may well be used for informing the reduced order methods, and may require thousands of runs to do proper uncertainty quantification. Continue developing

Didier Banner (EDF):

Impressed with how VERA has developed over five years, broad range of fundamental science and applications. Interest from the industry to use the tools has grown. EDF modeling approach is different, but there are similar developments. Benchmarking EDF models to CASL can be valuable (e.g. single phase flow) and compare all aspects of modeling including results, computer platforms, and program/project management implementation.

Jess Gehin (CASL):

We're listening to your feedback, and this has been helpful for the transition. Excited to see the industry led industry council.

Doug Kothe (CASL):

Key metric is a vibrant industry council, and this meeting demonstrated it. More NRC engagement could be useful. Early wins in Phase 2 will advance CASL greatly, seek ways to demonstrate CASL value. VMA work (e.g. with TH) is really important.

Scott Thomas (Duke Energy)

Scott thanked everyone for coming and noted the progress that has been made in the last year.

The meeting was adjourned.

Action Items

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

Action	Owner	Date
Prepare slides and distribute prior to IC/SC meeting	Dennis Hussey	

An additional comment was to have a half-day tutorial for VERA at the end of the next IC/SC meeting

Prepared: April 29th, 2015
Distributed to Senior Leadership Team for Review: May 1st, 2015

By Dennis Hussey, Industry Council Director

CASL Industry Council Meeting
Agenda
March 17-18, 2015
Location: EPRI Office Bldg 1 Rm 305, Charlotte, North Carolina

Tuesday, March 17

8:00	Gather and Coffee	
8:30	Welcome and Introductions	Scott Thomas, Duke Energy
8:45	CASL Phase 2 Renewal	Alex Larzelere
9:00	CASL Status and Phase 2 Plans	Doug Kothe Jess Gehin Paul Turinsky
9:45	Action Item Review	Dennis Hussey
10:00	**Break**	
10:15	VERA CS Development and Benchmarking	Ben Collins
11:00	Validation and Modeling Applications Update	Yixing Sung Vince Mousseau
12:00	**Working Lunch**	
1:00	EDF Advances in Thermal Hydraulics Simulation	Didier Banner, EDF
1:45	Thermal Hydraulics (THM) Update	Doug Kothe
2:30	DNB Challenge Problem Update	Yixing Sung
3:00	**Break**	
3:15	VERA Use Case Discussion	Dennis Hussey
3:45	Discussion of TVA Test Stand (Lower Plenum Flow Anomaly)	Bill Bird Rose Montgomery
4:30	**Adjourn**	

Wednesday, March 18

8:00	Gather and Coffee	
8:30	Review of Day 1	Scott Thomas
8:45	VERA Working Group Discussion	Rose Montgomery
9:15	Asymmetric RCS Flow/Temperature insights needed for Safety Analysis	Jeff Abbott, Duke Energy
9:45	**Break**	
10:15	FMC Update	Chris Stanek
11:00	Round Robin	All
11:30	Wrap Up – Action Items, Next Meeting	Dennis Hussey
12:00	Adjourn	Scott Thomas

Industry Council Attendees

1. Scott Thomas, Duke Energy, (Industry Council Chair) Scott.Thomas@duke-energy.com
2. Chris Lewis, AREVA, Christopher.Lewis@areva.com
3. Brad Black, Duke Energy, bradley.black@duke-energy.com
4. John Harrold, Dominion Resources, Inc.
5. Robert (Bob) Wall, KAPL, robert.wall@unnpp.gov
6. Alan Copestake, Rolls Royce, Alan.Copestake@rolls-royce.com
7. Ian Stevenson , Simulia, Ian.STEVENSON@3ds.com
8. Bob Oelrich, Westinghouse, oelricrl@westinghouse.com
9. John Hannah, GNF
10. Walter Schwartz, ANSYS
11. Tyrone Stevens, Exelon
12. Didier Banner, EDF

CASL Staff

1. Doug Kothe, ORNL, kothe@ornl.gov
2. Paul Turinsky, NCSU, turinsky@ncsu.edu
3. Doug Burns, INL, douglas.burns@inl.gov
4. Jess Gehin, ORNL, gehinjc@ornl.gov
5. Rose Montgomery, TVA, rmontgomery@tva.gov
6. Dennis Hussey, EPRI, dhussey@epri.com
7. Steve Hess , EPRI, shess@epri.com
8. Jeff Banta, ORNL, bantajp@ornl.gov
9. Scott Palmtag, Core Physics, palmtagsp@ornl.gov
10. Jeff Secker, WEC, seckerjr@westinghouse.com
11. Travis Lange, University of Tennessee
12. Andrew Godfrey, godfreyat@ornl.gov, ORNL
13. Ben Collins, collinsbs@ornl.gov, ORNL
14. Yixing Sung, Westinghouse
15. Vince Mousseau, SNL (remote)
16. Bill Bird, TVA (remote)

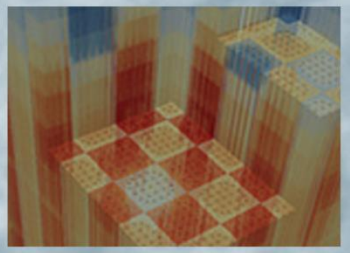
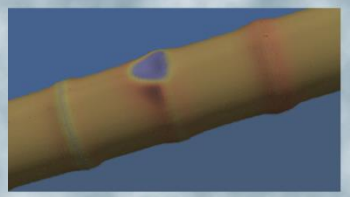
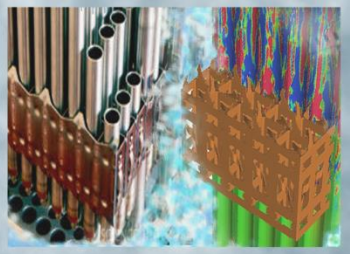
Department of Energy

1. Alex Larzelere, DoE-NE

A DOE Energy Innovation Hub

CASL Industry Council

Scott Thomas, Duke Energy
Charlotte, North Carolina
March 17th, 2015

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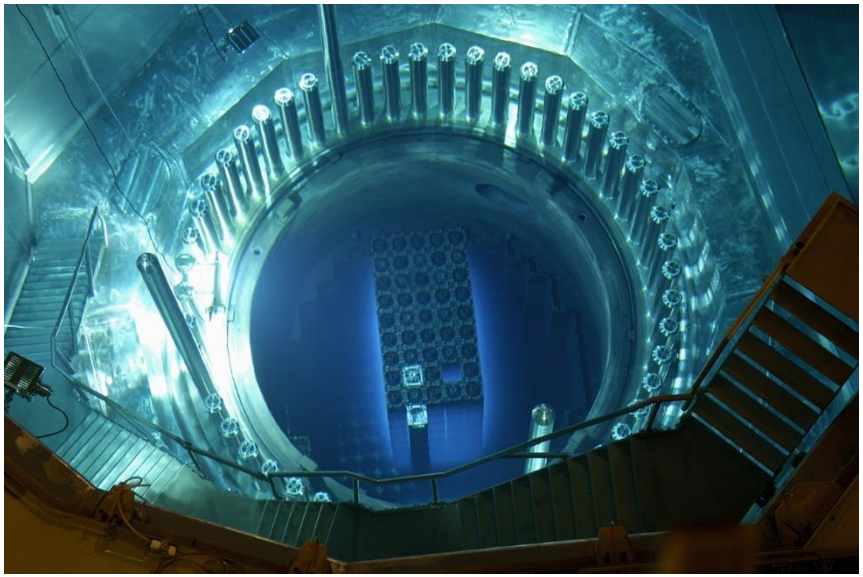
Industry Council

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

Objectives and Strategies

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



Outcomes and Impact

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

Industry Council Membership

Owner/ Operators of Nuclear Plants	Fuel and/or SMR Vendors	Engineering Design, Service Providers, R&D	Independent Software Vendor	Computer Technology Companies	Ex-Officio
Dominion	AREVA	Battelle	ANSYS	Cray	BOD
Duke Energy	GNF	Bettis /NNPP	CD-adapco	IBM	DOE
EDF	B&W Power Generation	EPRI	Dassault Systemes	NVIDIA	
Exelon	NuScale	Rolls Royce	GSE Systems		
TVA	WEC	Studsvik Scandpower			

Industry Council Updates

- Industry Council leadership change
  - Scott Thomas will chair the Industry Council
  - Dennis Hussey will serve as Director

- New Members are being recruited
  - Arizona Public Service has expressed interest.
  - Awaiting replies from Southern Nuclear and Vattenfall

Phase 2 expectations are increased collaboration between IC and CASL team

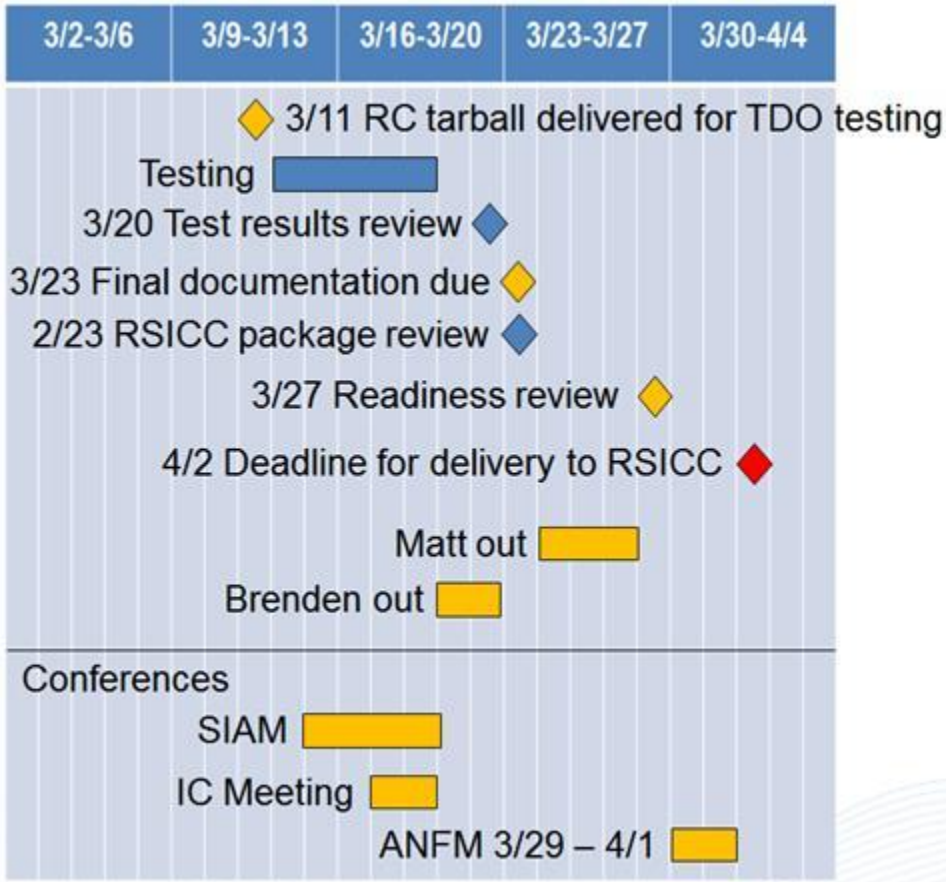
October 2015 IC Meeting

- Webcast to precede meeting for planning and updates to be scheduled for June-July 2015
- Joint Industry Council/Science Council Meeting
  - Dates are expected to be October 13-14 or 14-15
  - Location is Oak Ridge National Laboratory

VERA Release Plans

- VERA is scheduled for a release at the end of February
  - Inter-Institutional Agreement is near complete
  - Clears the path for licensing and VERA distribution
- During Phase 2, a working group model is proposed
  - Nominal fee is suggested
  - License terms still in development
- Post-CASL Phase 2 licensing options remain open

VERA Release Schedule



Revised release schedule on track

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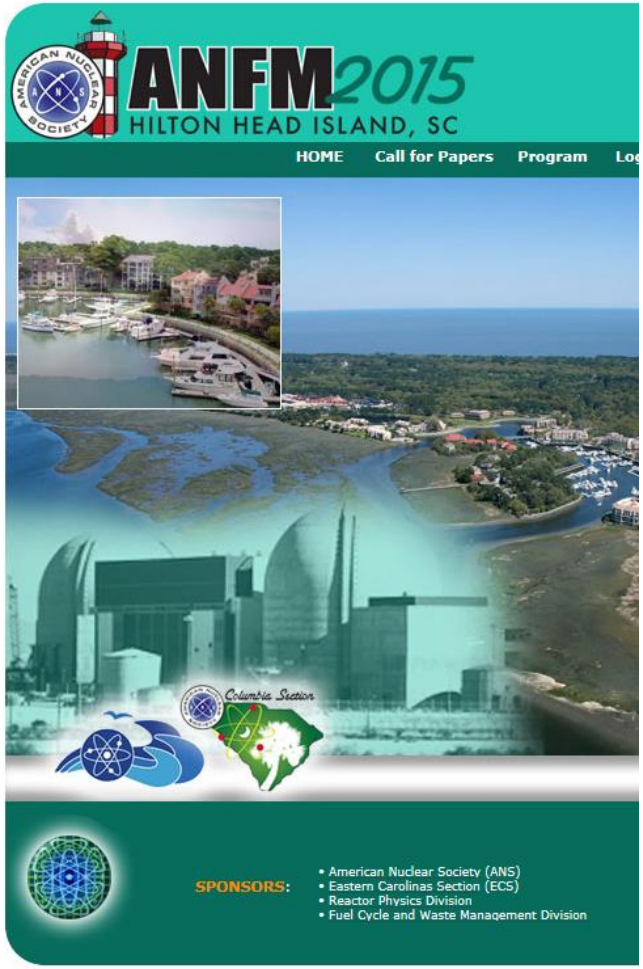
VERA Distribution

- VERA distribution via Working Group membership
  - Working Group members receive license (subject to export control)
  - Subscriptions open to utilities, vendors, academia and consultants
  - Nominal annual fee proposed to encourage early adoption
    - Fee supports Working Group activities and distribution costs
    - Membership fees will vary based on industry or academic applications
    - Founding partners will receive consideration for alternate fees
- Working Group fee structure and license terms will be subject to change annually

CASL's First VERA Training Opportunity

- Advances in Nuclear Fuel Management ANS Topical Meeting
  - March 29 to April 1
  - VERA Workshop will be all day on Wednesday, April 1
- Two Sessions presented
  - Physics and Methods
    - open to conference
  - Hands-on with VERA
    - limited to 20 pre-registrants



Register at *www.anfm2015.org*

Actions from September Industry Council Meeting

Action	Owner	Date	Status
Develop a strategy for meshing (pre-planning a meshing implementation guidelines).	TDO	IC meeting	Discussion for this meeting
Summary on Hydra progress/challenges, in particular with regards to BWR	Yixing, THM leadership	Deferred from webcast to this meeting	This meeting
Develop a table of use cases, needed VERA functionality, resource requirements, value added and timescale.	Dennis Hussey	Update at webcast, detail at meeting	Discussion for this meeting
Define plans for working group	Rose Montgomery	Webcast discussed, more this meeting	Discussion for this meeting

Actions from September Industry Council Meeting

Action	Owner	Date	Status
Develop a statement of Chairperson commitments.	Dennis Hussey	One month	Completed
Select an Industry Council Chairperson	IC Director	Before next webcast	Completed
Document distribution (tech notes, documents)	Dennis Hussey	Monthly	Tech Notes to be submitted by end of March

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Consortium for Advanced Simulation of LWRs

Phase 2 Renewal

Alex R. Larzelere,
Federal Director, Modeling and Simulation Energy Innovation Hub
Office of Nuclear Energy
U.S. Department of Energy

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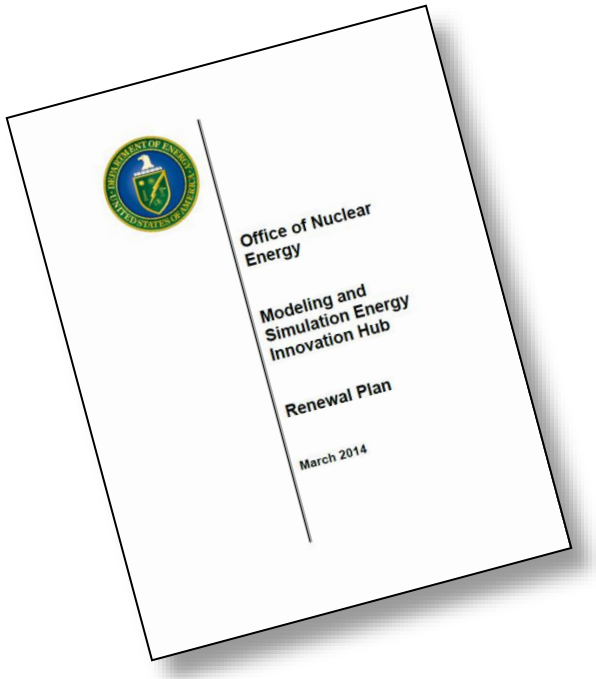
It's Done!

- **Announcement made on 1/30/15**
- **Accomplishment highlighted in the DOE FY-16 budget rollout.**

- **Culmination of a year long process**
- **Review goals**
  - Implement a creditable process
  - Have CASL create solid plans for 2nd phase work to allow continuation of light federal touch oversight



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The Energy Innovation Hub Concept & Basis for Renewal Review

- **"After five years, a Hub can apply for a five-year renewal, subject to it satisfying its goals and objectives and contributions to the overall mission of the Energy Innovation Hubs."**

- **Concept introduced by DOE Secretary Steven Chu in 2009**
- **Intended to develop and deploy game changing energy technology with a "fierce sense of urgency"**
- **Experiment in Three Areas**
  - Technology
    - Application of advanced, modern, modeling and simulation capabilities to address near term nuclear energy technology problems.
  - R&D Business Model
    - Bridge the traditional "valleys of technology transfer death" by tightly coupling national labs, universities and industry"
  - Collaboration
    - Create a multi-disciplinary, multi-institution collaborative environment to rapidly deliver results

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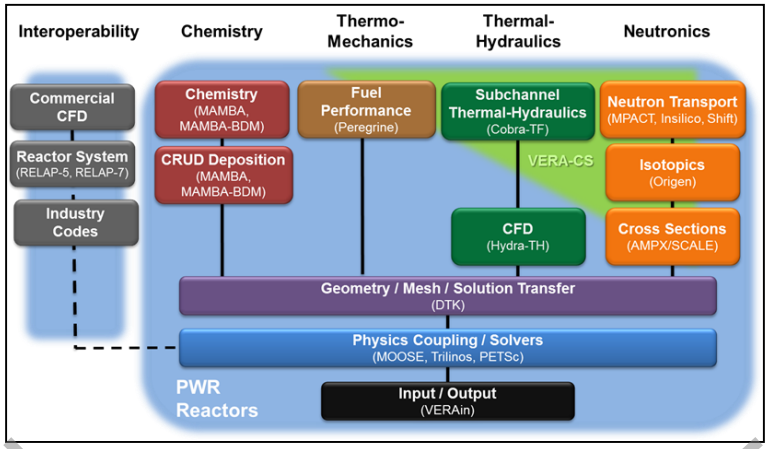
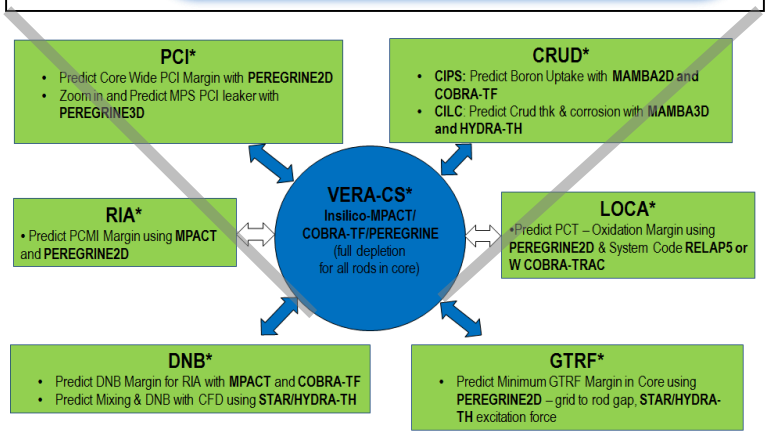
CASL Phase 1 Technology Experiment Results

- **Developed and Delivered the Virtual Environment for Reactor Analysis (VERA)**
  - Architecture and multi-physics code coupling software
  - Populated with advanced modeling and simulation tools that appropriately simulate physical behaviors found in nuclear reactors
  - Guided by "challenge problems" that ensured that VERA addressed current industry issues (i.e. useful)
  - Implemented with a "user environment" that is appropriate for an industry setting (i.e. usable)

CASL Built This - VERA





For Each Challenge Problem Apply DAKOTA using Coupled Tools for UQ

To Improve Industry's Ability to Address Performance & Safety Challenge Problems

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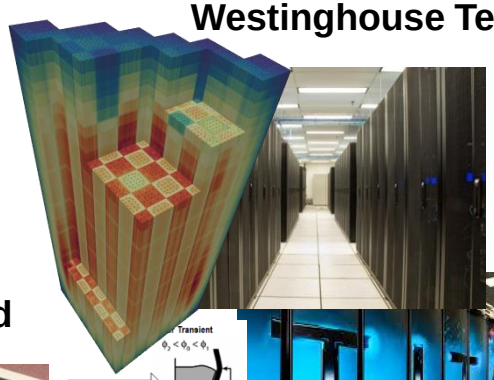
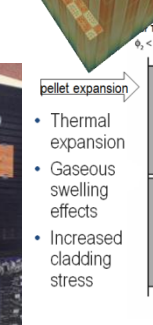
CASL Phase 1 R&D Business Model Experiment Results

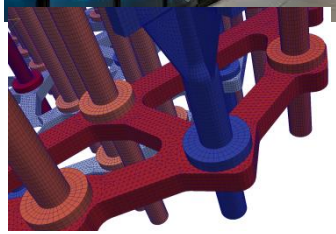
- **Focused on "use inspired" research**
  - Participation by industry partners in planning and executing R&D
  - Guided by outside Industry Council
- **Enabled Light (Right) Federal Touch**
  - Agility to quickly make technical course corrections when needed
  - Science Council to maintain technical quality
  - Board of Directors to set strategy
  - Very responsive to DOE annual reviews
- **Imbedded Educational Program**
  - Student researchers
  - Engagement with academia to move CASL technology into the classroom
- **Focused on Technology Deployment**
  - RSICC software releases
  - Use of "Test Stands" in industry settings to understand deployment issues

Westinghouse Test Stand



EPRI Test Stand





TVA Test Stand

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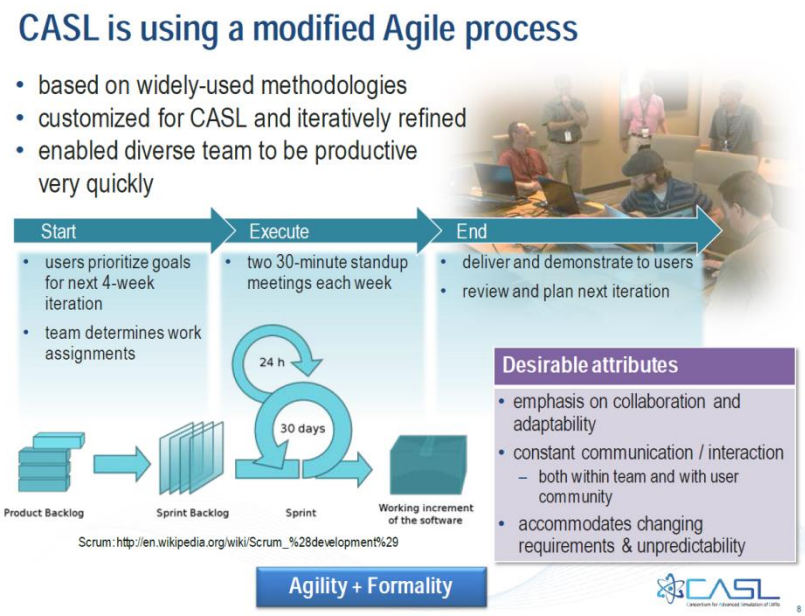
CASL Phase 1 Collaboration Experiment Results

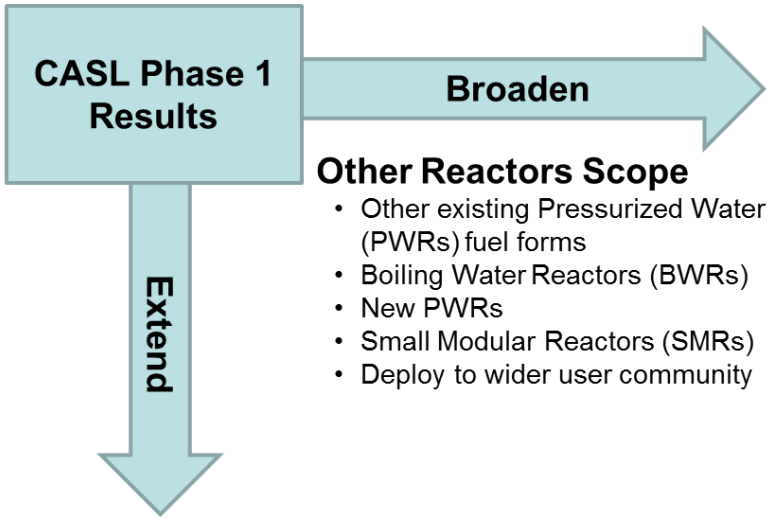
- **Created a "badgeless" multidisciplinary collaboration environment for a team of**
  - 4 national labs
  - 3 universities
  - 3 industry partners
  - Numerous associate members
- **Proactively assigned leadership roles to partners across the CASL organization**
- **Implemented an innovative mix of collaboration technologies and geographic co-location weeks to create a cohesive team**
- **Customized Trac tool enable distributed milestone creation, tracking, review, and completion**
- **Developed and implemented methodologies for distributed software development**



Review Factors

- **Significant Phase 1 Progress**
  - Milestone Completion
  - DOE-NE Annual Reviews
  - Impact on Science, Engineering & Education
  - Technology Deployment
- **Plans for Phase 2**
  - Technical Quality
  - Potential for Success
  - Team Capabilities

Requested Phase 2 Scope



Other Reactors Scope

- Other existing Pressurized Water Reactors (PWRs) fuel forms
- Boiling Water Reactors (BWRs)
- New PWRs
- Small Modular Reactors (SMRs)
- Deploy to wider user community

Watts Bar #1 Reactors Scope

- Extend modsim tools to address other PWR performance and safety issues
- Improve usability
- Extend and improve deployment of Phase 1 modsim products

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Phase 1 Performance Review Findings

- **Milestones**
  - CASL successful delivered 11 of the 12 milestones due on time (1 milestone missed was delivered one quarter late).
- **Annual Reviews**
  - CASL successfully completed all four annual reviews and addressed the review questions asked by DOE-HQ
- **Impact**
  - Published over 1,300 reports, journal articles, and conference papers.
  - CASL supported the participations of 20 undergraduates, 11 masters, and 57 doctoral students from 14 institutions.
- **Deployment**
  - Developed and implemented, via RSICC, a preliminary software licensing strategy.
  - Demonstrated deployment with 3 industry computational test stands.

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Summary of Phase 2 Proposal Review Finding and Comments

Technical Quality

- For its second Phase, CASL is proposing to move VERA to simulate some very difficult nuclear reactor modeling and simulation problems. This includes:
  - Multi-phase flow regimes
  - BWR geometries and fuels types
  - Convective (natural) flow
  - Transient/accident conditions
- The review team is concerned that given the fixed budget and five year limitation for Phase 2 of CASL, that these "aggressive" goals may not be achievable.
- However, given its success in Phase 1, the review team believes that CASL should be given the opportunity meet these "stretch goals."

Potential for Success

- CASL proposes that it will shift its development strategy to extending the use of VERA to other reactor types and fuels.
- In Phase 2, CASL proposes to continue to use the software engineering and quality practices established in Phase 1.
- Given the aggressive goals established in the renewal application, the review team recommends that CASL continues its proven task and milestone planning and tracking processes.
- Also, the review team recommends that CASL continues to actively manage its risks and where necessary define "trigger events" and "off ramps" to be exercised if the stretch goals become unachievable.

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Summary of Phase 2 Proposal Review Finding and Comments

Team

- The core CASL Team will remain the same in Phase 2.
- Anticipates adding industry members to guide VERA development to address new Challenge Problems.
- The review team recommends that CASL consider exploring ways to build and strengthen collaboration ties between its researchers at the overall team level.
- The review team recommends that CASL make the effort to document its experiences in creating a highly effective multi-disciplinary, multi-institutional collaboration and communicate those lessons to the other Energy Innovation Hubs and DOE.
- The review team suggests that CASL vigorously follow through with the suggestion that industry cost share increase from 20% to 50%.

Plans for Post Phase 2

- During Phase 2, CASL plans to establish the Advanced ModSim Working Group AMWG) to guide VERA development with the intent that it will continue beyond CASL.
- During Phase 2, the TDO will explore options for a “post-CASL” entity
- Create a business case for sustainability
  - Determine market for CASL tools
  - Develop revenue model
  - Determine support requirements
  - Build business plan for sustaining VERA indefinitely
- Post-CASL entity does not preclude DOE supported tech development and R&D if appropriate

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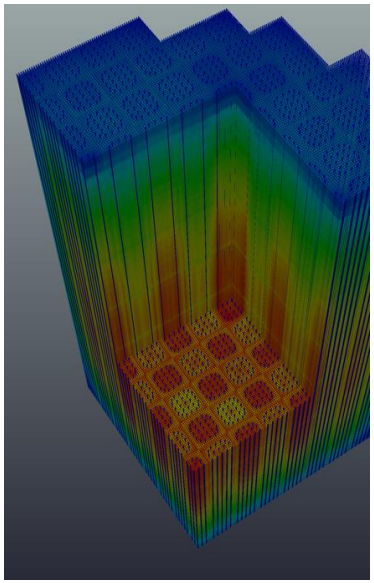
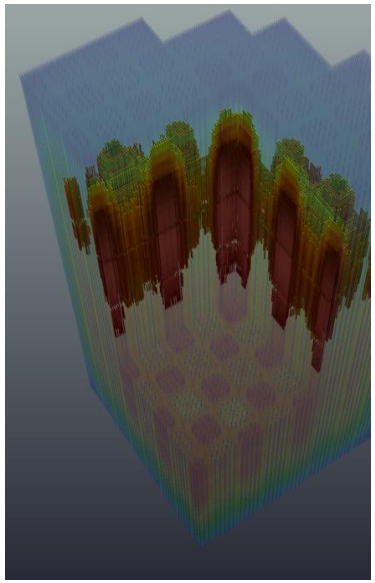
Renewal Review Conclusions

- **Overall – the federal review team found that CASL meets all of the criteria for renewal to a second phase.**
- **Therefore the review team strongly recommended that CASL be granted that opportunity.**
- **As CASL proceeds through its second phase, the review team recommended that CASL pay close attention to issues that will enable the taxpayer investment in the VERA technologies continues to be used and maintained after Phase 2.**
- **While the review team recommended continuation, there are a number of areas of concern. These include:**
  - The aggressive plans to broaden CASL tools to BWRs and iPWRs. The review team recommends that CASL be given the opportunity to attempt doing this, but also suggests that CASL closely monitor the risks and proactively implement mitigation plans if needed.
  - One of these risks is the limitation on funding and time. Therefore the review team recommends that CASL identify and peruse opportunities to shift work-scope to other funded programs (but only where appropriate).

A DOE Energy Innovation Hub





CASL 2.0

Doug Kothe

Deputy Associate Laboratory Director
Computing and Computational Sciences Directorate
Oak Ridge National Laboratory

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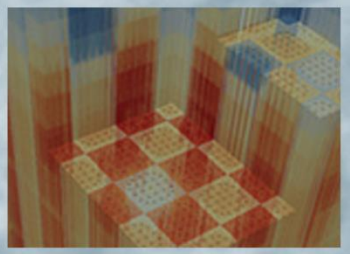
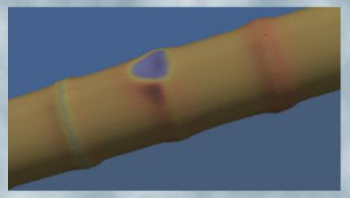
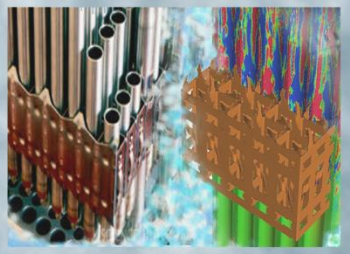






Energy Department Announces Five Year Renewal of Funding for First Energy Innovation Hub

Consortium for Advanced Simulation of Light Water Reactors (CASL) to Receive up to $121.5 Million Over Five Years (DOE Press Release Jan 30 2015)

In support of the President's call during his State of the Union Address to advance an all-of-the-above energy strategy, the U.S. Department of Energy announced on Jan 30, 2015 it would renew funding for CASL, an Energy Innovation Hub established in 2010 to develop advanced computing capabilities that serve as a virtual version of existing, operating nuclear reactors

"As President Obama made clear during his State of the Union address, reducing carbon pollution and protecting the climate has to be a top priority. CASL's work to help further our understanding of nuclear reactors, improving safety while also making them more efficient, will help the transition to a low carbon economy."

- **Energy Secretary Ernest Moniz**

"The work being done at the Energy Innovation Hub at Oak Ridge National Laboratory is an important part of our country's ability to innovate and safely maintain our nuclear reactor fleet. I'm glad to see the Consortium for the Advanced Simulation of Light Water Reactors remains a priority as we rely on nuclear power to provide the clean, cheap, reliable energy we need to power our 21st-century."

- Senator Lamar Alexander

Phase 1 Milestone Progress

Challenge Problem: Core Simulator (OR)

Challenge Problem & Year Planned [1]		Level 1 Milestone suggested in the Phase 1 Proposal [1]	Milestones executed by CASL (see Tables A-1 and A-2 of Appendix A for more detailed descriptions)
OR	3	Initial modeling of reactor operation; qualify with operational data.	L1:CASL.P7.01 delivered June 2013 - Demonstration with VERA-CS (CASL.003).
OR	5	Improved simulation of reactor operation; qualify with operational data.	L1:CASL.P9.04 planned delivery Sept 2014; Implementation of Operational Reactor Depletion Analysis Capability with TH Feedback (FY14.CASL.011)* Planned year 5 milestone: Qualify multi-cycle PWR core simulator capability.

- Notable deliverables
  - Developed VERA-CS with coupled neutronics, subchannel thermal hydraulics and fuel rod performance tool capability
  - Analyzed Watts Bar Unit 1 Cycle 1 startup physics tests using VERA-CS and Monte Carlo, showing excellent agreement
  - Deployed VERA-CS as a Test Stand and utilized to analyze AP-1000 Generation 3+ reactor core
  - Completing PCMM and UQ for VERA-CS with CASL reduced-order modeling
  - Continued Watts Bar Unit 1 Cycle 1 analysis to include prediction of initial power escalation
  - Added space-time kinetics capability to radiation transport component of VERA-CS

CASL did not fully understand or appreciate the importance of the Core Simulator as an integrated, usable, and standalone product.

The need for practical, engineering-scale simulations executable on industry-class computing platforms was not articulated.

VERA-CS requirements continue to evolve and undergo refinement as feedback is incorporated from users and R&D experiences.

Phase 1 Milestone Progress

Challenge Problem: CRUD

Challenge Problem & Year Planned [1]		Level 1 Milestone suggested in the Phase 1 Proposal [1]	Milestones executed by CASL (see Tables A-1 and A-2 of Appendix A for more detailed descriptions)
CRUD	1	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.	L1:CASL.P1.02 delivered Dec 2010. Baseline transport (e.g. DeCART) and CFD (e.g. STAR-CCM+) with loose coupling applied to a PWR sub-core scenario to demonstrate feedback coupling and contrast predictions with WEC coupled tool; and L2;RTM.P2.01 delivered June 30, 2011. Full-core 3D transport (DeCART, 2D/1D, pin-resolved) capability with single-phase T/H coupling (CFD, Star-CCM+).
CRUD	2	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness.	L1:CASL.P2.03 delivered Sept 2011. Deliver and demonstrate the utility of two-way multi-physics coupling in a VERA simulation of CRUD-based effects using actual reactor conditions.
CRUD	3	Model boron uptake from reactor coolant into CRUD on fuel rods.	L1:CASL.P4.02 delivered March 2012 - Conduct a CRUD investigation on representative clad surface regions within a 3D subassembly configuration; and L2:MPO.P3.01 delivered Aug 2011. Conduct 2-D, high resolution, coupled demonstration and assessment.
CRUD	4	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape.	L1:CASL.P7.05 delivered Sept 2013 - Multi-physics modeling of CRUD deposition on PWR fuel (CASL.009).
CRUD	5	Analyses to mitigate CRUD formation and minimize CIPS.	Planned Year 5 Milestone: Qualify core-wide PWR CIPS capability with corrosion product treatment.

- Notable deliverables
  - Developed/applied new CRUD evolution model with enhanced corrosion and boron products chemistry treatment utilizing FDT based thermodynamics.
  - Developed meso-scale CRUD evolution model (MAMBA-BDM) modeling CRUD structure (porosity and chimneys), two-phase Darcy flow, solubility/dissolutions, and cladding oxidation.
  - Integrated and coupled industry baseline components (ANC + VIPRE-W + BOA) within VERA and applied to multi-cycle operational reactor instances; results identify uncoupled baseline model errors.
  - Industry CRUD model (BOA) improved
  - Coupled advanced components (CFD + neutronics + CRUD) elucidate localized CRUD growth mechanisms completing assembly-level and full-core CIPS analysis

BOA capability and role; MAMBA; MAMBA-BDM; importance of coupling; driving force role of flow illuminated by CFD

Phase 1 Milestone Progress

Risks encountered and mitigated or being managed

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

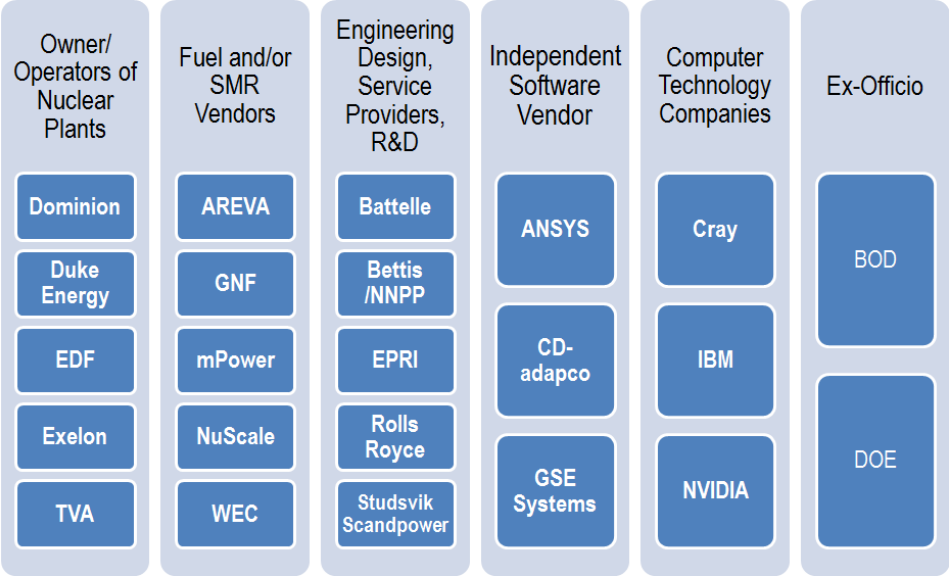
*** Denotes risks identified in the CASL Phase 1 proposal.**

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

CASL in Indebted to its Industry Council

And yet needs a more active role in Phase 2 for success

- When proposed in 2010, DOE Office of Nuclear Energy (NE) rightly viewed the CASL Industry Council (IC) as key for a successful public-private partnership
  - Not sure he CASL leadership appreciated this until later
  - And the fact that you likely "bit your tongue" is appreciated; witnessing plans rather than results does get old



- CASL has greatly benefitted from the strong engagement by the Industry Council
  - Fortunate to have an industry rep (Scott Thomas – Duke) now as the IC Chair
- CASL needs continued yet more critical feedback from the IC in Phase 2

CASL commits to a more active and engaged IC in Phase 2

Path Envisioned for Advanced Simulation Tools

Today
Early Deployment

- Integrate existing toolkit
- Selected applications and users
- Most of the applications on current LCF

Next 5 Years
Expansion

- Broaden applications and user basis as experience and computer power increase
- Most applications on Industry HPC
- Exascale computing facility for most demanding applications

Next 10 years
Integration

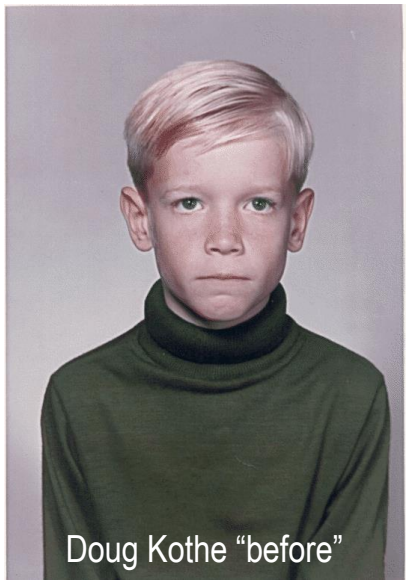
- Full integration of advanced tools in industry workflow
- Licensing with Nuclear Regulator

Next 20 years
Replacement

- Advanced simulation tools become a stand-alone design tool

Dr. Jess Gehin Named as CASL Director Effective April 1, 2015

- After a very successful Phase 1 and DOE approval of the CASL Phase 2 application, Doug Kothe is returning to the Computing and Computational Sciences Directorate
  - Initial focus: DOE Exascale Program, DoD Advanced Computing Program, decompression ☺


Doug Kothe "before"

- Gehin has been responsible for two CASL Focus Areas and delivery of key CASL accomplishments in the development and application of VERA
- Gehin's background well suited for Phase 2 applications of VERA research:
  - Ph.D. in Nuclear Engineering from MIT
  - Previous role as Reactor Technology R&D Integration in the Reactor and Nuclear Systems Division
  - Expertise is in nuclear reactor physics and reactor technology

Jess Gehin "before"

A DOE Energy Innovation Hub

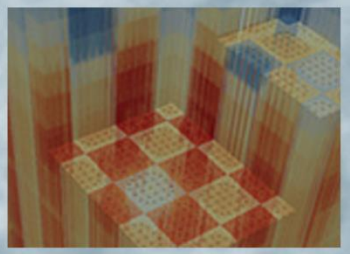
Current Status

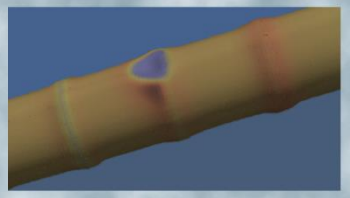
Organization updates

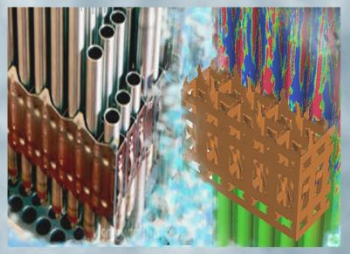
Progress on FY15 Milestones

Technical Capabilities Status

Jess Gehin, Director







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CASL Organization Update (Effective April 1)

Board of Directors
Jim Duderstadt, Chair

Oak Ridge National Laboratory
Thom Mason, Laboratory Director
Nuclear Science and Engineering Directorate
Alan Icenhour, Associate Laboratory Director

Science Council
Bill Oberkampf, Chair

Chief Computational Scientist
John Turner

Industry Council
Scott Thomas, Chair
Dennis Hussey, Executive Director

Technology Deployment & Outreach
Lead: Dennis Hussey
Deputy: Rose Montgomery
User Group: Rose Montgomery
Test Stands: Steve Hess
Education Program: Mike Doster, Director
Communications: Mark Uhran

Senior Leadership Team
CASL Director: Jess Gehin
Deputy Director: Doug Burns
Chief Scientist: Paul Turinsky
CASL Director Emeritus: Doug Kothe

Product Integrators

Challenge Problems
Integration Lead: Zeses Karoutas
CRUD: Jeff Secker
PCI: Robert Montgomery
RIA,LOCA: Gregg Swindlehurst
DNB: Yixing Sung
GTRF: Brian Wirth
BWR CPs: TBD

Validation Data
Nam Dinh

Technical Focus Areas

Fuel Materials & Chemistry
Lead: Chris Stanek
Deputies: Brian Wirth, Rich Williamson

Physics Integration
Lead: Jess Gehin (interm)
Deputy: Scott Palmtag

Radiation Transport Methods
Lead: Bill Martin
Deputy: Tom Evans

Thermal Hydraulics Methods
Lead: Marcus Berndt (interm)
Deputy: Emilio Baglietto

Validation & Modeling Applications
Lead: Vince Mousseau
Deputies: Brian Williams, Yixing Sung

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

Operations Support
Contracting: Jo Ann Fitzpatrick, Justin Keck
Information Technology: Brian Zachary
Program Administration: Linda Weltman
Safety Officer: Jeff Banta
Technology Control: Sam Howard
Web Design: Cheryl Richardson

VOCC
Collaboration & Ideation Officer: April Lewis
VOCC Support: A.J. Ierulli, Teresa Robison

Management and Administrative Functions
Technical Functions
Technology Useability and Distribution Functions

CASL Status and Looking Forward

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

Years 6-10: Phase 2 – Approved by DOE

Scientific Output thru Year 3

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

FY14 CASL Milestones

Formally reportable to DOE

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

Broad coverage of our committed plan
All milestones completed on time and within scope

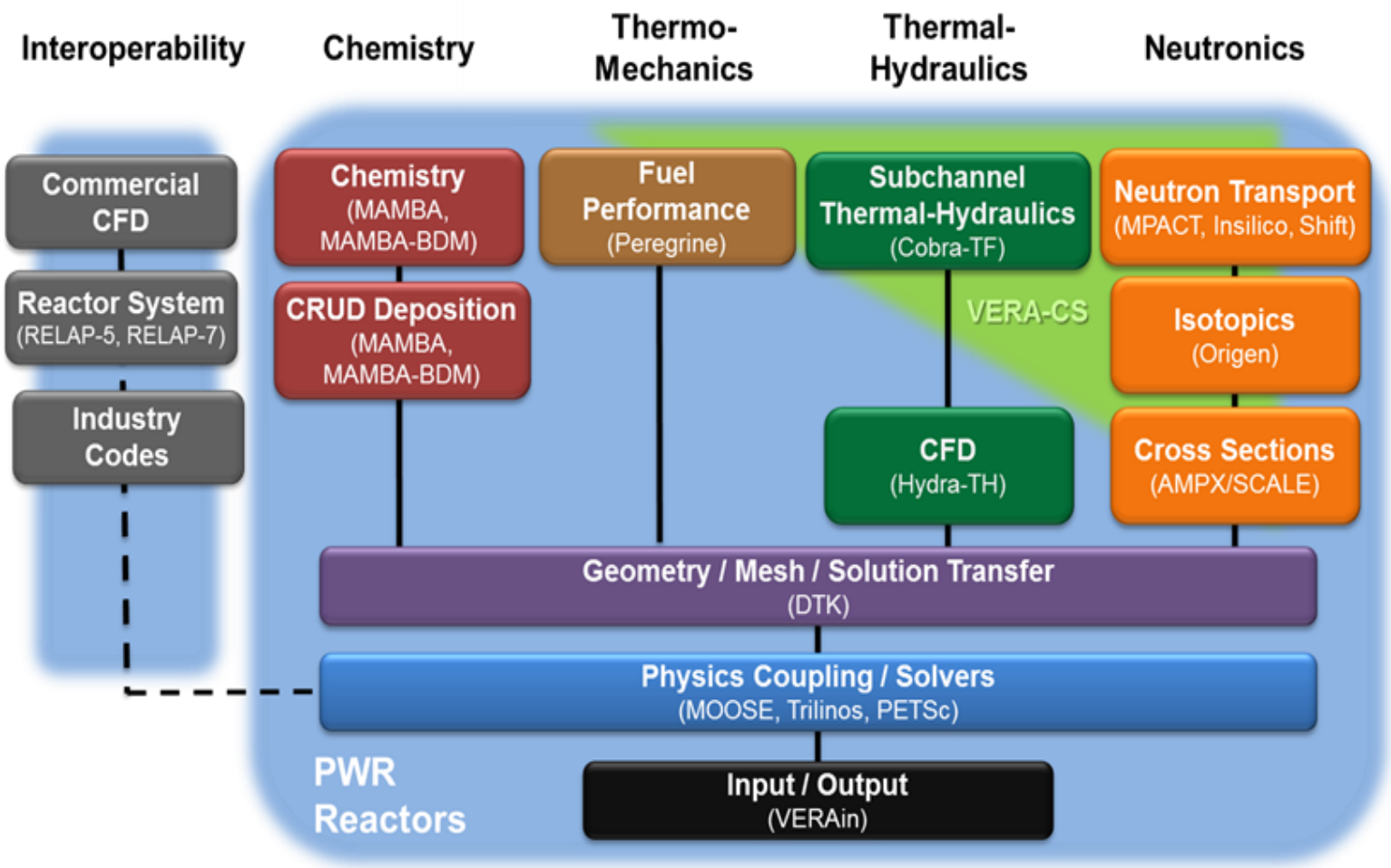
FY15 CASL Milestones

Formally reportable to DOE

Reportable #	Milestone ID	Milestone Description	Finish Date	Owner	Status
FY15.CASL.001	L3:SLT.MGMT.P10.01	Develop and document the CASL Management and Operations Plan for Phase 2	Dec 2014	Doug Kothe	Completed
FY15.CASL.002	**L1:CASL.P10.01**	**Demonstrate VERA-CS capabilities for a representative iPWR core**	Feb 2015	Rose Montgomery	Completed
FY15.CASL.003	L2.PHI.P10.01	Validate VERA-CS against the industry standard BEAVRS cycle depletion benchmark problem	Mar 2015	Ben Collins	On Track
FY15.CASL.004	L2:TDO.P10.01	Develop a preliminary deployment strategy for VERA that includes options for a post-CASL entity	Mar 2015	Dennis Hussey	On Track
FY15.CASL.005	**L1:CASL.P11.02**	**Qualify VERA-CS for a multi-cycle (w/fuel-reloading) PWR core simulation capability**	Jun 2015	Andrew Godfrey	On Track
FY15.CASL.006	L2:RTM.P10.01	Demonstrate a BWR subregion neutronics capability using a planar pin-resolved MOC methodology	July 2015	Brendan Kochunas	On Track
FY15.CASL.007	L2:VMA.VUQ.P11.04	Demonstrate an uncertainty quantification analysis of VERA-CS for a PWR fuel assembly with depletion	Sept 2015	Vince Mousseau	On Track
FY15.CASL.008	**L1:CASL.P11.03**	**Qualify a core-wide PWR CIPS capability that includes an initial corrosion product treatment**	Sept 2015	Jeff Secker	On Track
FY15.CASL.009	L2:FMC.P11.01	Demonstrate 3D PCI analysis with BISON-CASL on a relevant operating plant that experienced PCI failures	Sept 2015	Brian Wirth	On Track
FY15.CASL.010	L2:THM.P11.02	Experimenetally determine the effects of CRUD on sub-cooled boiling	Sept 2015	Jacopo Buongiorno	On Track
FY15.CASL.011	L3:THM.CFD.P11.07	Document the progress made on developing multi-phase capabilities in Hydra-TH	Sept 2015	Mark Christon	On Track

- 11 milestones with a broad coverage of CPs and FA capability development
- Initial Phase 2 scope represented (BWR neutronics, iPWR benchmark)
- DOE Review concerns addressed in part (multiphase CFD, etc.)
- Highest risk likely resides in PWR CIPS milestone (culmination of a large body of work)

VERA: Virtual Environment for Reactor Applications



Technical Capabilities Status

Core Simulator (VERA-CS: MPACT + CTF + ORIGEN)

- MPACT restart & fuel shuffle capability functional but still immature and in need of more rigorous testing;
  - Core Simulator Progression problems 1-9 completed, 10 nearly completed
- Code Camp in January focused on status of code and highlighted need for more attention to many-group cross-section preparation & resonance treatment
- Significant progress in reducing computer resource requirements, however, they are still larger than desired (target is for 4x reduction)
- Early Applications continue…
  - SMR demonstration (DOE reportable milestone completed in February)
  - MIT BEAVRs Benchmark (DOE reportable milestone due in March)
  - Watts Bar Multicycle (DOE reportable milestone due in June)
  - Single assembly UQ (DOE reportable milestone due in September)
  - CIPS Analysis (DOE Reportable milestone due in September)

Ben Collins will discuss VERA-CS Validation

Technical Capabilities Status

Fuel Performance (BISON-CASL)

- Tighter integration with NEAMS Program via addition of second Deputy Lead for FMC Focus Area
- Fuel pellet-cladding contact model difficulties mainly resolved (convergence, preconditioner & memory requirements)
- Continued effort on improving incorporation of viscoplastic self consistent (VPSC) model for cladding growth and creep
- New path being pursued for cladding oxidation and hydriding model development
- Key milestone in FY15 on predicting onset of PCI fuel failure that occurred in operating PWR

Chris Stanek will provide an update on Fuel Materials & Chemisty FA tomorrow

Technical Capabilities Status

Multiphase CFD (Hydra-TH)

- Single phase capabilities developed (additional turbulence models being added)
- Numerical methodology for multi-field CFD developed and appears robust
- Focus in FY15 is to add capability to model subcooled boiling and bubble flow regime
  - Work on closure relationships (lift, drag, turbulence & bubble origination, growth, detachment, etc.) via conducting and interpreting experimental and DNS results
  - Addition of closure models to Hydra-TH solution algorithm
  - Key milestones in Sep and Dec 2015 for implementation of subcooled boiling/bubble flow regime modeling
- Work on completing integration of MAMBA (CRUD model) delayed

Doug Kothe will provide a THM Update later today

Technical Capabilities Status

Uncertainty Quantification & Data Assimilation (DAKOTA)

- Development of Best Practice Guidelines applicable to CASL problems for non-UQ experts
- Incorporation of data assimilation capabilities to more efficiently address multi-parameter problems
- Development of rank reduction and surrogate model generation methodologies for multiphysics problems, making possible efficient UQ and DA for high fidelity simulators
- FY15 DOE reportable milestone on UQ of 3D fuel assembly with T-H feedback and depletion

Vince Mousseau will provide a VMA update later today

Current Technical Challenges

Known risks for remaining FY15 milestones

1. **Qualify VERA-CS**

   Delays in establishing restart and shuffling capabilities and large computational requirements.

2. **UQ Analysis for Fuel Assembly using VERA-CS**

   Delays in providing software access to key researcher [Export Control clearance] and large computational requirements.

3. **Qualify PWR CIPS Capability**

   Delays in gaining access to MAMBA source code, and integrating MAMBA into CTF and VERA-CS.

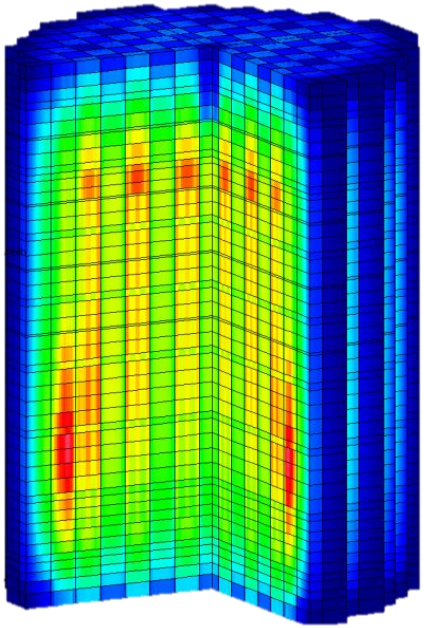
Items 1 & 2 have fall back paths.

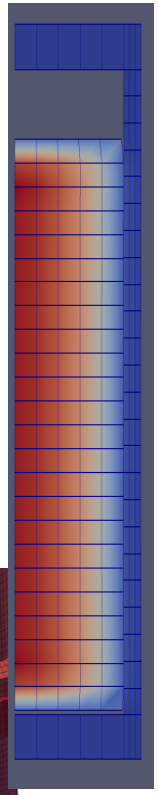
Item 3 fall back path not obvious.

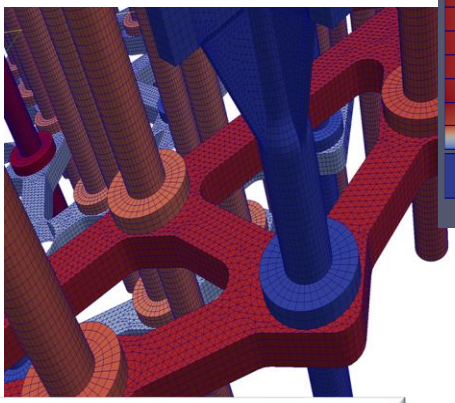
Deployment & Outreach Activities

3 deployed with more anticipated moving forward

- CASL Test Stands
  - Westinghouse (Mar 2013**):** Test VERA **core simulator's** ability to analyze AP1000 first core startup
  - EPRI (Nov 2013**):** Benchmark VERA fuel performance on **PCI** applications
  - TVA (Mar 2014): Test VERA CFD capability on **lower plenum flow anomaly**
- More Test Stands on the horizon
- Next VERA release planned for April 2015
- First VERA workshop to be held at Advances in Nuclear Fuel Management Conference (ANFM-V) on April 1
- Continued Planning for VERA Working Group





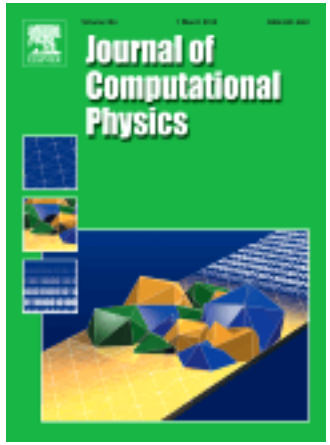


Rose Montgomery will cover the TVA Test Stand and Working Group

Kudos: Special CASL Issue in the Journal of Computational Physics

Articles featuring R&D advances (coming in fall 2015)

- *The Journal of Computational Physics* (JCP) "thoroughly treats the computational aspects of physical problems, presenting techniques for the numerical solution of mathematical equations arising in all areas of physics. The journal seeks to emphasize methods that cross disciplinary boundaries."
- >15 targeted CASL articles spanning many topics (current list):
  - CASL: Overview
  - PHI: VERA architecture and infrastructure; multi-physics coupling
  - RTM: Insilico; Shift; MPACT; cross sections; reactor physics; transport methods
  - THM: Hydra-TH (algorithms, turbulence, GTRF forcing); adjoint-based analysis
  - FMC: MAMBA-BDM
  - VMA: Surrogate models for calibration; software verification
- Good opportunity for staff professional development and CASL overall: plan to pursue these types of avenues again

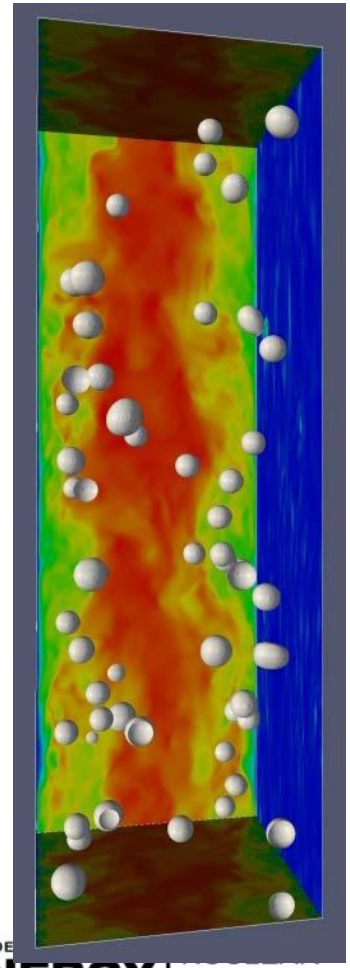


Paul Turinsky (NCSU) and Bill Martin (UM) are guest editors of this special issue. Anticipate other journal special issues to target deeper dives into specific focus areas.

Kudos: NCSU Researchers Receive IDC HPC Innovation Excellence Award

For Innovative Research Performed in the CASL Thermal Hydraulics Methods Focus Area (Lead: Igor Bolotnov, NCSU)

International Data Corporation (IDC) HPC Innovation Excellence Awards recognize noteworthy achievements by users of high performance computing technologies, thereby showcasing return on investment (ROI) and scientific success stories involving HPC. "IDC research has confirmed that HPC can greatly accelerate innovation and in many cases can generate ROI. The award program aims to collect a large set of success stories across many research disciplines, industries, and application areas," said Earl Joseph, Program Vice President for HPC at IDC. "The winners achieved clear success in applying HPC to improve business ROI, scientific advancement, and/or engineering successes. Many of the achievements will also directly benefit society."



Igor Bolotnov, NCSU

Researchers from NCSU conducted innovative research that will allow better prediction of thermal hydraulic behavior for current and future nuclear reactor designs. They analyzed the turbulence anisotropy in single-phase and two-phase bubbly channel flows based on DNS data. These novel simulations will help academia and later industry. Multiphase flow model development for computational fluid dynamics already benefits from high fidelity simulations presented in this work.

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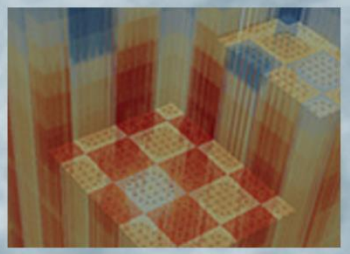
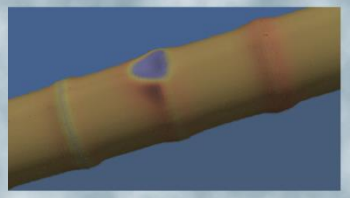
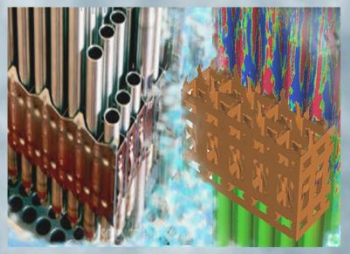
Phase 2

Overview of Roadmap Challenges

Paul Turinsky, Chief Scientist







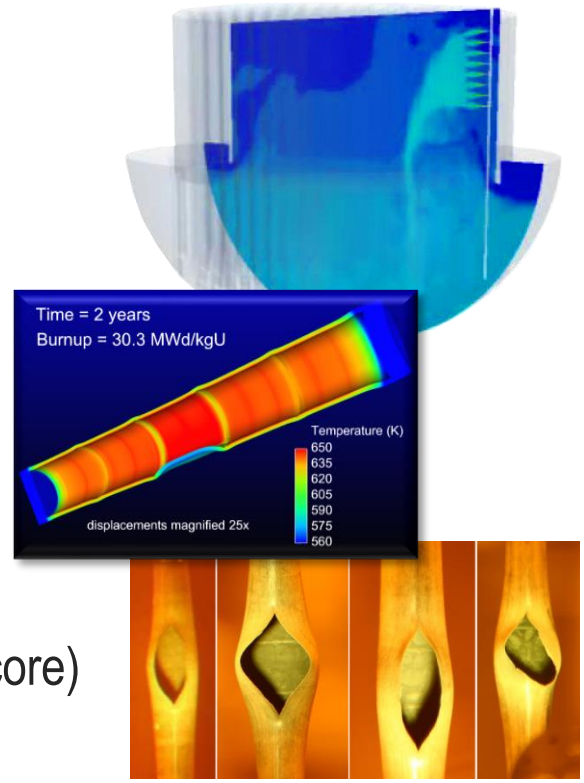
U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Phase 2 Philosophy

- **Direction**
  - Phase 1 R&D targets PWRs and steady state conditions to build a versatile capability
  - In Phase 2, broaden and deepen the Phase 1 technology
  - Continue in Phase 2 the successful *Challenge Problem* strategy to target simulation capability for the R&D effort
- **Guiding Principles**
  - Enhance the maturity level of VERA's predictive fidelity to allow industry to incorporate and build upon CASL's capabilities for industrial usage
  - Broaden the applicability of the capabilities developed in Phase 1 so that they can be applied to a wider class of LWR types
  - Deepen the capabilities developed in Phase 1 and their applicability to new challenge problems.

Phase 2 Plans

- **Expand capabilities for PWR Challenge Problems**
- **Extend and apply capabilities to SMRs (iPWRs)**
  - Natural circulation
  - DNB in low-flow conditions
  - CRUD for long-cycle operations
- **Extend capabilities to BWR challenge problems**
  - Thermal-hydraulic flow regimes
  - Core simulation (sub regions and potentially full core)
  - Fuel performance – PCI, cladding integrity
  - Convective and solute flows and mixing
- **Continued releases and deployment to potential end users**



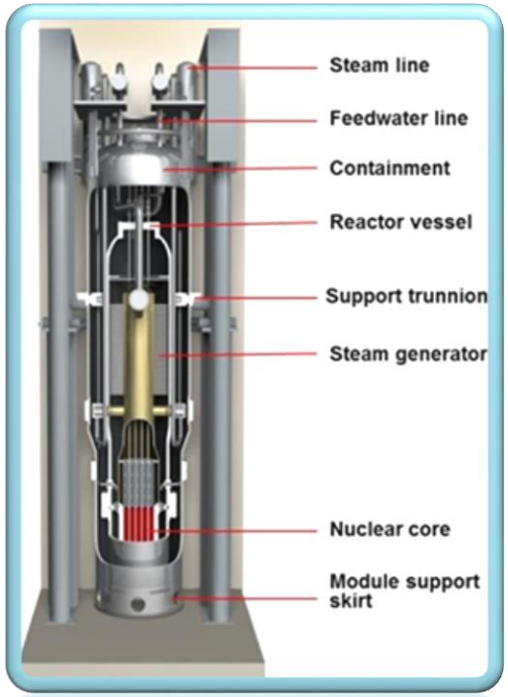
Five-year $121.5M renewal extends CASL into FY20!

Broaden Reactor Types in Phase 2

Move beyond a sole PWR focus

BWRs

iPWRs



BWRs will require considerable T-H flow regime and neutronics geometry broadenings

Phase 2 Challenge Problems

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

Combination of broadening and deepening

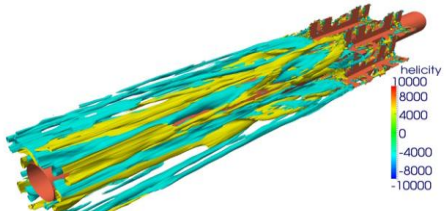
We Have an Aggressive Phase 2 Plan for VERA

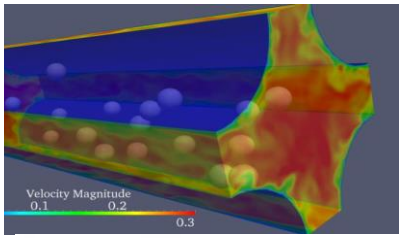
Year	Planned Capability Progression	Coupled / Interoperable Component Progression	CP Supported
1	• VERA-CS for PWR multi-cycle simulation • VERA-CS + MAMBA for PWR CIPS • MAMBA with improved CRUD source terms • VERA-CS & Shift for iPWRs • Hydra-TH for subcooled boiling & bubbly flow regime • Peregrine-3D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

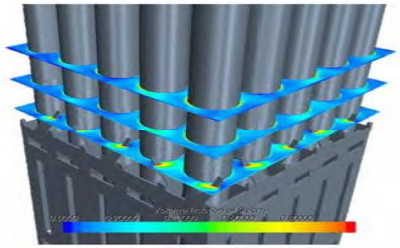
Phase 2 Challenge Problems

Thermal Hydraulics Category

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

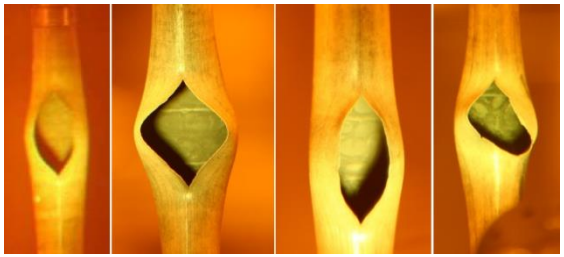


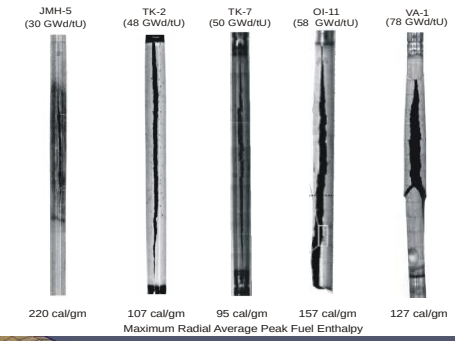


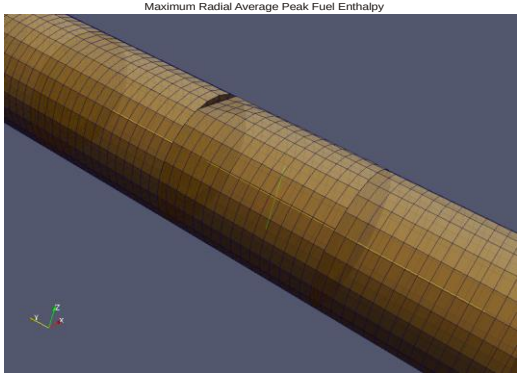


Phase 2 Challenge Problems
Cladding Performance Category

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



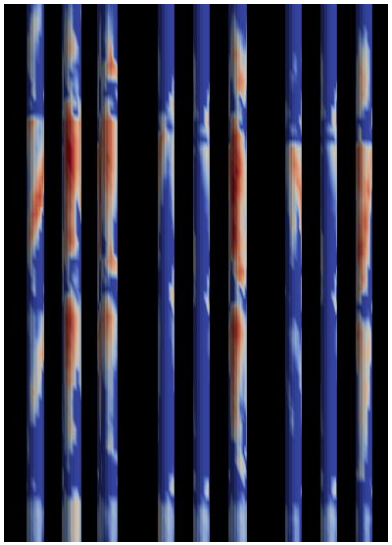


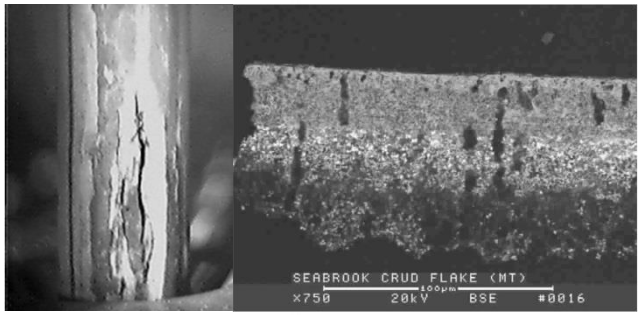


Phase 2 Challenge Problems

Coolant/Corrosion Chemistry Category

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

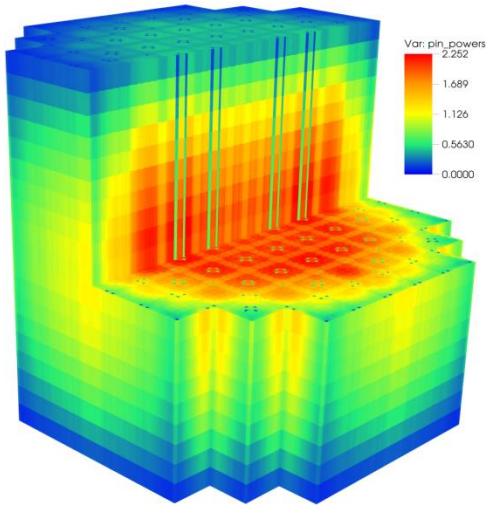


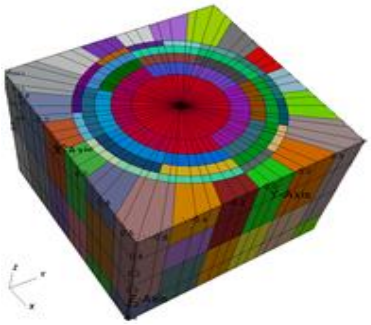


Phase 2 Challenge Problems

VERA Core Simulator

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



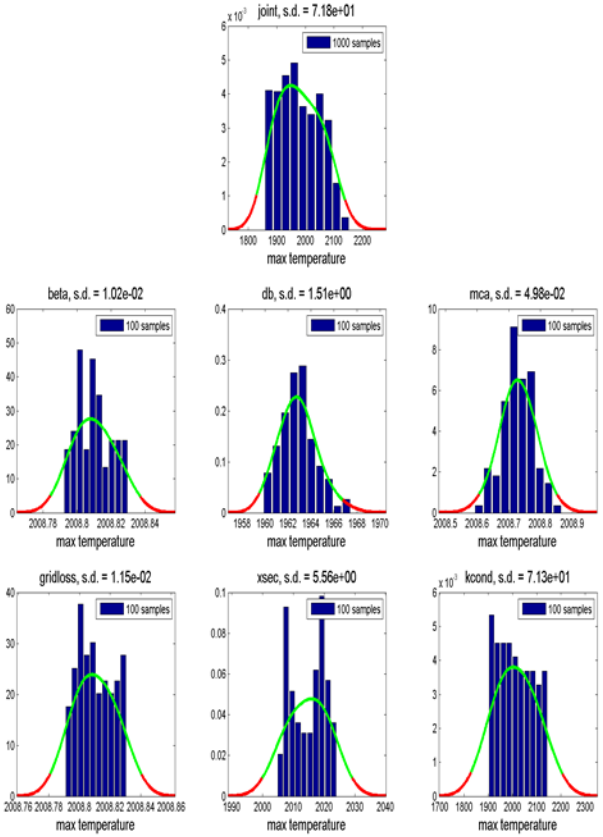


Phase 2 Challenge Problems

Data Assimilation & UQ

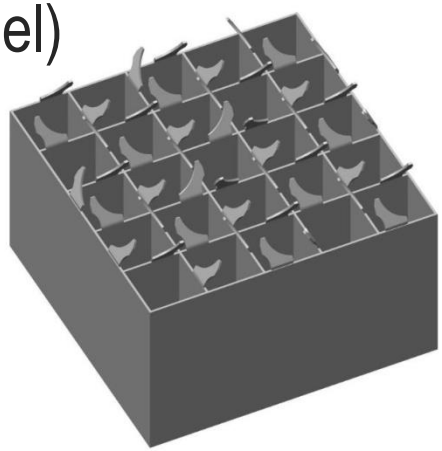
- Targeted applications to Challenge Problems
  - ❑ PWR CIPS
  - ❑ PWR PCI
  - ❑ PWR DNB
- Data Assimilation (DA) required to obtain uncertainty distributions used as input to UQ analysis
  - ➢ Parameter dimensional reduction and surrogate models needed to facilitate DA

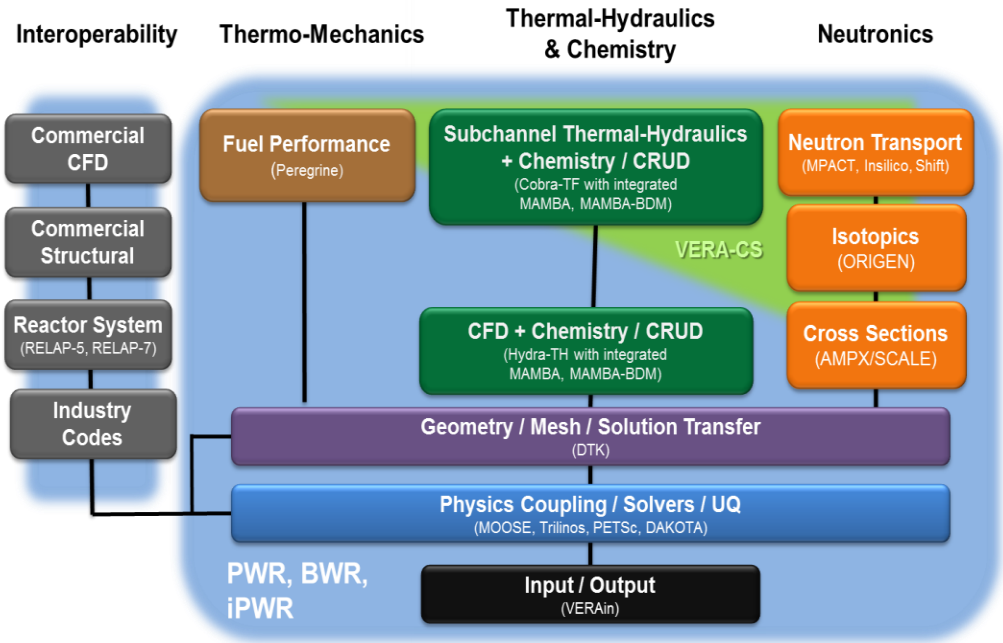
Maximum Temperature Uncertainty



Phase 2 Challenge Problems
Interoperability Category

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





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Phase 2 L1 Milestone Roadmap

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

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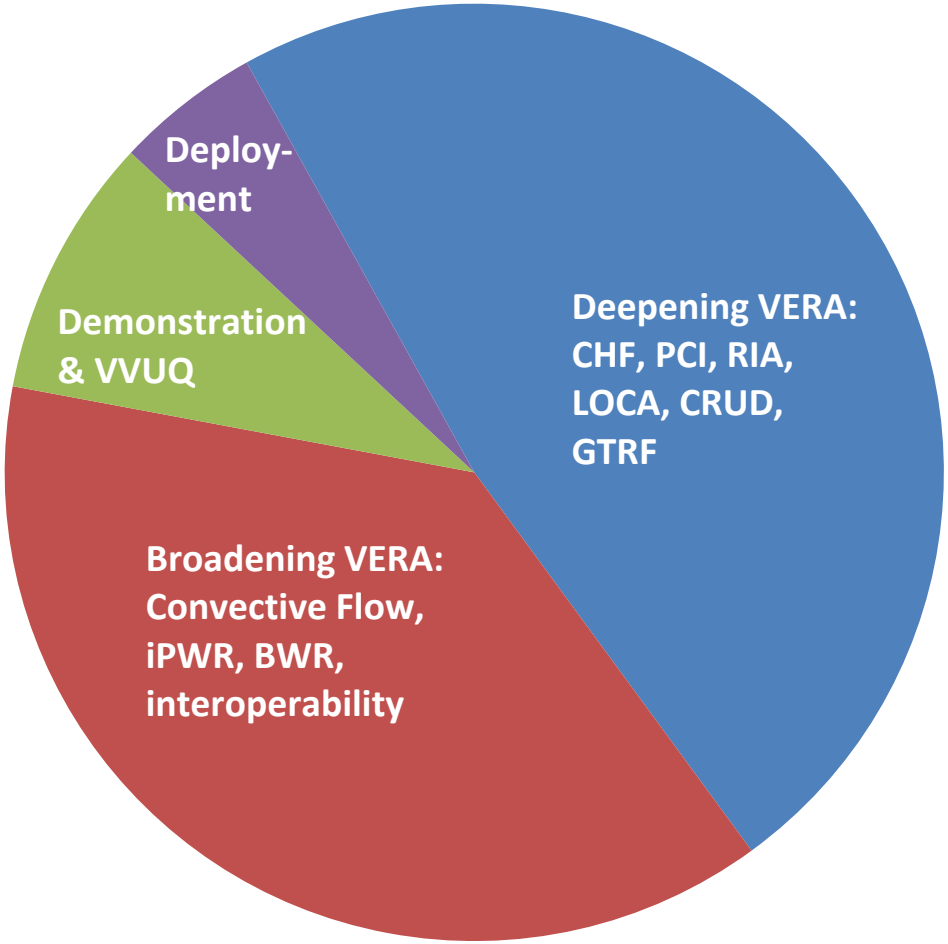
Phase 2 Anticipated Resource Allocations



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

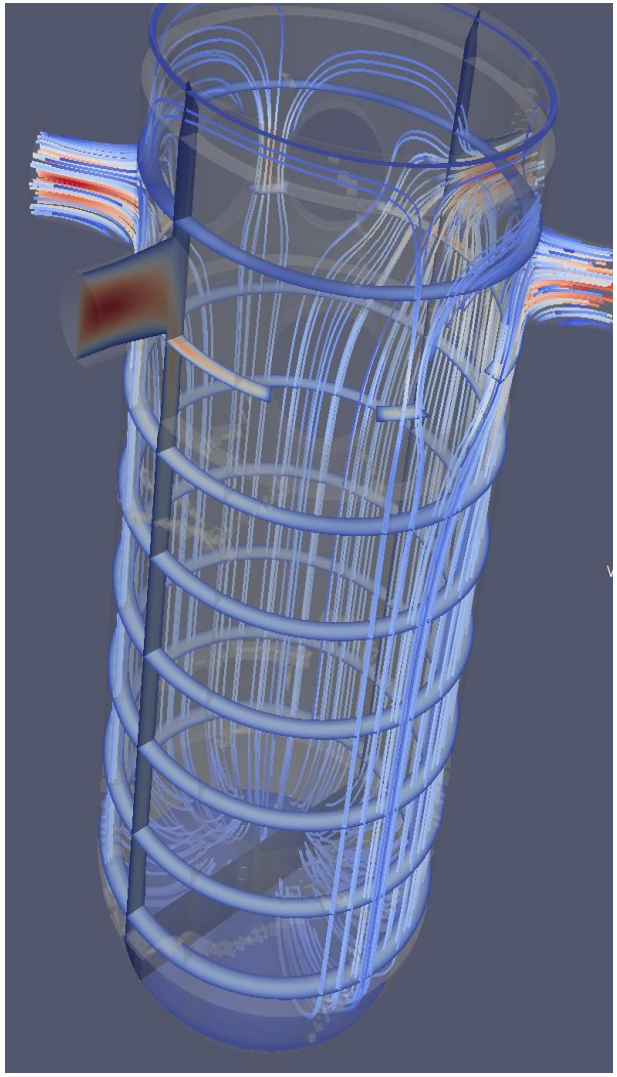
End-of-Phase 2 Simulation Targets

- **VERA-CS**
  - PWR & iPWR full-core, pin resolved, depletion & transient capability
  - BWR sub-core (stretch full-core), pin resolved, depletion capability
- **PCI**: PWR, iPWR and BWR capability
- **CRUD**: PWR & iPWR capability
- **DNB**: PWR & iPWR core-wide (subchannel) & M-CFD
- **LOCA**: PWR, iPWR & BWR fuel response (IC, corrosion and ballooning)
- **RIA**:
  - PWR & iPWR full-core, pin resolved, transient neutronics, subchannel, fuel performance capability
  - BWR sub-core (stretch full-core), pin resolved, transient (stretch neutronics), subchannel, fuel performance capability
- **GTRF**: PWR & iPWR pin behavior (stretch gap opening), wear, fluid forces & interoperability (structural mechanics)
- Other Thermal-Hydraulics (M-CFD)
  - Thermal & solutal driven flows (single phase) & BWR nominal operating conditions flow regimes
- **Interoperability**: Structural mechanics, systems simulation & core simulator
- Uncertainly Quantification & Data Assimilation: Capabilities integration

Phase 2 Technical Challenges

A few rise to the top

1. VERA compute requirements amenable to platforms accessible to industry
2. Verification & Validation of VERA to a stage that industry is willing to adopt and complete the necessary validation
3. Advancing CFD capabilities to the level that meaningful two-phase flow calculations can be completed



Engagement with industry is essential to understand Items 1 and 2

Phase 2 Technical Challenges

Known risks and expected mitigations

Risk Description	Risk Mitigation
Multiphase CFD closure relationships beyond bubbly flow require more effort than planned. Extensions to Gen-I/Gen-II closure models and BWR-like flow regimes lead to excessively complex models and numerical algorithm challenges.	Establish evolution and maturity of Hydra-TH effort as the singular focus of THM with highest priority for resources as early as possible. Seek and extend existing Gen-1/Gen-II closure models and numerical algorithms. Reduce scope on depth of closure modeling if necessary. Communicate this is an immature and active area of research to temper expectations.
Transient neutronics capability is too compute intensive.	Have trigger to implement interoperability with existing industry transient neutronics capability to minimize delay of dependent work; engage computer science expertise if necessary in scrutinizing and implement compute efficiency opportunities.
COBRA-TF subchannel T-H model for BWRs is not sufficiently validated for predicting void distribution and unable to model BWR features such as water rods and bypass flow are insufficient. Also not able to yield acceptable steady-state full-core BWR solutions.	Address physical models and computational algorithms in COBRA-TF to correct issues by drawing in part on existing BWR work as guided by validation results. If not feasible, develop new steady-state subchannel T-H capability.
Unable to devise compute-efficient, accurate, and robust multi-physics coupling models, algorithms and software implementations, especially for the BWR core simulator.	Perform research on advanced coupling methods as a backup to standard Picard iteration to provide an alternative approach with improved convergence properties.
Run times for MPACT full-core, multi-cycle depletion with TH-feedback are too high for industry class clusters.	Several efforts are underway to improve MPACT run times, with expected gains of 5-10. If these fail, Moore's Law continues to make computing cheaper and may allow re-definition of "industry class cluster".

This list does not include unknown unknowns, which will surface based on past experience

Phase 2 Non-Technical Challenges

- Overall scope outpaces constrained budget and schedule for the BWR core simulator, where development proves more difficult than planned and results in delays in delivery of capability
- Insufficient availability of experimental and operational reactor data for validation and insufficient effort available for validation activities
- **Inability to expand industry interest and engagement through the effective deployment of CASL-developed technologies**
- Post-CASL entity not ready or not capable of accepting ownership of CASL processes
- IP Management Plan is unable to accommodate potentially conflicting requirements and priorities of DOE and consortium partners

This list was articulated in the Renewal Application

Questions?

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

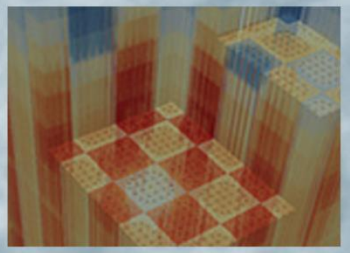
A DOE Energy Innovation Hub

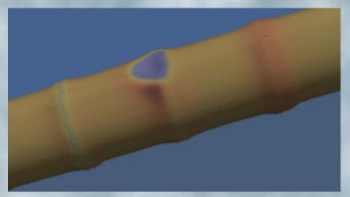
Benchmarking and Validation of VERA-CS

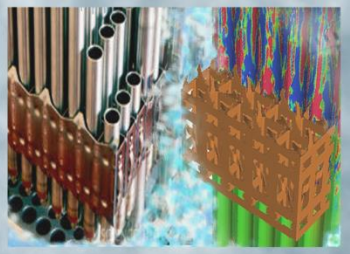
Ben Collins, RTM/PHI Developer

Jess Gehin, PHI FA Lead

Scott Palmtag, PHI FA Deputy Lead







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Overview

- VERA-CS Status Update
- VERA-CS Validation Plan
- Critical Experiments
  - B&W 1484
  - B&W 1810
- Reactor Benchmarking
  - BEAVRS
  - Watts Bar Cycle 1
  - AP1000
- Looking Forward

Key Capability Developments Since September 2014

- VERA is being optimized to a stable set of components to support challenge problem analysis
- Key Additions
  - MPACT is directly coupled with CTF to increase performance
  - MPACT-CTF-ORIGEN used to deplete cycle 1 of Watts Bar and BEAVRS
  - MPACT-CTF-Peregrine coupling under development to support PCI
  - CTF-MAMBA coupling under development to support CIPS
  - Shuffling has been added to allow multicycle depletion
  - Many improvements to individual components
- Additional adjustments are anticipated in the future, but most effort will be in improving individual components and their coupling

Progression Problems Progress

FY11

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

FY12

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

FY13

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

FY14

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

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

Performance Improvements

- Milestone L2.AMA.P7.02 (Dec 2013)
  - Insilico/CTF – 56/8 energy groups
  - 18,769 cores, 17.5 hours wall time
- Milestone L3:RTM.PRT.P7.05 (Apr 2014)
  - MPACT/CTF – 56 energy groups, P2 Scattering
  - 2,784 cores, 12.25 hours wall time
- Milestone L3:RTM.PRT.P9.02 (Aug 2014)
  - MPACT/CTF – 56 energy groups, Transport Correction
  - 2,784 cores, 3.75 hours wall time
- Current (March 2015)
  - MPACT/CTF – 47 energy groups, Transport Correction
  - Direct Coupling
  - 4,234 cores, 36 minutes wall time

328,457 CPU-hr

↓

34,104 CPU-hr

↓

10,440 CPU-hr

↓

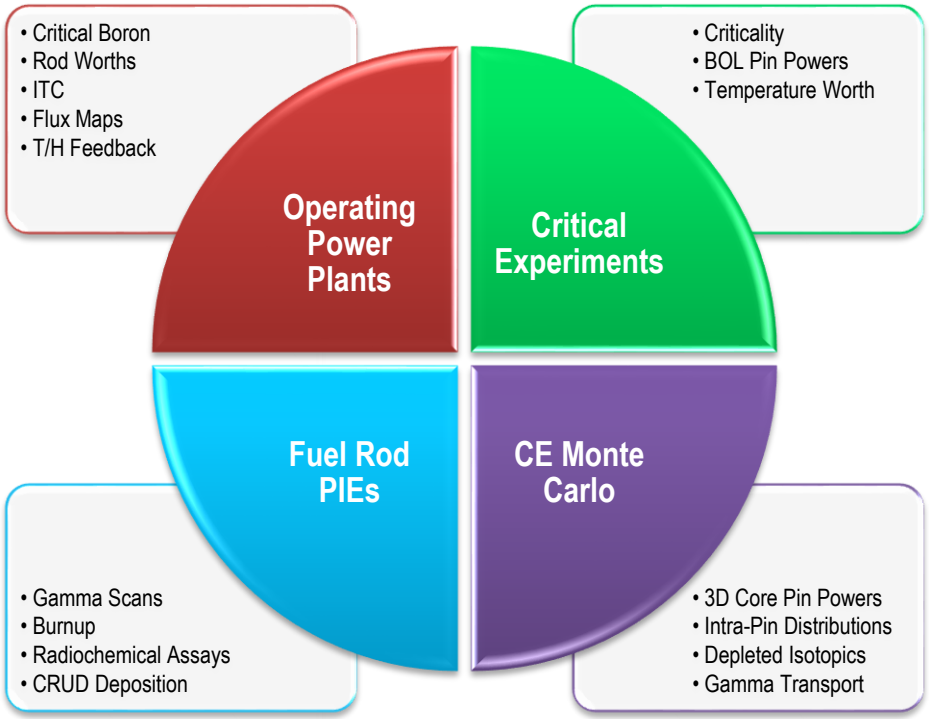
2,540 CPU-hr

↓

More Improvements in Progress

VERA-CS Validation

- Review of validation data that can be used for VERA-CS
  - Datasets chosen to demonstrate capability and accuracy
  - Not intended to support licensing
- Four components provide extensive coverage of validation scope

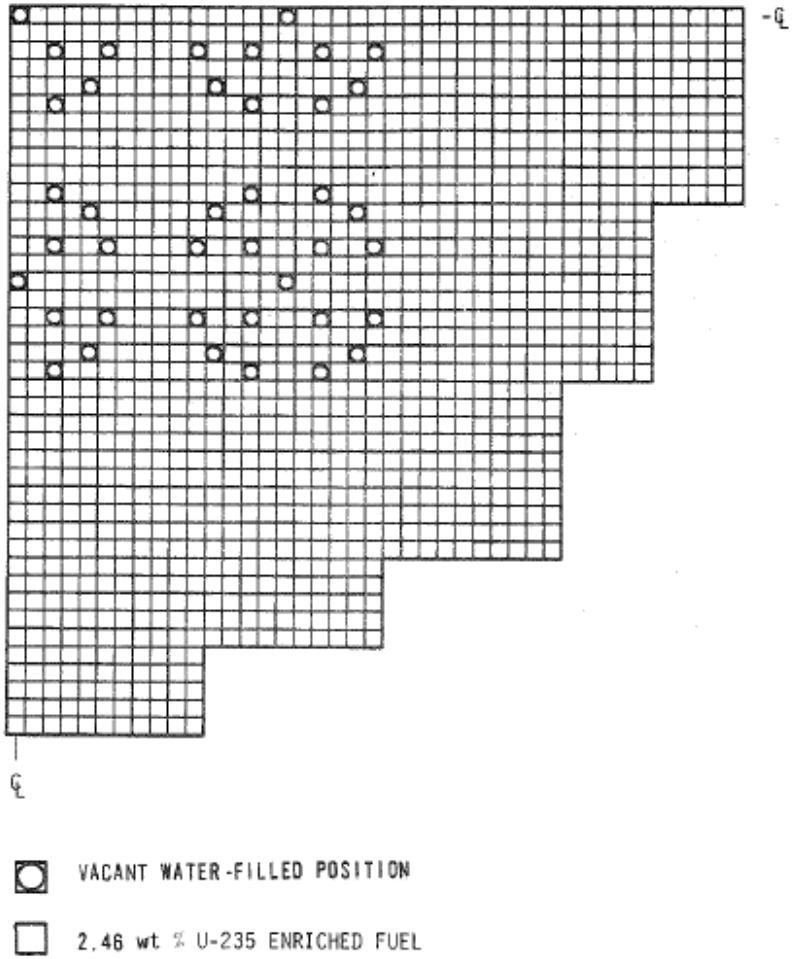


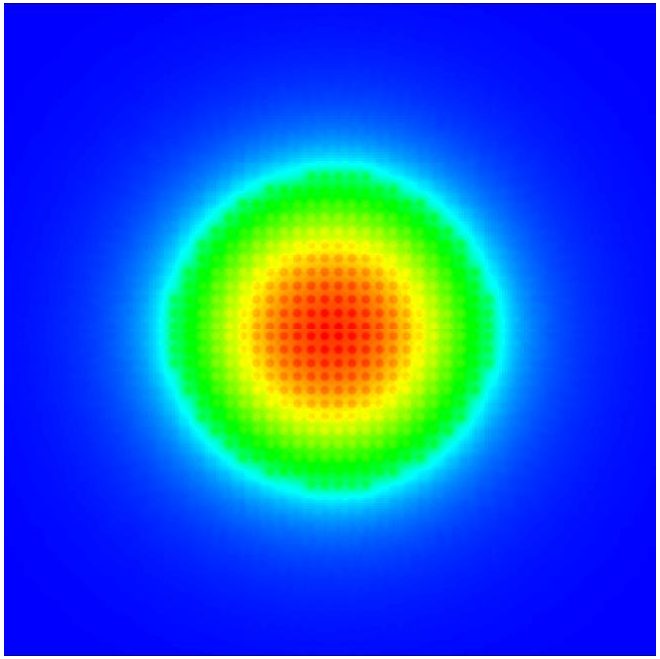
VERA-CS Validation

- Potential sources of validation data includes 8 power plants, 8 experiments, 5 post-irradiation programs, and various Monte Carlo models

Capabilities	Validation Activities																															
	Operating Power Plants								Critical Experiments																	Post-Irradiation Exams					CE Monte Carlo			
	Watts Bar	BEAVRS	Catawba	McGuire	Westinghouse 3-Loop	Krsko	B&W-Type	CE-Type	B&W	Halstrand	KRITZ	DIMPLE	VENUS	IPEN/Vb-01	RPI	SPERT III	Strawbridge & Barry	Saxton	CREOLE	EPCLIPE	CAVEBON	CROCUS	JAER TCA	ICSBP	Catawba/VDK LTAs	Three Mile Island	MALIBU	Robinson	Calvert Cliffs	Pin-by-Pin Fission Rates	Intra-Pin Distributions	Depleted Isotopics	Misc. Applications
PWR Types																																	
Westinghouse 4-Loop	X	X	X	X																					X					X			
Westinghouse 3-Loop					X								X															X					
Westinghouse 2-Loop						X																								X			
Babcock & Wilcox (B&W)							X																			X							
Combustion Engineering (CE)								X							X														X				
Fuel Assembly Types																																	
17x17	X	X	X	X	X				X										X						X					X	X	X	
16x16						X																								X			
16x16 CE								X	X						X																		
15x15					X																						X	X					
15x15 B&W							X		X																	X							
14x14 CE								X							X														X				
Mixed Oxide Fuel (MOX)			X								X		X					X	X	X					X		X						
Burnable Poison Types																																	
Pyrex	X	X	X	X	X	X			X											X										X			
IFBA	X		X	X	X	X																			X					X			
WABA	X		X	X	X																				X					X			
Solid B4C-AL2O3							X	X																	X	X			X				
Gadolinia							X		X				X							X	X		X			X	X						
Erbia								X							X																		
Control Rod Types																																	
AIC	X	X	X	X	X	X	X		X					X				X		X	X					X				X			
B4C	X		X					X	X					X						X	X	X											
Hybrid	X		X																						X					X			
Gray							X														X					X				X			
Hafnium					X																												
Incore Instrument Types																																	
Moveable	X	X	X	X	X	X																			X					X			
Fixed	X						X	X	X																	X							
Radial Reflector Types																																	
Thin Baffle	X	X	X	X	X	X	X	X				X	X												X	X				X			
Thick (Heavy) Shroud																																	X
Physics Components																																	
Neutron Transport	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Gamma Transport																																	X
Coolant Density Feedback	X	X	X	X	X	X	X	X			X								X				X		X	X	X	X	X	X			
Fuel Temperature Feedback	X	X	X	X	X	X	X	X			X								X				X		X	X	X	X	X	X	X		
Isotopic Depletion	X	X	X	X	X	X	X	X																	X	X	X	X	X		X	X	
Xenon Concentration	X	X	X	X	X	X	X	X																								X	
Shutdown Decay	X	X	X	X	X	X	X	X																	X	X	X	X	X				
Physics Results																																	
Reactivity	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X					X	X	X	
Assembly Power Distribution	X	X	X	X	X	X	X	X																	X					X			
Pin Power Distribution									X		X	X	X	X	X			X	X	X	X									X	X	X	
Intra-Pin Power Distribution																															X		
Pin Burnup Distribution																									X	X	X	X	X		X		
Intra-Pin Burnup Distribution																													X		X		
Incore Instrumentation Response	X	X	X	X	X	X	X	X	X				X						X						X	X							
Excore Instrumentation Response			X	X								X	X																				X
Control Rod Worth	X	X	X	X	X	X	X	X	X									X		X	X	X			X					X			
Temperature Coefficient	X	X	X	X	X	X	X	X			X			X					X				X		X								

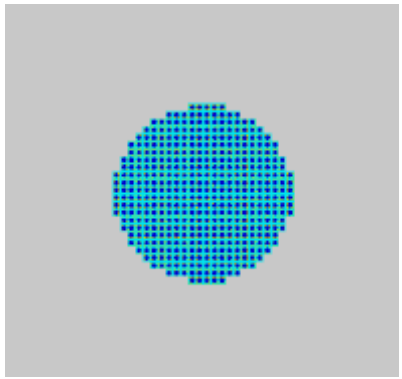
Critical Experiments

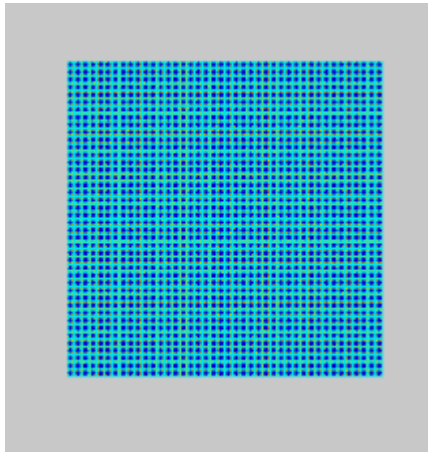




B&W 1484 Benchmarks

- B&W 1484 critical experiments modelled with MPACT in 2D using input axial buckling
- Core 1 - small circular core without soluble boron
- Core 2 – larger square core with soluble boron

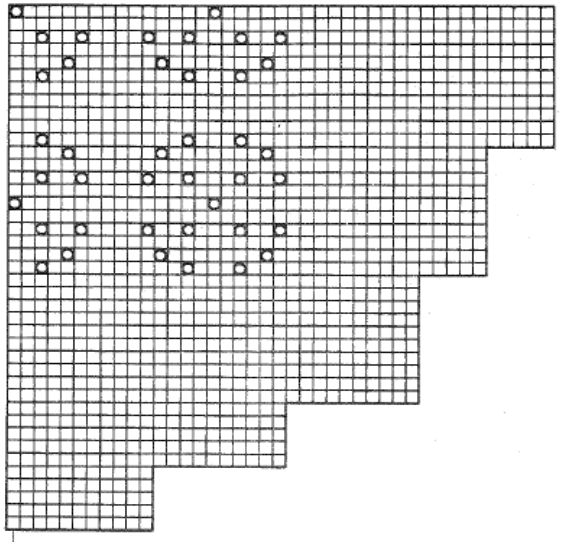




	Core 1	Core 2	Difference
Transport Corrected	0.99838	0.99597	241
P2	0.99993	0.99761	232
Deviation from Critical			
Transport Corrected	162	403	
P2	7	239	

B&W 1810 Benchmarks

- B&W 1810 critical experiments are also run with MPACT
- Fission rate measurements for 4 configurations
- 20 different configurations
  - Two enrichments
  - Gad pins
  - AIC/B4C pins



	2.46% Pins	4.02 Pins	Gd Pins	B_4C Pins	AIC Pins	Water Holes	Boron Conc.
1	4808	0	0	0	0	153	1337.9
2	4808	0	0	0	16	137	1250.0
3	4788	0	20	0	0	153	1329.3
4	4788	0	20	0	16	137	1171.7
5	4780	0	28	0	0	153	1208.0
5A	4776	0	28	0	0	153	1191.3
5B	4780	0	32	0	0	153	1207.1
6	4780	0	28	0	16	137	1155.8
6A	4776	0	32	0	16	137	1135.6
7	4780	0	28 (ann.)	0	0	153	1208.8
8	4772	0	36	0	0	153	1170.7
9	4772	0	36	0	16	137	1130.5
10	4772	0	36	0	0	137	1177.1
12	3920	0	0	0	0	153	1899.3
13	3920	888	0	16	0	137	1635.4
14	3920	888	28	0	0	153	1653.8
15	3920	860	28	16	0	137	1479.7
16	3920	852	36	0	0	153	1579.4
17	3920	852	36	16	0	137	1432.1

B&W 1810 Benchmarks

Core	Short Description	TCP0		P2	
		Eig.	Diff. (pcm)	Eig.	Diff. (pcm)
1	0 Gd	0.99809	-191	0.99981	-19
2	0 Gd, AIC Rods	0.99757	-243	0.99915	-85
3	20 Gd	0.99778	-222	0.99933	-67
4	20 Gd, AIC Rods	0.99840	-160	0.99990	-10
5	28 Gd	0.99749	-251	0.99899	-101
5A	32 Gd	0.99739	-261	0.99888	-112
5B	28 Gd	0.99755	-245	0.99905	-95
6	28 Gd, AIC Rods	0.99770	-230	0.99918	-82
6A	32 Gd, AIC Rods	0.99765	-235	0.99912	-88
7	28 Gd (annular)	0.99749	-251	0.99899	-101
8	36 Gd	0.99762	-238	0.99910	-90
9	36 Gd, AIC Rods	0.99752	-248	0.99900	-100
10	36 Gd, Void Rods	0.99743	-257	0.99889	-111
12	0 Gd	0.99886	-114	1.00092	92
13	0 Gd, B4C Rods	0.99901	-99	1.00056	56
14	28 Gd	0.99854	-146	1.00024	24
15	28 Gd, B4C Rods	0.99887	-113	1.00030	30
16	36 Gd	0.99851	-149	1.00015	15
17	36 Gd, B4C Rods	0.99848	-152	0.99990	-10
Cores 1-10	2.46% Enriched Throughout	STDDEV	29	STDDEV	32
		RMS	235	RMS	87
		MAX	261	MAX	112
Cores 12-17	4.02% Enriched Inner Core, 2.46% Outer	STDDEV	23	STDDEV	35
		RMS	131	RMS	47
		MAX	152	MAX	92
Total		STDDEV	56	STDDEV	64
		RMS	208	RMS	77
		MAX	261	MAX	112

B&W 1810 Benchmarks

0.08	0.28						
-0.48	-0.42						
0.43	0.63	0.36	1.08				
0.61	0.62	-0.31	0.01				
-0.82	-0.99		-0.20	-0.25	-0.27		
-0.16	-1.32	0.42	0.33	0.05	0.44	-0.03	
-0.26	0.23	0.21	0.11	0.05	-0.02	-0.18	-0.02

Core 1

RMS 0.48%

MAX 1.32%

Gd Pins

-0.23	0.66						
0.14	0.10						
0.80	-0.74	-0.34	0.14				
0.08	0.29	-0.35	-0.26				
1.31	-0.47		0.43	-1.17	0.35		
1.01	0.42	-0.43	0.63	-0.09	-0.27	-0.12	
1.15	0.05	-0.17	-0.04	-0.28	-0.25	-0.08	-0.03

Core 5

RMS 0.53%

MAX 1.31%

0.08	0.18						
-0.32	-0.82						
0.58	0.13	1.40	0.72				
-2.00	-0.08	0.30	0.15				
-0.75	-0.13		0.66	-0.35	1.10		
-0.47	-0.45	1.32	0.21	0.21	0.87	-0.33	
-0.48	-0.47	-1.44	0.51	0.00	-0.72	-0.01	-1.03

Core 12

RMS 0.74%

MAX 2.00%

Gd Pins

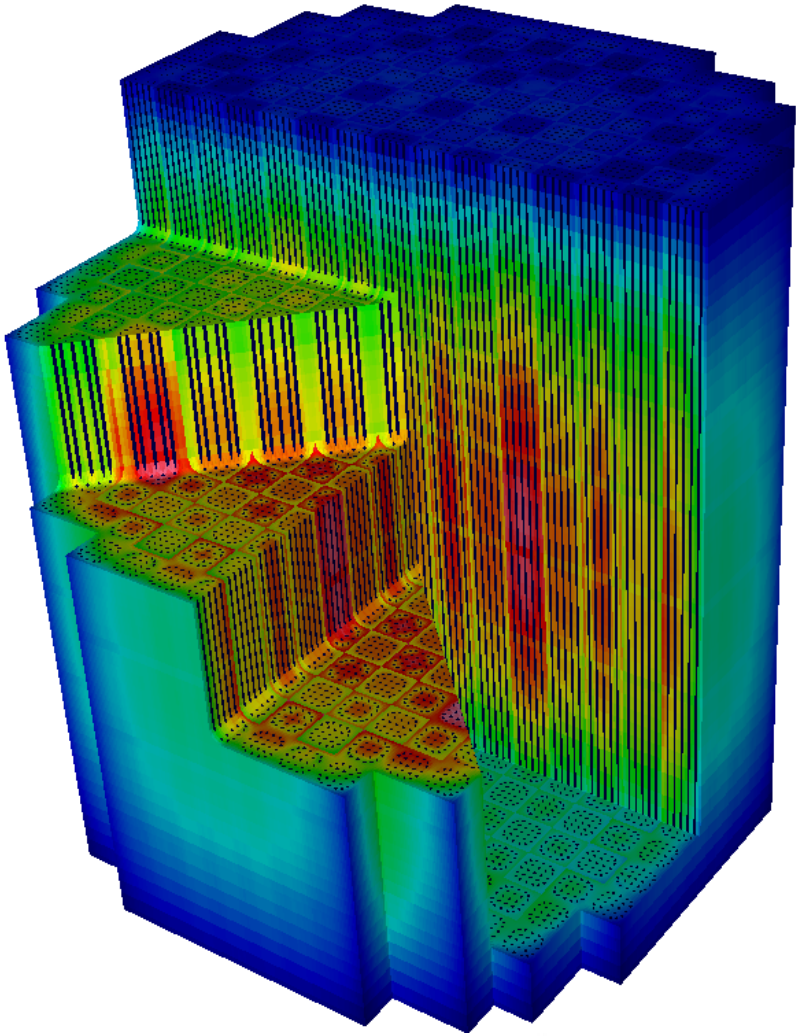
-0.90	-0.44						
-0.32	-1.16						
-0.34	-0.25	0.79	-0.32				
-0.02	-0.45	0.66	0.91				
-0.61	-1.35		2.11	-0.05	-0.31		
0.58	-1.61	0.72	1.12	-0.35	-0.39	-0.48	
-0.10	0.41	0.08	0.96	-0.21	0.34	-0.80	0.07

Core 54

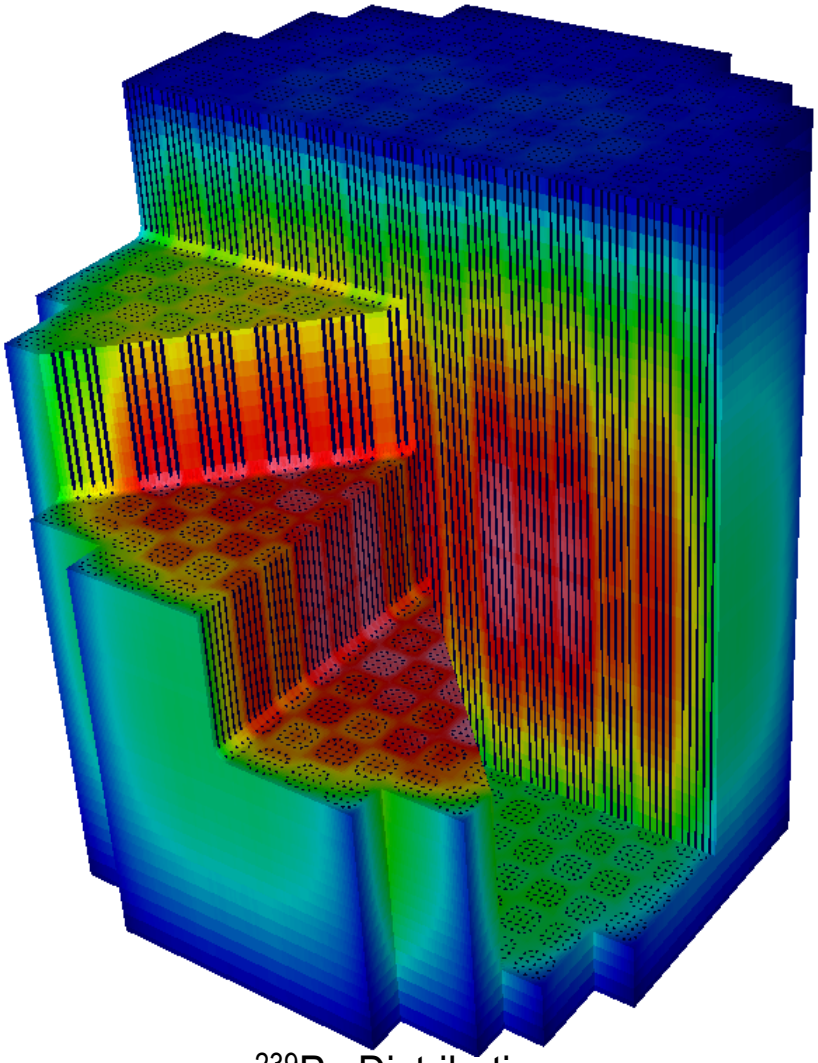
RMS 0.76%

MAX 2.11%

Reactor Benchmarking



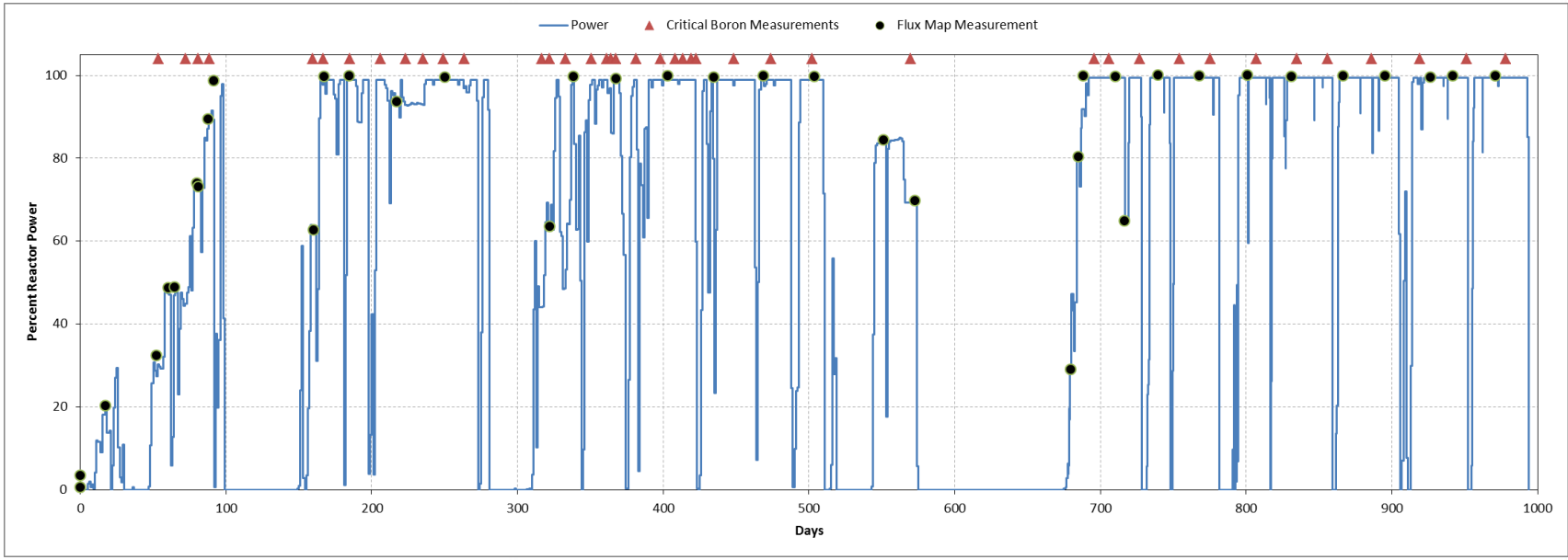
Power Distribution



^{239}Pu Distribution

BEAVRS Benchmark

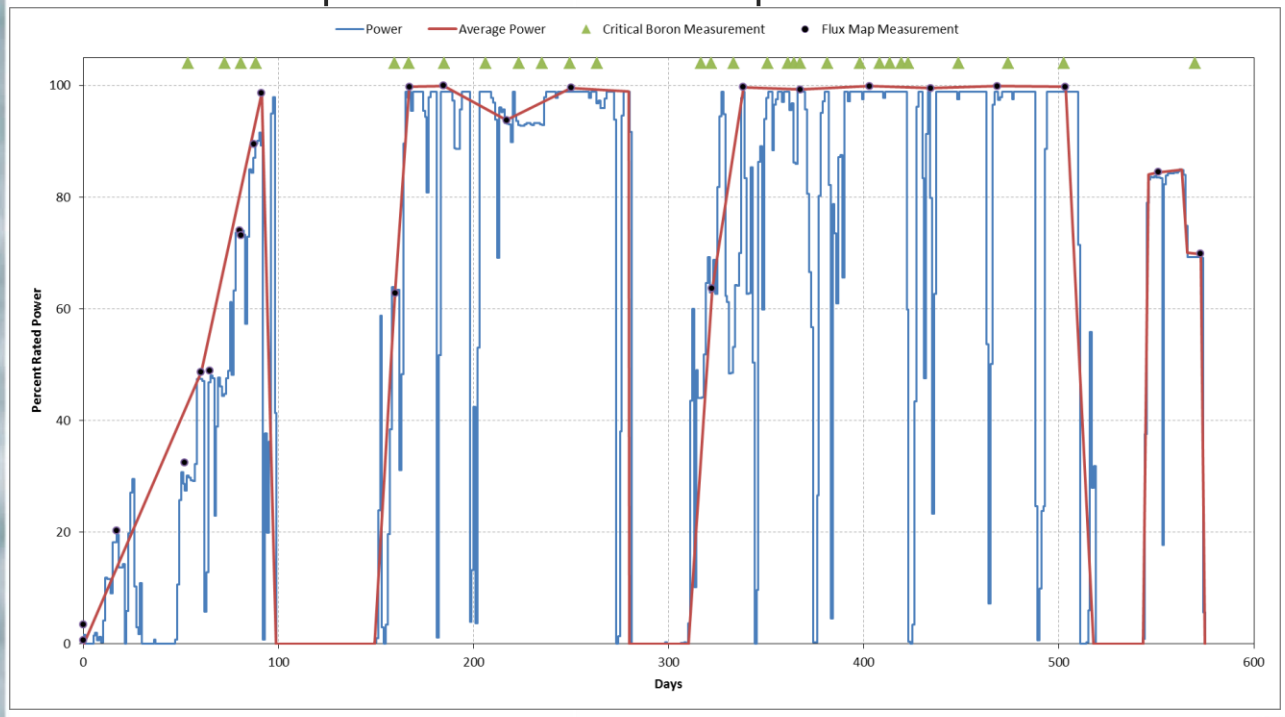
- Benchmark for Evaluation and Validation of Reactor Simulations
- Provides 2 cycles of data
  - Detailed assembly designs and core loading
  - Daily power history
  - Boron letdown curve and 61 level flux map data



N. Horelik, B. Herman, B. Forget, and K. Smith. Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS), v1.0.1. *Proc. Int. Conf. Mathematics and Computational Methods Applied to Nuc. Sci. & Eng.*, 2013. Sun Valley, Idaho

Cycle 1 Model

- Cycle 1 Power history very difficult to model
  - Capacity factor - 57%
- Approximate power history is developed
  - Attempt to capture major features of operating history
  - Get data points close to flux map measurements



Cycle 1
Zero Power Physics Tests

- Critical positions

	K-eff	Difference [pcm]
ARO	0.99819	-181
D In	0.99972	-28
C/D In	0.99913	-87
A/B/C/D In	0.99769	-231
SE/SD/SC/A/B/C/D in	0.99660	-340

ITC [pcm/°F]

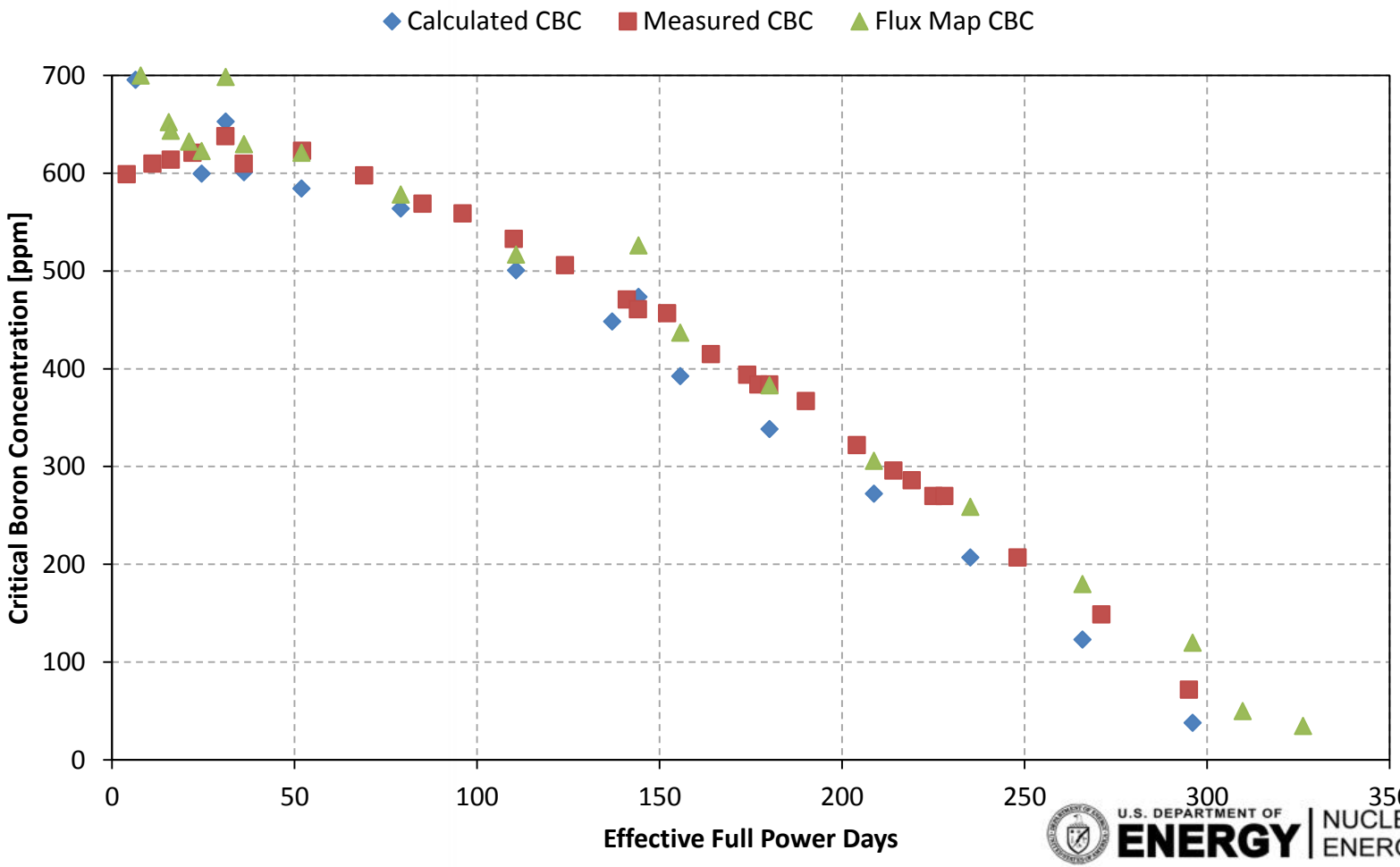
Calculated	Measured
-2.09	-1.75
-3.47	-2.75
-8.34	-8.01

- Control Rod Worth Measurements

	Calculated	Measured	Difference
D	780	788	-1.1%
C with D In	1252	1203	4.1%
B with C/D In	1175	1171	0.3%
A with B/C/D In	568	548	3.6%
SC with A/B/C/D In	477	461	3.5%
SD with SC/A/B/C/D In	765	772	-1.0%
SE with SD/SC/A/B/C/D In	1071	1099	-2.5%

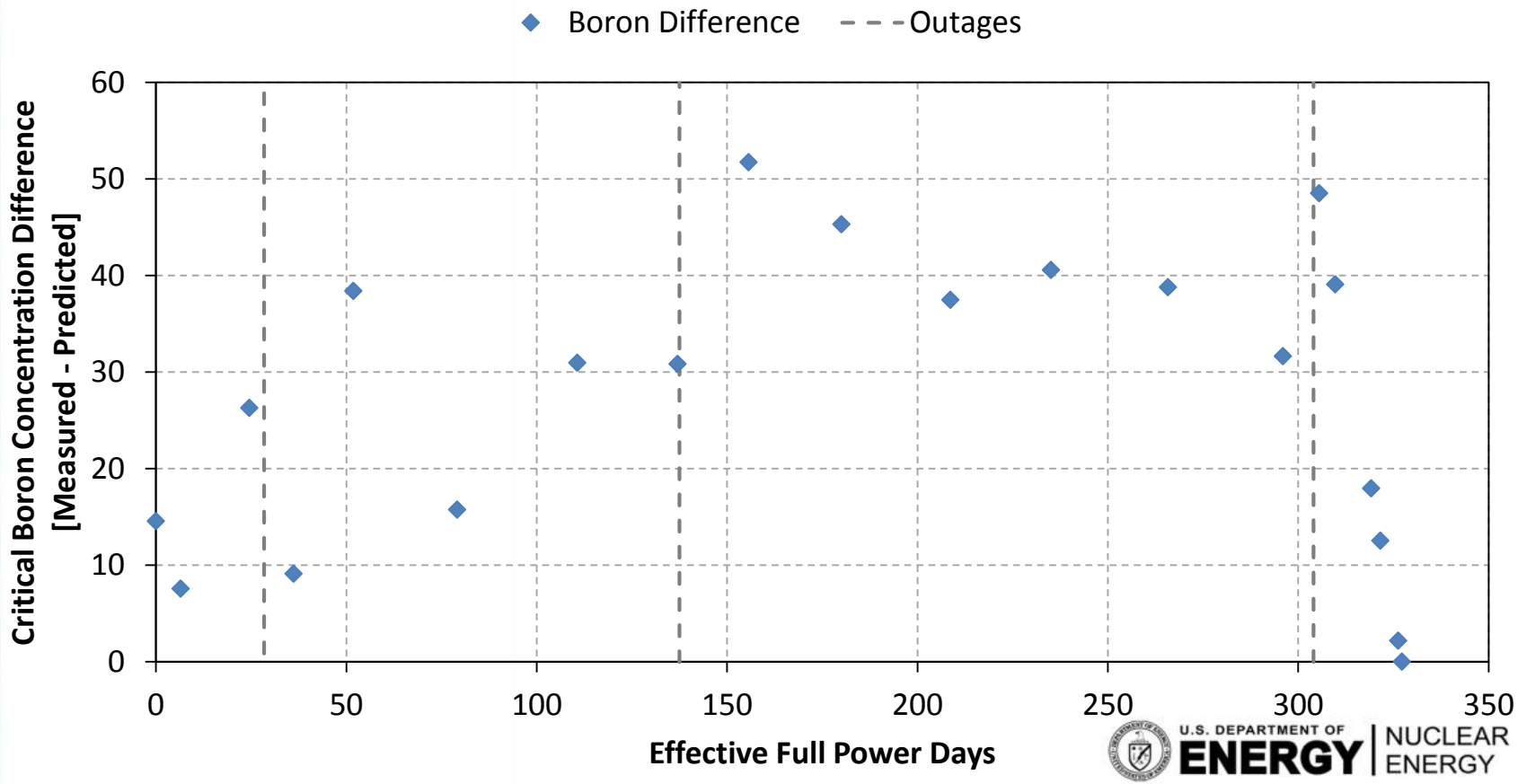
Cycle 1 Boron Letdown

- Cycle 1 is simulated with simplified power history, rods out, and equilibrium Xe



Cycle 1 Boron Letdown

- VERA-CS under predicts boron throughout cycle
  - Maximum difference – 52 ppm
  - Average Difference – 27 ppm

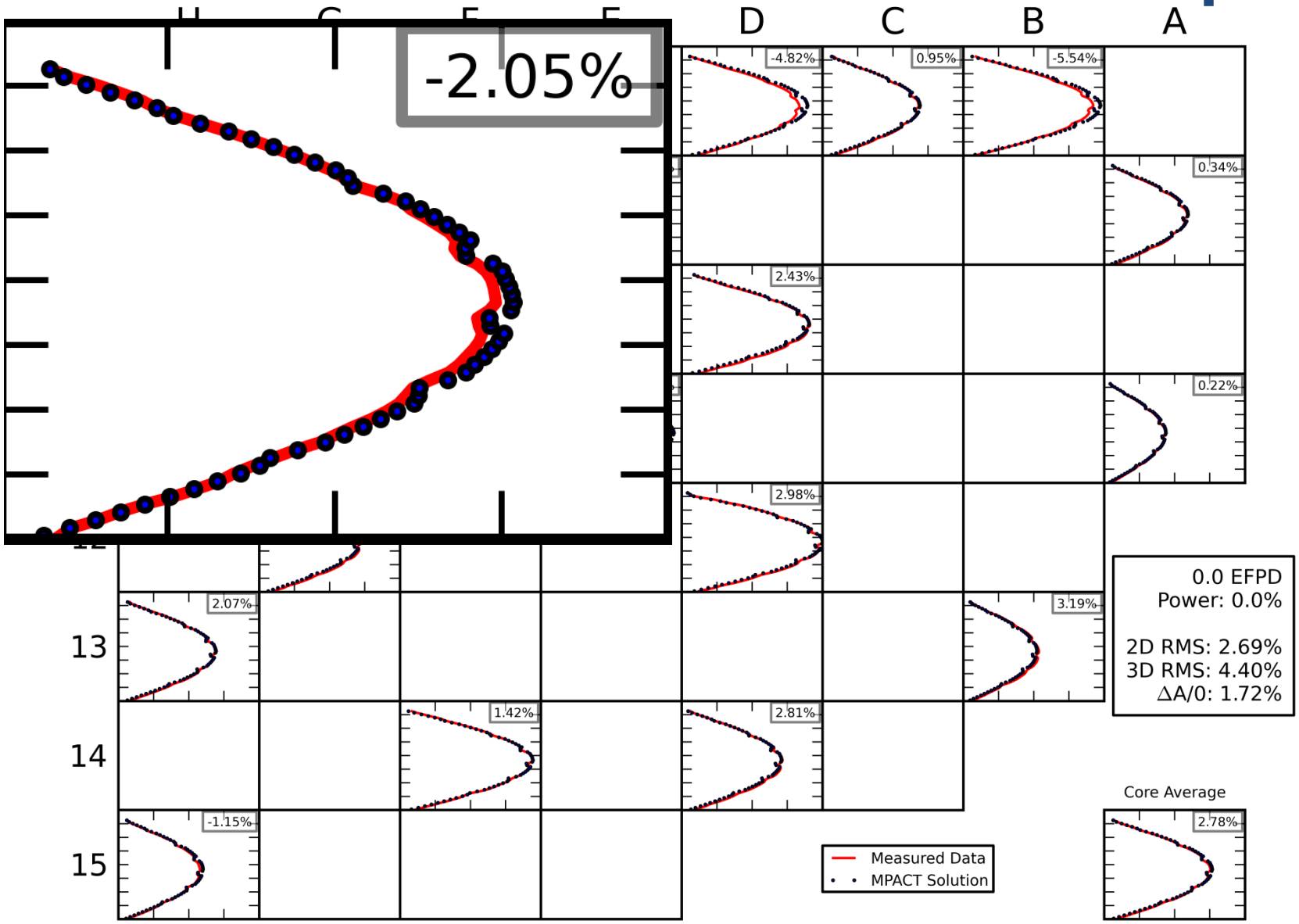


Cycle 1 Flux Maps

- MPACT extracts detector signal using local flux in the detector thimble with the fission cross-section for ^{235}U
- Detector signals are normalized and saved for post processing

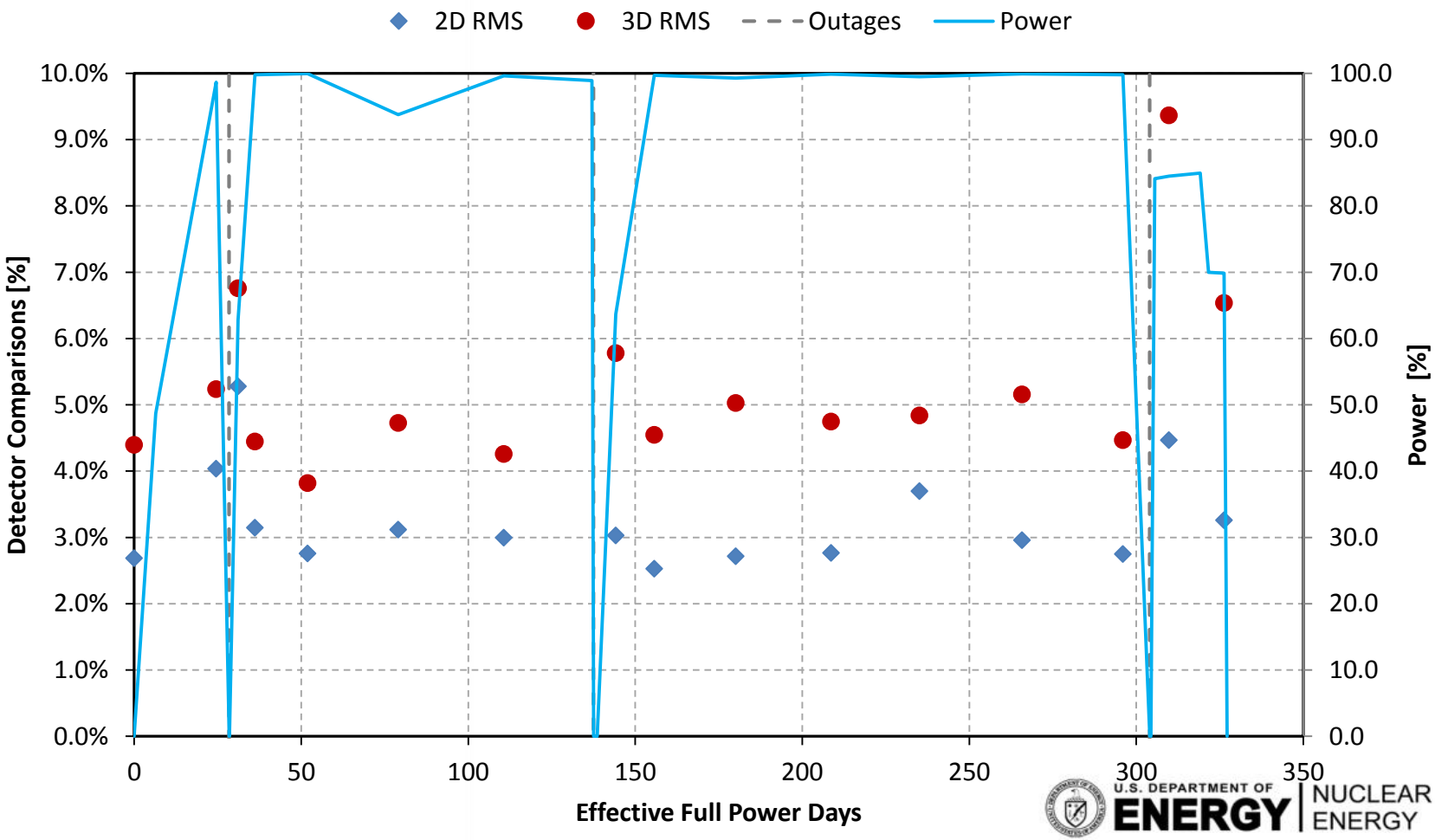
- Detector data is fit using a cubic spline and mapped onto 61 equal spaced levels for comparison with measured data
- A script performs this mapping and compares local and integral comparisons
  - 3D RMS of detector signal
  - Axially integrated RMS of detector signal
  - Measured vs Predicted Axial Offset from detector signals

Cycle 1
Zero Power Flux map



Cycle 1 Flux Map Comparisons

- Average 2D RMS – 3.03%
- Average 3D RMS – 4.8%



Watts Bar – Zero Power

Criticality (pcm)

	KENO-VI†	MPACT
Initial	-67	-144
ARO	-25	-98
D	-149	-234
C	-153	-255
B	-121	-228
A	-177	-275
SD	-160	-267
SC	-159	-262
SB	-125	-222
SA	-155	-267
Average	**-129**	**-225**

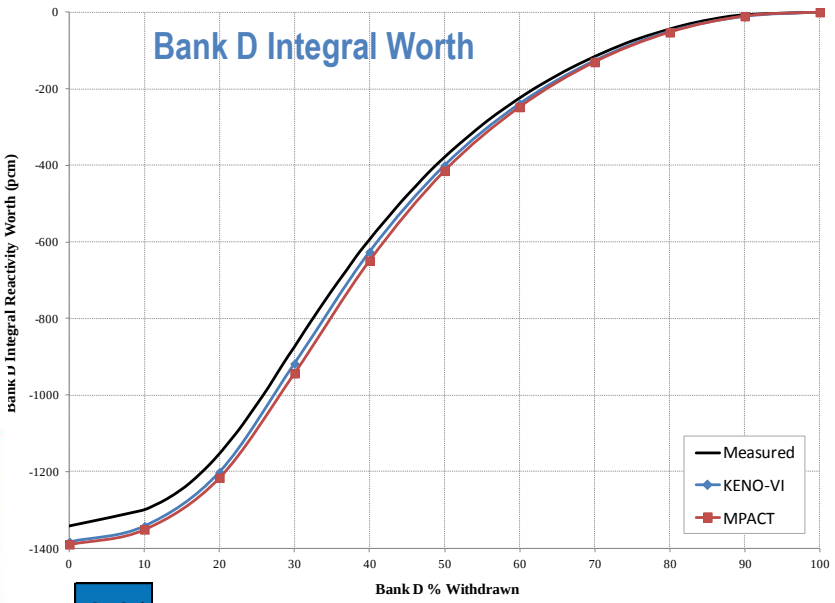
†σ <= 1 pcm

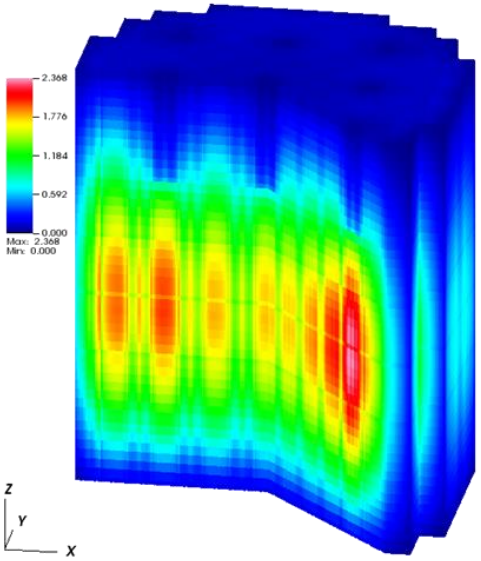
Bank Worths

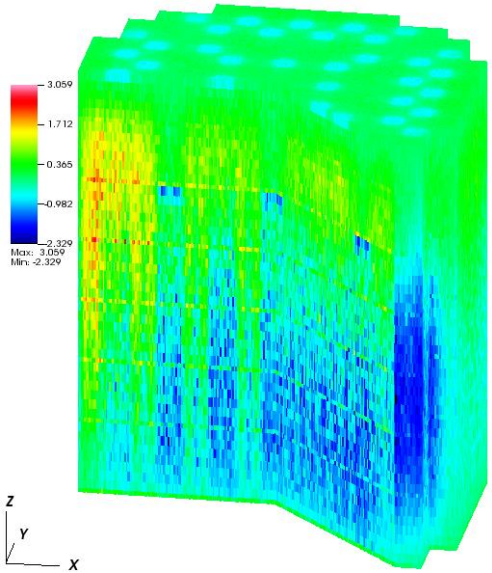
Bank	Measured (pcm)	KENO-VI	MPACT
D	1342	3.3 ± 0.1%	3.6%
C	951	3.5 ± 0.1%	4.2%
B	879	-0.5 ± 0.2%	1.2%
A	843	6.4 ± 0.2%	5.7%
SD	480	4.0 ± 0.4%	3.8%
SC	480	3.9 ± 0.4%	2.9%
SB	1056	1.0 ± 0.2%	1.4%
SA	435	2.6 ± 0.4%	3.9%
Total	**6467**	**2.9 ± 0.1%**	**3.3%**

Reactivity Coefficients

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







-0.48%					
-0.10%	-0.39%				
-0.37%	-0.05%	-0.39%			
-0.03%	-0.35%	-0.03%	-0.40%		
-0.35%	0.06%	-0.27%	-0.02%	-0.50%	
0.28%	-0.06%	0.19%	-0.23%	-0.04%	-0.18%
0.23%	0.59%	0.09%	0.27%	-0.15%	-0.44%
0.62%	0.54%	0.44%	0.11%		

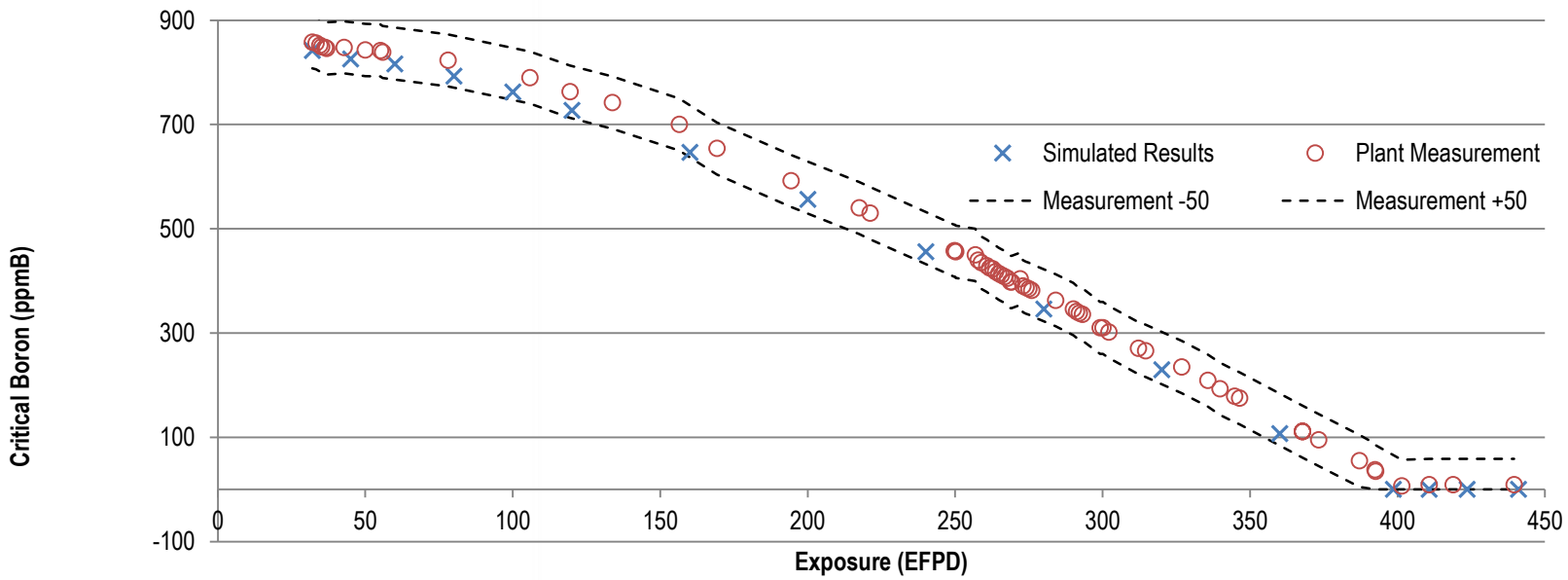
Initial Criticality Radial Core Fission Distribution

RMS=0.36%

75 mins
2784 cores

Watts Bar Cycle 1 Depletion

- Primary analysis run at full power with a small coast down at end of life
  - Further analysis of Watts Bar 1 Cycle 1 will occur during the multicycle depletion L1 milestone due in June 2015



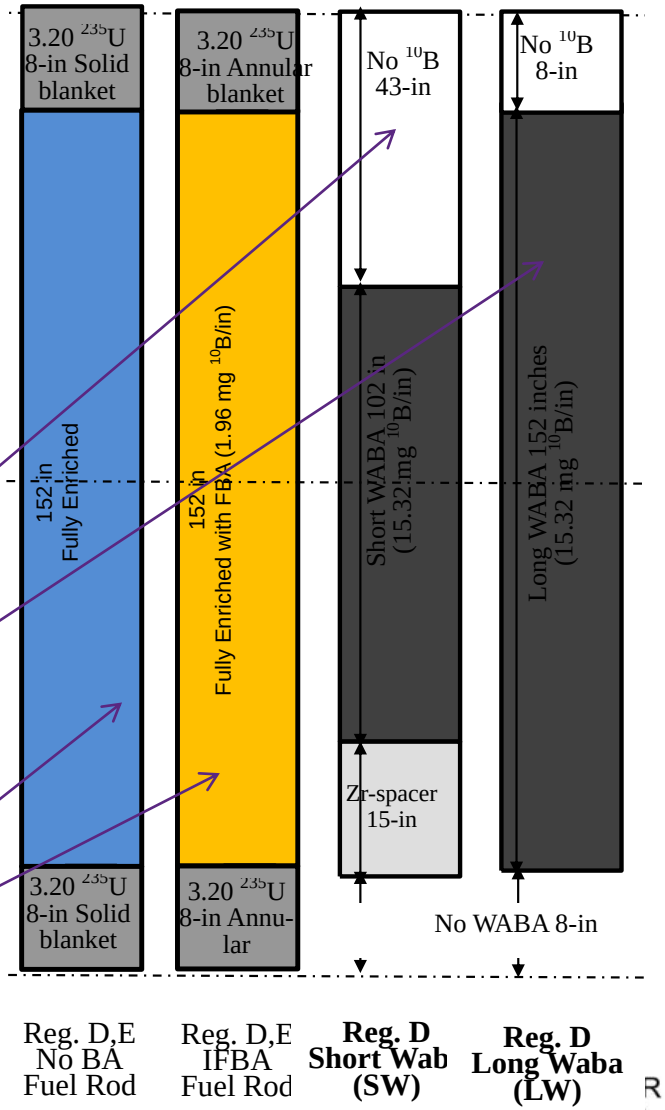
AP1000

- Aggressive design
  - Heterogeneous core (radially, axially)
  - Rodded operation (MSHIM™)
  - Ag-In-Cd and Tungsten CRs
  - IFBA and WABA inserts

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

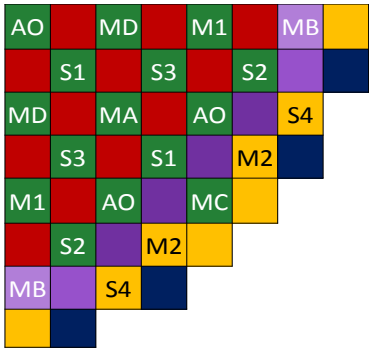
Region
IFBA
WABA

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

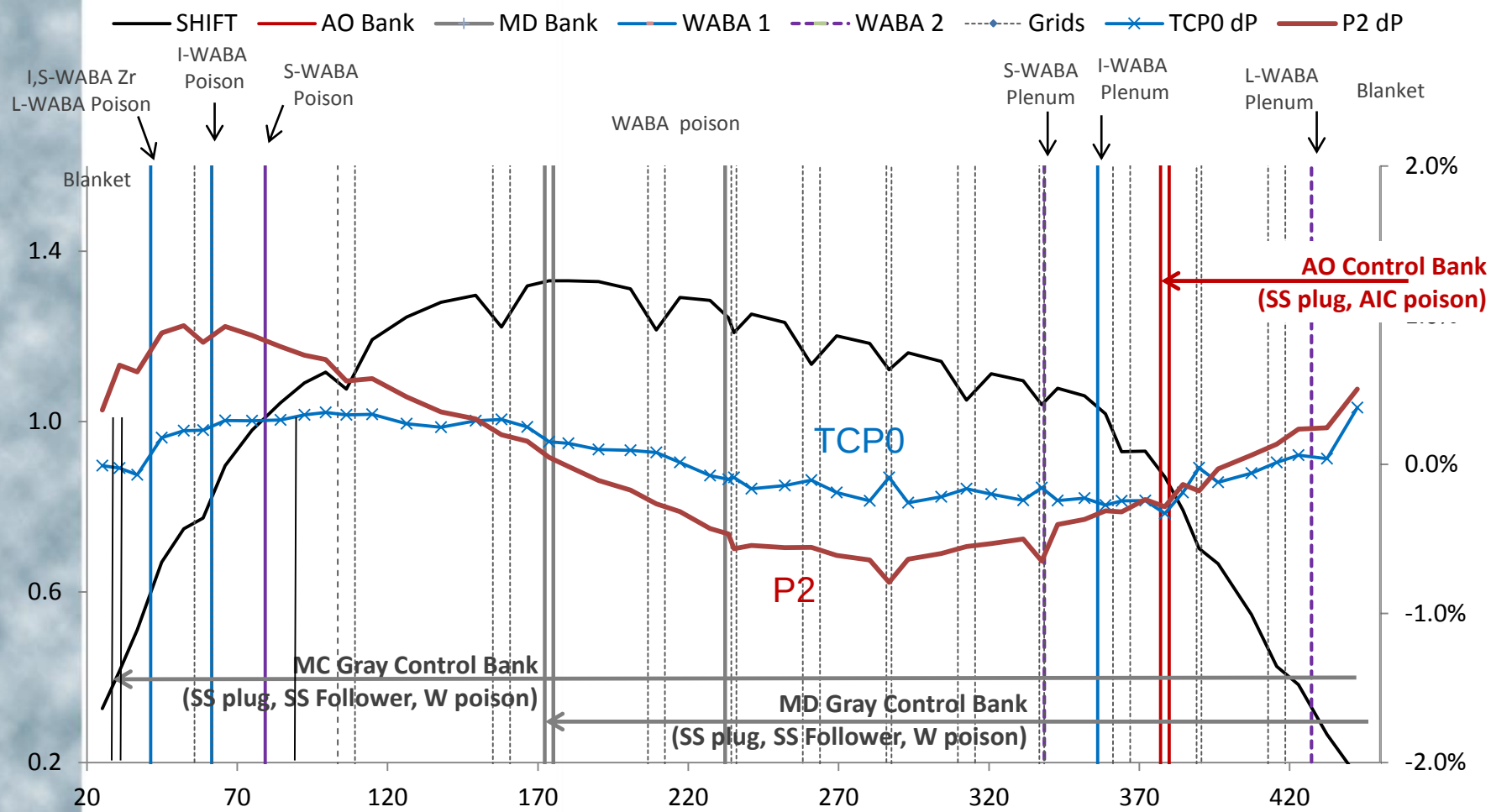


AP1000
Rod Worth – Zero Power Physics

		KENO	SHIFT		MPACT TCP0	
Rod Worth	Material	Worth (pcm)	ΔWorth (pcm)	ΔWorth (%)	ΔWorth (pcm)	ΔWorth (%)
MA	Tungsten	258	4	1.6%	1	0.5%
MB	Tungsten	217	-5	-2.3%	-6	-2.6%
MC	Tungsten	188	0	0.0%	1	0.4%
MD	Tungsten	234	5	2.1%	3	1.3%
M1	Ag-In-Cd	651	0	0.0%	-8	-1.2%
M2	Ag-In-Cd	887	4	0.5%	6	0.7%
AO	Ag-In-Cd	1635	17	1.0%	-11	-0.7%
S1	Ag-In-Cd	1079	14	1.3%	1	0.1%
S2	Ag-In-Cd	1096	-2	-0.2%	-11	-1.0%
S3	Ag-In-Cd	1124	16	1.4%	1	0.1%
S4	Ag-In-Cd	580	-4	-0.7%	-2	-0.4%
		RMS Max	9 17	1.3% 2.3%	6 11	1.1% 2.6%



AP1000
3D Core Multi-Rodded



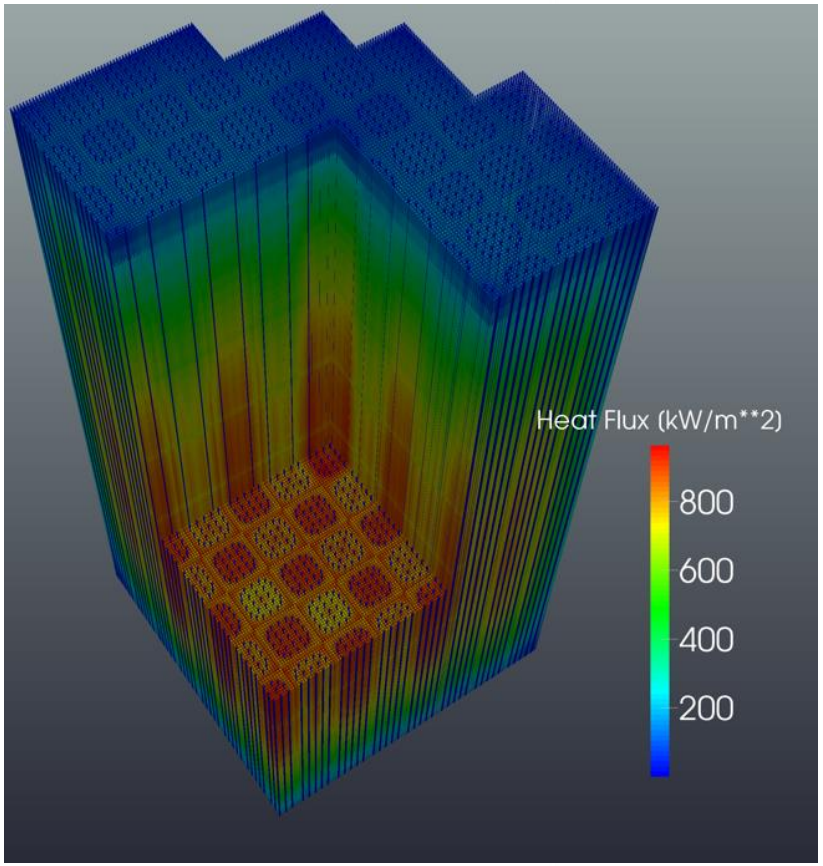
TCP0: ΔK = -118 pcm (600/900K) P2: ΔK = -94 pcm (600/900K)

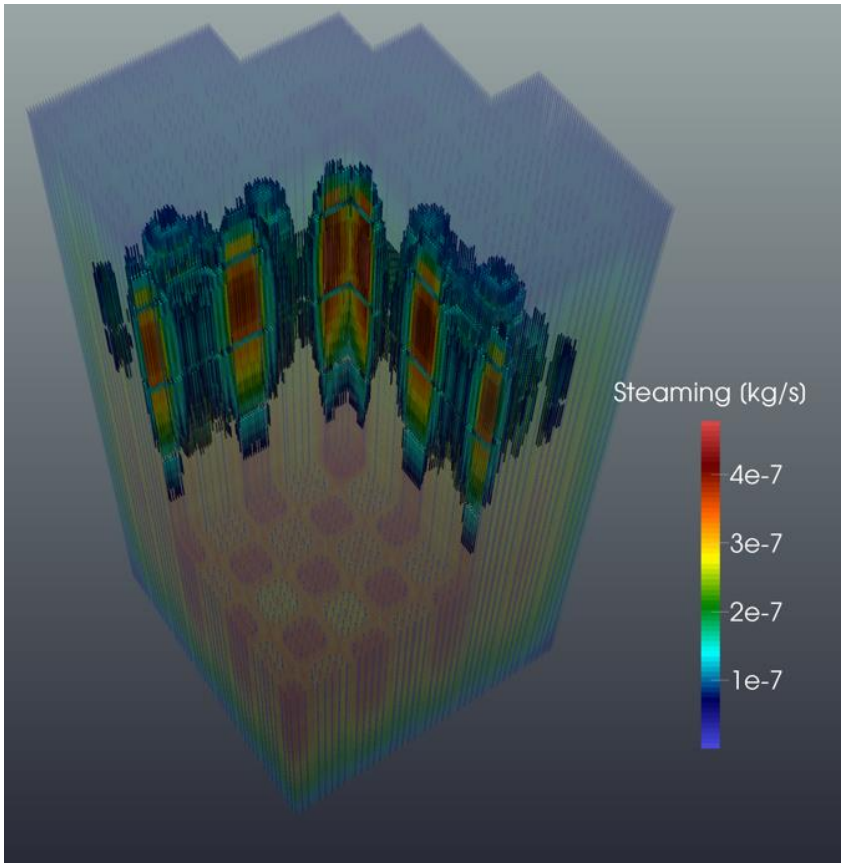
RMS 0.5% Max 2.6% RMS 0.7% Max 3.1%

Looking Forward

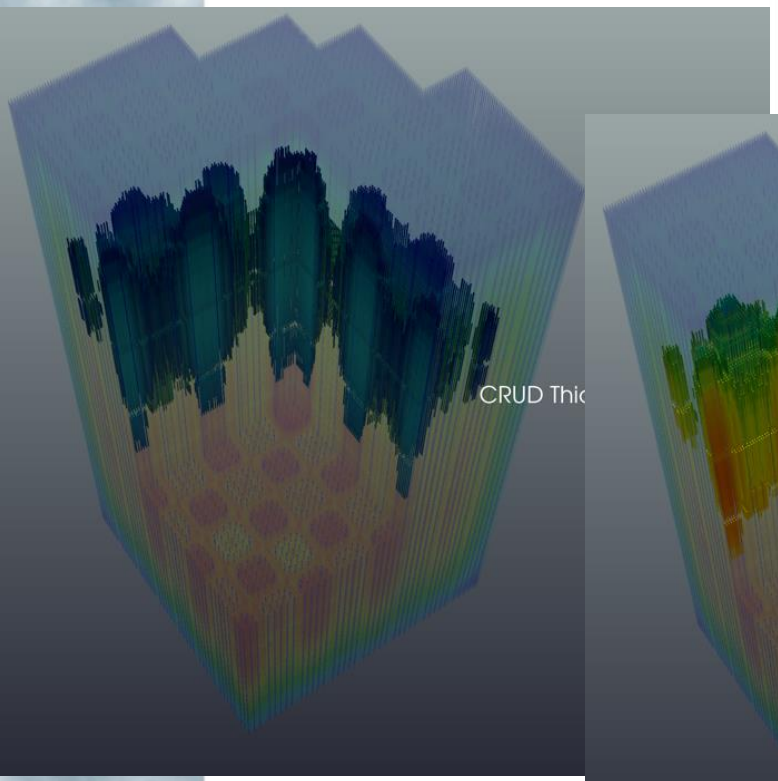
- Capability
  - Multicycle Depletion of Watts Bar
  - Completion of BEAVRS Benchmark
  - CIPS analysis
  - BWR Geometry
  - AP1000 Depletion
- Accuracy Improvements
  - Library verification for depleted fuel
  - Burnup dependent fuel temperatures
- Code performance improvements
  - Increase parallelism for COBRA-TF
  - Optimization of MPACT solvers

Extras
COBRA-TF – MAMBA Coupling

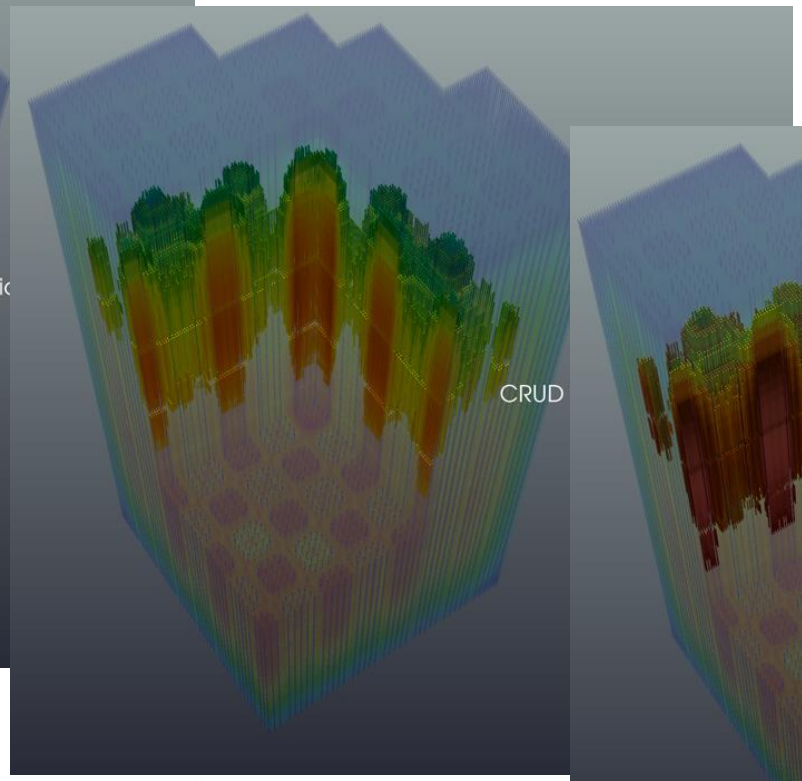




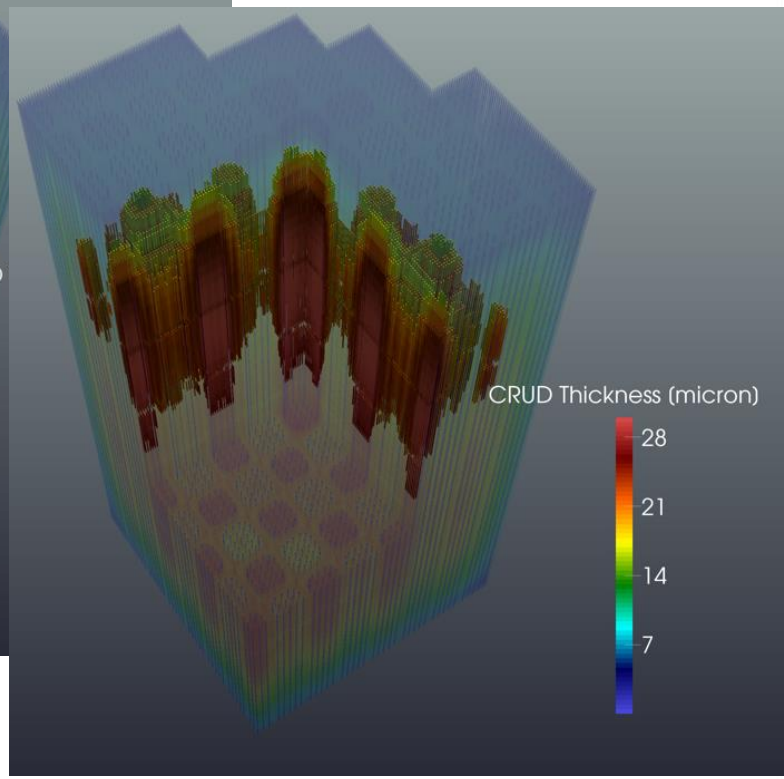
Extras
COBRA-TF – MAMBA Coupling



90 EFPD



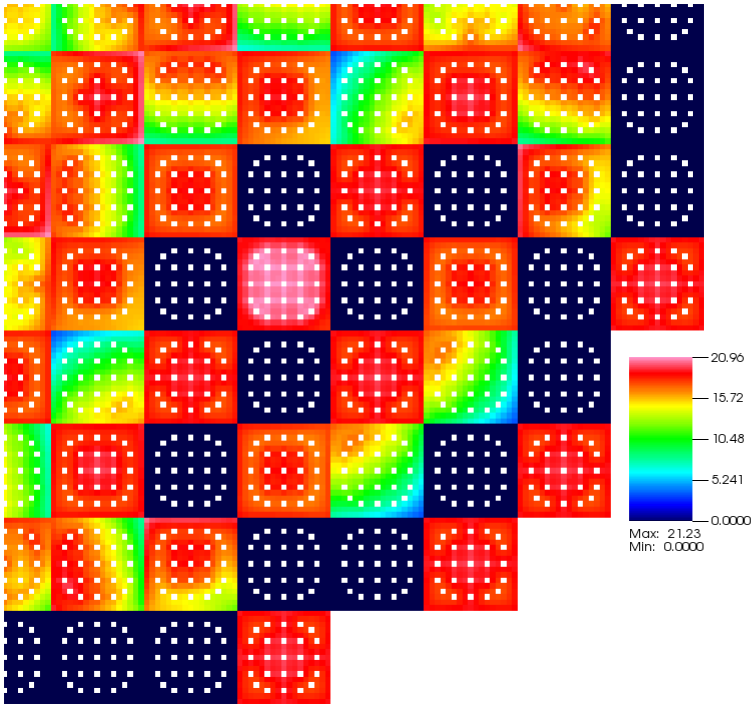
270 EFPD



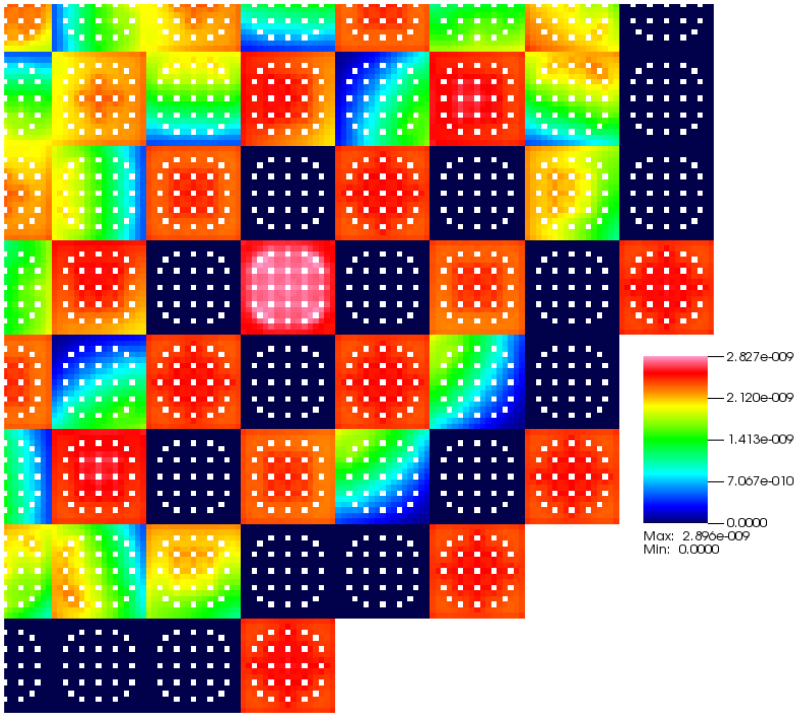
360 EFPD

Extras
Beginning of Cycle 2 Burnup

- Shuffling currently under acceptance testing



Pin Average Exposure



Pin Average ^{241}Pu Density

Questions?

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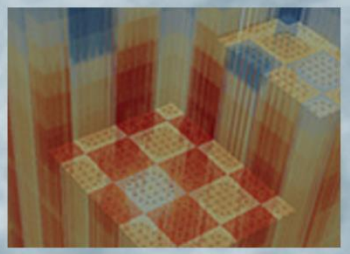
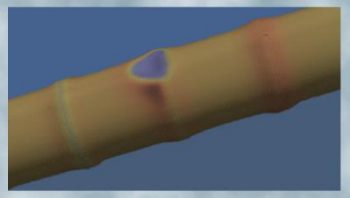
Update on Validation and Modeling Applications (VMA)

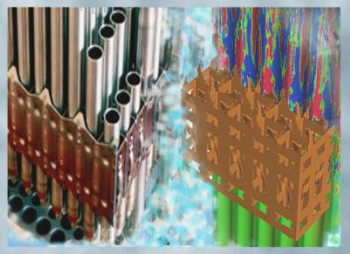
Vince Mousseau

Yixing Sung

Brian Williams







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Outline

- Phase I accomplishments
- VUQ application examples
- Phase 2 strategy and data challenges

Validation and Modeling Applications (VMA)

Achieving Credible, Science-based Predictive Simulation Capabilities

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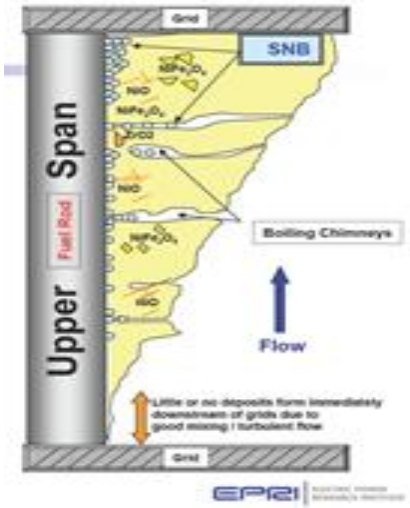
Objectives and Strategies

- VMA = VUQ + AMA: Validation and Modeling Applications has been formed by combining Validation and Uncertainty Quantification with Advanced Modeling Applications.
- This provides a much tighter coupling between the assessment and application of VERA with its VVUQ.
- This improves technology development and product delivery to address the industrial Challenge Problems.



Requirements Drivers

- Software related to reactor safety analysis must meet quality requirements.
- Provide a clear justifiable case that the software is appropriate for the intended application.
- PCMM, CSAU, SQA, and VVUQ are the key tools to define new standards for software development and application.

Outcomes and Impact

- The DAKOTA software will be delivered as part of VERA and it will introduce modern tools for VVUQ for use by Industry.
- We will help to define VVUQ plans and processes for the CASL challenge problems and for the VERA components.
- These plans and processes when implemented will provide confidence in VERA for industry use by clearly defining value added work.

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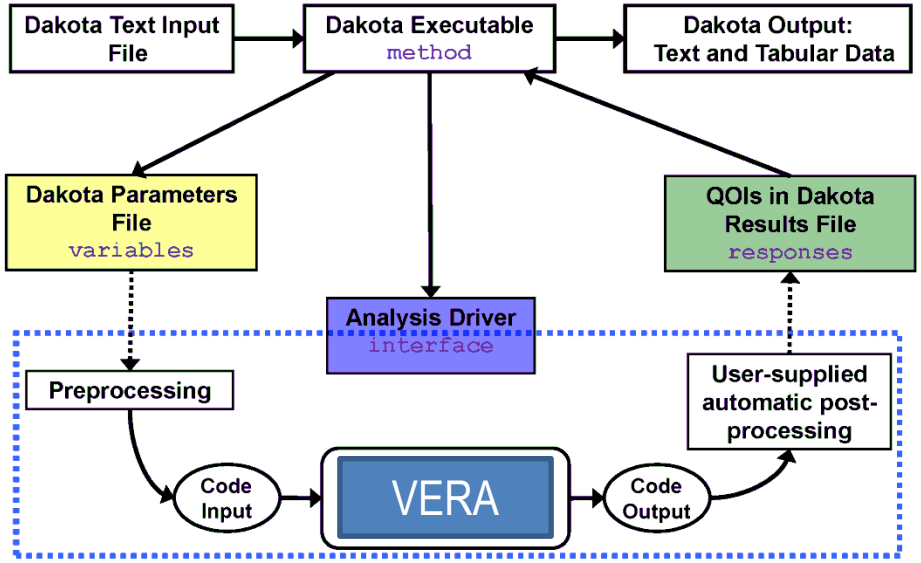
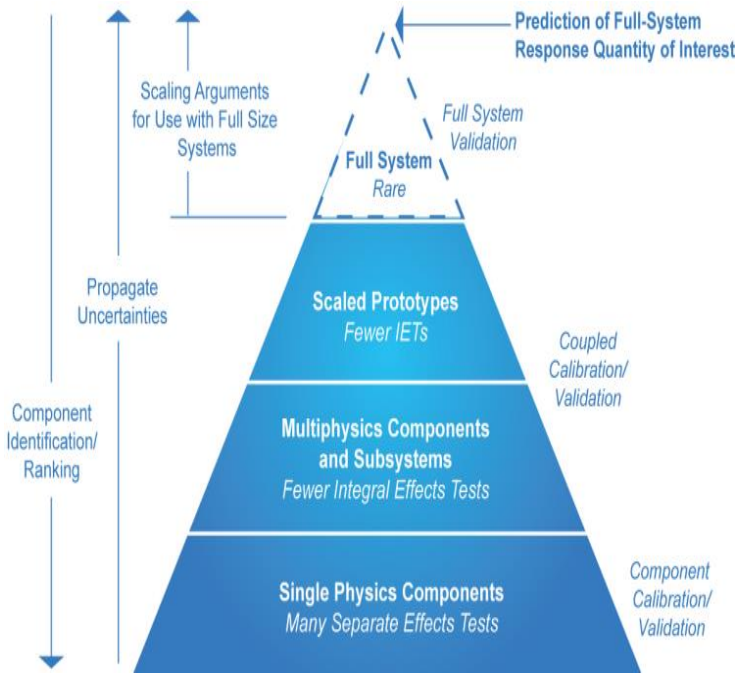
Phase I Accomplishments (1)

- Provided DAKOTA tools and user guidelines to automate and guide VVUQ for code development and challenge problem applications
  - DAKOTA contains tools for optimization, uncertainty quantification, parameter estimation, and sensitivity/variance analysis
- Completed initial VVUQ assessments of CASL tools
  - Revealed simulation and DAKOTA weaknesses have been improved
  - Some of the work has been on "one-off" studies
  - Early work with industry codes



Phase I Accomplishments (2)

- Performed VERA-CS component code VUQ studies
  - Parameter exposure work in subchannel T/H code CTF to improve sensitivity and UQ
  - Initial PCMM analysis of CTF to measure documentation and testing
  - Initial PCMM analysis of neutronic code Insilico to measure documentation and testing
- Worked with CASL partners to collect industry-quality data to address code and model validation needs



Better VUQ engagement in CASL

VUQ Application Examples

- VERA Progressive Problem 6 Study
  - Geometry: Single Westinghouse 17x17 fuel assembly
  - Condition: hot full power (HFP) and Beginning of Life (BOL)
  - Modeling and Simulation: VERA-CS neutronic and subchannel thermal-hydraulic (T/H) code plus DAKOTA

- Turbulent mixing parameter calibration under DNB CP
  - Geometry: 5x5 rod bundle mixing test
  - Condition: Single phase flow and heat transfer for channel exit temperature measurements
  - Modeling and simulation: VERA-CS T/H code CTF plus DAKOTA for calibrating empirical constant

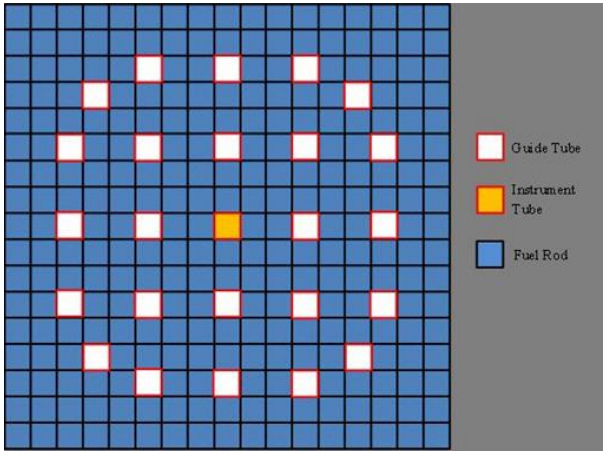
VUQ Example Summary

Initial VERA-CS Problem 6 Multi-scale Multi-physics VUQ

- Phenomenon Identification Ranking Table
  - Define phenomena for fuel, thermal hydraulics, and neutronics
- Quantified Parameter Ranking Table
  - Top down approach (test the trees not branches)
- Low level calibration work with Dittus-Boelter (single phase heat transfer) and McAdams (single phase friction) and neutronics
  - Challenge to get "appropriate" calibration data
  - Key result is the importance of capturing the "joint" distributions between parameters
- Initial Uncertainty Quantification results
  - Problem 6 is single phase liquid: thermal hydraulic uncertainties are small
  - Need to address cross section uncertainties with reduced order modeling and calibration to reduce uncertainties

Problem 6 is a VUQ surrogate for CPs

VUQ Analysis of Cobra-TF for Progression Problem 6

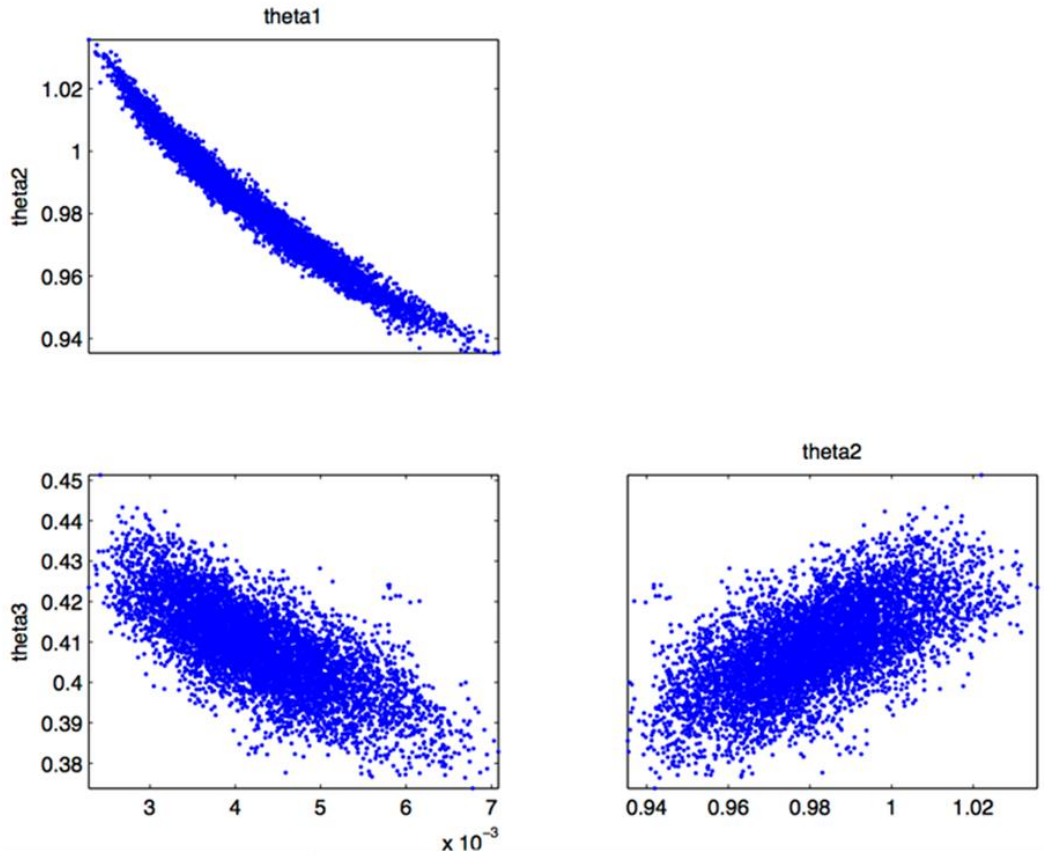


- Simulation of a single PWR assembly
  - Hot Full Power, T/H feedback
  - Boron concentration of 1300 ppm, 100% power
  - Power supplied by neutronics held constant
- Quantity of Interest is maximum fuel temperature
- We have three parameters distributions to construct
  - Expert opinion
  - Marginal (independent)
  - Joint distribution

$$Nu = 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4} = \theta_1\,\mathrm{Re}^{\theta_2}\,\mathrm{Pr}^{\theta_3}$$

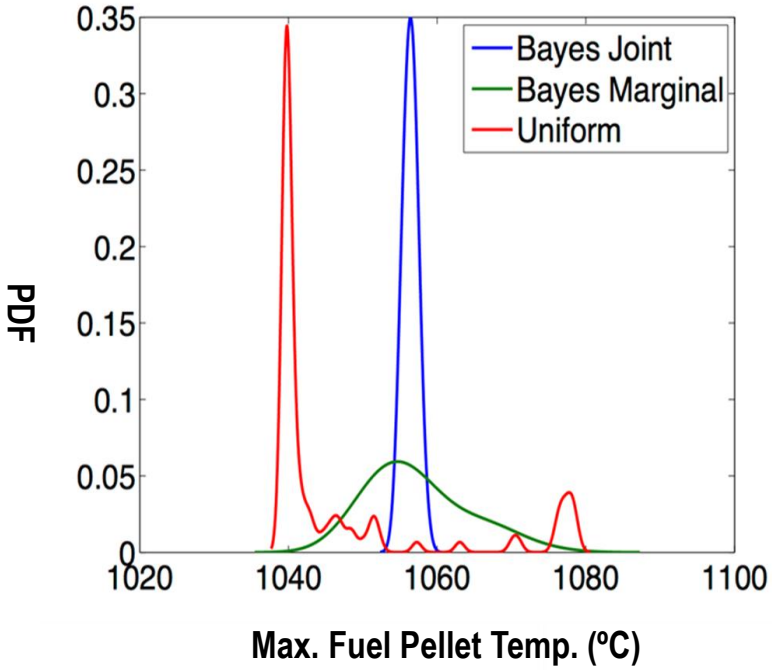
Single phase heat transfer

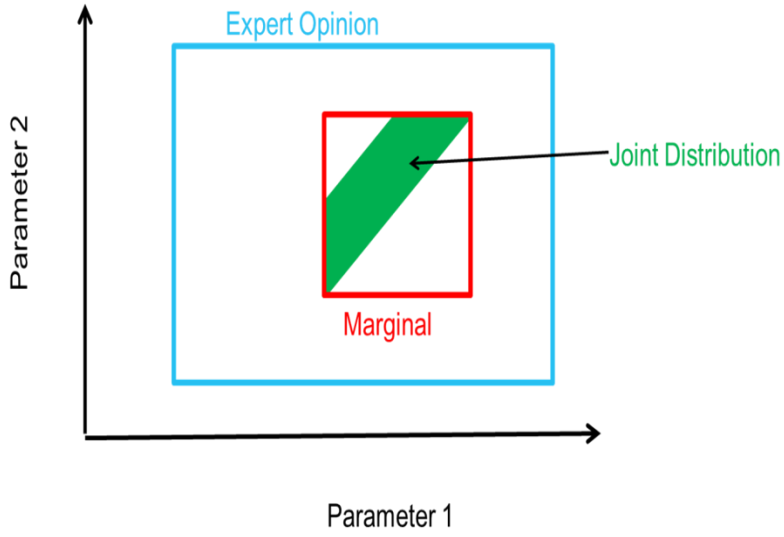
Dittus-Boelter -Bayesian Calibration Reveals Parameter Interactions



Experts assume independent

Dittus-Boelter Calibration





Capturing the joint distribution

Problem 6 UQ Summary

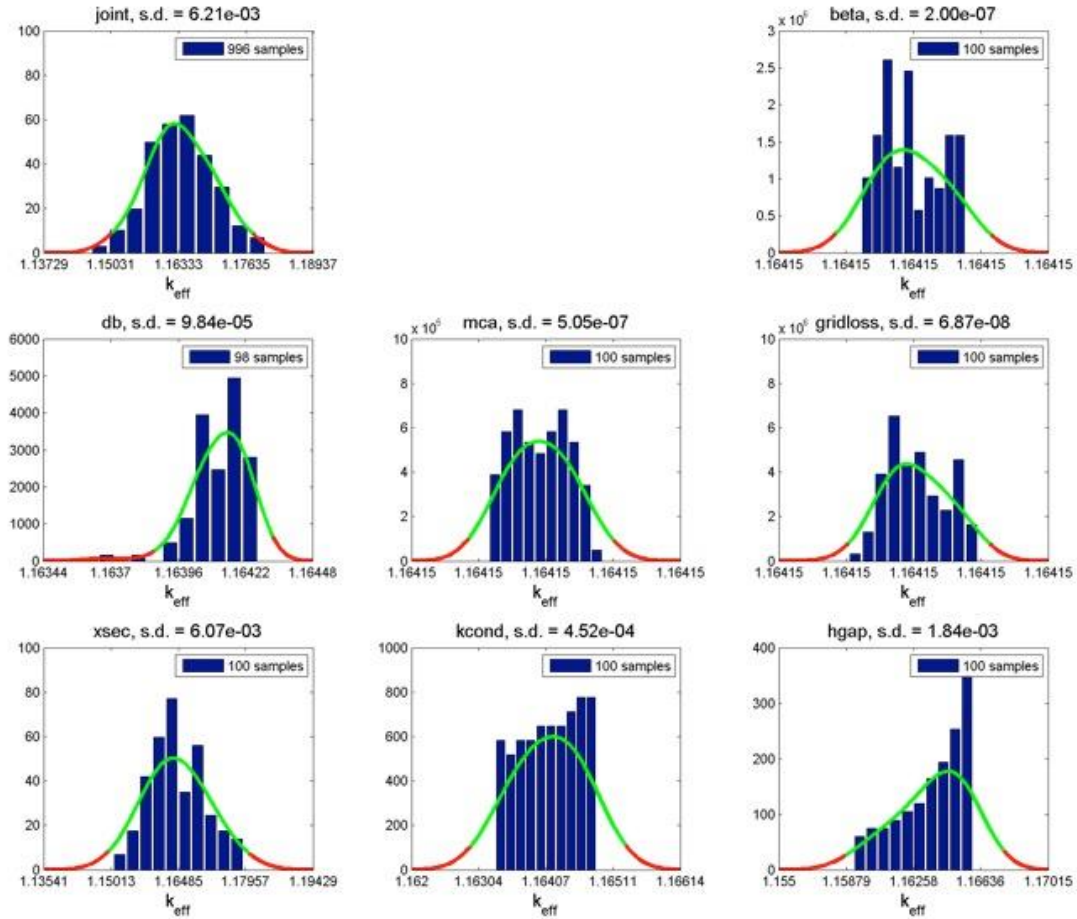
- ***Keff*** – is mainly a function of the cross section uncertainty, and followed by gap conductivity.

- ***Max Pin Temperature*** – Is dominated by gap conductivity, and followed by pellet thermal conductivity. Note we assumed a 10% uncertainty in the thermal conductivity of fresh fuel.

- ***Max Pin Power*** – Is dominated by gap conductivity, and followed by the cross section and fuel pellet thermal conductivity uncertainties

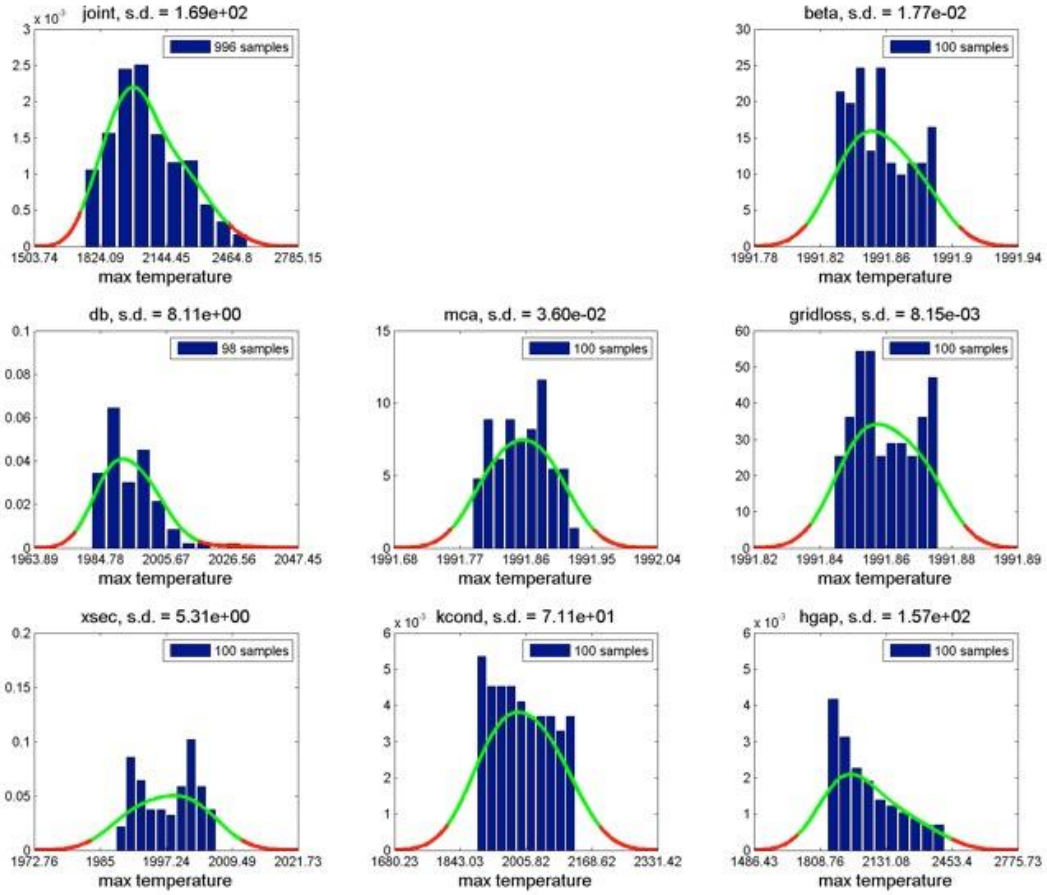
Coupled code BEPU on QoIs

Keff Study



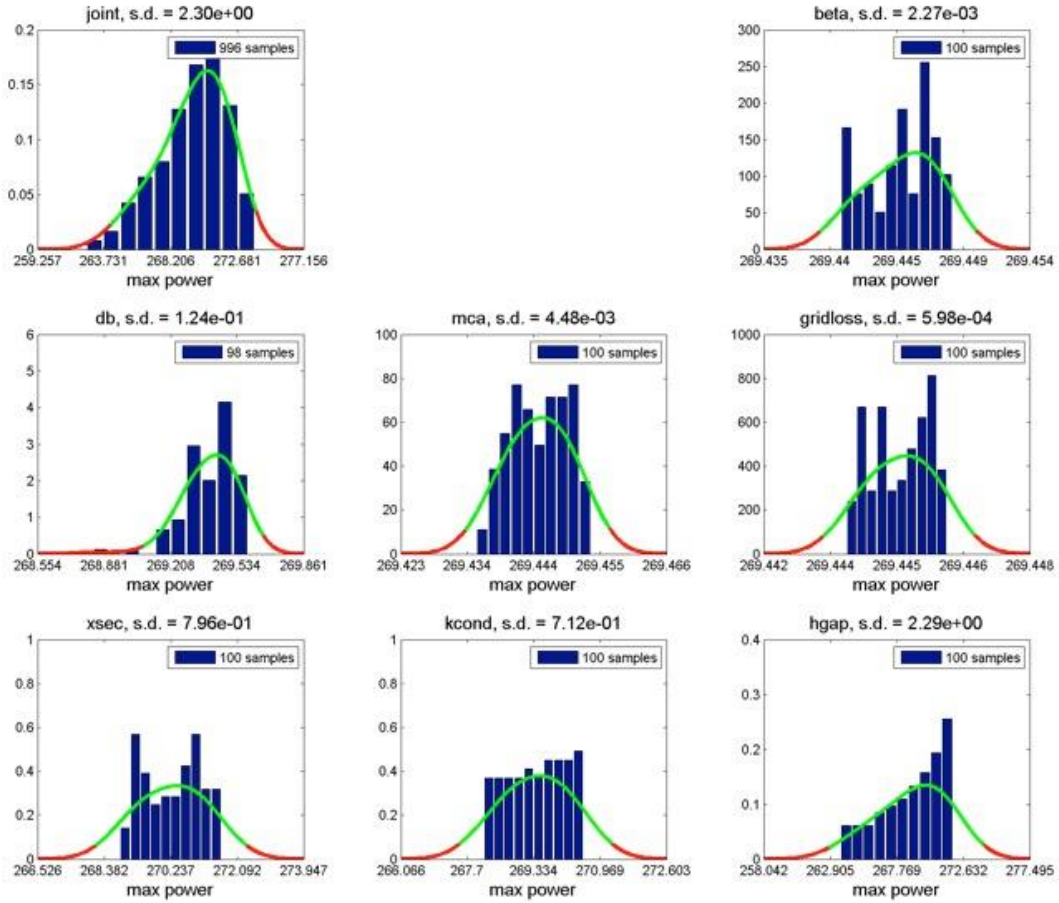
VERA Problem 6 UQ

Max Pin Temperature Study



VERA Problem 6 UQ

Max Pin Power Study



VERA Problem 6 UQ

Initial VUQ DNB CP Study

- T/H solution Verification – quantitatively established that CTF results were mesh converged. Numerical uncertainty approximately zero. Single phase results are almost linear
- Analysis of the experimental data – the code results are symmetric by design. The data are not symmetric
- Initial calibration of turbulent mixing using DAKOTA with data
  - WEC provided proprietary rod bundle mixing and DNB data for CASL validation use
  - This large amount of experimental data allows for both validation and calibration
- Data and calibration are fuel design specific:
  - Initial calibration based on data for non-mixing vane grid spacer

Subchannel Turbulent Mixing Model – Initial DNB Study

The turbulent mixing in subchannels was modeled using the following empirical correlation:

$$\Delta Q = -w' \times \Delta h \times \Delta X \qquad (5\text{-}1)$$

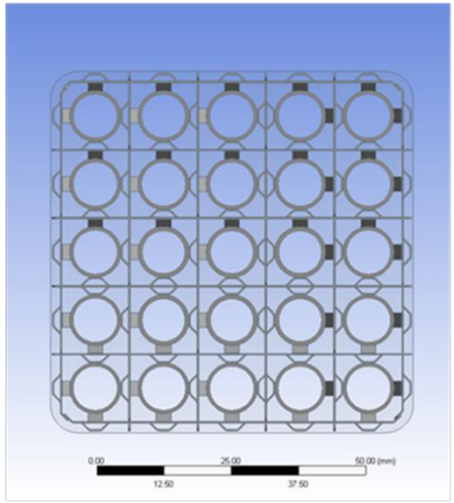
where ΔQ = energy exchange due turbulent mixing (W or Btu/hr)
w' = lateral turbulent flow per unit length (kg/s/m or lbm/hr-ft)
Δh = enthalpy difference between two subchannels (J/kg or Btu/lbm)
ΔX = axial nodal length (m or ft)

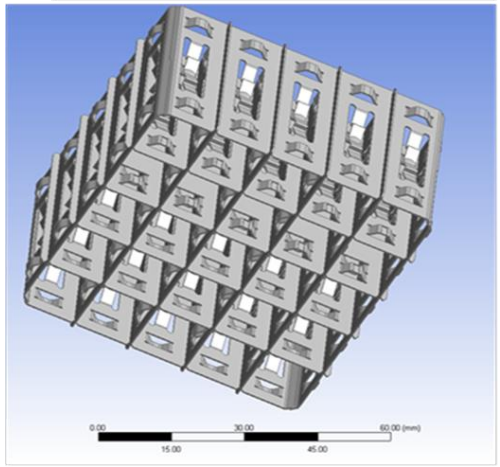
$$w' = ABETA \times G_{AVG} \times S \qquad (5\text{-}2)$$

where $ABETA$ = empirical coefficient,
G_{AVG} = average axial mass flow in the connected channels (kg/s/m^2 or lbm/s/ft^2)
S = rod-to-rod gap width (m or ft)

Mixing Model and Empirical Coefficient

Calibration of CTF Mixing with Rod Bundle data





Eval #	BETA	wRSS
1	0.00600000	17.6802
2	0.00100000	18.566
3	0.00496073	17.57965
4	0.00392327	17.57847
5	0.00408976	17.57021
6	0.00442246	17.56284
7	0.00440553	17.56482
8	0.00442077	17.56318
9	0.00442229	17.56307
10	0.00442244	17.56284
11	0.00442245	17.56284
12	0.00442245	17.56284
13	0.00442246	17.56284

DAKOTA used to calibrate CTF

VVUQ Strategy in Phase II

- PIRT (expert opinion) and QPRT (code sensitivity) “iterated to convergence” (What the experts think are important and what the code thinks is important match) for a challenge problem.
- Validation Data Integrator constructs a validation pyramid that separates low level code validation (bottom) from coupled code validation (top).
- Code VVUQ and Challenge Problem VUQ done in 2 steps
  - Code VVUQ during software development
  - Validation and uncertainty quantification during application
- Initial uncertainty quantifications focus on three CPs; CIPS, PCI, and DNB.
- VUQ requires strong team work in CASL and **support of IC**

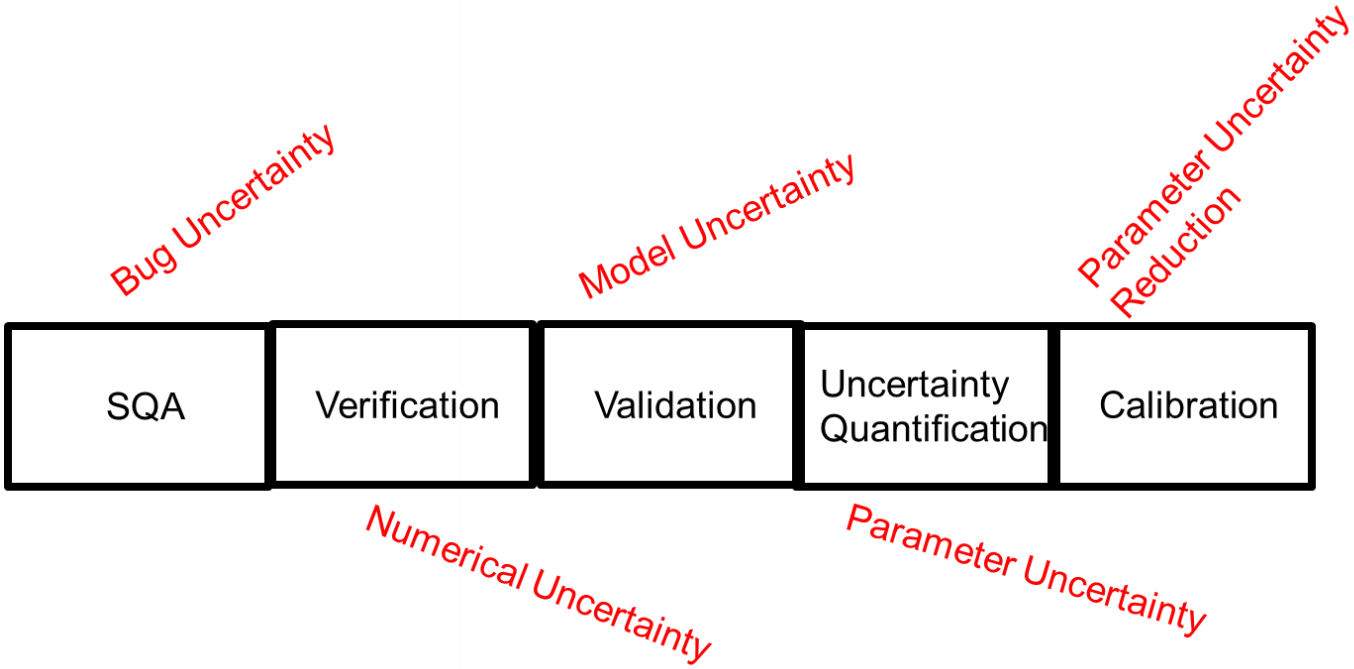
It takes a village to raise a child

Total Uncertainty

- **Verification:** $\left\| QOI_{exact} - QOI_{computed} \right\|$
- **Validation:** $\left\| QOI_{experimental} - QOI_{computed} \right\|$
- **Uncertainty Quantification:** $\left\| QOI_{perturbed} - QOI_{computed} \right\|$
- **Impacts of numerical, model, and parameter uncertainties should be compared and evaluated.**

Holistic view of uncertainty

Predictive Capability Maturity Model (PCMM)



CASL has chosen PCMM which is an iterative process to measure software quality and maturity where one continually works on the lowest score.

The process that connects the tools

CASL VUQ Impacts

- PCMM helps to justify new software application to meet regulatory requirements
  - A “modernized” CSAU.
  - The total uncertainty approach.
  - Improvement of the Wilks formula approach.
- DAKOTA use by CASL
  - Provide better frequentist tools (better statistics).
  - Provide Bayesian tools.
  - Use of HPC when needed for VVUQ (~1000 runs).
- In addition to CASL applications, DAKOTA is coupled to all NRC codes through SNAP (the NRC graphical user interface)

CASL VUQ Benefits Industry

Current Validation Work

- A large amount of validation work being performed for the CASL codes:
  - CTF: PSBT, BFBT, FRIGG, Harwell, GE3x3, CE 5x5, PNNL 2x6, and Westinghouse Mixing Tests.
  - Peregrine: Comparisons with Halden, Studvik SuperRamp, and RIS0.
  - Bison, Abaqus, WEC Vitran: Wear model GTRF data from ORNL.
  - Hydra Validation: TAMU 5x5, MIT subcooled boiling data.
  - Hydra Benchmarks: Erturk, Moser, Prasad, Elmadi, de vahl Davis, and Ghia.
  - Insilico: Validation - Watts Bar; Benchmarks - SHIFT and KENO.
  - MPACT Validation: Watts Bar, SPERT, B&W 1484,1810 and Takahama.
  - MPACT Benchmarks: KENO, Insilico, and Shift.
  - Shift: Watts Bar, B&W 1484,1810.
  - Mamba: Comparison with WALT data and comparison with CRUD pictures and CRUD scrapings from Seabrook.

Large amount of validation work currently underway

Validation Data Hierarchy

- When we do not have the quantity, quality, or relevancy of the validation data we need, we will leverage those who have it or can get it for us.
  - DOE projects, NEUP and the new validation database
  - ***Industrial partners current and new.***
  - "Data mining" of the literature.
- New integral effects experiments designed with CASL software, CPs, and VVUQ in mind from DOE or industry partners.
- New separate effects experiments with CASL in mind from DOE or industry partners.
- The value of validation data increases significantly when the simulation and experiment happen simultaneously.

No rock unturned when looking for validation data

Data from Industry Partners

- Phase I partners provided data critical to CASL software development and CP applications
  - Industry sponsored test and plant data (EPRI)
  - Plant data and measurements (TVA)
  - Fuel design and test data (WEC)
- CASL has well defined process and procedure for data management and control
  - Technology Control Plan (TCP)
  - Protection of proprietary data under nondisclosure agreements (NDA)
- New data continue to be identified and collected in Phase II
  - Separate effects tests to validate individual models.
  - Integral effects tests validate coupled physics and coupled codes.
  - High fidelity test data to validate CFD, fuel, and chemistry codes.

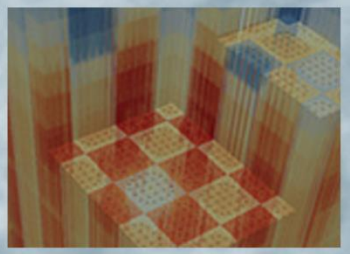
Industry Data Critical to CASL Success

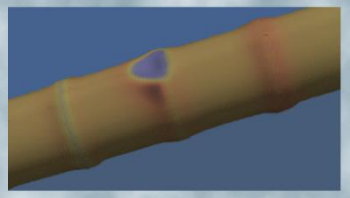
Summary

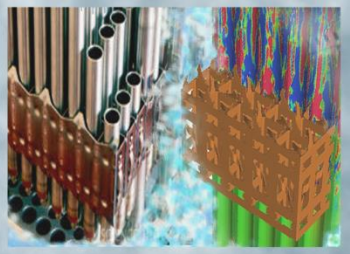
- Phase I in CASL has been very dynamic and focused on bringing capability of VERA tools to a mature level.
- Advanced VUQ techniques and tools have been applied to code development and challenge problems
- Phase II will move from capability development to production deployment - application driven
- VVUQ tools and methods improve software development and applications to challenge problems
- Data from industry partners are critical to successful application of CASL technology

A DOE Energy Innovation Hub

Additional Information on VVUQ Concept and Approach







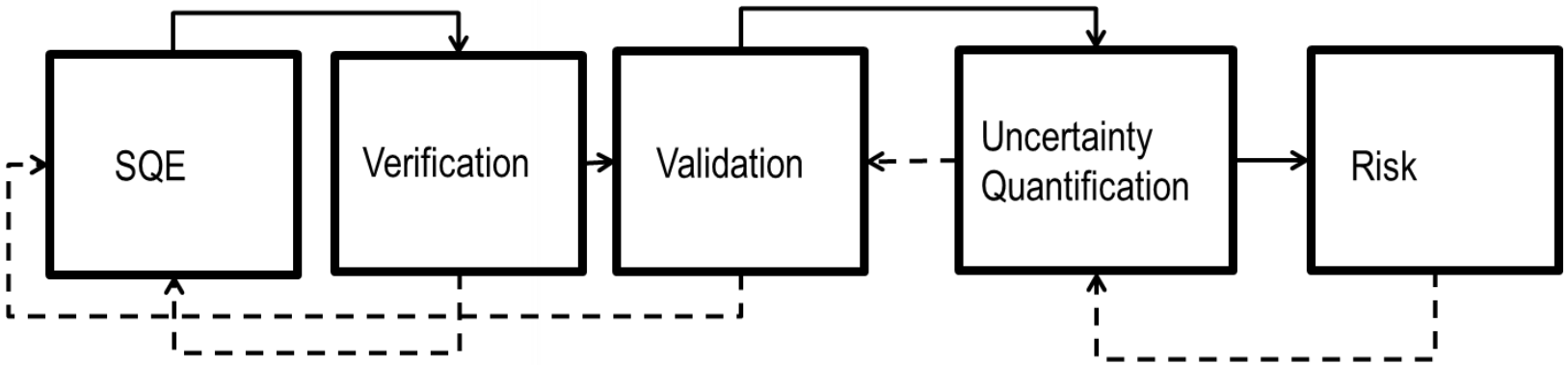
U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Vocabulary

- It is more important that the work gets done than what it is called.
  - **Software Quality** – Do you know what's in your code?
  - **Verification** – Did you solve the equations correctly?
  - **Validation** – Are you solving the correct equations?
  - **Uncertainty Quantification** – do you know the parameters in your models?
- The names vary form field to field but knowing the answer to these four questions is key.
- These processes depend on each other. Just doing one of these has limited value.

Don't get hung up on names

Dependencies



UQ is an iterative process

Total Uncertainty

This equation is wrong. However, it is better than assuming the first two are zero. We will be happy when new versions of this equation that are better are implemented proving us wrong.

$$\mathrm{UQ}_{\mathrm{total}} = \min \left\{ \begin{array}{l} \left\| \mathrm{QoI} - \mathrm{QoI}_{\Delta x \to 0} \right\|, \\ \left\| \mathrm{QoI} - \mathrm{QoI}_{\mathrm{exp}} \right\|, \\ \left\| \mathrm{QoI} - \mathrm{QoI}_{2\sigma} \right\| \end{array} \right\}$$

Need to account for all modes of uncertainty

Thermal-hydraulics simulation at EDF

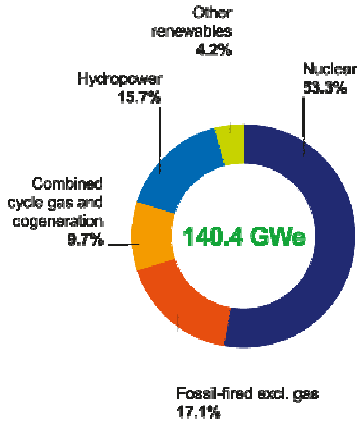
Didier BANNER

CASL Industry Council March 17-18 2015 Meeting

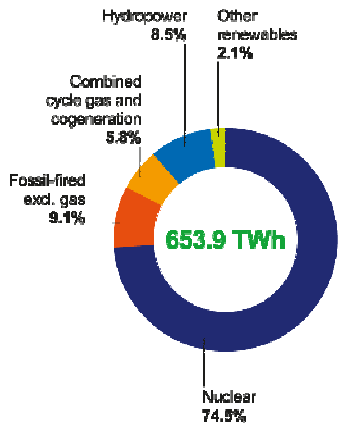
ABOUT EDF

- **€75.6**
  - billion in sales
- **39.1**
  - million customers
- **158,467**
  - employees worldwide
- **85.1%**
  - generation without CO_2

INSTALLED CAPACITY



GENERATION



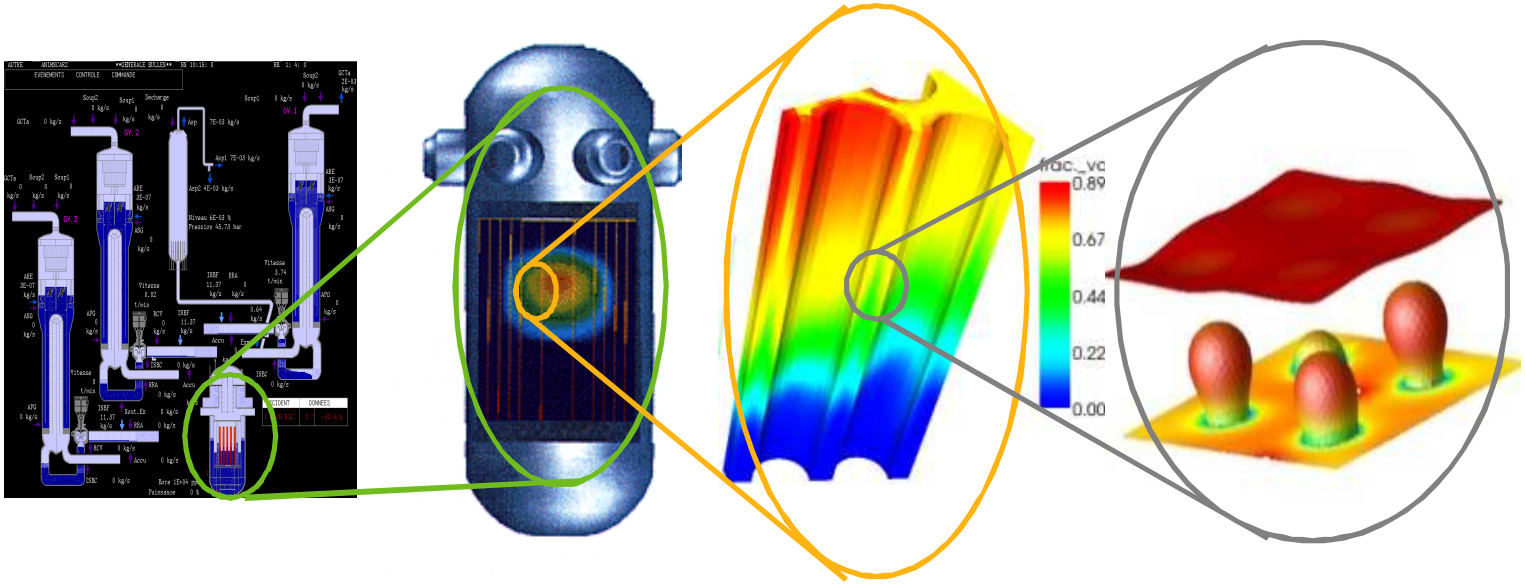
Modeling and simulation - what for ?

Need for Thermal-hydraulic modeling?

- **Justifying installations**
  - Identification of **new safety margin** ie. thermal shock on vessel, DNB
  - Analysis of accidental situations non reproducible by experiments
    - i.e, severe accidents, fire propagation, geological disposal
- **Understanding physics or system response**
  - **Ageing** of materials and installations i.e loads,
  - Addressing the issue of uncertainties and identifying the prominent parameters (regulatory V&V requirements)
- **Qualifying and optimizing processes**
  - NDT methods or instrumentation: i.e temperature distribution
  - **Optimizing** equipment i.e cooling systems

EDF

Thermal-hydraulics Modeling
Scales to be considered



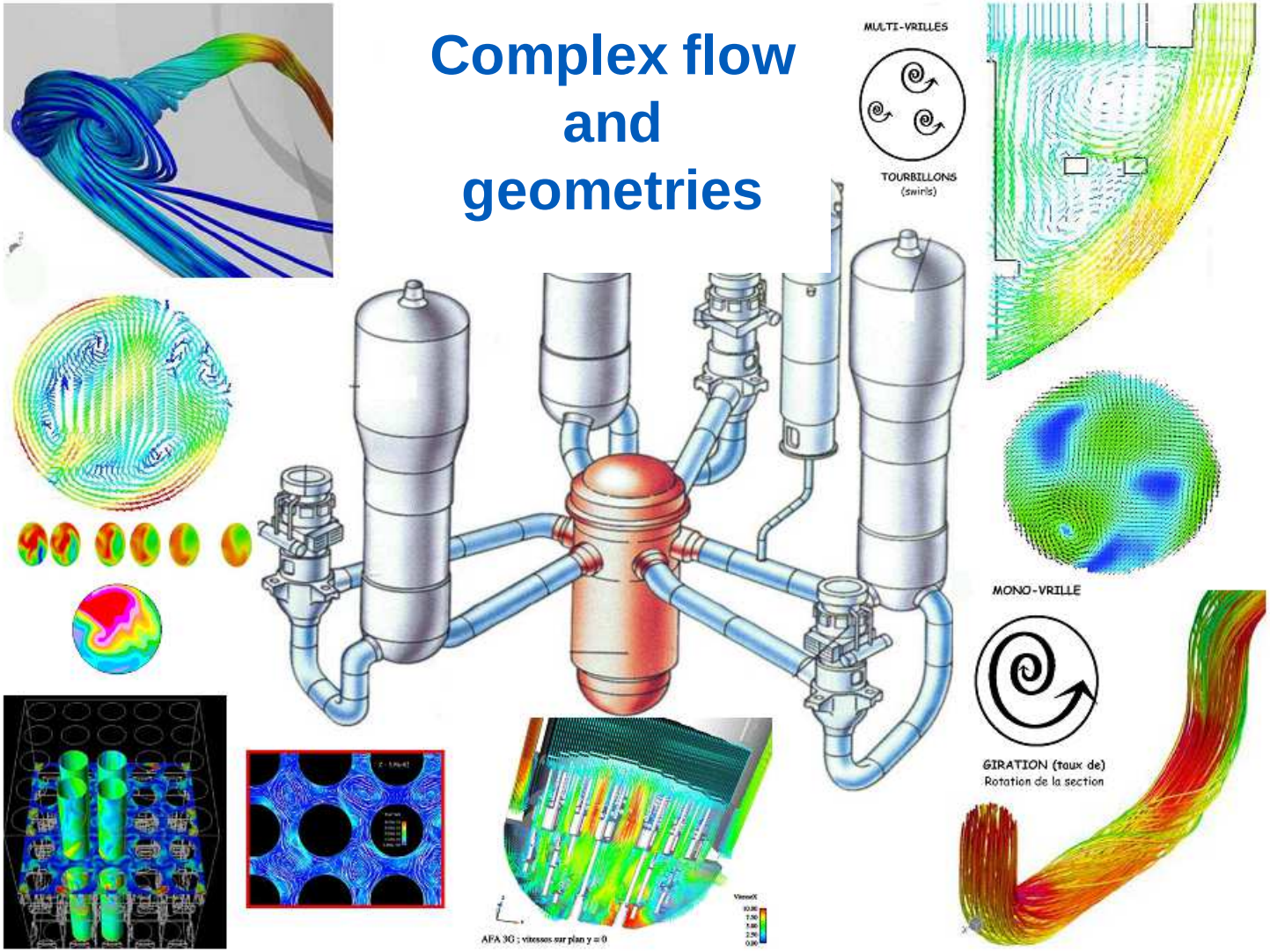
System (RELAP, CATHARE,..)

Component (COBRA, THYC,..)

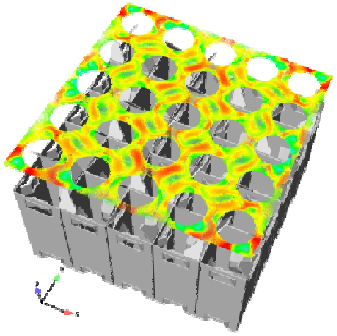
CFD (Star CCM, Code Saturne,..)

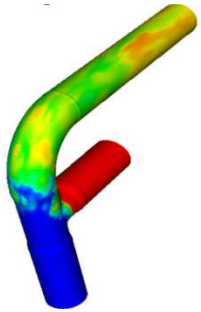
Direct Numerical Simulation

Focus on CFD (local scale)

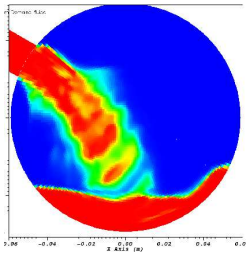


T/H codes: Developement at EDF

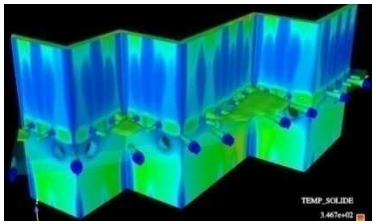




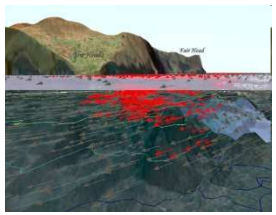
- **Code_Saturne**
  - General usage single phase CFD, plus specific physics
  - Property of EDF, open source (GPL)
  - http://www.code-saturne.org

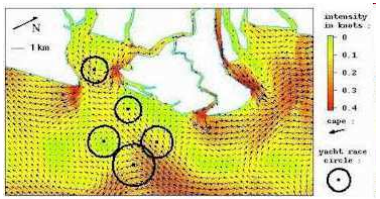


- **Neptune-CFD**
  - Multiphase CFD, esp. water/steam
  - Property of EDF/CEA/AREVA/IRSN (proprietary)



- **SYRTHES**
  - Thermal diffusion in solids and radiative transfer
  - property of EDF, open source (GPL)
  - http ://rd.edf.com/syrthes



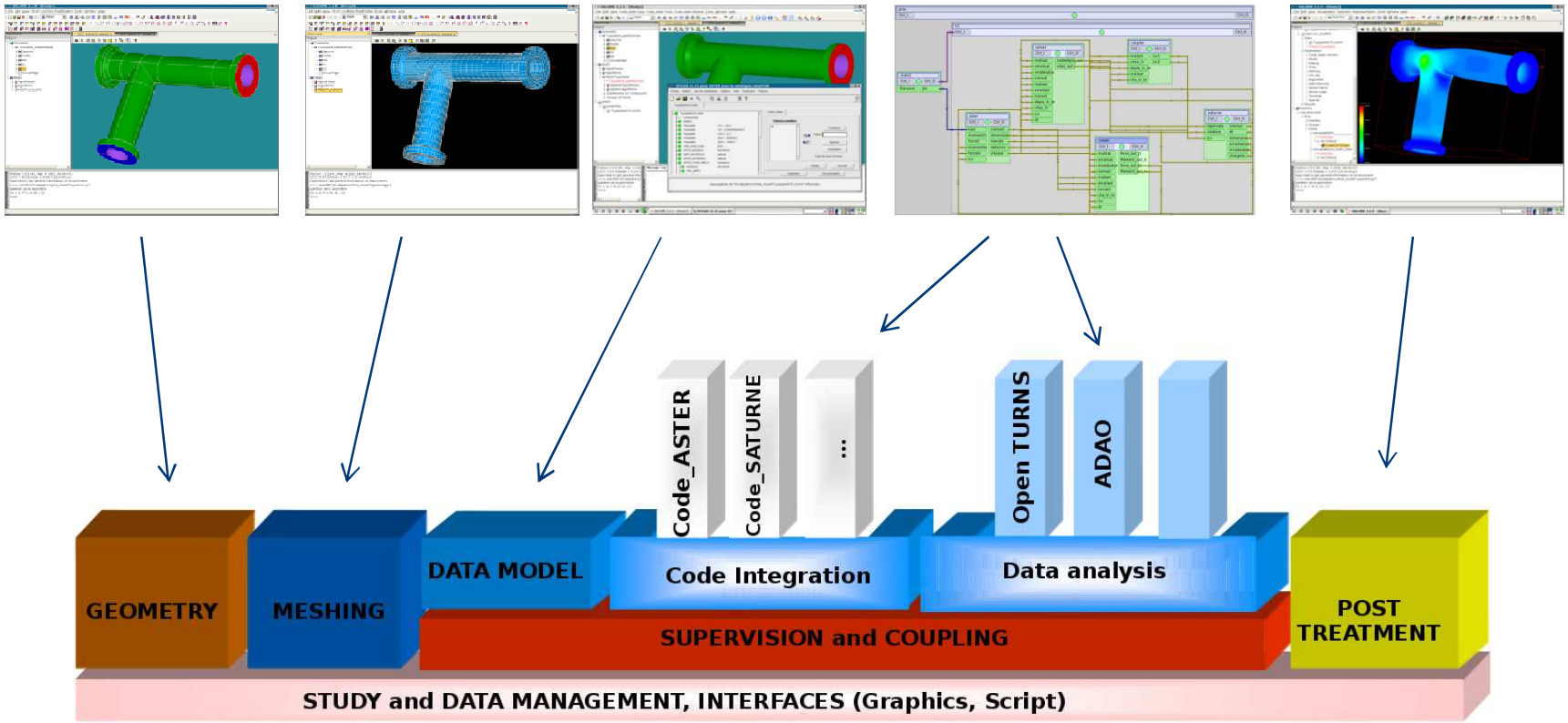


- **TELEMAC system**
  - **Free surface flows**
  - **Many partners, mostly open source (GPL, LGPL)**
  - http://www.opentelemac.org

And many others: neutronics, electromagnetics, structural mechanics, component codes, system codes, …

Interoperability -SALOME

- **SALOME is**
  - an EDF-CEA development
  - Opensource: http://www.salome-platform.org



Applications based on SALOME for nuclear energy

- **EDF and CEA are integrating their scientific codes in SALOME in order to obtain a common simulation framework for their applications**
- **Each application provides a pre/post processing and computation environment integrated in SALOME platform**

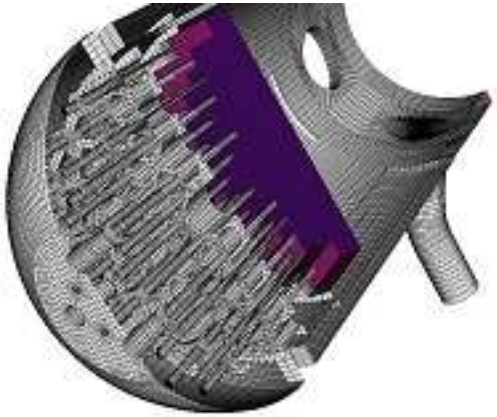
Thermal-Mechanics	Thermal-Hydraulics
Neutronics	Radioprotection
Electromagnetism	Materials
Nuclear Fuel science	Waste repository

Integration platform

SALOME

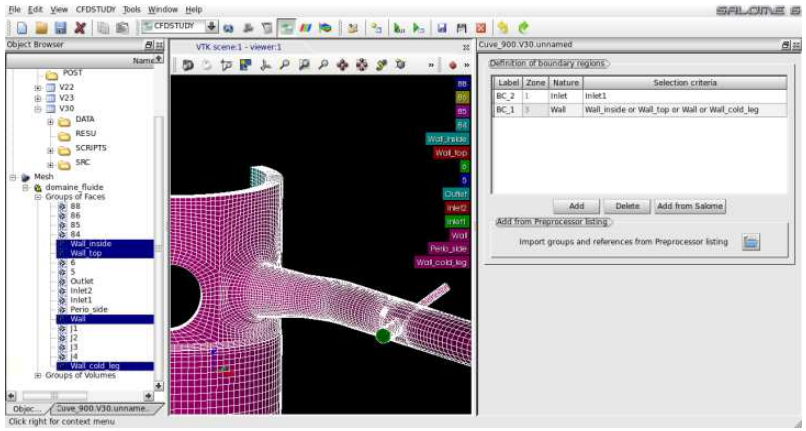
(pre/post and supervision)

Code_Saturne
EDF's general purpose CFD software



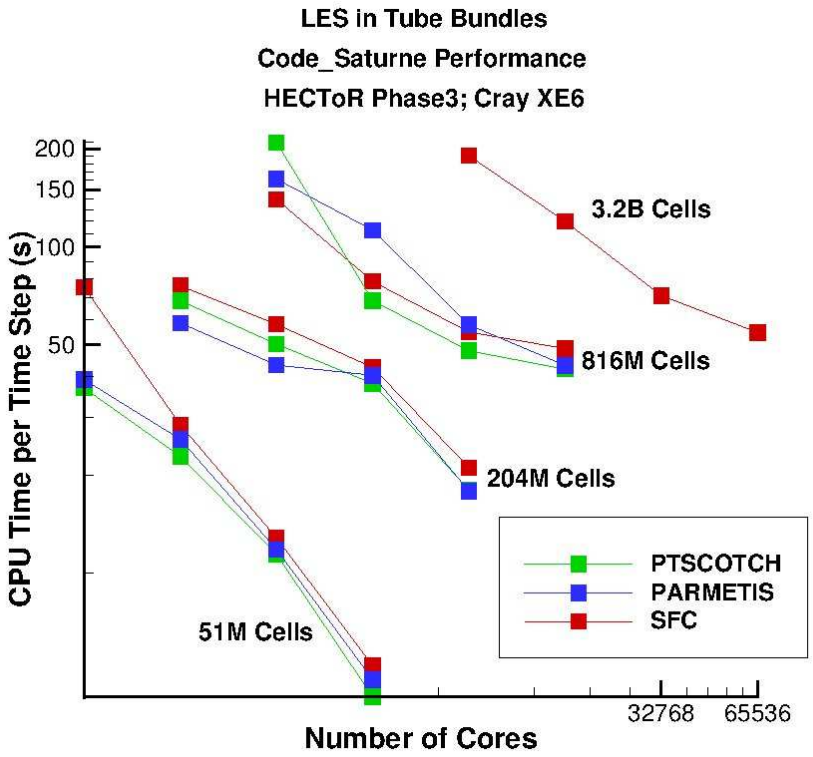
- **Technology**
  - **Co-located unstructured finite volume, predictor-corrector method**
  - **450 000 lines of code,**

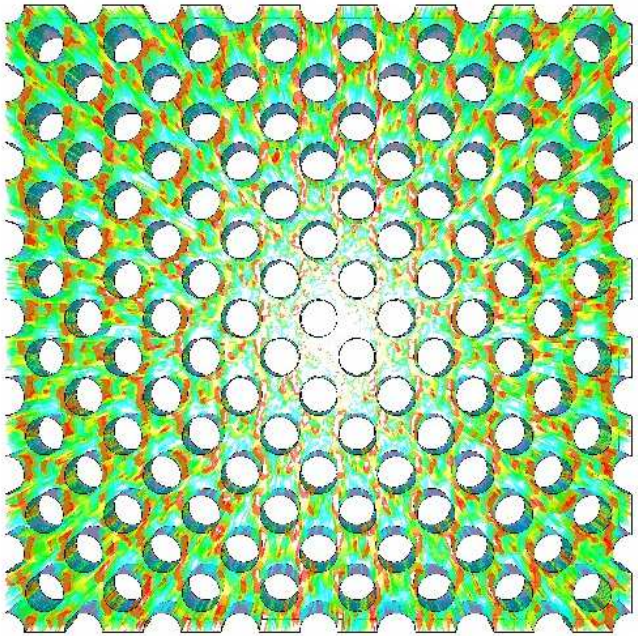
- **Physical modeling**
  - **Laminar and turbulent flows: k-ε, k-ω SST, LES**
  - **Radiative transfer**
  - **Lagrangian module for particles tracking**
  - **Rotor / stator interaction for pumps modeling**
  - **Conjugate heat transfer (SYRTHES & 1D)**
  - **Common structure with NEPTUNE_CFD (2phase Flow) for Eulerian multiphase flows**
  - **Accepts large range of unstructured meshes with arbitrary interfaces**
    - **generated with SALOME, STAR-CCM+, ANSYS Meshing, GMSH, GAMBIT, …**
  - **Coal, heavy-fuel and gas combustion, Atmospheric modeling**



Scalability of *Code_Saturne*

- Scalability as a function of mesh size
  - here, comparing partitioning options
  - At 65 000 cores and 3,2 billion cells, about 50 000 cells / core



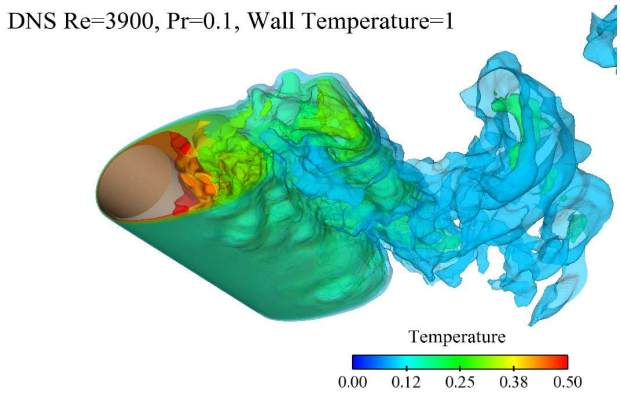


Experiment of Simonin and Barcouda.

2-D section: 100,040 cells; 3rd direction: 128 layers -> 13M cells

High Performance Computing with *Code_Saturne*

- *Code_Saturne* used extensively on HPC machines
  - EDF clusters (IBM Idataplex, Blue Gene/Q)
  - CCRT calculation center (CEA based)
  - PRACE machines
    - Archer (EPCC), Jugene (FZJ), Curie (GENCI)
  - DOE machines (through INCITE access)
    - Jaguar (ORNL), Mira (ANL)



- *Code_Saturne* used as reference in PRACE European project
  - reference code for CFD benchmarks on 6 large European HPC centers

APPLICATIONS (see animations)

- Pressurized Thermal Shock
- Flow downstream of a mixing grid
- Boron Dilution

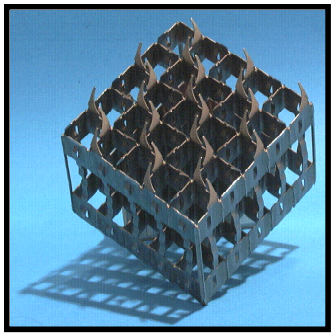
NEPTUNE_CFD: Multi-phase local CFD

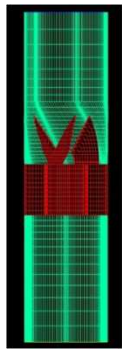
EDF CEA IRSN AREVA

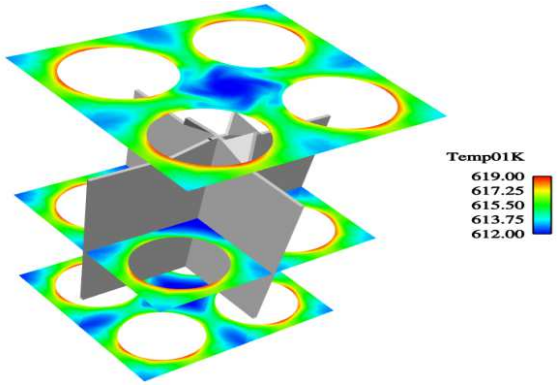
NEPTUNE

INDUSTRIAL ISSUES CONCERNED WITH TWO PHASE FLOWS (1)

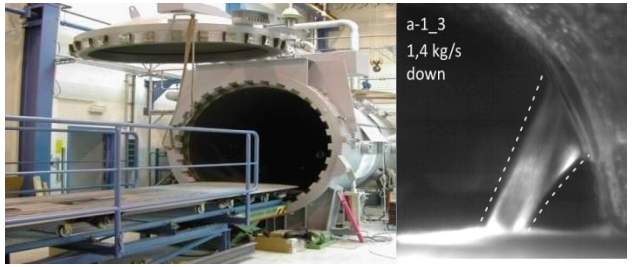
Heat Flux for PWR cores



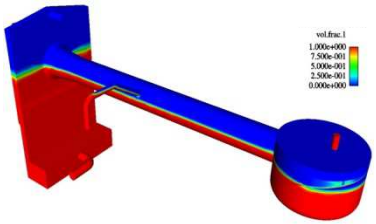


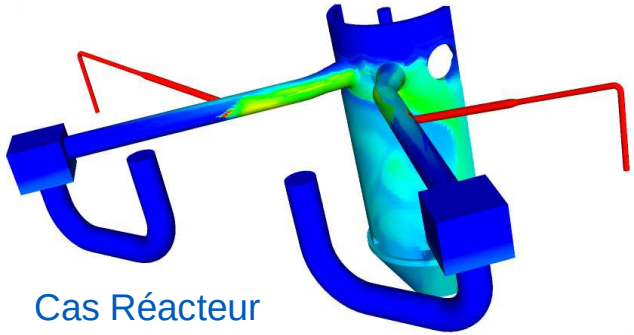


Pressurized Thermal Shock



Expérience TOPFLOW

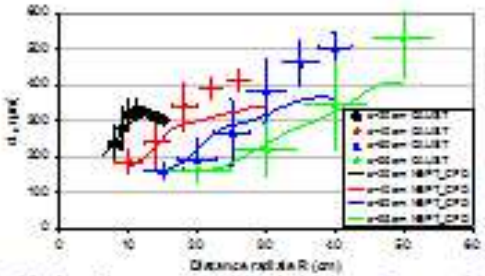


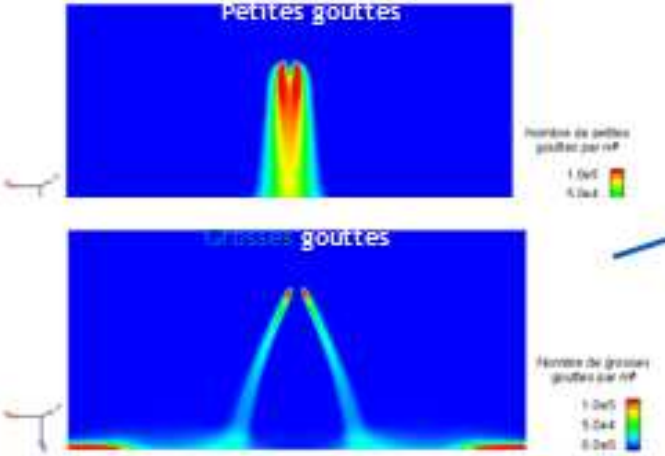


Cas Réacteur

INDUSTRIAL ISSUES CONCERNED WITH TWO PHASE FLOWS (2)

Analysis of Mitigation Means for Severe Accidents (Sprinklers, Recombiners)

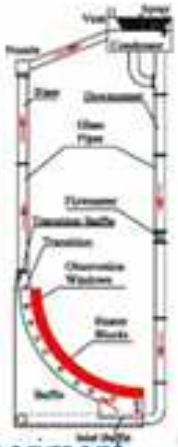


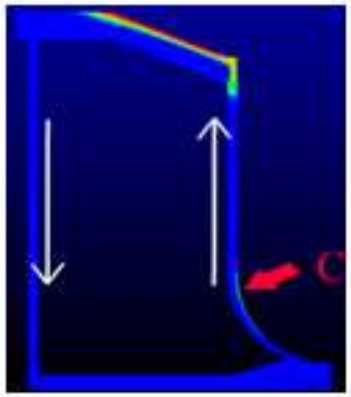


Validation test-case for droplet flows

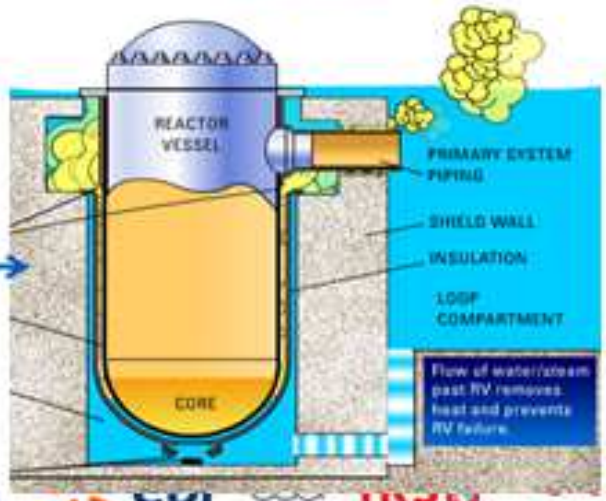
Reactor case

Analysis of IVR mitigation means



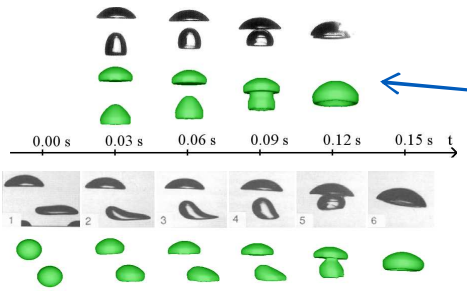


ULPU Experiment
Validation test case for natural circulation



NEPTUNE AREVA

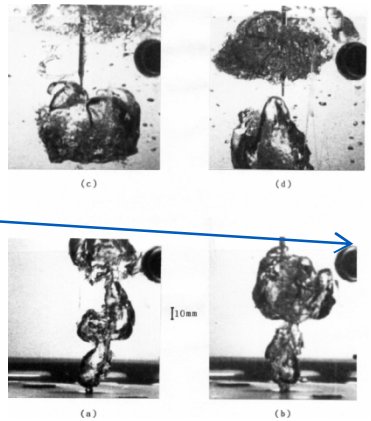
Vibration in Steam Generator => all range two phase flows

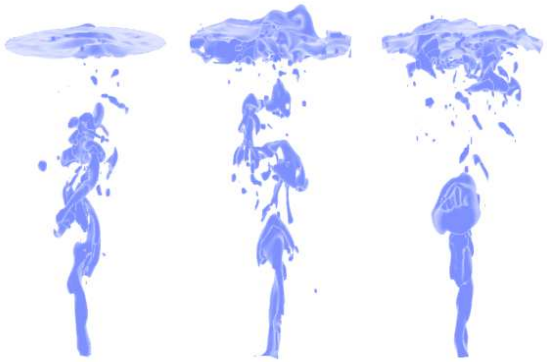


Comparison between the predicted coalescence phenomena (in green) and the experimental observations for in line and oblique two bubble rising

Validation analytique

Validation de régime d'écoulements plus complexe



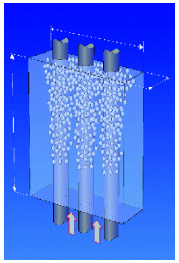


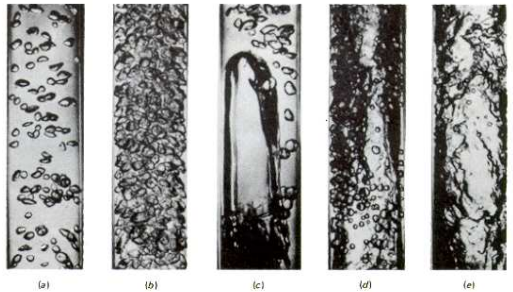
Overview of NEPTUNE_CFD

- Development team: EDF and CEA
  - Development, validation, maintenance, installation, training, hot-line
  - Pioneering applications

- Users
  - EDF, CEA, IRSN, AREVA-NP
  - European project partners (NURESIM=>NURISP,=>NURESAFE)
  - Academic collaborations (IMFT)

- Main features (current version: 1.2)
  - 3D and local two-phase flow analysis
  - Generalized multi-field model
  - Physical models
    - Turbulence (k-ε and RSM)
    - Interfacial area and polydispersion models
    - Set of models for boiling bubbly flows
    - Set of models for stratified steam-water flows
    - Set of models for droplet flows
    - Conjugate heat transfer

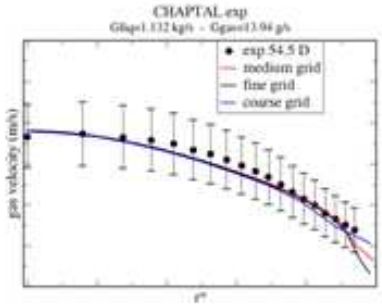


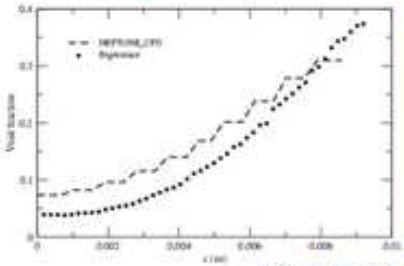


Verification & Validation strategy

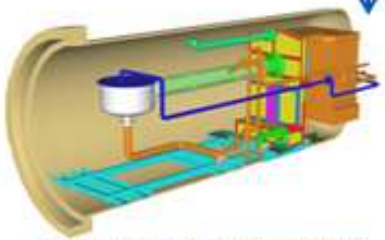
- Physical and numerical benchmarks
  - Aiming to show the ability to handle a broad range of situations
  - Classical benchmark and more complex cases
  - Verification tests
- Physical validation for boiling bubbly flows (for DNB)
  - Existing data for adiabatic and boiling bubbly flows
  - Comprehensive experimental programs
    - **Adiabatic bubbly flow (CHAPTAL, in progress)** **tube**
    - **Adiabatic bubbly flow** **bundle+grid**
    - **Condensation (TESS, in progress)** **tube**
    - **Convective boiling flow, refined** **tube**
    - **Global** **tube**
    - **Global** **bundle+grid**
- Physical validation for PTS-related models
  - Validation on existing experiments
  - Dedicated international program (TOPFLOW-PTS, in progress)
- Validated against several other available data
  - Stratified flow
  - Bubbly flow

CHAPTAL (gas velocity profile)





DEBORA (void profile)



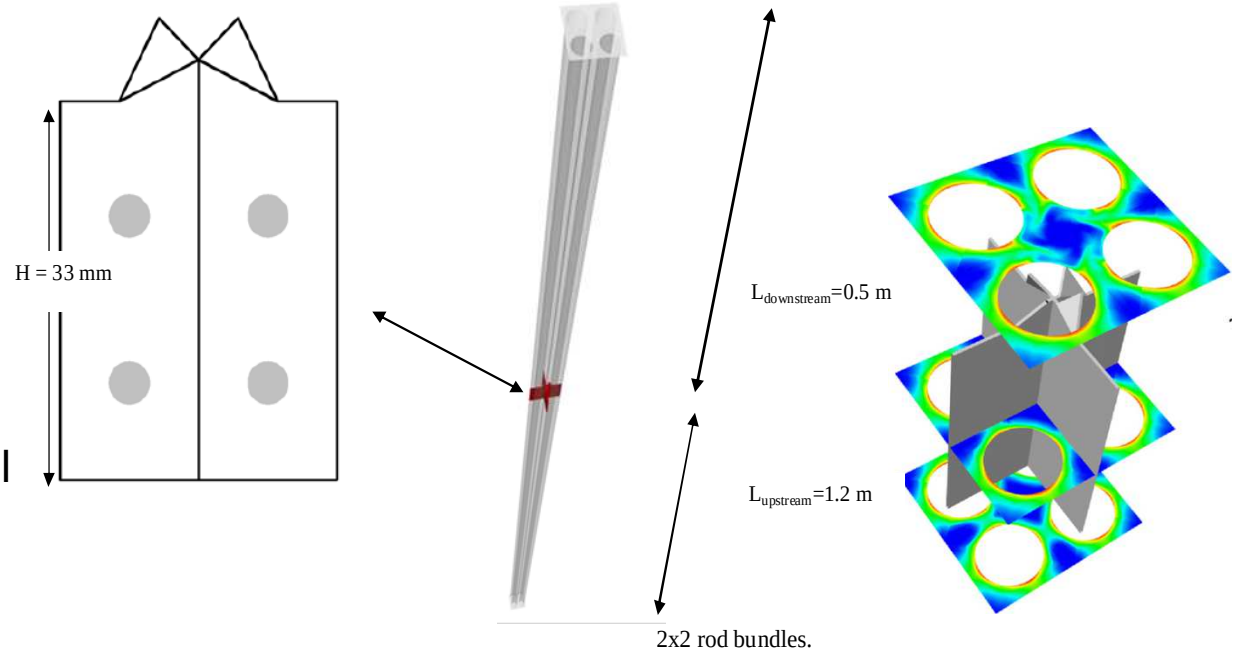
TOPFLOW-PTS experiment

Application to mixing grid analysis

- Objectives
  - Gain knowledge about the two-phase boiling flow through a spacer grid with mixing vanes
  - Assess the impact of turbulence models on the target variables supposed to be related to DNB (max void fraction at the wall, max wall temperature, mixing efficiency,…)
  - Impact of vane orientation on the target variables

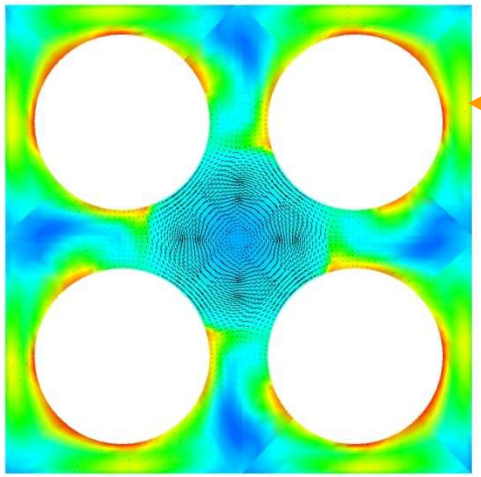
- Configuration
  - 2x2 bundle, simple specer grid
  - PWR core conditions penalised to cause boiling
    - 155 bar; 330 °C; 3000 kg/m^2/s;1.6 MW/m^2
    - Vapour fraction up to 70%

- Meshes: 1.5 to 7.6 Mcell



Application to mixing grid analysis

- Void fraction and liquid velocity
  - Downstream mixing vanes

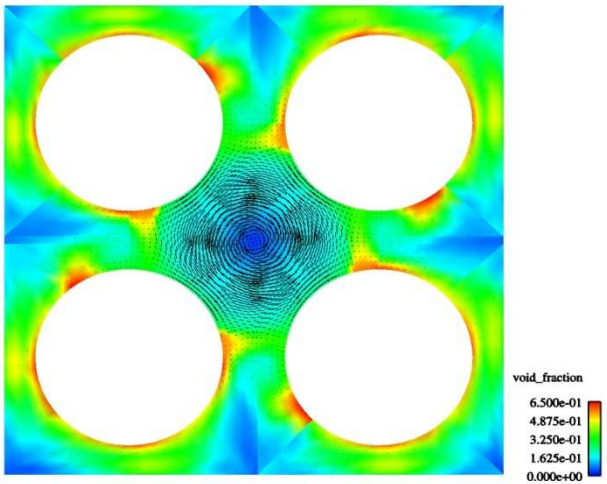


$EVM \quad (K-\varepsilon)$

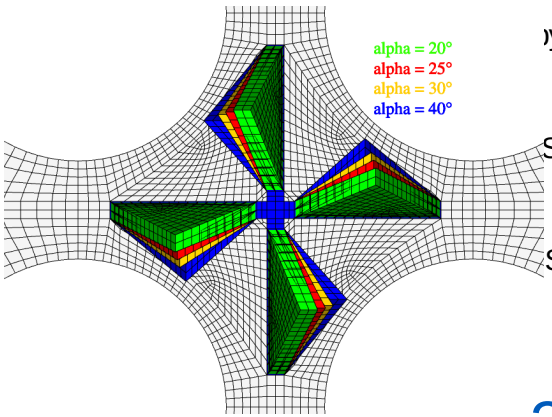
ti-void" effect

2 turbulence

$RSM \quad (R_{ij}-\varepsilon)$



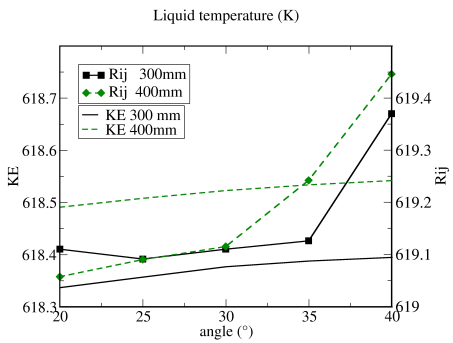
models results



y k-ε

SM

SM

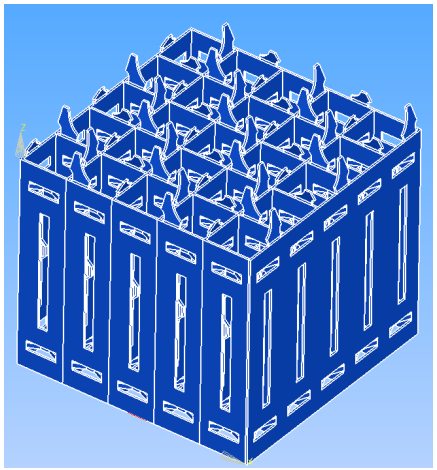


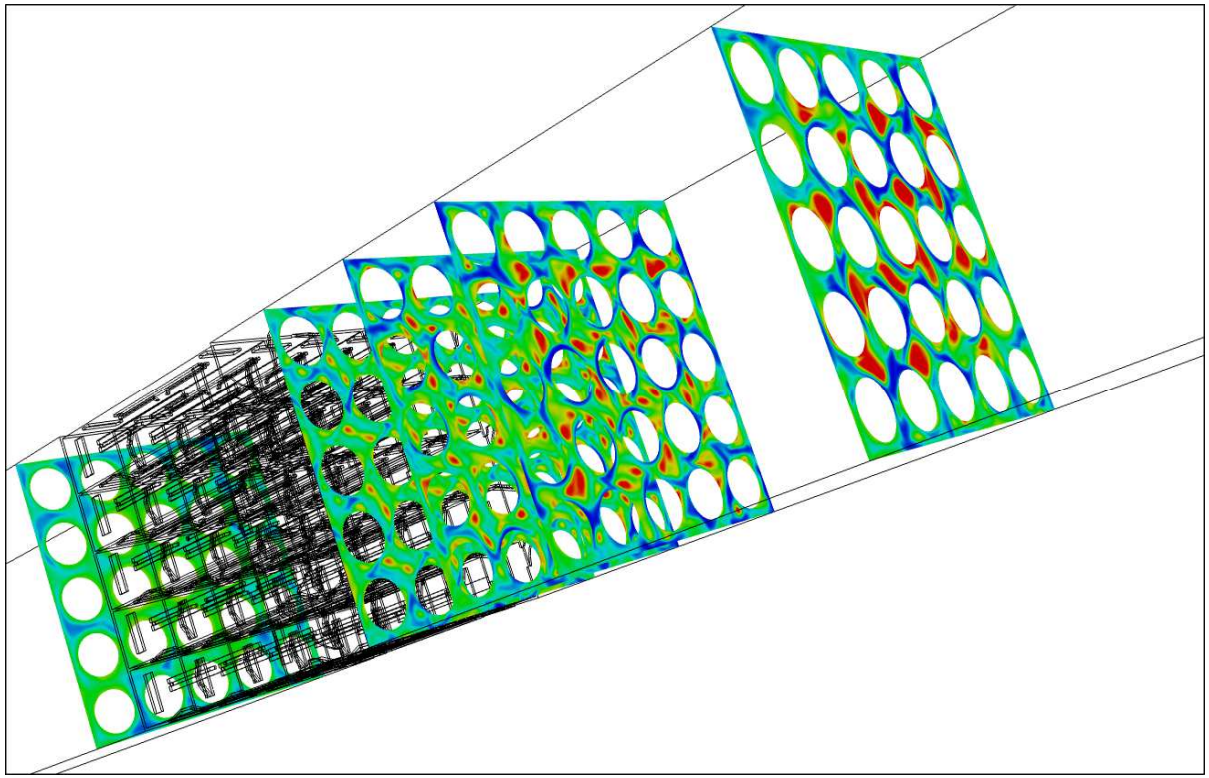
Maximum liquid temperature in a cross-section as a target variable

-> *identification of a minimum around 30°*

Application to mixing grid analysis

- Full length 5x5 bundle with detailed grid ~ up to 800,000,000 cells

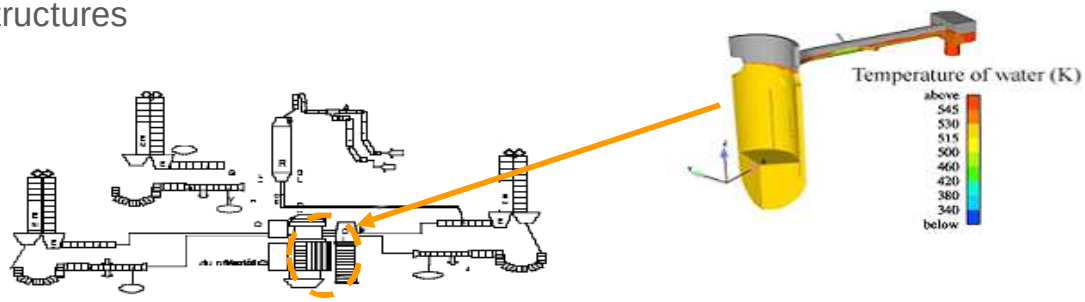




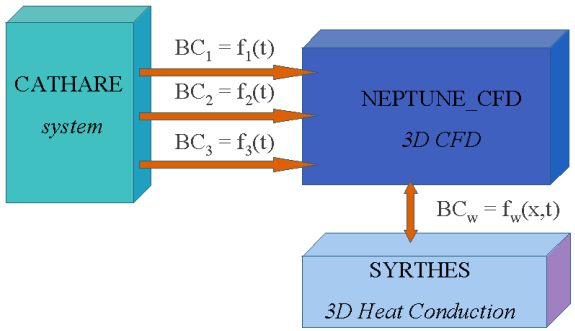
Void fraction map

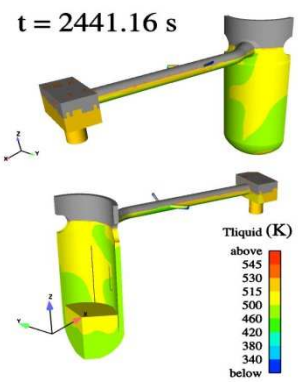
Application to PTS analysis

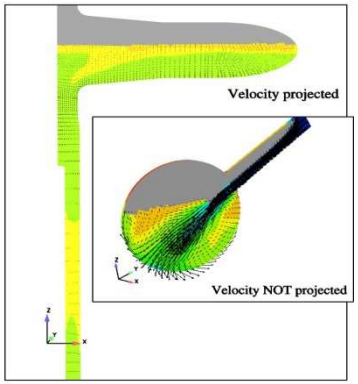
- Reactor application: a multi-scale and multi-physics issue
  - 2 TH scales invoved: **System** and **local CFD** -> handled by chained computations (one-way coupling)
  - 3 physics: **fluid** – **heat transfer in structures** – **fracture mechanics** -> handled by
    - coupled fluid –heat transfer in structures
    - chained to fracture mechanics



- TH step
  - System scale (CATHARE) one way coupling requires
    - same thermodynamics tables if mass transfer is taken into account
    - "compatible" heat & mass transfer closure laws
  - NEPTUNE_CFD coupled to SYRTHES (heat transfer in structures)







Application to 900 & 1300 MW LOCA reactors transient

APPLICATION

European projects : NURESIM (2005-2008) =>NURISP (2009-2011) => NURESAFE (2013-2015)

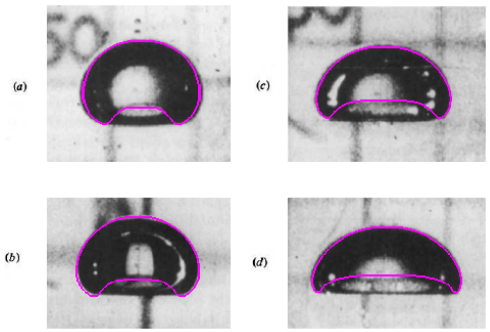
- NEPTUNE_CFD promoted in the framework of the E.U. projects NURESIM, NURISP and NURESAFE now (Thermal-Hydraulics sub-project)
  - 15 partners have worked in two-phase CFD on PTS & CHF with NEPTUNE_CFD

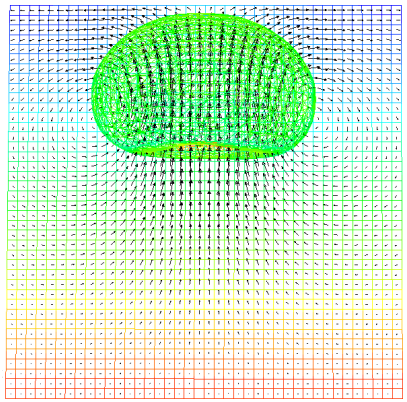
- Fruitful outcome for the NEPTUNE project and NEPTUNE_CFD
  - **Verification**: a more robust code with extended group of european users
  - **Validation**: more than 20 experiments calculated
  - **Benchmarking**: numerous benchmarks with FLUENT & CFX. NEPTUNE_CFD supports the comparison to FLUENT and CFX. e.g. : 3 users mention its good numerical performance
  - **Exchange of experimental data**
  - **Developments** in NEPTUNE_CFD: wall functions, surface tension, …
  - NEPTUNE_CFD gained more at the international level: numerous journal and conference papers
  - Creation of a network on CFD with fruitful technical exchanges

- Examples of valuable contributions from NURESIM partners
  - Horizontal Air-Water Channel (HAWAC) simulated by UCL (University Catholique de Louvain)
  - Use of LES for bubbly flow: DEEN Bubble column simulated by PSI (Paul Scherrer Institute)
  - Simulation of CHF Experiments (LWL) by NRI (Nuclear Research Institute, Czech Republic)

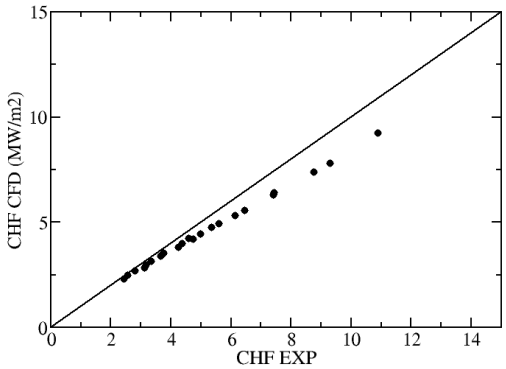
Perspectives

- Enlarge flow regimes capabilities
  - Simulation of large bubbles
  - Slug flow

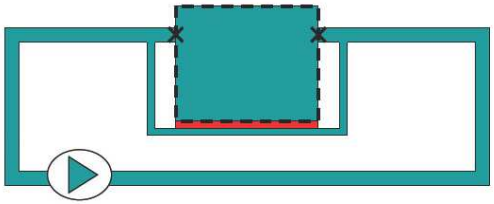




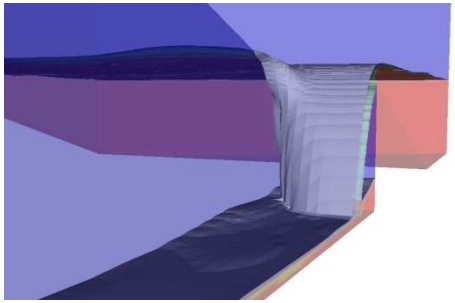
- Improvement of CHF prediction
  - Flow in pipe
  - Flow through mixing grid

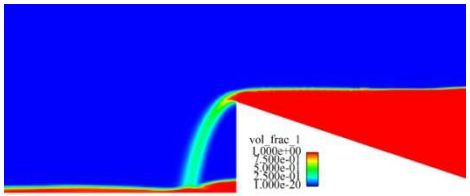


- Coupling NEPTUNE_CFD / CATHARE
  - LOCA applied to PTS issues



- Non nuclear: free surface flow for complex configurations





Thanks for your attention

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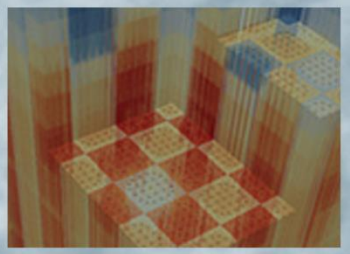
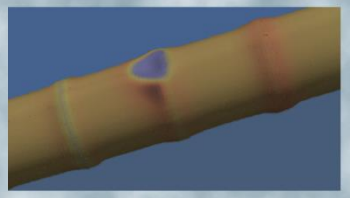
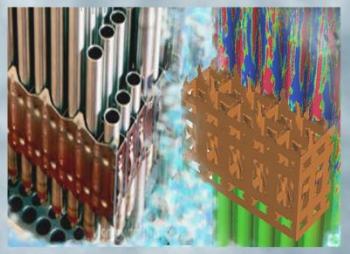
Industry Council Meeting - Update on DNB Modeling and Simulation

Yixing Sung
DNB Challenge Problem Integrator

March 17, 2015
Charlotte, NC

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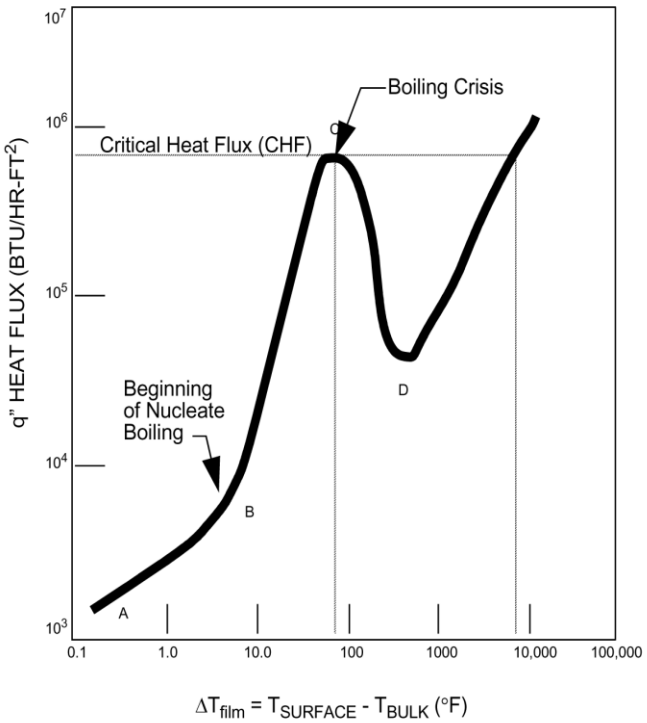
DNB Challenge Problem Progress

- Review of Challenge Problem
- CASL Path Forward
- Accomplishments in Phase 1
- Work in Progress in Phase 2
- Summary

Departure from Nucleate Boiling (DNB)

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

Boiling Curve



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

- Fuel hardware design improvement
  - Higher fidelity of M&S capabilities (multi-phase) to predict fluid and fuel surface conditions and effects of fuel design features (e.g., grid spacer)
  - Applications of advanced data assimilation and uncertainty quantification methods on test design, data collection and analysis
  - Control and optimization of fuel cladding surface morphology and properties during reactor operation
- Margin quantification in accident analysis
  - Multi-scale and multi-physics M&S capabilities
  - Technical basis for DNB-related fuel failure (e.g., DNB during Reactivity Insertion Accident (RIA))

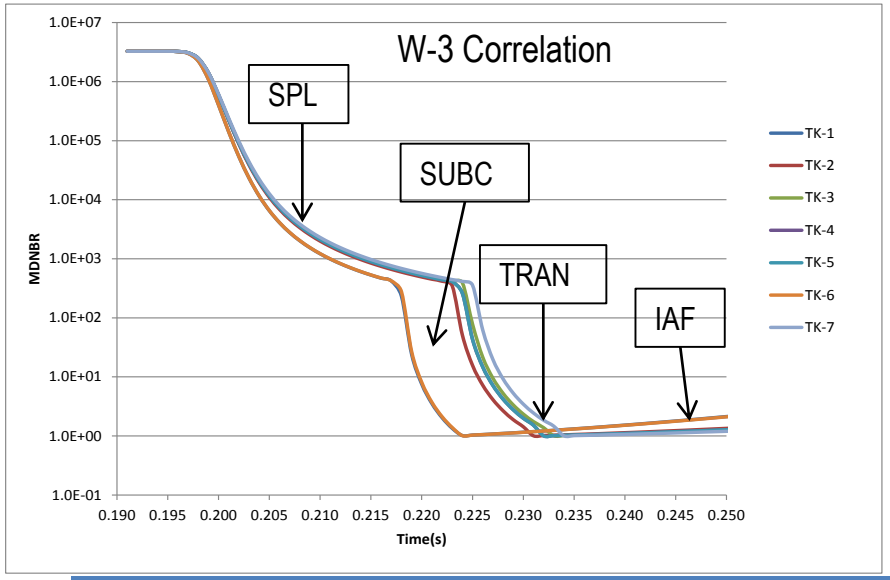
Phase 1 Accomplishments

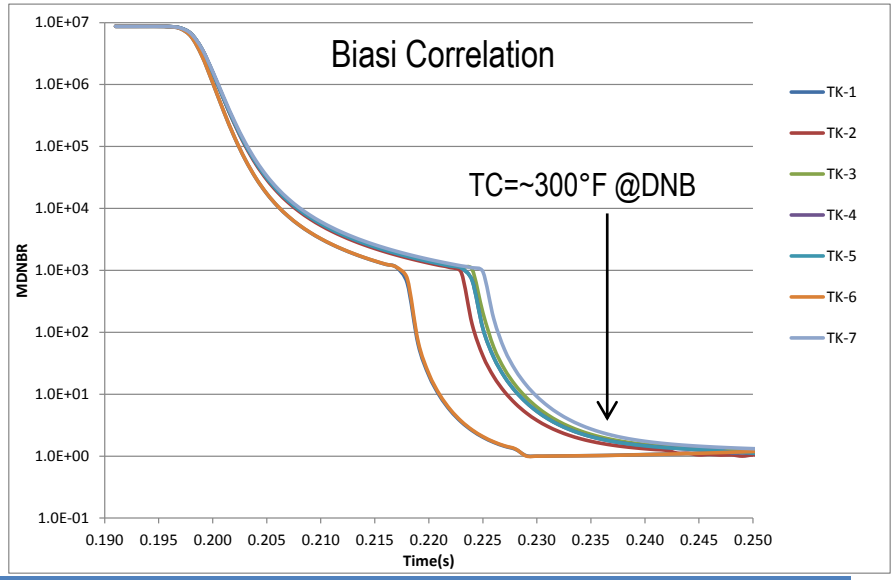
- COBRA-TF (CTF) subchannel code
  - Rod bundle mixing and DNB test simulations
  - RIA experiment simulation
  - Reactor core modeling under DNB limiting conditions (LOF, Steamline Break and RIA)
- Hydra-TH CFD code
  - Rod bundle single-phase mixing initial study
- VUQ study initiated on code and CP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

NSRR RIA Experiment –Results and Analysis

- Onset of DNB, indicated by the Minimum DNB ratio (DNBR)

$$MDNBR = \frac{q''_{CHF}}{q''_{actual}} \leq 1.0$$

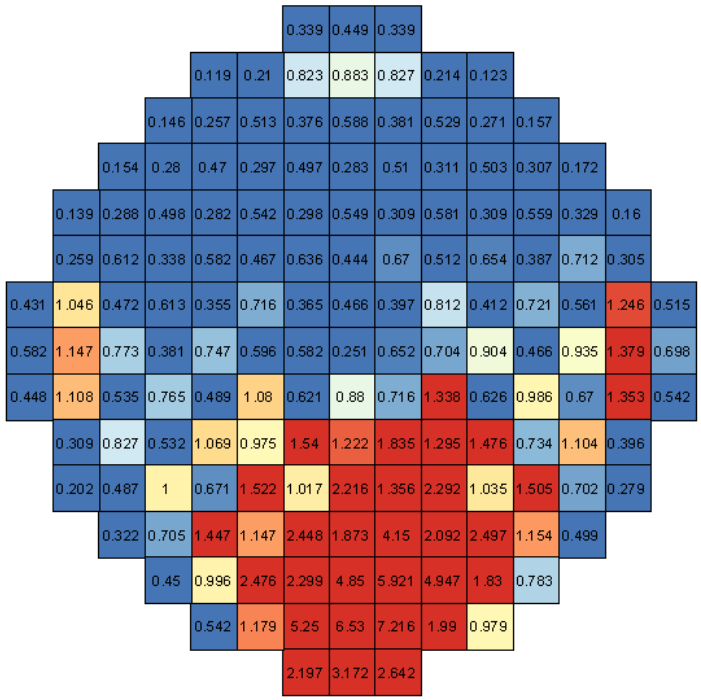


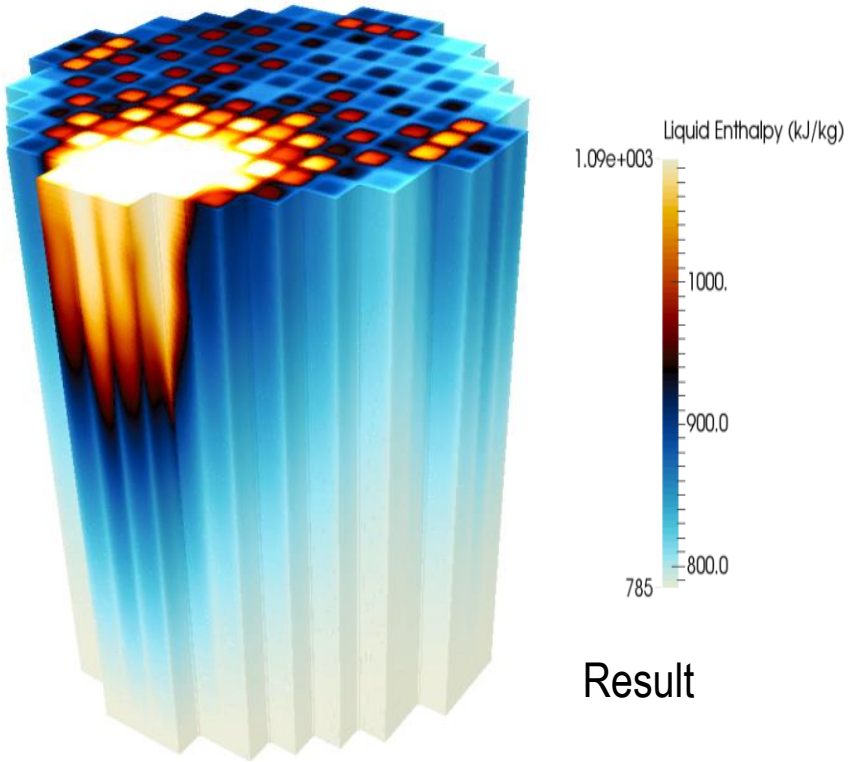


- DNB occurrences predicted for all cases (DNBR ≤ 1)
- Only 2 cases experienced fuel cladding failure (not DNB related)
- DNBR is a poor indicator of fuel cladding failure during fast transients

CTF Simulation of Low Flow Steamline Break

Input





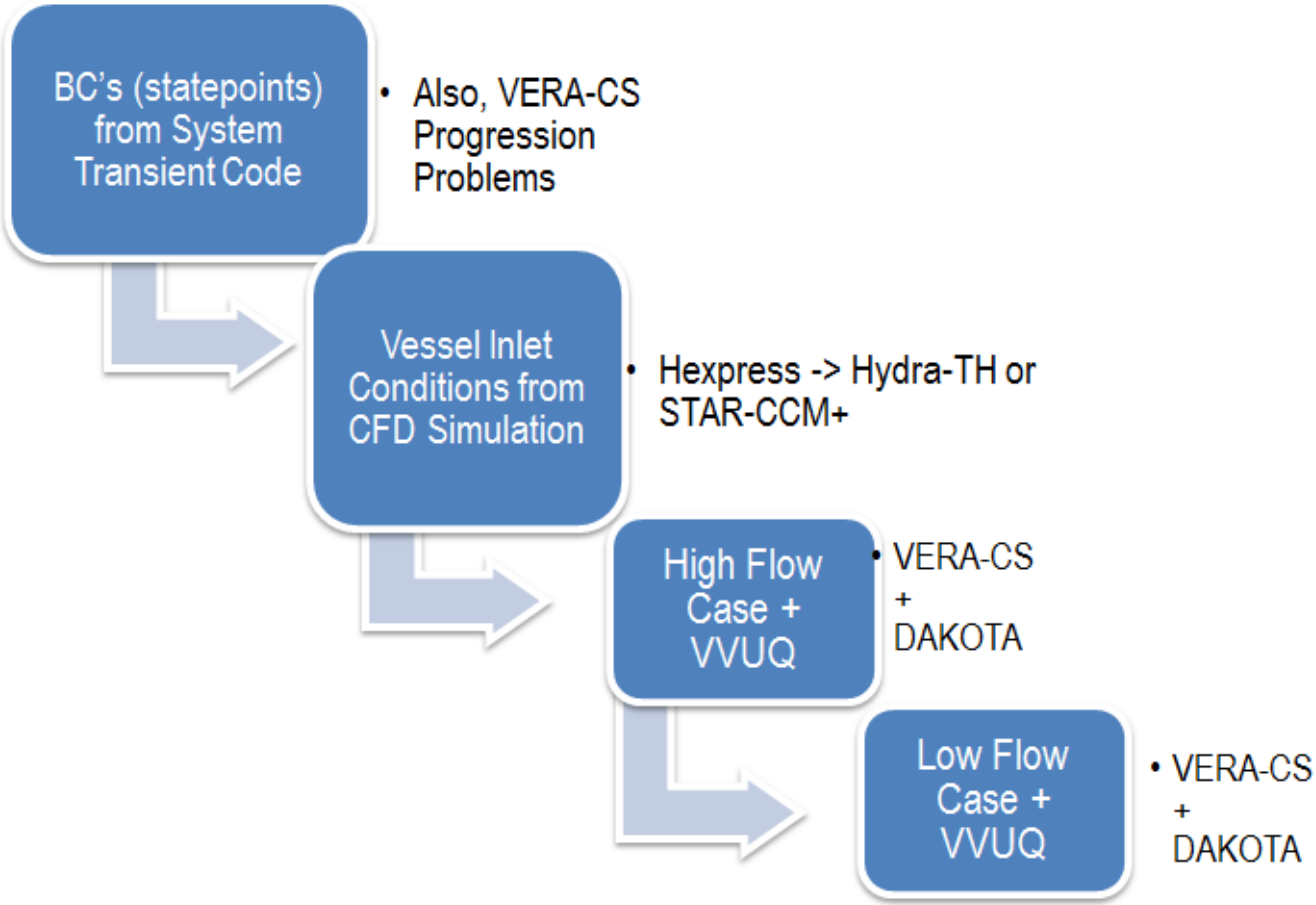
Result

- PWR DNB event - steamline break without offsite power
- Large model of reactor core simulating asymmetric distributions
- ~45000 channels x 151 axial nodes = ~6.8M control volumes
- Simulation of DNB limiting time step (low pressure/low flow)
- High void predictions in hot channels without VERA neutronic coupling

Work in Progress

- Apply coupled neutronic and T/H code system VERA-CS for evaluating core response to DNB
  - Main steamline break limiting case study (steady state)
- Apply CFD software for evaluating fuel bundle DNB-related performance
  - Turbulent mixing (single phase flow)
  - DNB occurrence (two-phase flow)
- Learn and apply advanced UQ technology to quantify uncertainty and conservatism
- Pursue complete success of Desirable Level and Ultimate End Game in Phase 2
  - Coupled VERA-CS code system with kinetic and VUQ capabilities
  - Application of multi-physics and high fidelity modeling and simulation and VUQ capabilities to resolve DNBR margin prediction as an unknown barrier in safety analysis

Work in Progress



VERA Application to PWR Steamline Break

Summary

- Phase 1 accomplishments include CASL T/H tool applications to multi-scale modeling and simulations
  - Test bundles
  - Fast transient
  - Reactor core response

- In Phase 2 Work is in progress following Implementation Plan
  - Applications of multi-physics coupled code system (VERA-CS)
  - VVUQ study
  - Research and development on high resolution (CFD) DNB modeling

DNB Modeling & Simulations

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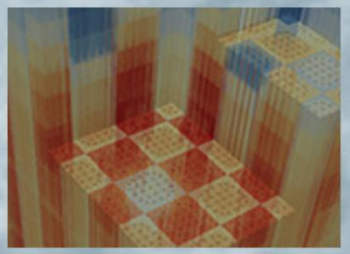
Thermal Hydraulics Methods (THM) Update

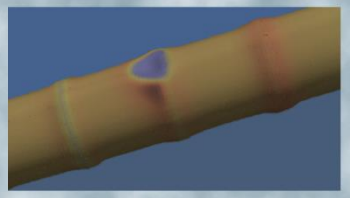
The Closure (CLS) Project

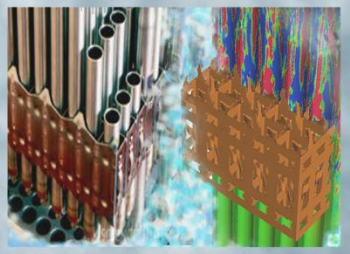
Emilio Baglietto (MIT)

THM Deputy Lead, CLS Project Lead

Mark Christon, Markus Berndt (LANL)







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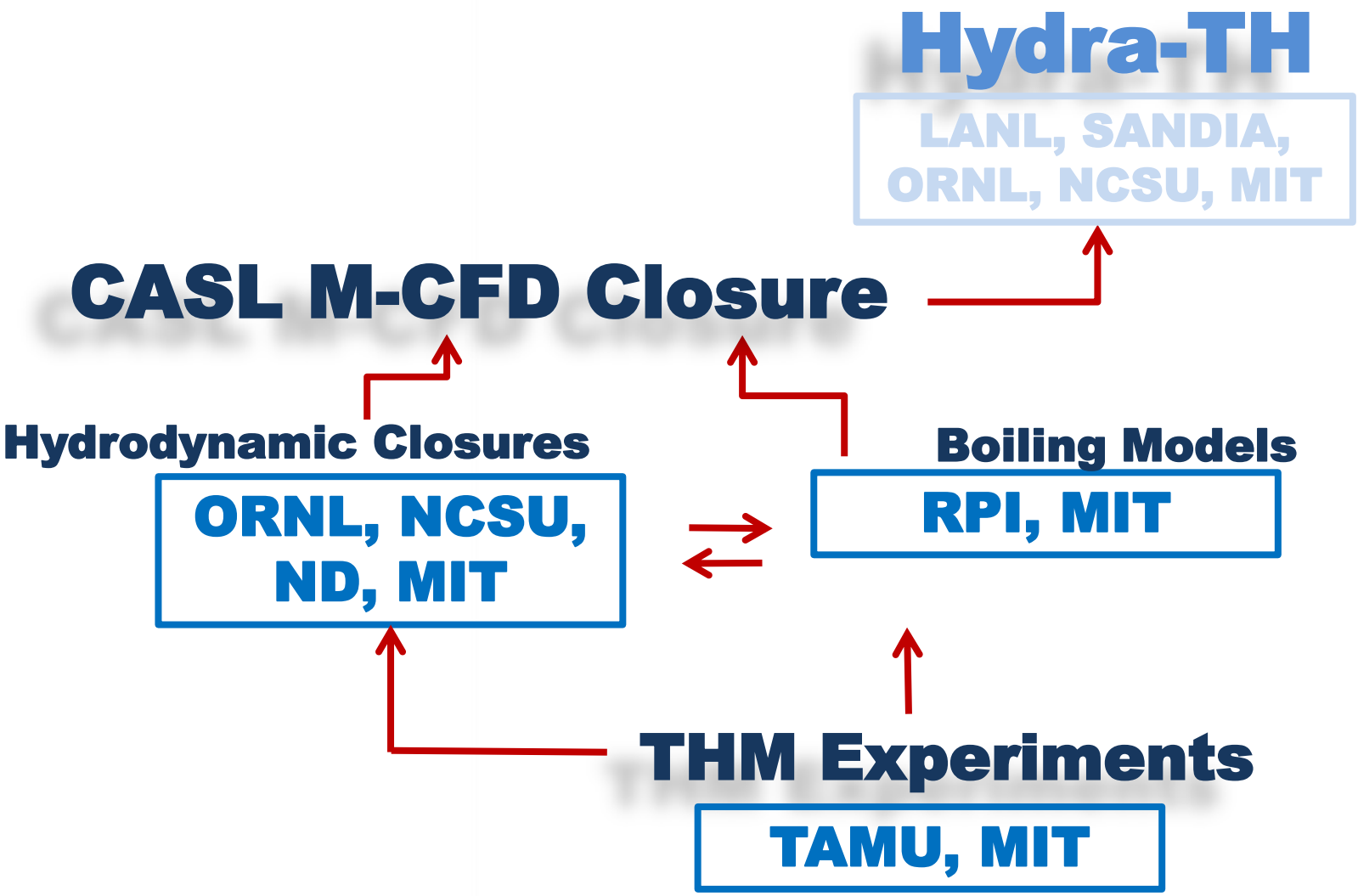
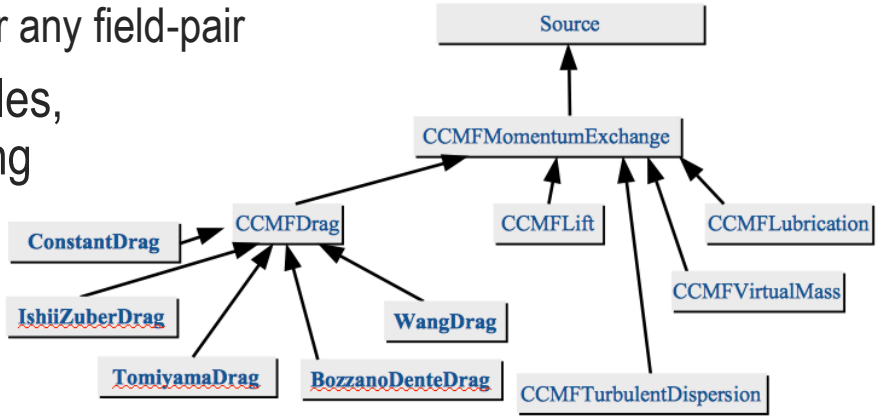
The CLS Team Roles



Multiphase Flow Target

- Generic N-field multiphase capability that is extensible for:
  - Lahey's 4-field model
  - Gen-I, Gen-II boiling closures (and beyond) for DNB and CHF calculations
  - BWR-regimes with breakup/coalescence effects, interface effects on large consolidated bubble regions
  - Accommodating new turbulence models beyond the "hacked" version of k-ε currently used, e.g., the BHR model
  - Well-behaved phasic volume-fraction preservation (i.e., the GCL)
- High-performance and scalable, e.g., beyond the demonstrated 36,000 cores
- Generic and virtual interface for phasic-exchange source terms
  - User can specify different closure for any field-pair
- Integrated IAPWS-IF95/97 steam tables, general EOS interface of other working fluids
- Verified algorithms to the extent possible with CASL resource constraints



Multiphase Status – Two Algorithms for the p-α-ρ Update

- Requires fully-implicit method, i.e., an outer iteration, inner p-α-ρ solution
- Option-1: The Simple PPE Approach (Performance)
  - Uses: Source-term anti-symmetry $\sum_k \Gamma_k$, and $\sum_k a_k = 1$

$$\text{Macro-Density}: \hat{\rho}_k = a_k \rho_k$$

$$\text{Lagrange Multiplier}: \lambda = q \Delta t\, dp$$

$$\nabla \cdot \nabla \lambda = \sum_k \nabla \cdot \left(\hat{\rho}_k^{n+1*} v^{n+1*} \right) + \frac{(1-q)}{q} \sum_k \nabla \cdot \left(\hat{\rho}_k^{n} v^{n} \right) + \frac{1}{q} \sum_k \left\{ \frac{\hat{\rho}_k^{n+1*} - \hat{\rho}_k^{n}}{\Delta t} \right\}$$

$$\rho_k^{n+1*} = \rho_k(p^*, T_k^{n+1*})$$

$$a_k^{n+1} = \frac{\hat{\rho}_k^{n+1*}}{\rho_k^{n+1*}}$$

May require renormalizing volume fractions

- Option-1: The CartaBlanca Approach
  - Guarantees: $\sum_k a_k = 1$

$$q^2 \Delta t^2 \sum_k \left\{ \frac{\nabla \cdot a_k^{n+1*} \nabla p^{n+1*}}{\rho_k^{n+1*}} \right\} = \sum_k \left\{ \frac{\hat{\rho}_k^{n+1*}}{\rho_k^{n+1*}} \right\} - \sum_k \left\{ \frac{\hat{\rho}_k^{n}}{\rho_k^{n+1*}} \right\} + q \Delta t \sum_k \left\{ \frac{\nabla \cdot \left(\hat{\rho}_k^{n+1*} v_k^{n+1*} \right)}{\rho_k^{n+1*}} \right\} + (1-q) \Delta t \sum_k \left\{ \frac{\nabla \cdot \left(\hat{\rho}_k^{n} v_k^{n} \right)}{\rho_k^{n+1*}} \right\} +$$

$$q^2 \Delta t^2 \sum_k \left\{ \frac{\nabla \cdot a_k^{n} \nabla p^{n}}{\rho_k^{n+1*}} \right\} + \Delta t \sum_k \left\{ \frac{q \Gamma_k^{n+1*} + (1-q) \Gamma_k^{n}}{\rho_k^{n+1*}} \right\}$$

$$\rho_k^{n+1*} = \rho_k(p^*, T_k^{n+1*})$$

$$a_k^{n+1} = \frac{\hat{\rho}_k^{n+1*}}{\rho_k^{n+1*}}$$

Multiphase Flow in Hydra-TH

The Goal for FY15 (by Oct 2015)

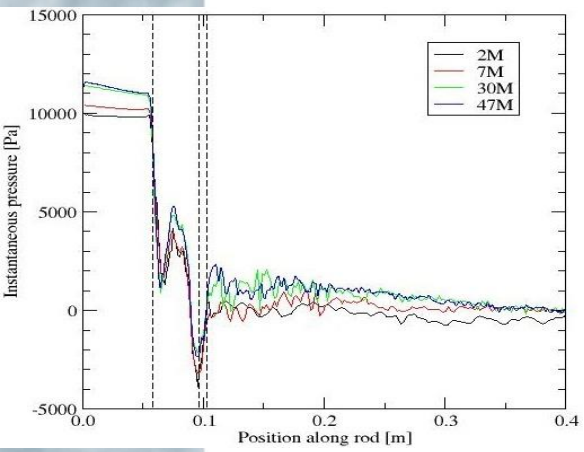
- Goal for Capabilities by the end of PoR-11 (Oct 2015)
  - Complete fully-implicit algorithm with lift/drag and assess on verification problems (constant density)
  - Steam table integration, extensions and cleanup of Material class
  - Add wall-lubrication, virtual-mass, turbulent-dispersion to momentum-coupling
  - Add mass-, and energy-exchange classes
  - Integrate k-ε model with Lahey mod's
  - Testing and initial verification studies

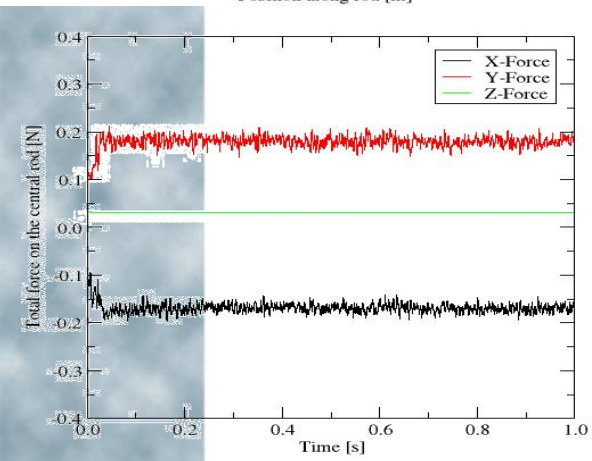
- Staffing
  - Christon –technical direction, completion of multiphase algorithm
  - Bauer, Kitware – close range development support
  - Berndt – consulting, logistics, coordinate dev team
  - Nadiga – multiphase and finishing work on Hydra-MAMBA deployment
  - Stagg – Multispecies prototype, conjugate heat transfer, multiphase
  - Zhang – formulation of boiling closures, consulting

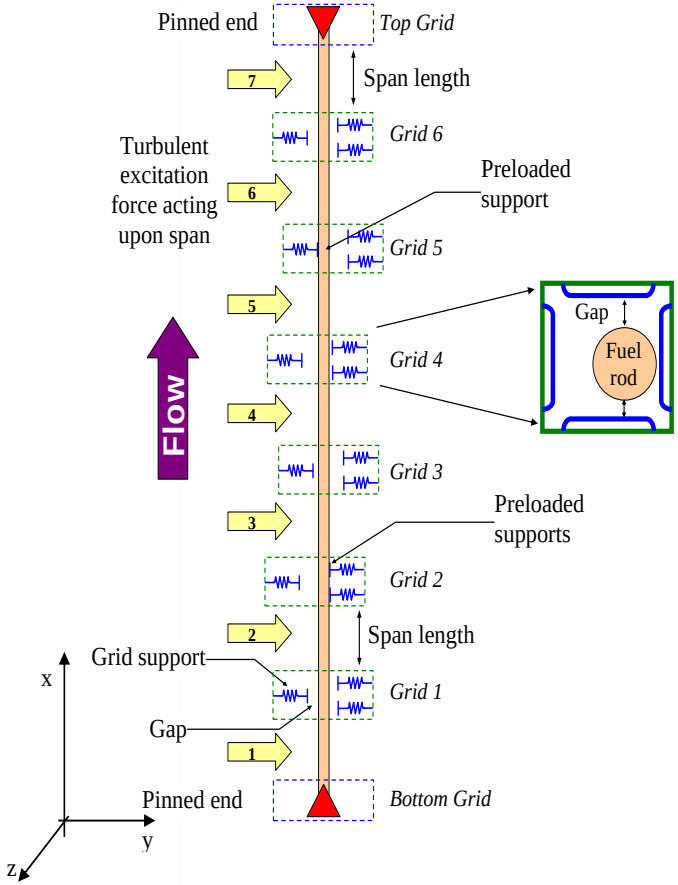
The Hydra-TH Single Phase Capability is Relatively Mature

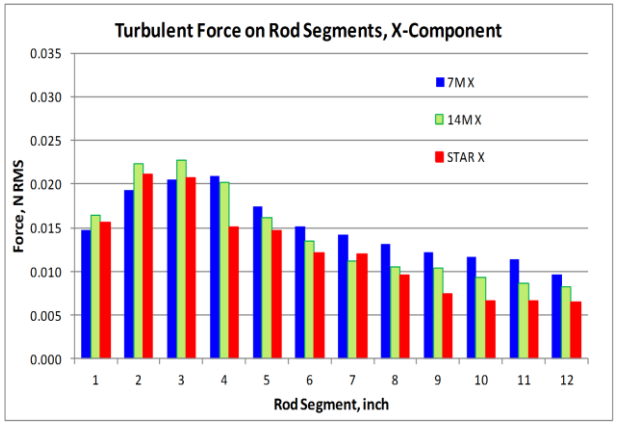
More to do in V&V, turbulence model breadth, compute efficiency

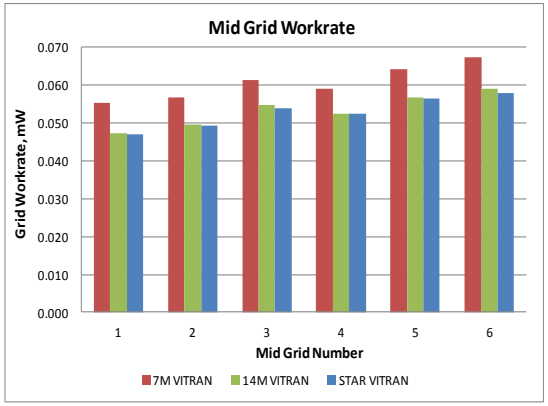
- Pressure Profiles and Rod Forces are extracted from Hydra-TH for the 3x3 Rod Bundle
- The data are used as input to VITRAN to compute rod acceleration/displacement
- 7 to 14M meshes required for reasonable fidelity in design analysis ~ 8 – 24 hour calculations











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

Integration of Surface Chemistry Capability as Sub-Grid model in Hydra-TH

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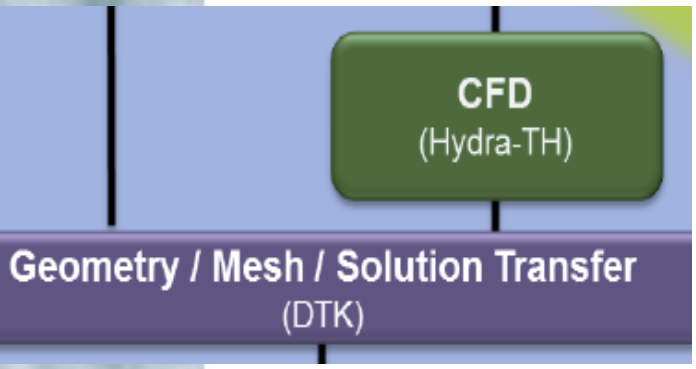
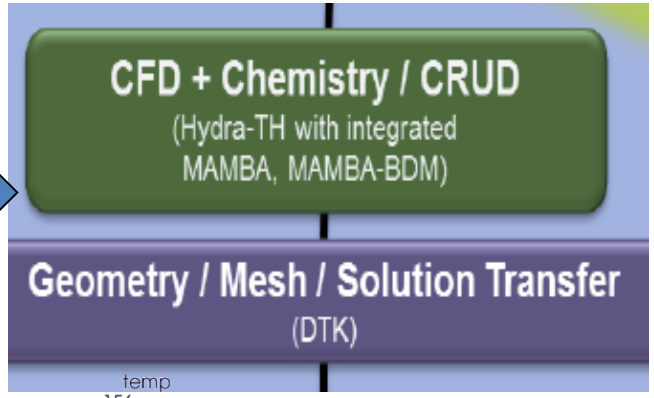
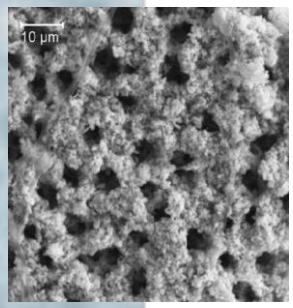
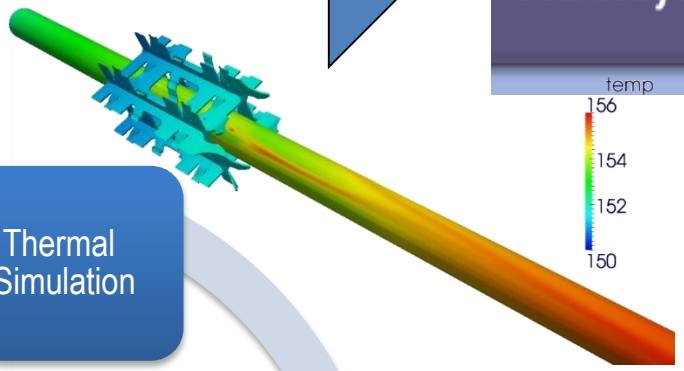


Evolution of Hydra-TH in VERA From End of Phase 1 to Phase 2





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



Fully-Implicit Projection

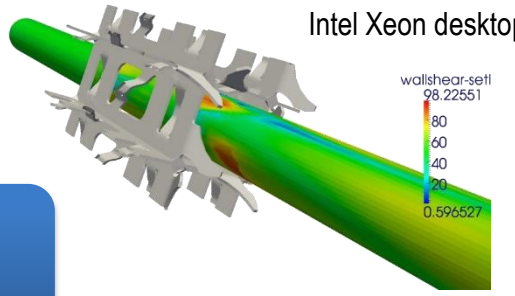
- RNG k-ε model
- Re ~ 4.0×10^5
- $q_w = 10^6$ W/m^2
- 2.4M elements, ~18M DoF
- ~ 4.75 hours on 16-core Intel Xeon desktop

Hydra-TH Thermal Hydraulics Simulation

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

MAMBA Sub-Grid Scale Model

Wall-Shear, Temperature, Heat Flux



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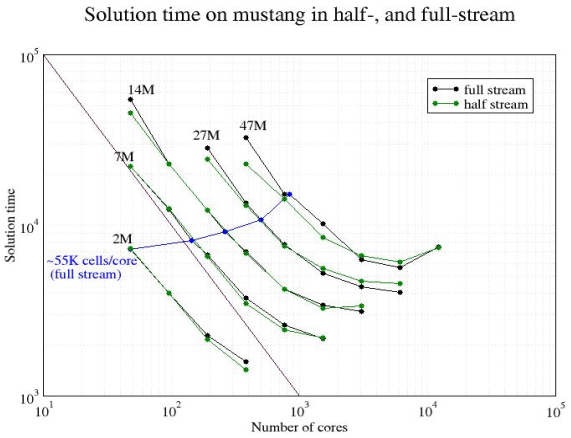
Performance Assessment, Memory Improvements and Linear Algebra

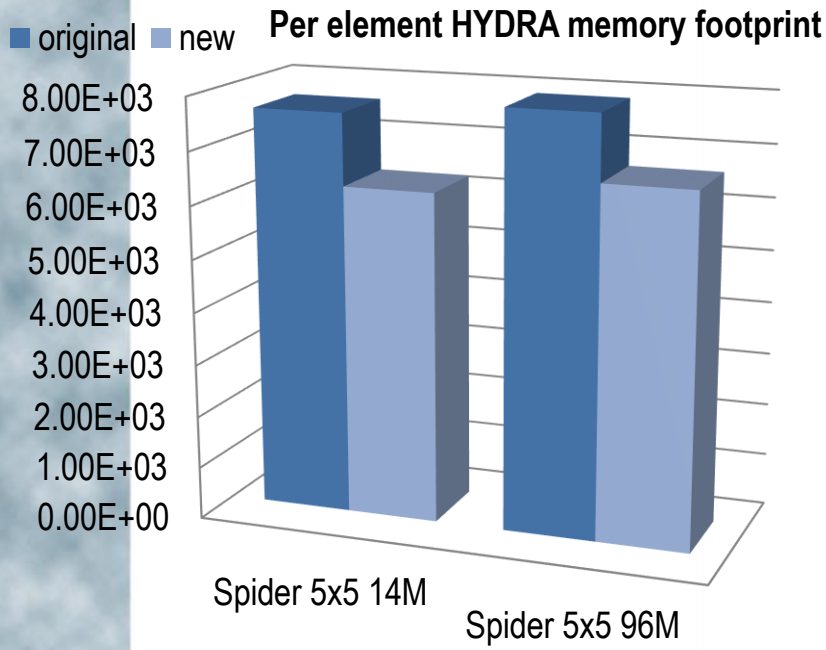
Assessment of computational performance using existing MPI-parallelism on Titan and LANL Turquoise HPC clusters using V5H GTRF problem

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



Implementation of nvidia AMGX solver for TITAN

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



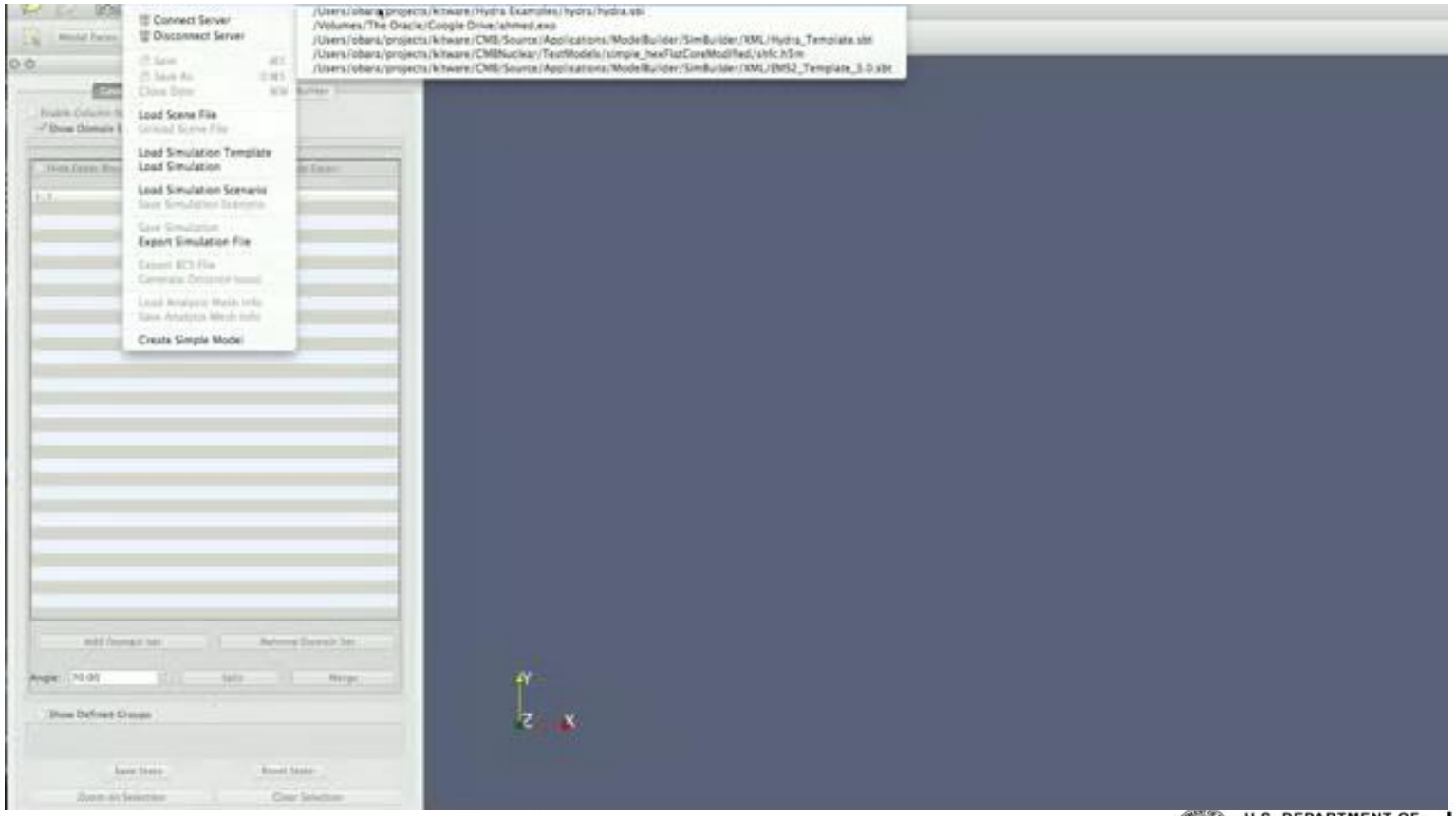
PETSc → Trilinos

Conversion to Trilinos/ML for PPE

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

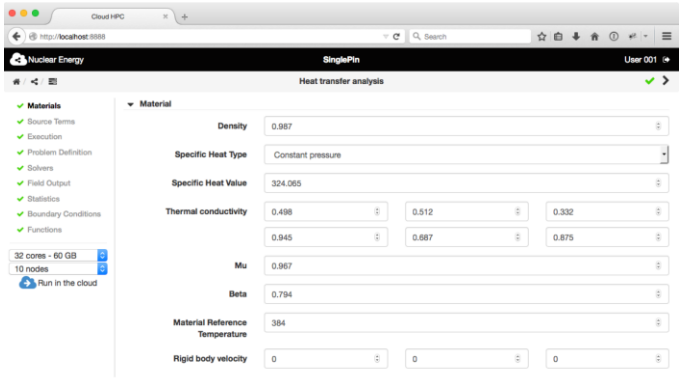
Computational Model Builder (CMB) for Setup, BC spec's, Material Properties, Generation of "cntl" file

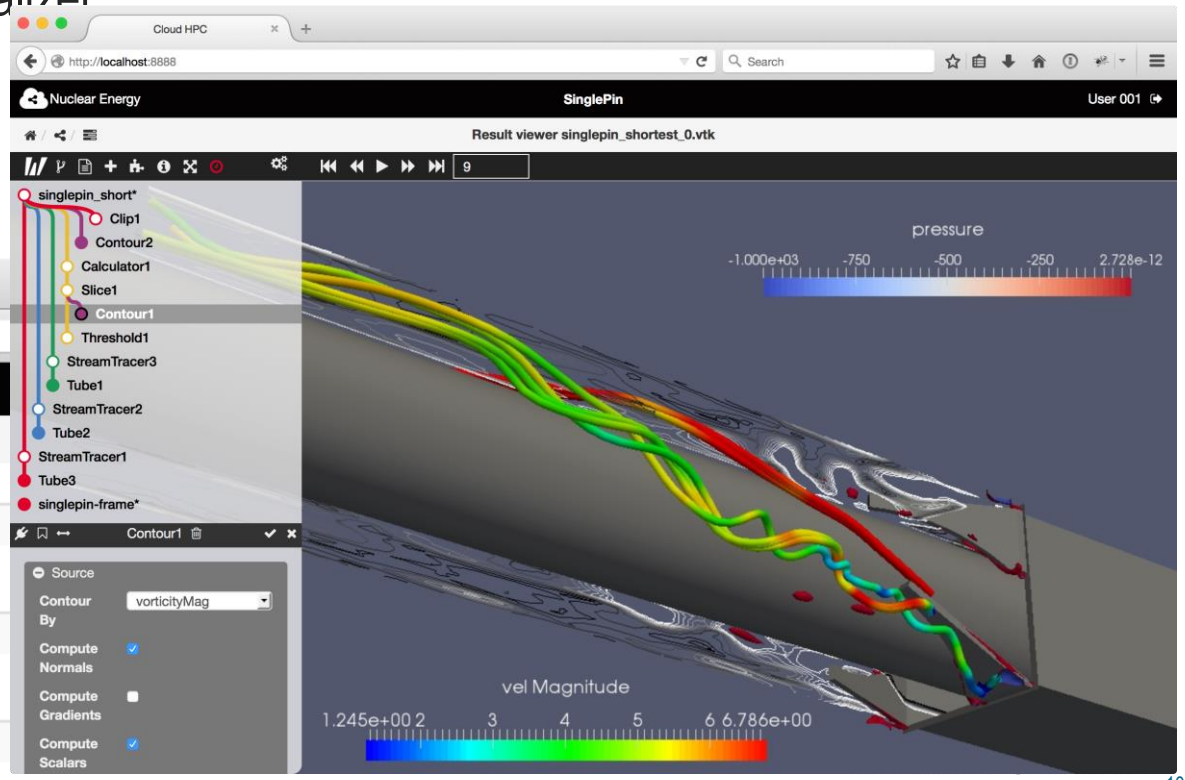
- Computational Model Builder Movie at: http://get-hydra.lanl.gov
- Tutorial from Hydra dev team or Kitware

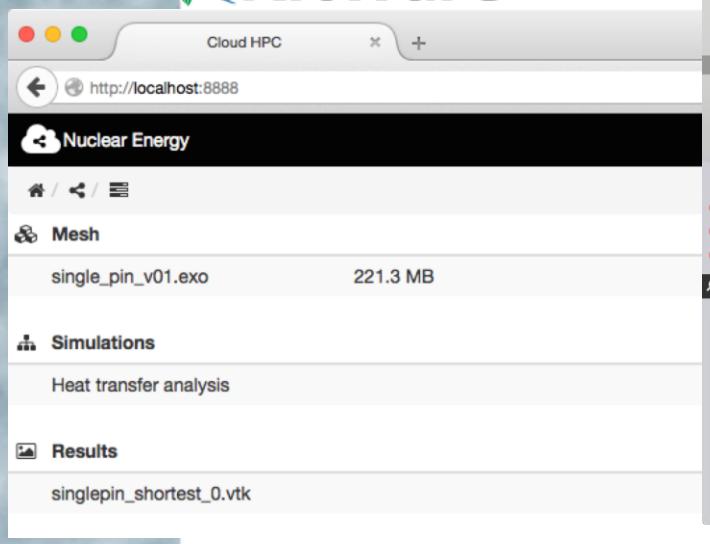


CMB-Web: Cloud based computing interface

- Cloud/Web HPC Infrastructure
- Simulation Asset Management
- Features:
  - Mesh viewing, model setup
  - Simput to generate Hydra-TH cntl file
  - Cloud job submission, e.g., on Amazon cloud
  - ParaView Web visualizer



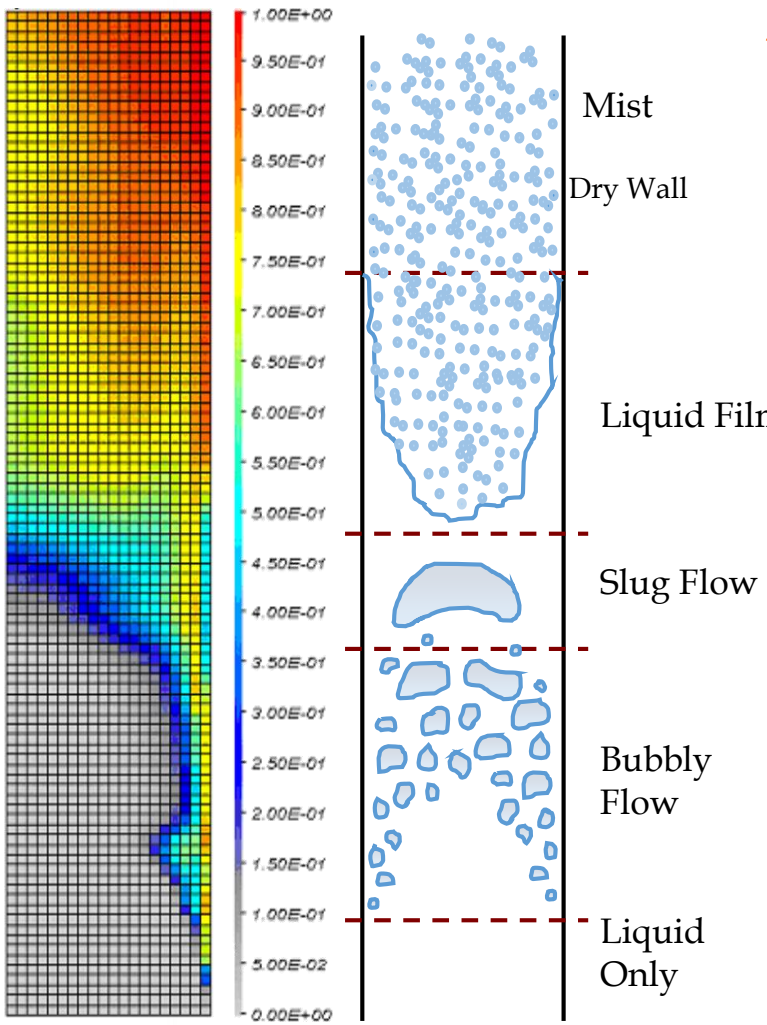




The CASL way to M-CFD

Challenges:

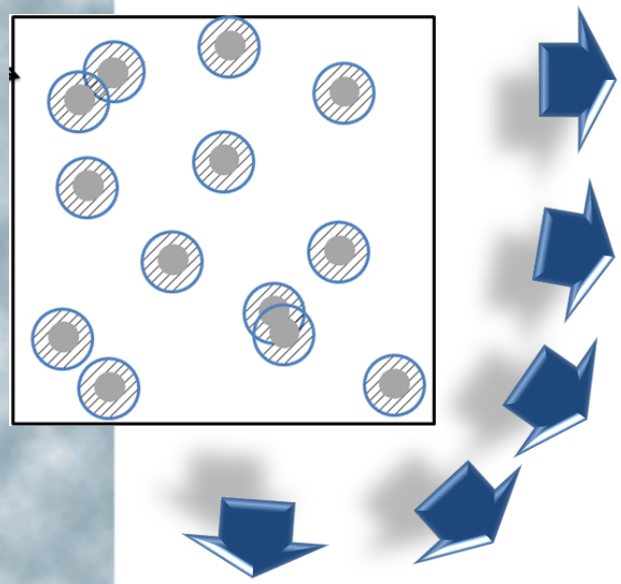
- Complex physical phenomenon
  - Complex interfaces
  - Multiple flow regimes
- Undeveloped physical laws & mathematical treatment of two phase phenomena
  - Lack consistent experimental validation
- Complex interaction of numerics and closure forces
  - Unstable solutions, oscillatory behavior, etc.



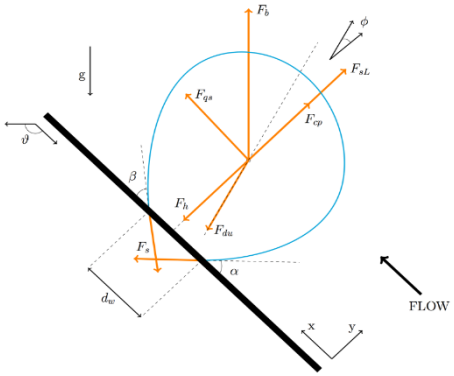
Approach:

- Wall Boiling
  - Novel Physical Representation
  - Extension to CHF
  - Multiple flow regimes
- Hydrodynamic Closures
  - Account for vapor morphology
  - Account for group behavior
  - Implement physical under-relaxation
- 2-Phase wall Functions
  - Extend to include unresolved lubrication effect
- Multiphase turbulence
  - Leverage recent work on ITM/DNS and experimental data

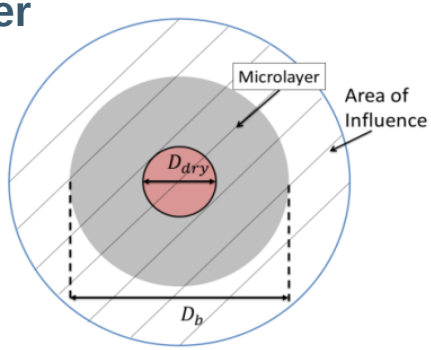
GEN-II Heat Partitioning
Quick Overview



1. Mechanistic Representation of Bubble Lift off and Departure Diameters

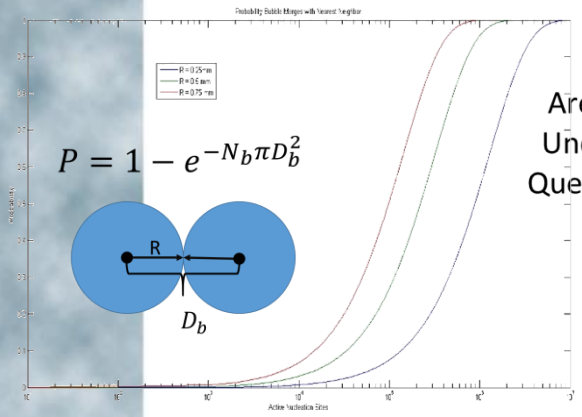


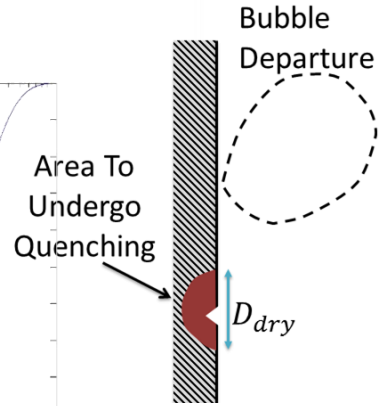
2. Accurate evaluation of evaporation heat flux by modeling effective microlayer

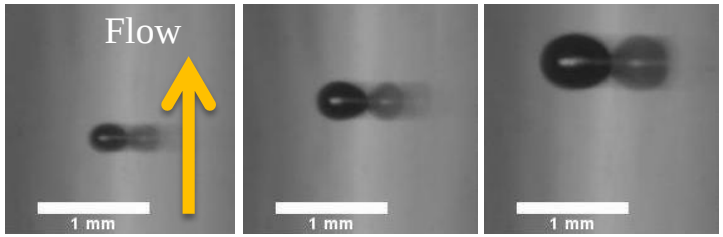


3. Account for sliding bubble effect on heat transfer and nucleation sites

5. Account for bubble interaction on surface







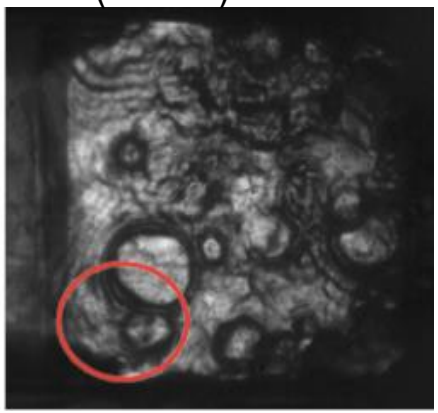
4. Account surface quenching after bubble departure

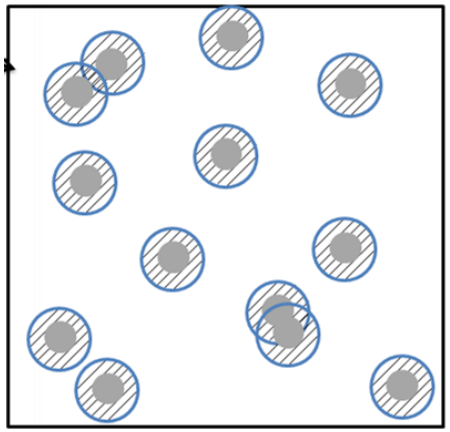
Demonstration of GEN-II M-CFD → Closure for onset of DNB

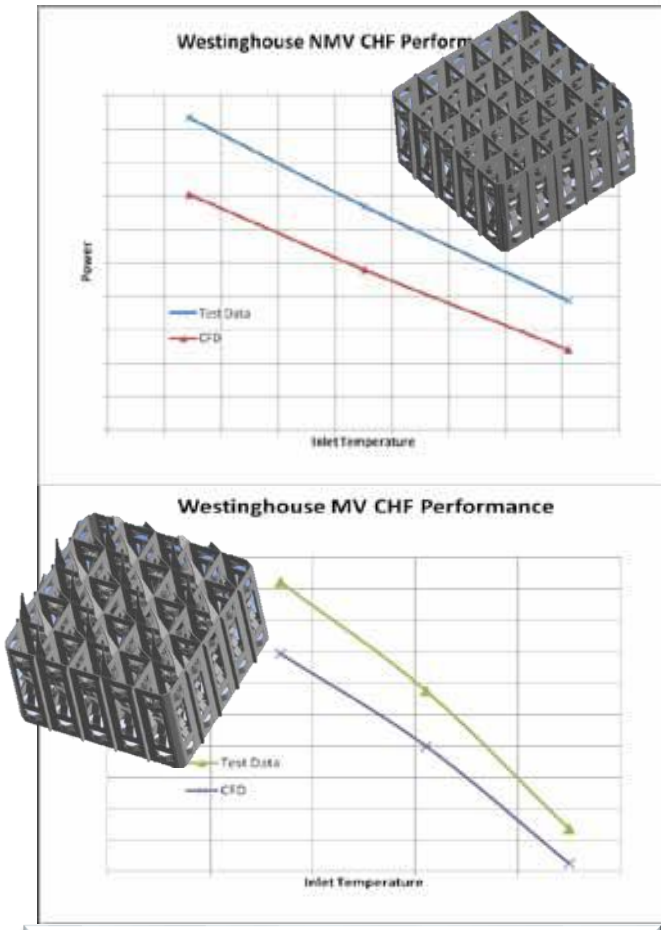
GEN-II

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

DNB inception -
Nam Dinh (NCSU)







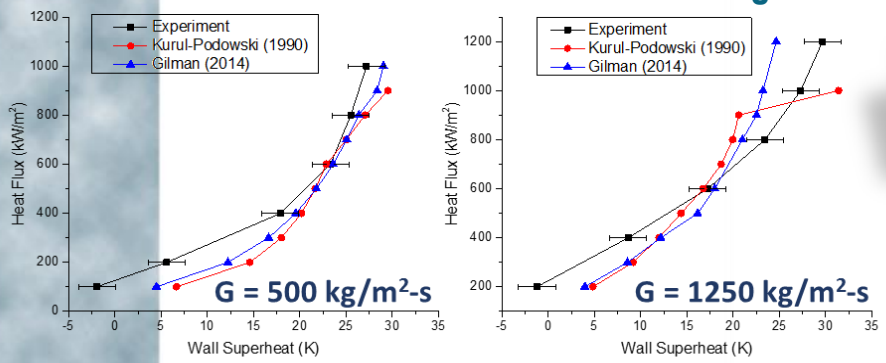
Current State of the Art

Jin Yan -ISACC-2013, Xian, China

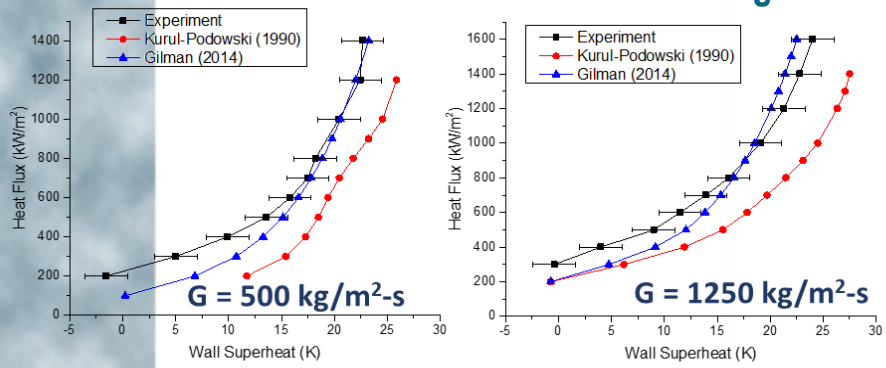
GEN-II Heat Partitioning: Assessment

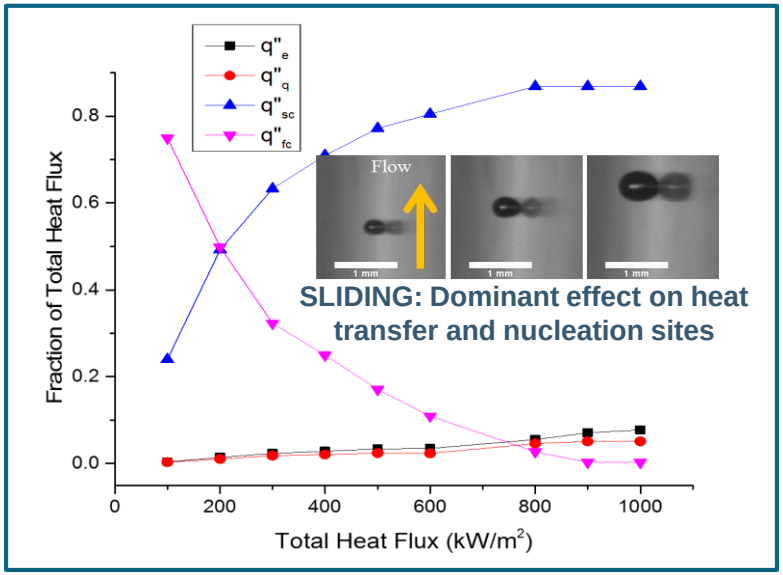
- Validation performed against MIT boiling curves
- Allows validating separate model components
- **Calibration-free – demonstrated generality deriving from improved physical representation**

Pressure = 1.0 bar and 10°C Subcooling



Pressure = 2.0 bar and 15°C Subcooling





- Evaporation term is not dominant contribution
- **Effect of bubble sliding dominates Flow Boiling Heat Transfer** *(previously postulated by Basu)*
- The new model demonstrates improved predictions at all conditions
- **Enhanced robustness** at higher heat fluxes

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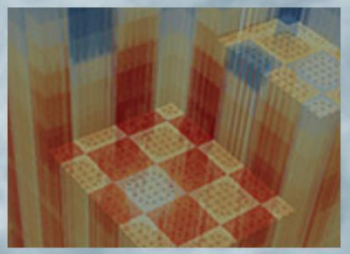
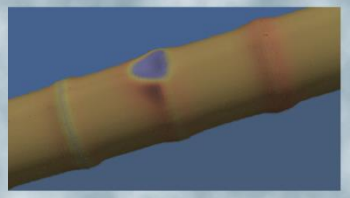
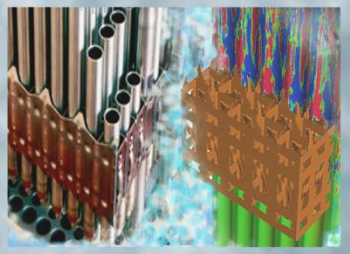
GEN-II Boiling going forward

- Extension to DNB
- Validate against TAMU data *
- *Move towards fast running approach*
- *Validate Heat Partitioning*
- *Test on artificial CRUD*







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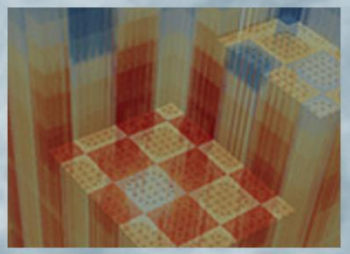
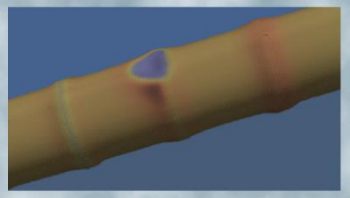
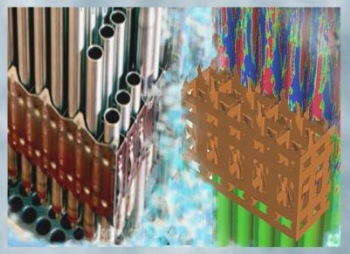
Hydrodynamic Closure Update







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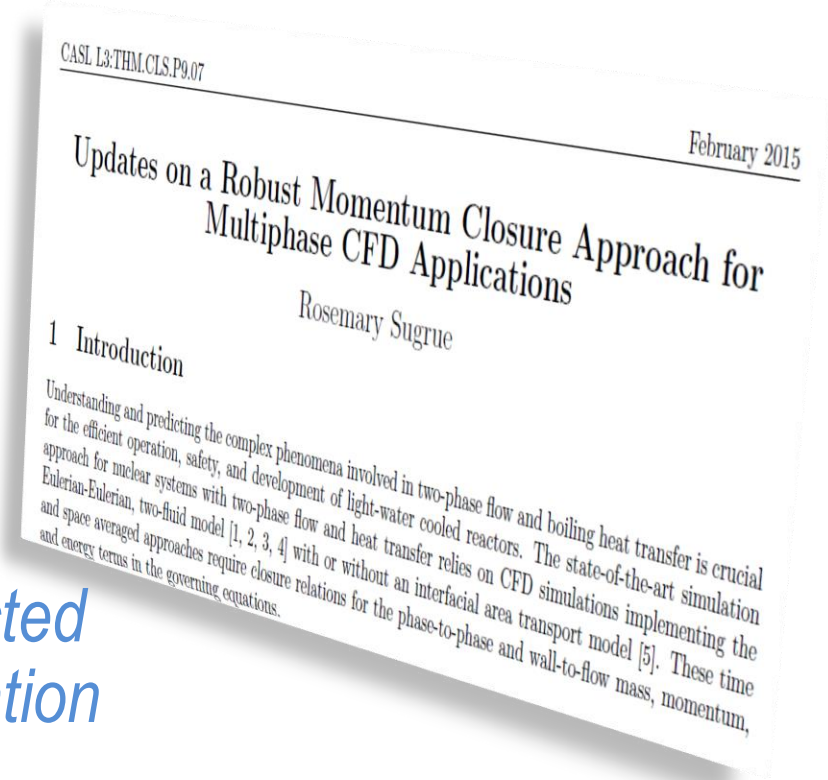
L3:THM.CLS.P9.07

- Overarching goal is to assemble a fully consistent closure for PWR application
- Everything went well up to Drag force testing
- *Testing of lift shows unexpected inconsistence of Lift Formulation*
- *Currently Leveraging ITM work (Bolotnov) to supplement experimental data from literature to re-evaluate Lift formulation*



CASL L3:THM.CLS.P9.07

February 2015

Updates on a Robust Momentum Closure Approach for Multiphase CFD Applications

Rosemary Sugrue

1 Introduction

Understanding and predicting the complex phenomena involved in two-phase flow and boiling heat transfer is crucial for the efficient operation, safety, and development of light-water cooled reactors. The state-of-the-art simulation approach for nuclear systems with two-phase flow and heat transfer relies on CFD simulations implementing the Eulerian-Eulerian, two-fluid model [1, 2, 3, 4] with or without an interfacial area transport model [5]. These time and space averaged approaches require closure relations for the phase-to-phase and wall-to-flow mass, momentum, and energy terms in the governing equations.

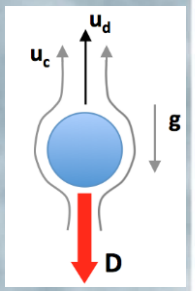
Momentum Closures are Complex

The general expression for the conservation of momentum for a given phase k [19] is given by

$$\frac{\partial}{\partial t}\left(\alpha_k \rho_k u_k\right) + \nabla \cdot \left(\alpha_k \rho_k u_k u_k\right) = -\alpha_k \nabla p + \alpha_k \rho_k g + \nabla \cdot \alpha_k \left(\tau_k + \tau_k^t\right) + M_k \tag{1}$$

where α is the volume fraction, ρ is the density, u is velocity, p is pressure, g is gravity, τ is the shear stress, and M is the sum of the interfacial forces and momentum transfer associated with mass transfer:

$$M = F_B + F_D + F_{TD} + F_L + F_{VM} + F_{WL} + \sum_{j=1}^{N} \left(\dot{m}_{jk} u_j - \dot{m}_{kj} u_k\right) \tag{2}$$



$$F_D = \frac{1}{2} C_D \rho_c A |u_r| u_r \tag{4}$$

where u_r is the relative velocity ($u_r = u_c - u_d$, with subscript c for the continuous phase and subscript d as the dispersed phase), A is the projected area ($A = \pi d^2/4$), and C_D is the drag coefficient. There are many formulations for the drag coefficient, which is a function of the particle Reynolds number:

$$Re_d = \frac{\rho_c |u_r| d}{\mu_c} \tag{5}$$

where d is the particle diameter and μ_c is the viscosity of the continuous phase. The various expressions for drag coefficient are based on the flow regime, the shape of particles considered (spherical, etc.), and amount of bubbles (single vs. multi particle).

Rosemary Sugrue, *Updates on a Robust Momentum Closure Approach for Multiphase CFD Applications (CASL Milestone Report L3:THM.CLS.P9.07)*

Momentum Closures are Complex

Turbulence dispersion, or turbulent drag, has the effect of dispersing the particles as a function of the particle concentration gradient. One common expression for this force was proposed by Antal et al. (1991) as a function of turbulent kinetic energy in the continuous phase and the gradient of the volume fraction:

$$F_{TD} = C_{TD}\rho_c k_c \nabla\alpha_c \tag{6}$$

where C_{TD} is the turbulence dispersion coefficient and k_C is the turbulent kinetic energy of the continuous phase. The lateral lift force on bubbles rising in a liquid is due to the horizontal velocity gradient. It originates from the inertia effects in the viscous flow around the particle and is expressed as:

$$F_L = C_L \alpha_d \rho_c \left[u_r \times (\nabla \times u_c)\right] \tag{7}$$

where C_L is the lift coefficient. There are many expressions for the lift force and lift coefficient, which depend on bubble shape (e.g. spherical vs. deformed bubbles).

Rosemary Sugrue, *Updates on a Robust Momentum Closure Approach for Multiphase CFD Applications (CASL Milestone Report L3:THM.CLS.P9.07)*

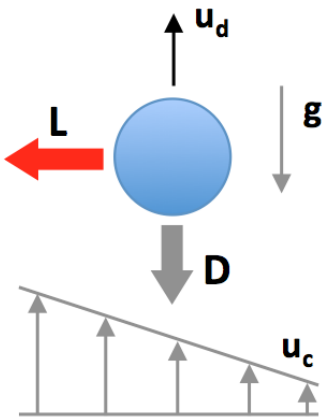


Figure 3. Schematic of the lift force on a bubble.

The virtual mass, or added mass, force arises as a consequence of the relative acceleration between phases and is particularly important in accelerating flows (swirling bubbles). It is typically taken to be proportional to the relative phase acceleration:

$$F_{VM} = C_{VM}\alpha_d \rho_c \left(acc_c - acc_d\right) \tag{8}$$

where C_{VM} is the virtual mass coefficient.

Momentum Closures are Complex

The Basset force is due to the temporal delay in boundary layer development as the relative velocity changes with time. This force is commonly neglected as it is difficult to quantify and implement, and it is typically negligible unless strong accelerations are present. Finally, the wall lubrication force prevents bubbles from attaching onto the solid wall. It results in a low void fraction in the vicinity of the wall, and disappears away from the wall. The wall lubrication is expressed as:

$$F_{WL} = -C_{WL}\alpha_d\rho_c\left(u_c - u_d\right)^2 \cdot n_w \tag{9}$$

where C_{WL} is the wall lubrication coefficient and n_w is the unit outward normal vector on the surface of the wall.

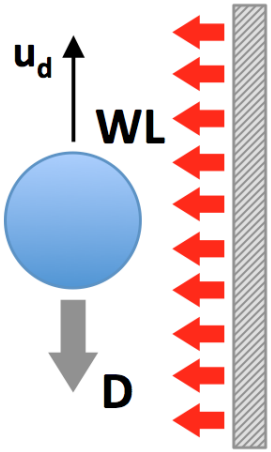


Figure 5. Schematic of the wall lubrication force on a bubble.

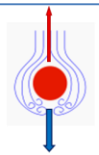
Rosemary Sugrue, Updates on a Robust Momentum Closure Approach for Multiphase CFD Applications (CASL Milestone Report L3:THM.CLS.P9.07)

CFD-BWR formulation

- Extremely Complex Closure
- Lack of physical under-relaxation limits robustness

Drag force (1)

$$F_D = \frac{1}{2} C_D \rho_c u_r^2 a_d$$



(when bubbly or mist topology)

$$a_d = \frac{A_i}{4} \rightarrow F_D = \frac{1}{8} C_D \rho_c u_r^2 A_i$$

(when bubbly topology)

Schiller & Neumann correlation

$$\begin{cases} C_D = \frac{24}{Re_d}\left(1 + 0.15 Re_d^{0.687}\right) & 0 < Re_d \leq 1000 \\ C_D = 0.44 & Re_d > 1000 \end{cases}$$

(when mist topology)

$$C_D = \frac{24}{Re_d} + \frac{5.48}{Re_d^{0.573}} + 0.36$$

(when sharp interface topology)

$$a_d = A_i \rightarrow F_D = \frac{1}{2} C_D \rho_d u_r^2 A_i$$

$$C_D(\varphi) = C_{d,tan} + (C_{d,ort} - C_{d,tan})|cos\varphi|$$

$C_{d,tan} = 0.005 \quad C_{d,ort} = 1$

φ angle between the relative phase velocity vector and the normal to interface

Lift force (2)

(only in bubbly and mist topologies)

$$F_{Ld} = -\boldsymbol{u_r} \times \left(\xi_b \zeta_b C_{Lb} \alpha_d \rho_c (\nabla \times \boldsymbol{u_c}) - \xi_m \zeta_m C_{Lm} \alpha_c \rho_d (\nabla \times \boldsymbol{u_d})\right)$$

$= 0$

$$\boxed{F_{Ld} = -\boldsymbol{u_r} \times \left(C_{Lb} \alpha_d \rho_c (\nabla \times \boldsymbol{u_c})\right)}$$

$$\xi_b = \begin{cases} 1, & \alpha < \alpha_{g,bc} \\ \frac{1}{2}\left(1 - cos\left(\pi \frac{\alpha - \alpha_{g,cm}}{\alpha_{g,cm} - \alpha_{g,bc}}\right)\right), & \alpha_{g,bc} < \alpha < \alpha_{g,cm} \\ 0, & \alpha > \alpha_{g,cm} \end{cases}$$

$$\zeta_b = \begin{cases} 1, & \gamma < \gamma_1 \\ \frac{1}{2}\left(1 - cos\left(\pi \frac{\gamma - \gamma_2}{\gamma_2 - \gamma_1}\right)\right), & \gamma_1 < \gamma < \gamma_2 \\ 0, & \gamma > \gamma_2 \end{cases}$$

$$\xi_m = \begin{cases} 0, & \alpha < \alpha_{g,bc} \\ \frac{1}{2}\left(1 - cos\left(\pi \frac{\alpha_{g,cm} - \alpha}{\alpha_{g,bc} - \alpha_{g,cm}}\right)\right), & \alpha_{g,bc} < \alpha < \alpha_{g,cm} \\ 1, & \alpha > \alpha_{g,cm} \end{cases}$$

$$\zeta_m = \begin{cases} 0, & \gamma < \gamma_1 \\ \frac{1}{2}\left(1 - cos\left(\pi \frac{\gamma_2 - \gamma}{\gamma_1 - \gamma_2}\right)\right), & \gamma_1 < \gamma < \gamma_2 \\ 1, & \gamma > \gamma_2 \end{cases}$$

Lift Closure in M-CFD

Deformable Particles: $-0.25 < C_L < +0.25$

e.g. Tomiyama (2002); Hibiki & Ishii (2007)

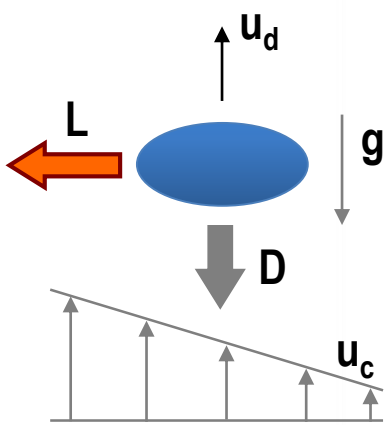
$$C_{L,T} = \begin{cases} 0.288\tanh\left(0.121\max\left[\mathrm{Re}, 7.374\right]\right), & Eo_d < 4 \\ 0.00105Eo_d^3 - 0.0159Eo_d^2 - 0.0204Eo_d + 0.474, & 4 \le Eo_d \le 10 \\ -0.27, & 10 < Eo_d \end{cases}$$

$$Eo_d = \frac{g\left(r^c - r^d\right)D_H^2}{s}$$

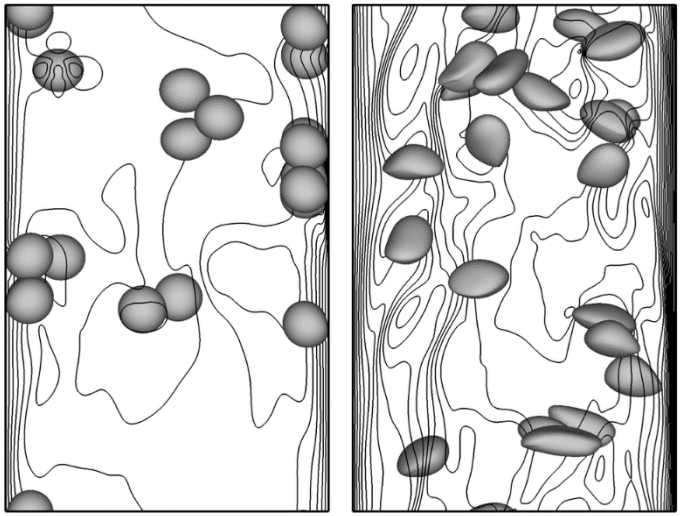
$$D_H = D_s\left(1 + 0.163Eo^{0.757}\right)^{1/3}$$

$$C_{L,H} = 0.010 + \frac{0.490}{p}\cot^{-1}\left(\frac{\log z + 9.3168}{0.1963}\right) \approx 0.02 + 0.6\left(\log z + 10.67\right)^{-2.605}$$

$$z \approx e^{-a_g}\frac{d_b}{v_r}\frac{dv_f}{dr}\left(\frac{d_b}{D}\frac{m_f}{m_n}\frac{1}{N_{\mathrm{Re}}}\frac{v_g}{1.18(s g / r_f)^{1/4}}\right)^2$$



G. Tryggvason, ND



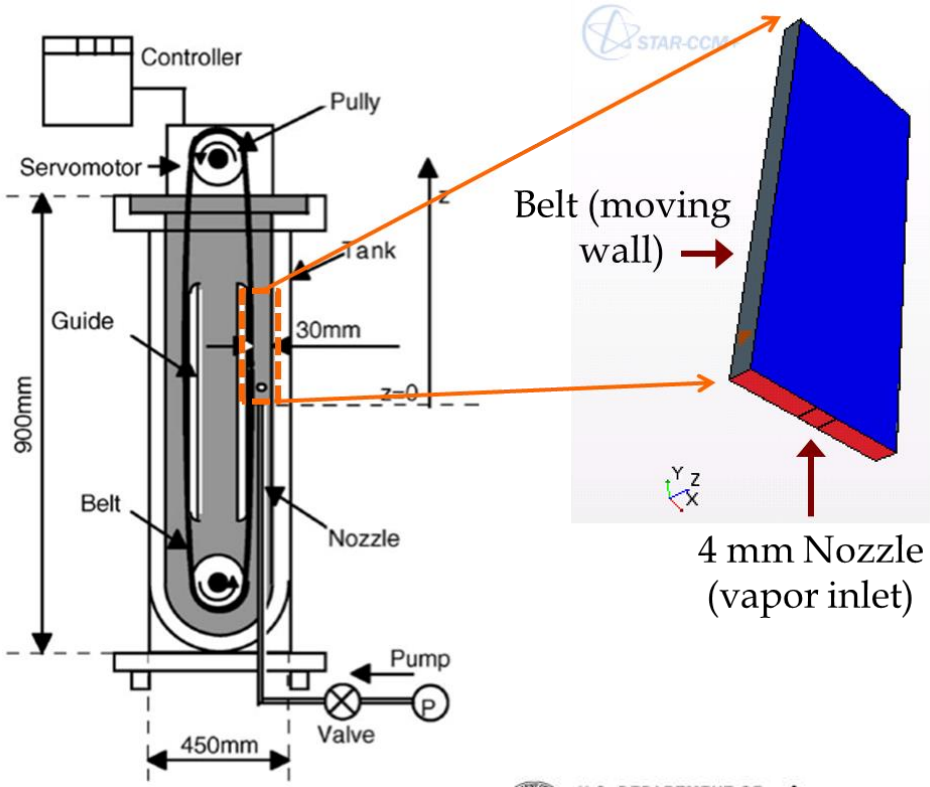
Low Eotvos # **High Eotvos #**

Unit testing for LIFT

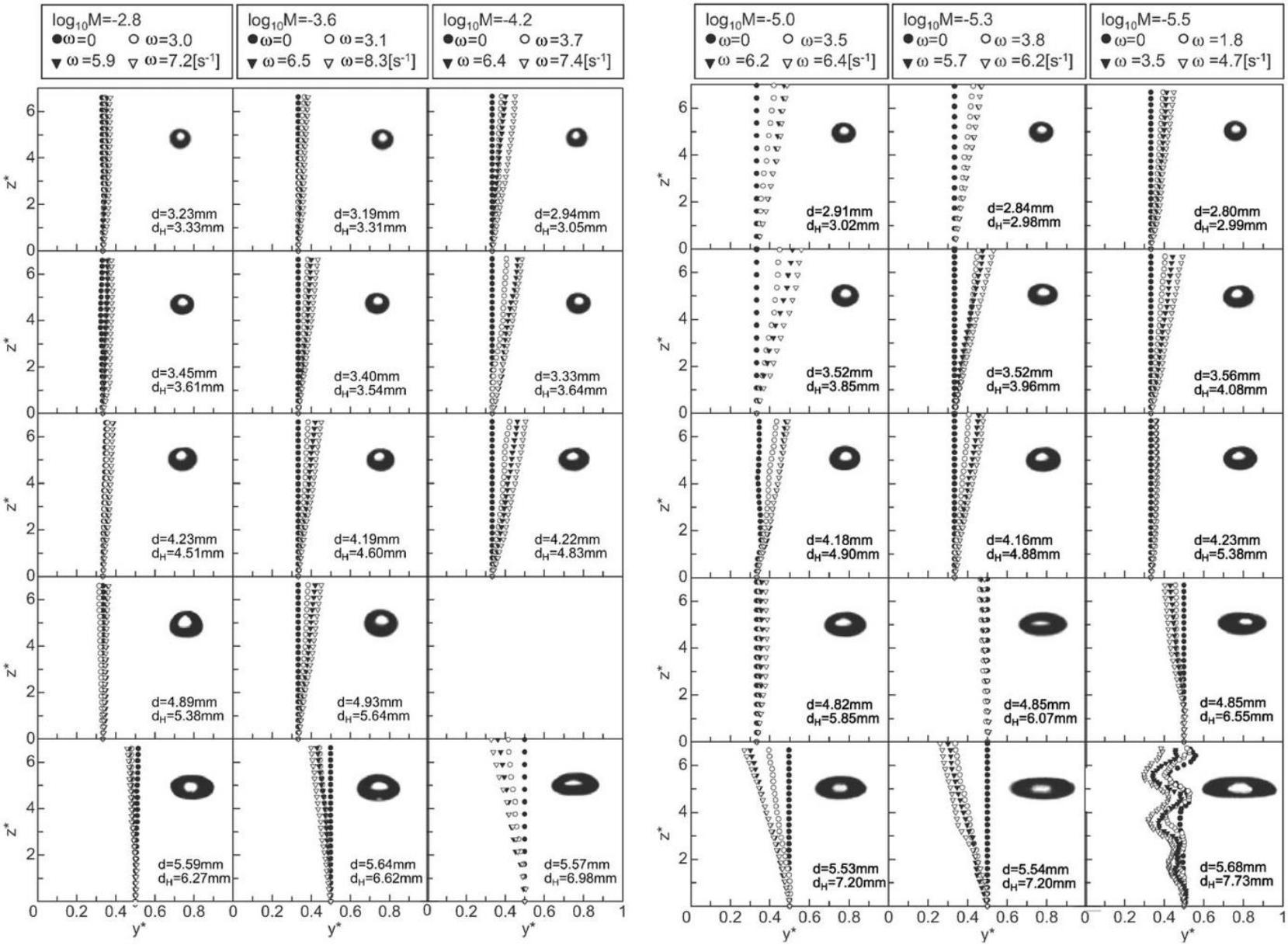
- Luck of unit testing for Lift force during code development
- Lift is only evaluated a posteriori
- Our first question: does it really work?

APPROACH

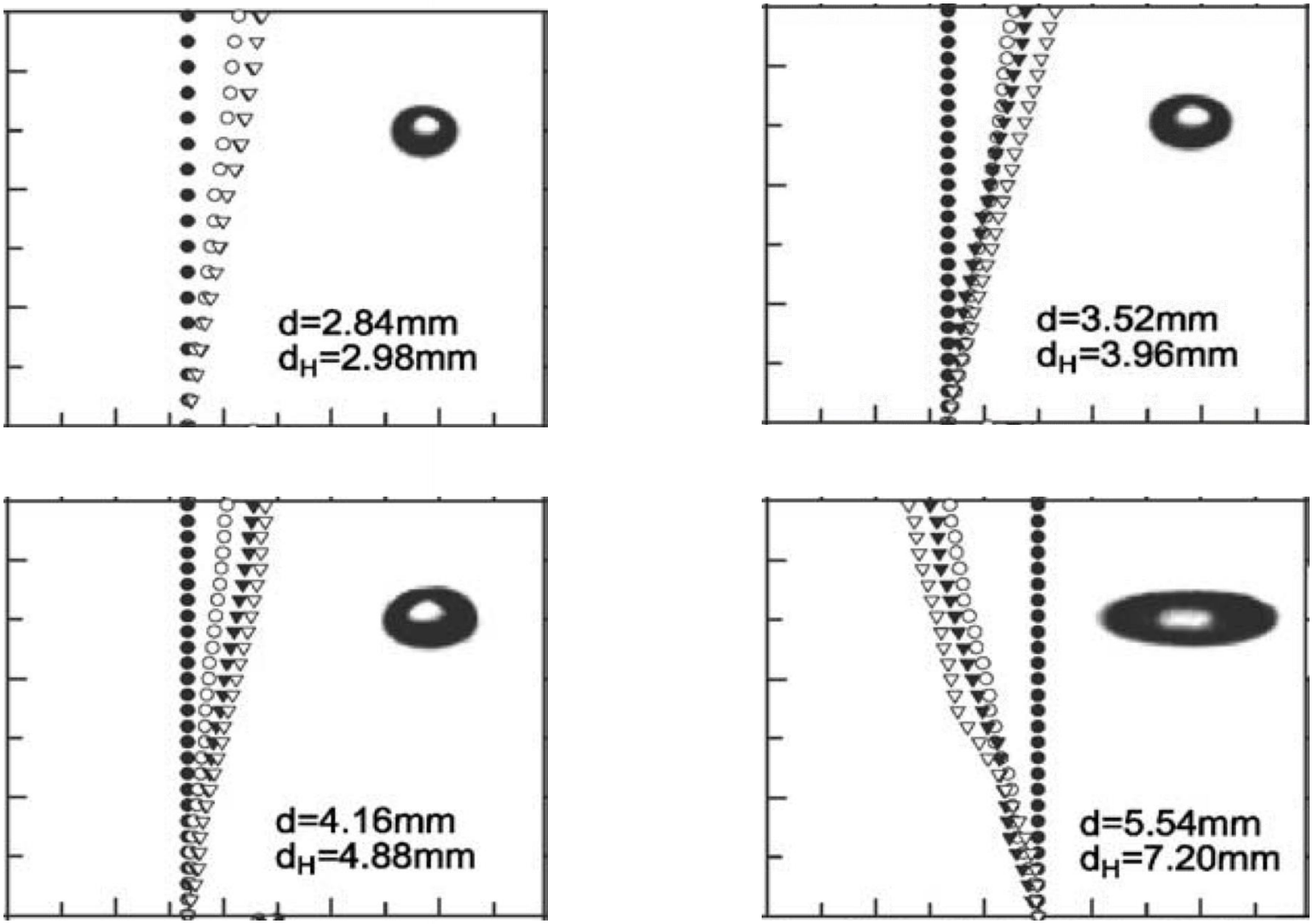
- Reproduce in M-CFD Tomiyama's single bubble tests



Tomiyama Experimental Results



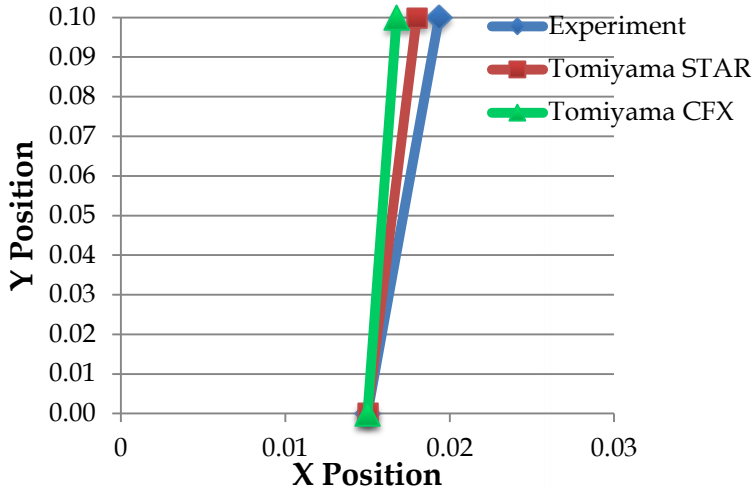
Tomiyama Experimental Results



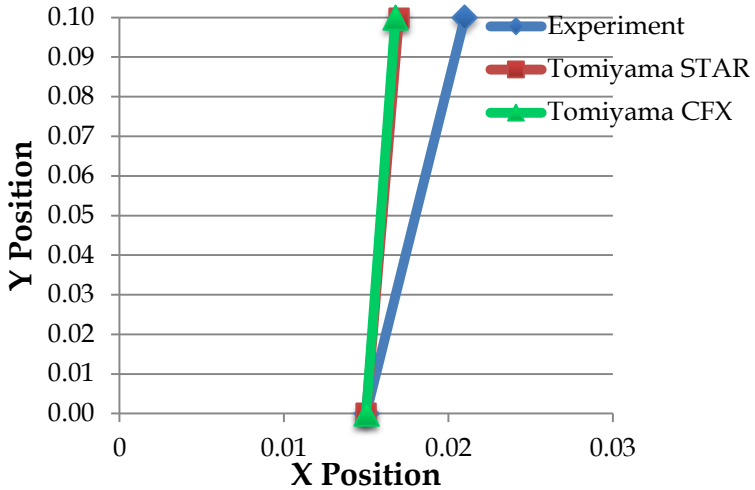
d_H = maximum horizontal dimension of bubble

Lift Testing: STAR-CCM+ vs. CFX

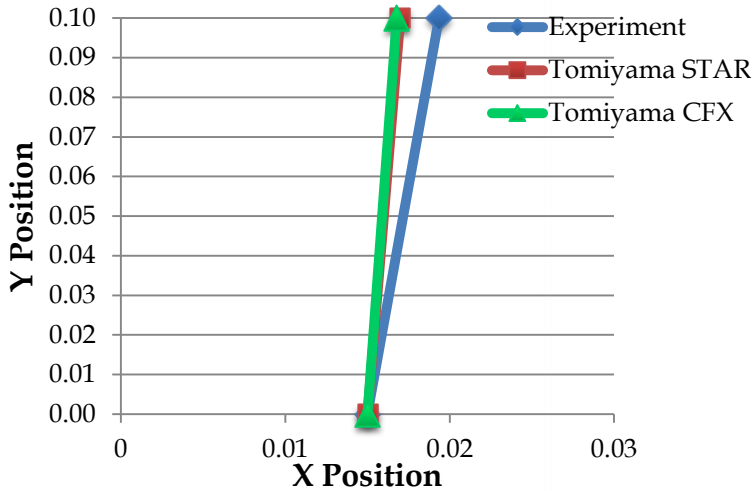
2.84mm



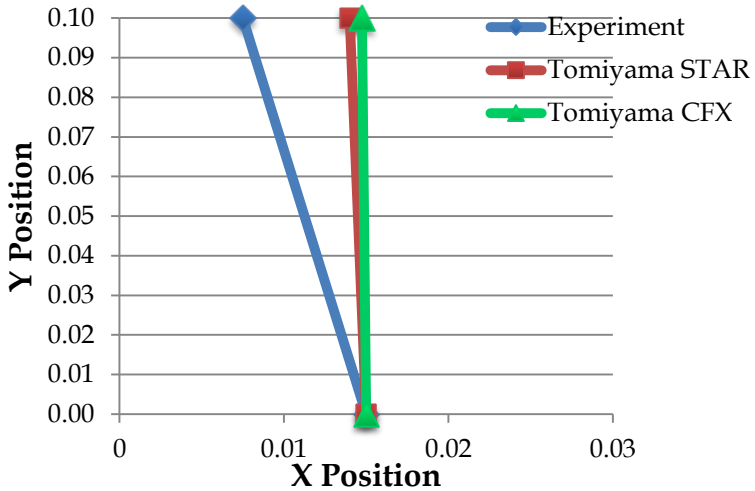
3.52mm



4.16mm

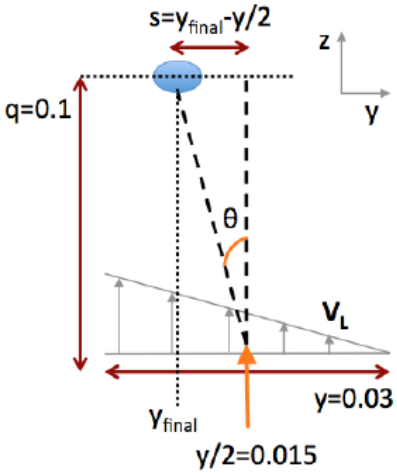


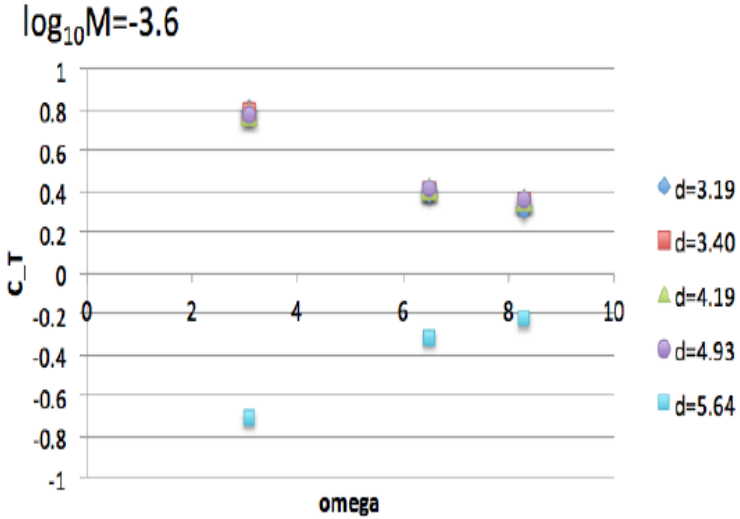
5.54mm

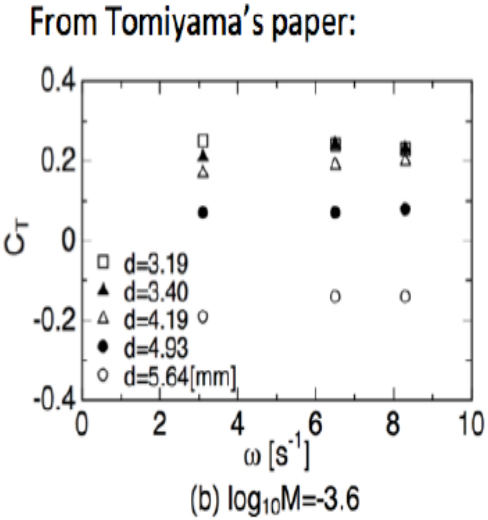


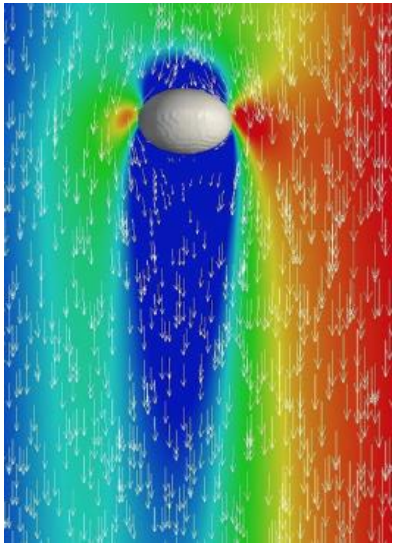
ITM Methods + Tomiyama Data

- Current work is leveraging ITM data (extended database, Bolotnov)
- Re-evaluate forces from Tomiyama data
- *Test new formulation on Unit test*









Consistent and Validated Closure

DEVELOPMENT PHASE

SPHERICAL BUBBLES

Drag Force ✓
Lift Force ✓

DEFORMED BUBBLES

Drag Force ✓
Lift Force ←

GROUP BEHAVIOR

Length Scales
Drag & Lift ←

INTEGRAL VALIDATION

TOPFLOW

Test Case Setup ✓
HZDR Benchmark ✓
WH 5x5

CRIEPI (?)

Test Case Setup
Full Closure Testing

A DOE Energy Innovation Hub

Synthesis of CRUD and its Effects on Subcooled Flow Boiling

Carolyn Coyle, Jacopo Buongiorno, and Thomas McKrell
Department of Nuclear Science and Engineering, MIT

Massachusetts Institute of Technology

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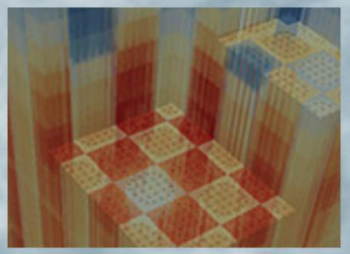
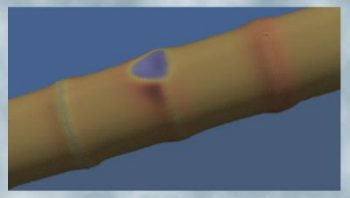
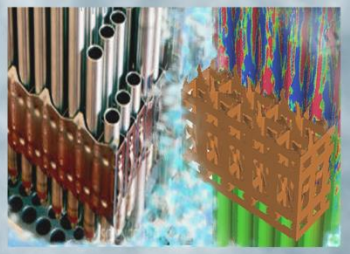
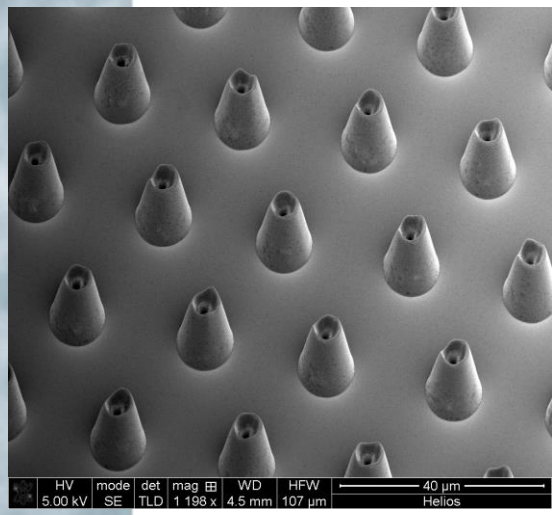
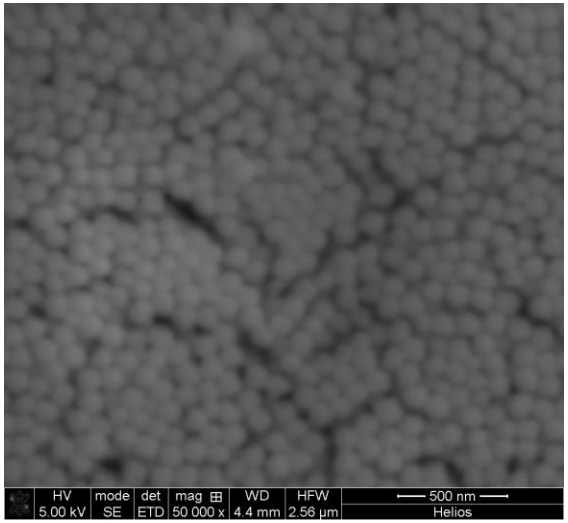




Current Status



Photolithography



Electrophoretic Deposition

Using photolithography (chimneys) and electrophoretic deposition (porous structure) to create synthetic CRUD

Massachusetts Institute of Technology

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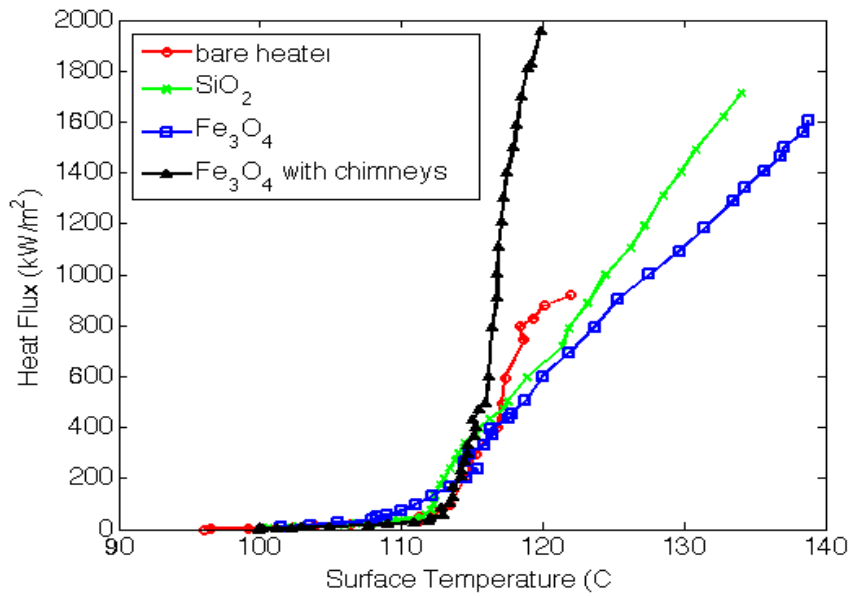
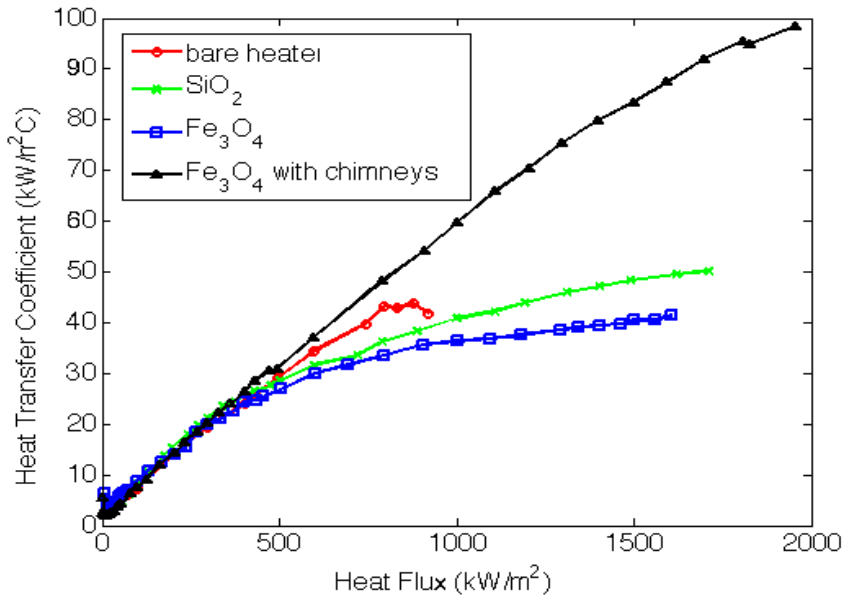
Initial Results





- Fe_3O_4 and SiO_2 behave similarly
- CRUD enhances CHF and HTC roughly 100%

*Apparatus uncertainty ~1.5%

Deliverables (Test Matrix)

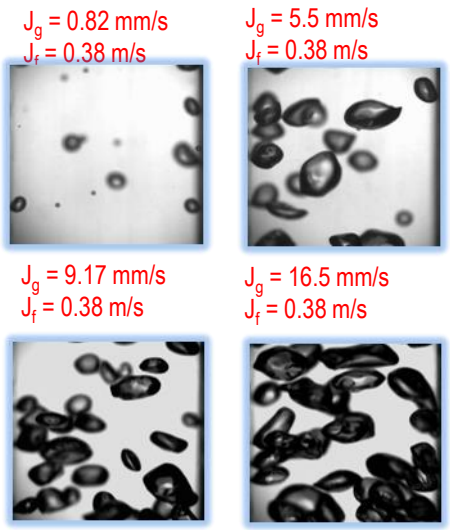
- The following test matrix will be run in a subcooled flow boiling loop to determine the effects of the parameters and test conditions below on boiling quantities of interest
  - Mass Flux: 150, 250, 500, 750, 1000, 1250 kg/m^2s
  - Heat Flux: 100-1600 kW/m^2
  - Pressure and Subcooling: 1.05 bar and 5, 10, 15°C

Parameter	Reactor CRUD	Synthetic CRUD
Composition	Fe_3O_4, NiO, $NiFe_2O_4$, ZrO_2	SiO_2
Thickness	10-100 µm	5, 10, 15 µm
Chimney Diameter	2-10 µm	5, 10 µm
Chimney Pitch	5-20 µm	10, 25, 100 µm

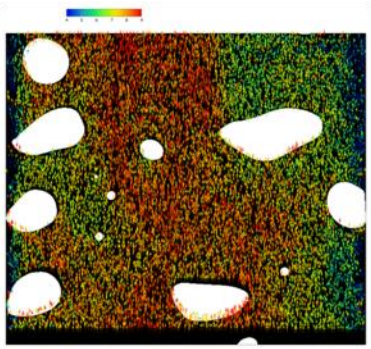
TAMU Status

Flow Boiling

- **Performed two-phase flow experiments**
  - Subcooled flow boiling experiments
  - Bubble plume experiments (bubble driven flow)
  - Isothermal bubbly flow experiments.
- **Feasibility studies to**
  - Quantify and reduce uncertainty
  - Identify experimental techniques limitations
  - Develop rigorous experimental protocols
- **Studied**
  - Important two-phase flow turbulence parameters (liquid and gas velocities and bubbles dynamics)
  - Liquid and bubble dynamics interaction.
  - Effects on the wall heat transfer



Bubbly Flow



- **Publications**

A proper observation and characterization of wall nucleation phenomena in a forced convective boiling s
Yoo, CE **Estrada-Perez**, YA Hassan - … Journal of Heat and Mass Transfer, 2014 - Elsevier

An accurate wall temperature measurement using infrared thermometry with enhanced two-phase flow visualization in a convective boiling system J Yoo, CE **Estrada-Perez**, YA Hassan - International Journal of Thermal …, 2015 - Elsevier

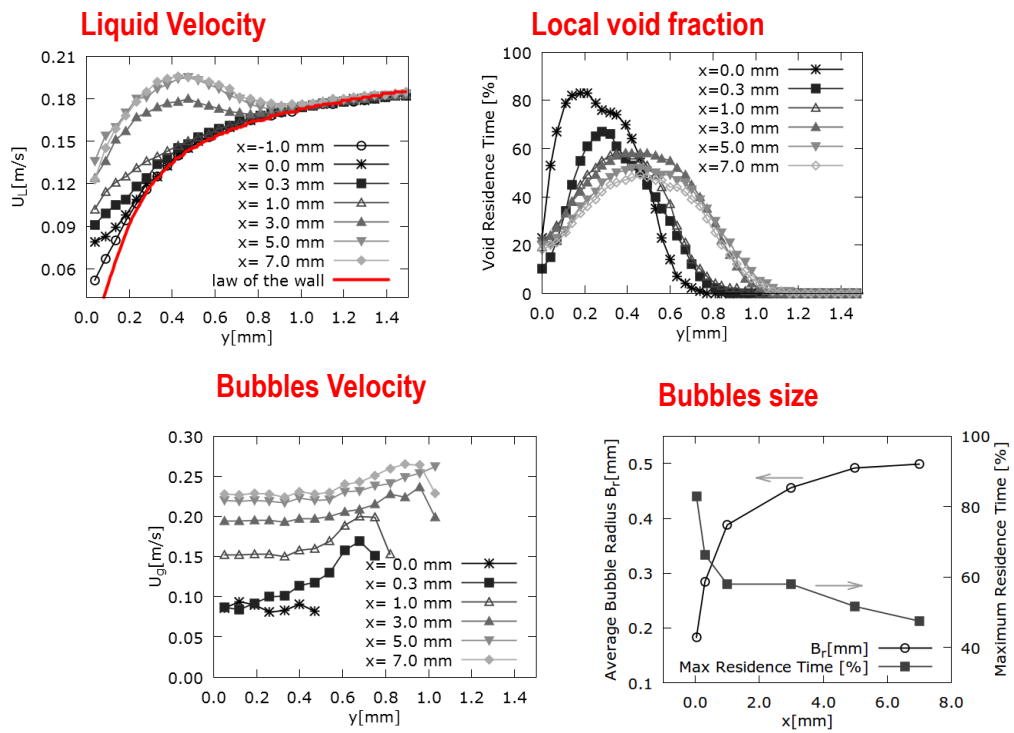
Feasibility Investigation of Experimental Visualization Techniques to Study Subcooled Boiling Flow CE **Estrada-Perez**, J Yoo, YA Hassan - International Journal of Multiphase …, 2015 – Elsevier

Measurement of subcooled flow boiling using Particle Tracking Velocimetry and infrared thermographic technique YA Hassan, CE **Estrada-Perez**, JS Yoo - Nuclear Engineering and Design, 2014 - Elsevier

TAMU Currently

Experimental Benchmark

- **First experimental benchmark in the release process** (under review)
  - From the subcooled flow boiling experiments
  - Out of the hundreds of terabytes of information, meaningful cases were selected
  - Simplified data delivery through the internet
- **Second experimental benchmark on the making**
  - From the isothermal bubbly flow experiment
  - Currently selecting meaningful cases aligned with CASL needs.



TAMU Future Work

- **Improving experimental facilities and exploring innovative measuring techniques**
  - Expand the experimental matrix with conditions more relevant with CASL requirements
  - Explore the proper implementation of LIF for liquid temperature fields measurements
  - Experimental facility modifications to accommodate demanding conditions and new measuring techniques
  - Development and improvement of empirical models for the prediction of two phase flow behaviour.

Supplemental Material

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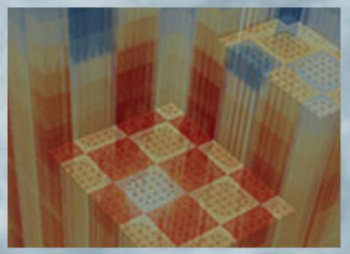
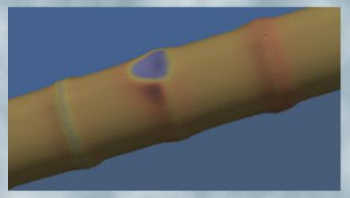
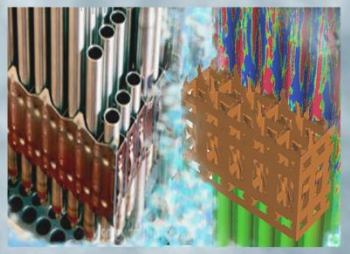
Extension to BWR







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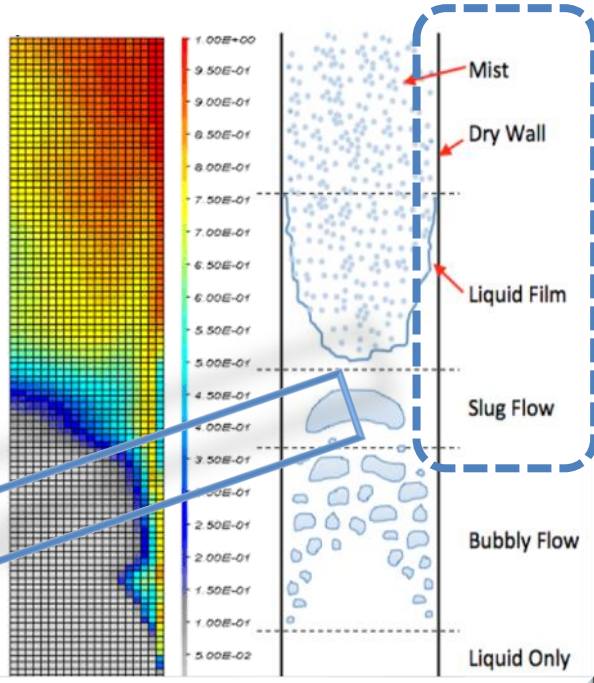
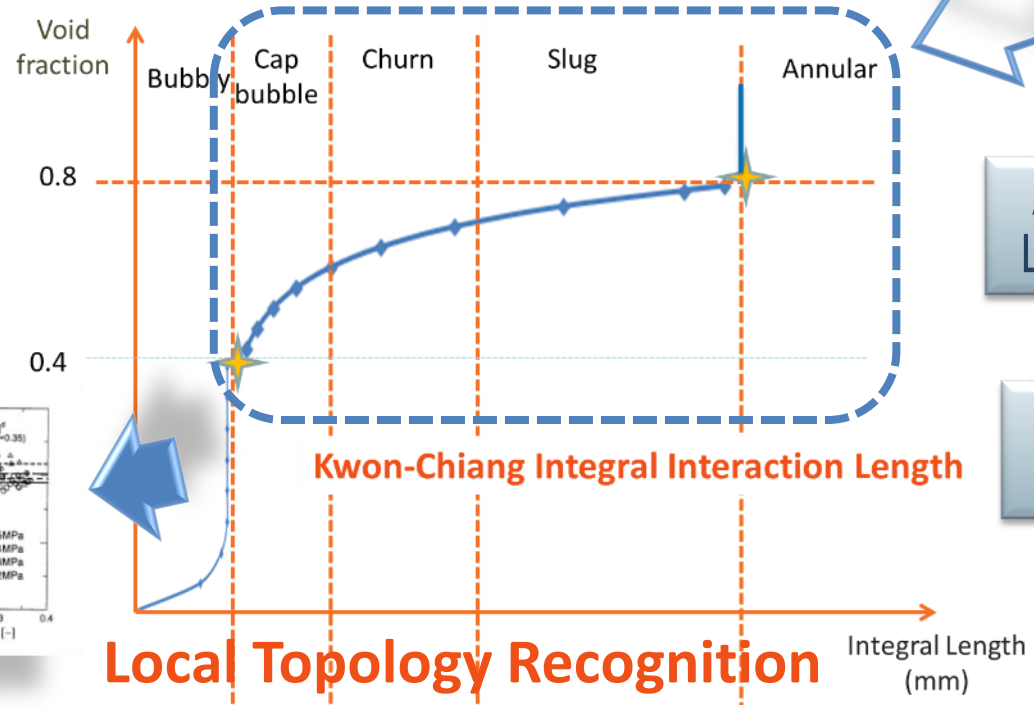
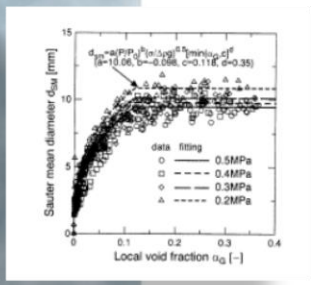
Extension to BWR Application

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



A fundamental distinction:
Local topology vs flow regime



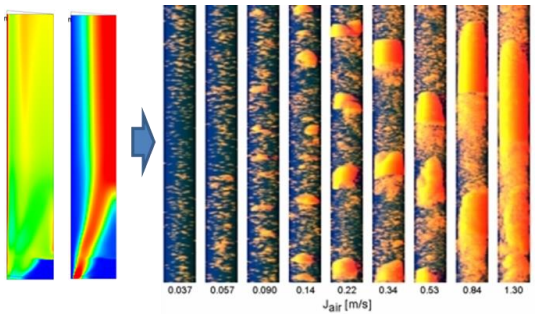


Confidence based on experience and validation

Step 1 – baselines & portability

- Demonstrate portability
- Evaluate Robustness and applicability of current state of the art
- Selected Benchmarks:
  - BFBT (OECD/NEA)
  - TOPFLOW (HZDR)

HZDR Baseline Closure

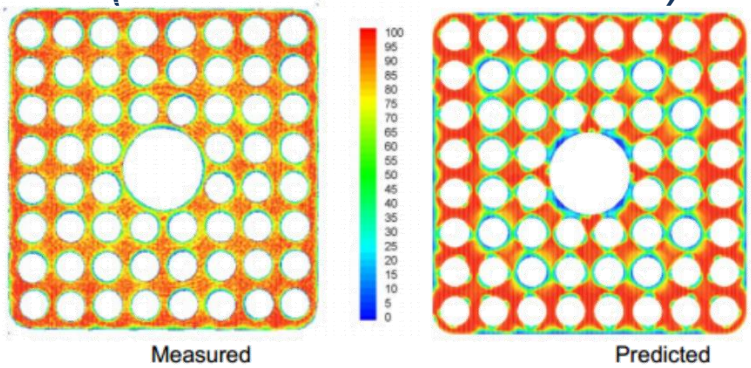


Massachusetts Institute of Technology

HZDR

Collaboration with G. Montoya, D. Lucas – (HZDR)

CFD-BWR (ANL,CD-adapco)
(OECD/NEA BFBT Benchmark)



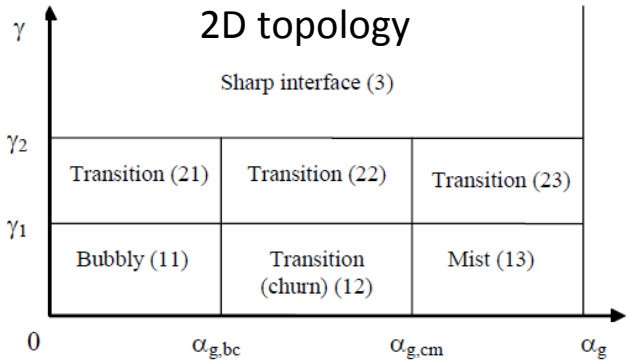
- Collaboration with Adrian Tentner (ANL)

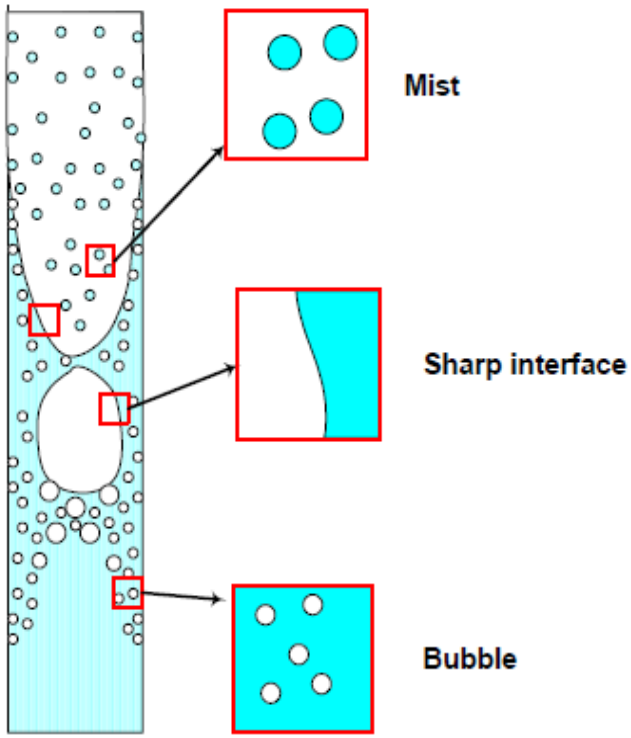
CFD-BWR formulation - I

- Adopts 2D Flow Topology approach (not flow map)
- 3 basic flow topologies with blended transition

LOCAL RECOGNITION BASED ON

- void fraction α_g
- void fraction increment $\gamma = \delta \cdot |\nabla \alpha_g|$ at a distance of characteristic cell size δ



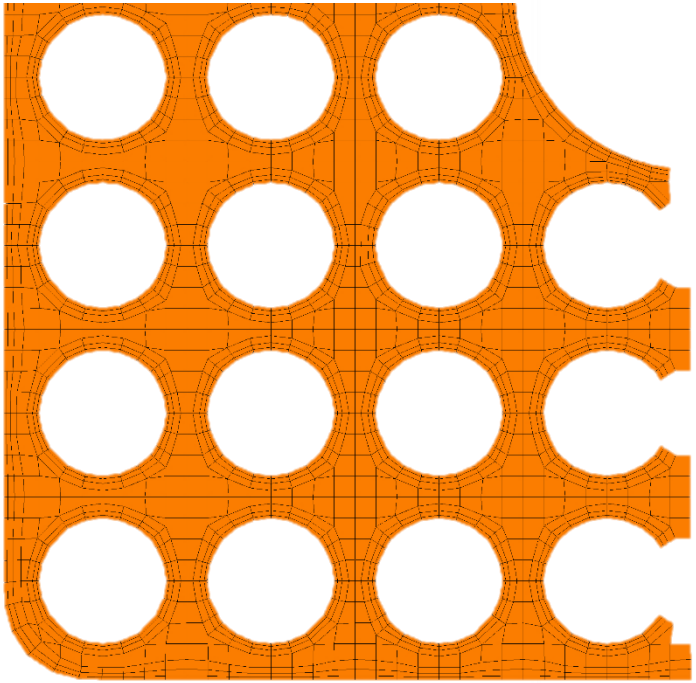


OECD/NEA BFBT Benchmark

- Fast testing (spacer are not resolved)
- Run time 3 hours on 10 cores

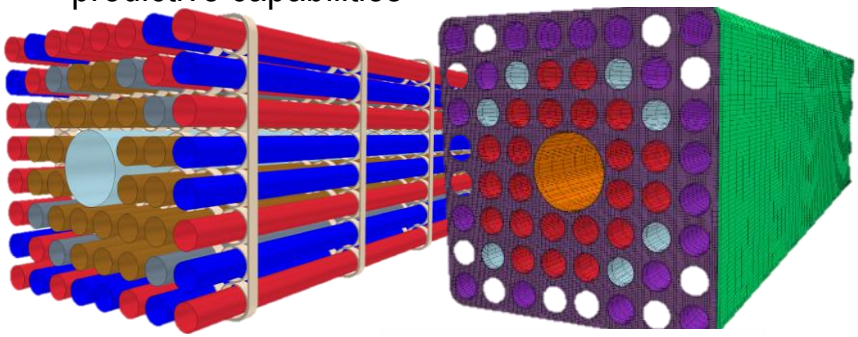
MESH

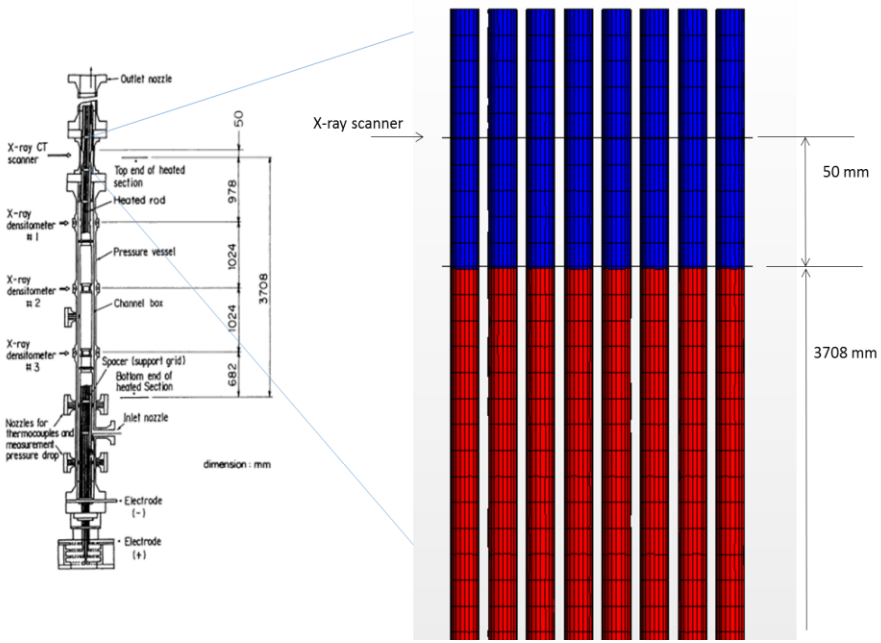
2,631,073 hexa (dominant) cells



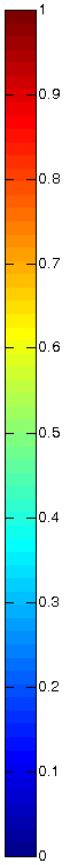
NUPEC BWR Full-size Bundle Test (BFBT)

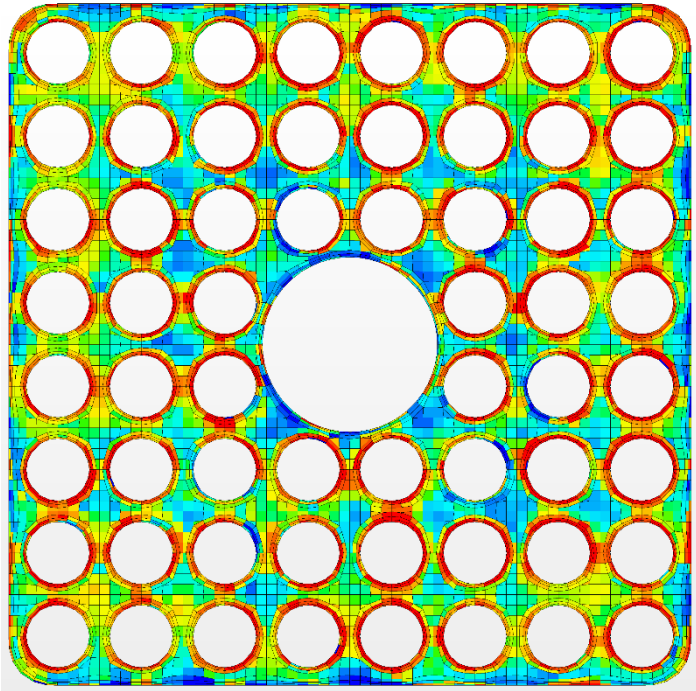
- Provides robust validation of closures predictive capabilities

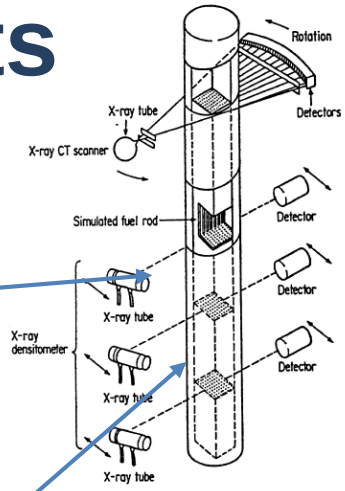


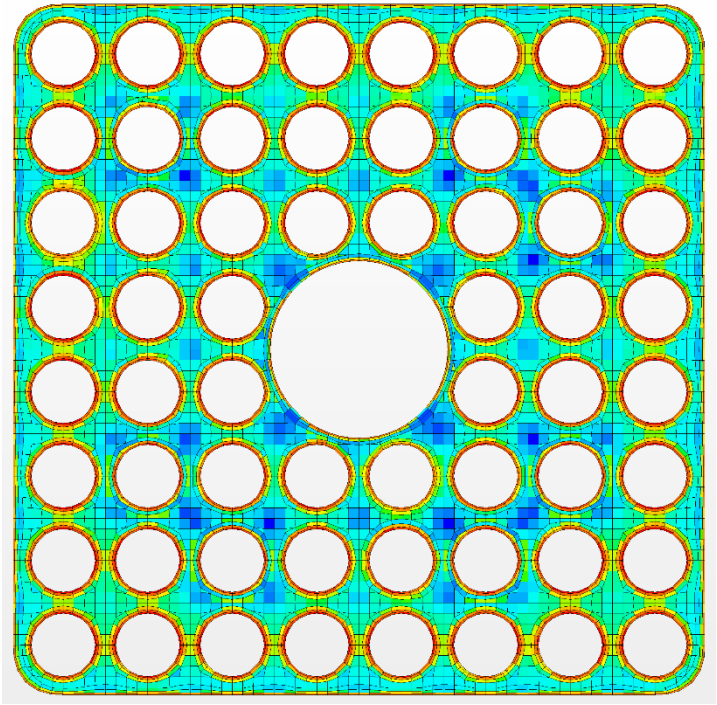


Sample Results

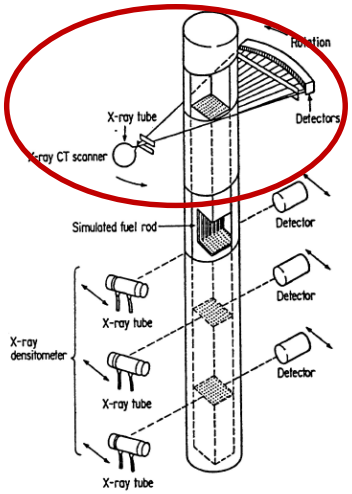






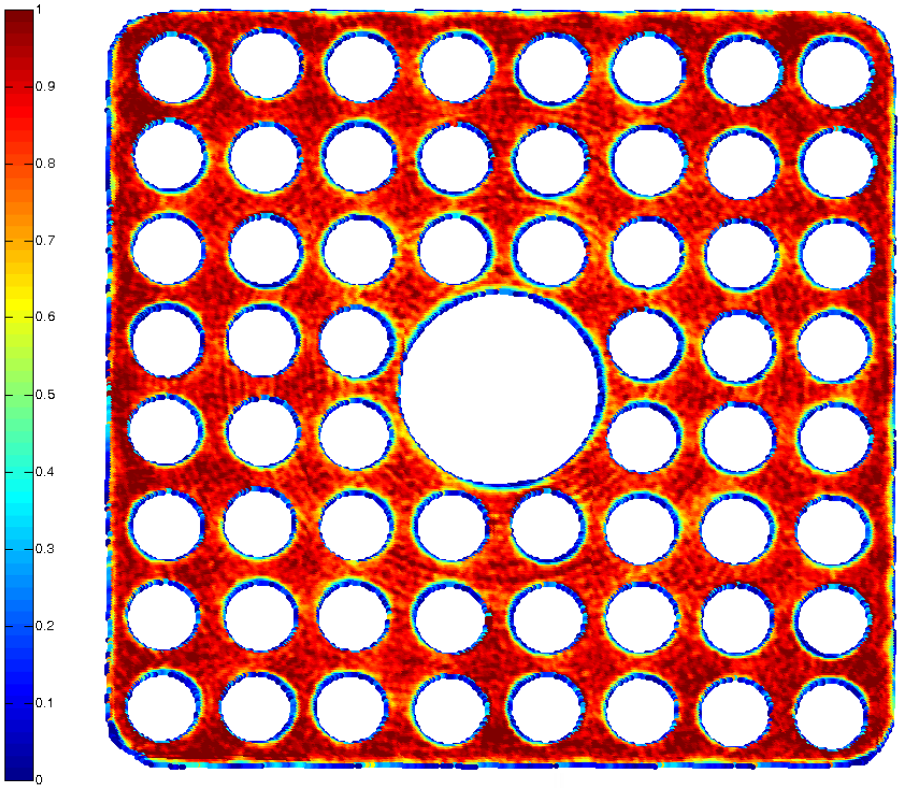


Sample Comparison

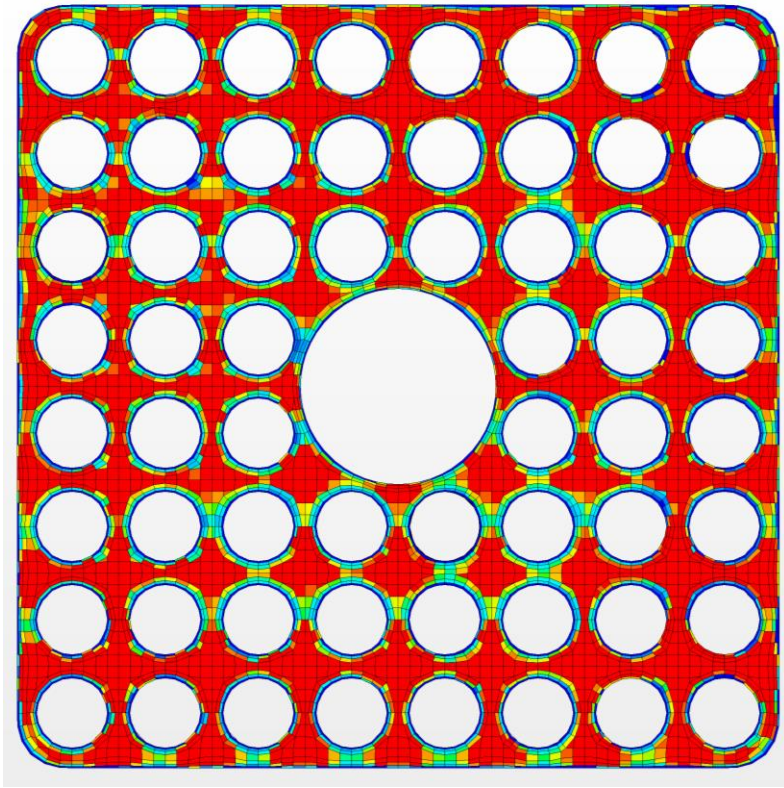


X ray Scanner: pixel-void fraction (%)

Experiment

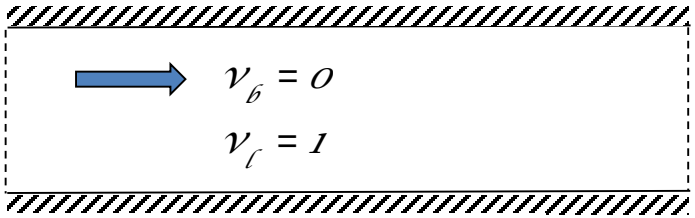


Predicted



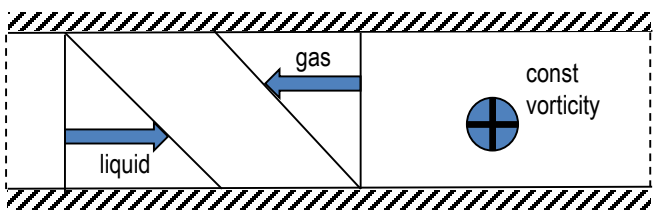
Multiphase Flow in Hydra-TH – Verification

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



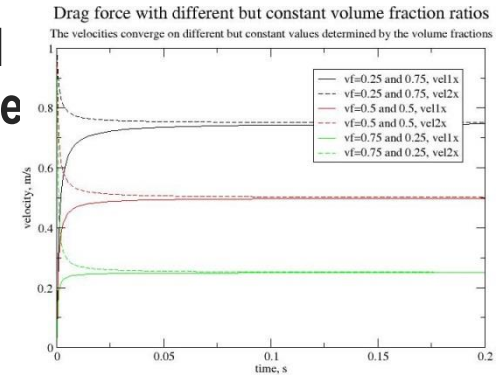
$$\mathbf{F}_d^D = -\frac{3}{8r_d} C_D \alpha_d \rho_c \left|\mathbf{v}_r\right| \mathbf{v}_r$$

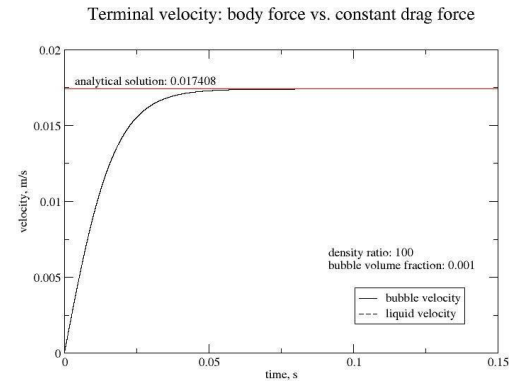
- Lift verification

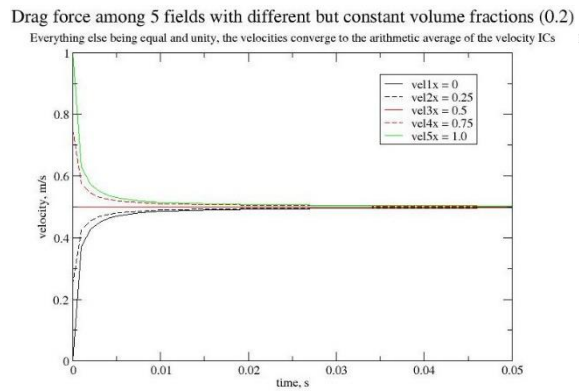


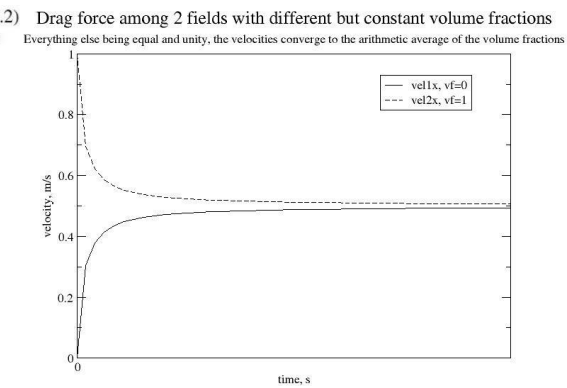
$$\mathbf{F}_d^L = -C_L \alpha_d \rho_c \mathbf{v}_r \times (\nabla \times \mathbf{v}_c)$$

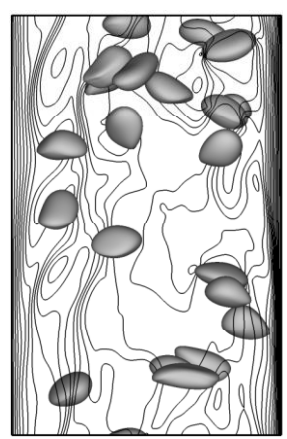
- More complex cases testing lift from:
  - Emilio Baglietto, Star-CCM+
  - Gretar Tryggvason's interface tracking code









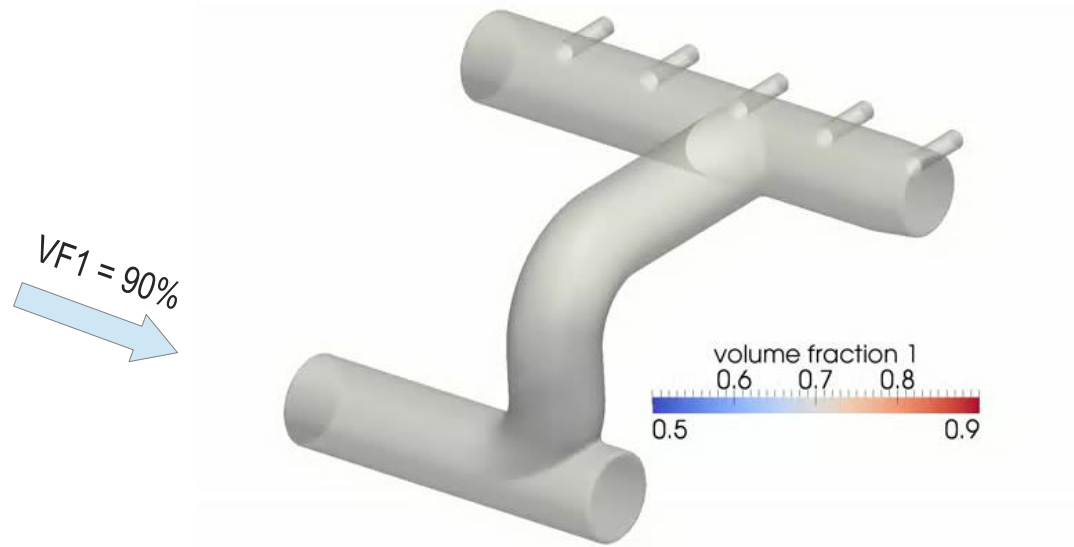


- Vary bubble diameter
- Vary spatial directions
- Vary volume fractions
- Vary number of fields
- Validation: balance of drag and body force results in terminal velocity with analytical solution

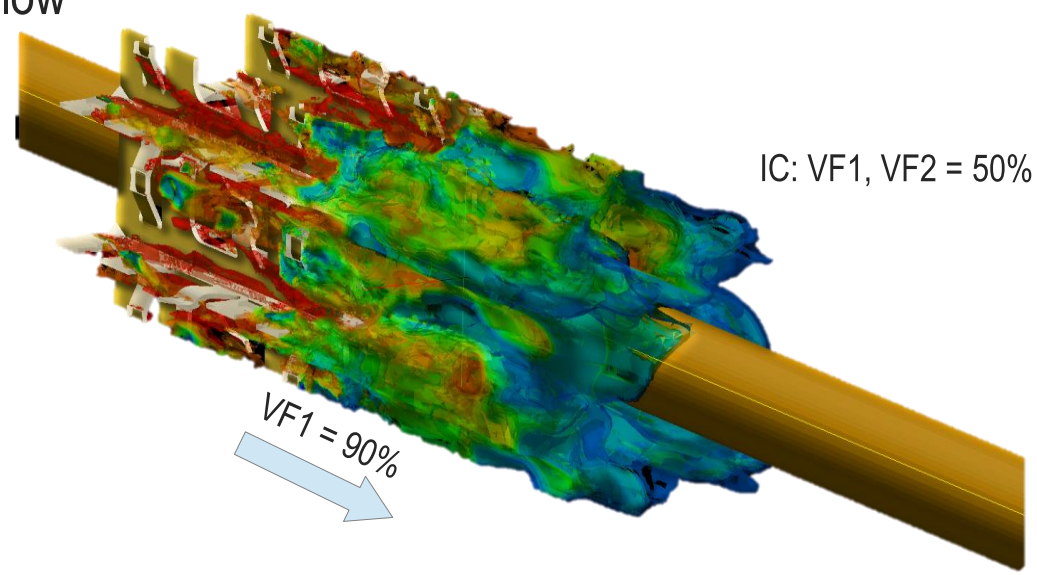
Some Multiphase Flow Calculations

IC: VF1, VF2 = 50%

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

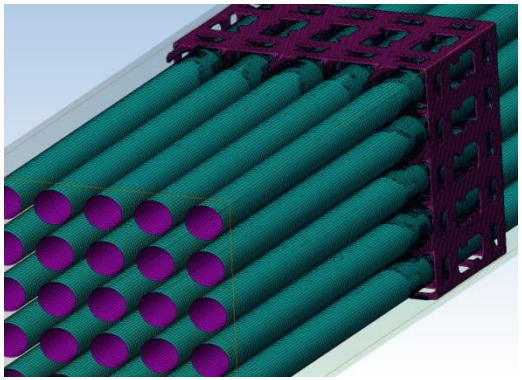


- V5H GTRF 3x3
- Same conditions as previous pipe flow
- Titan (400 CPU cores)

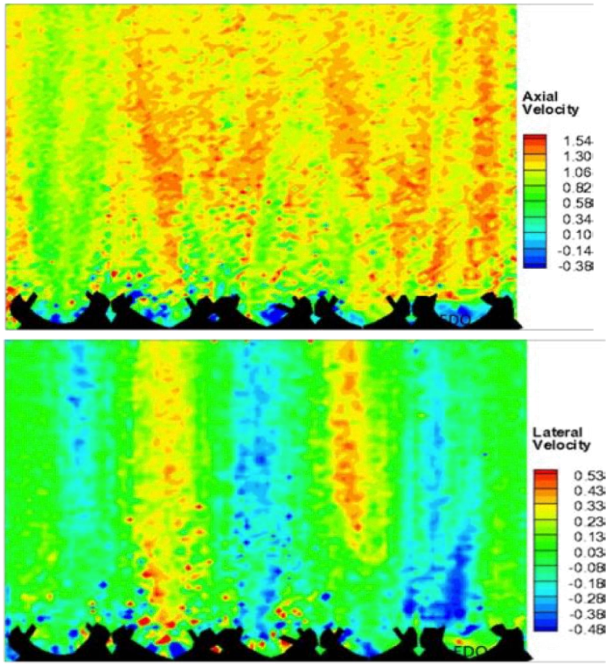


Scaled to 36,000 cores on Titan,
192 Million element mesh

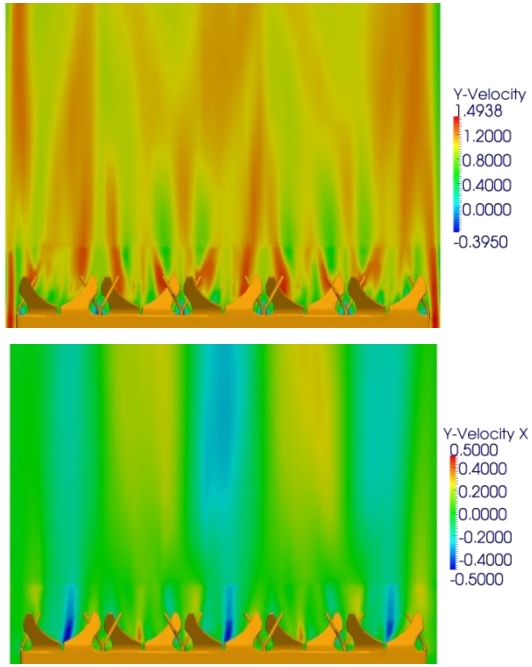
5x5 V5H study shows good agreement with experimental data



- Predicted mean peak velocities within 5% of experiments

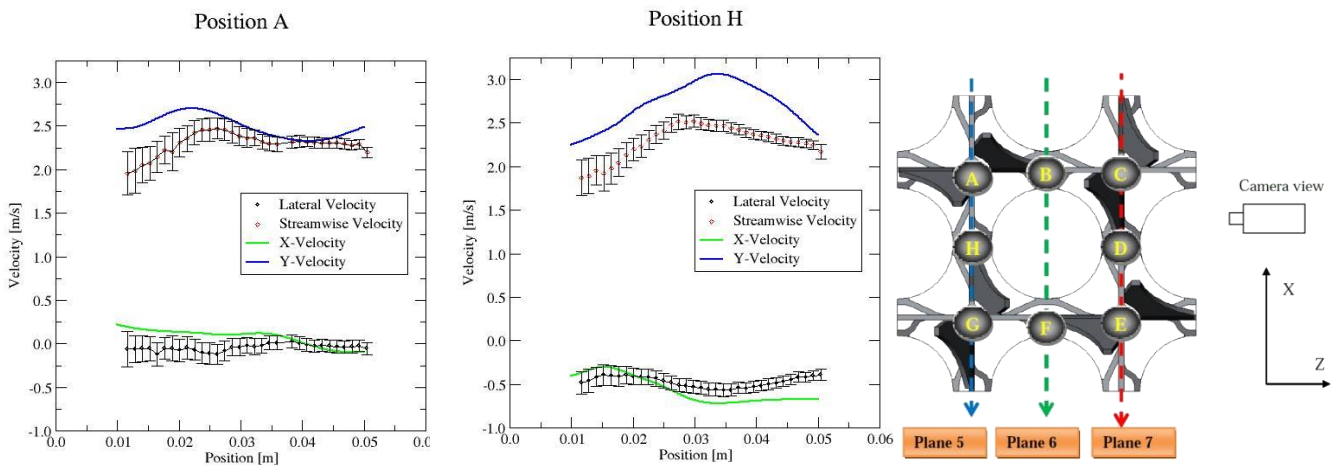


Texas A&M experiments

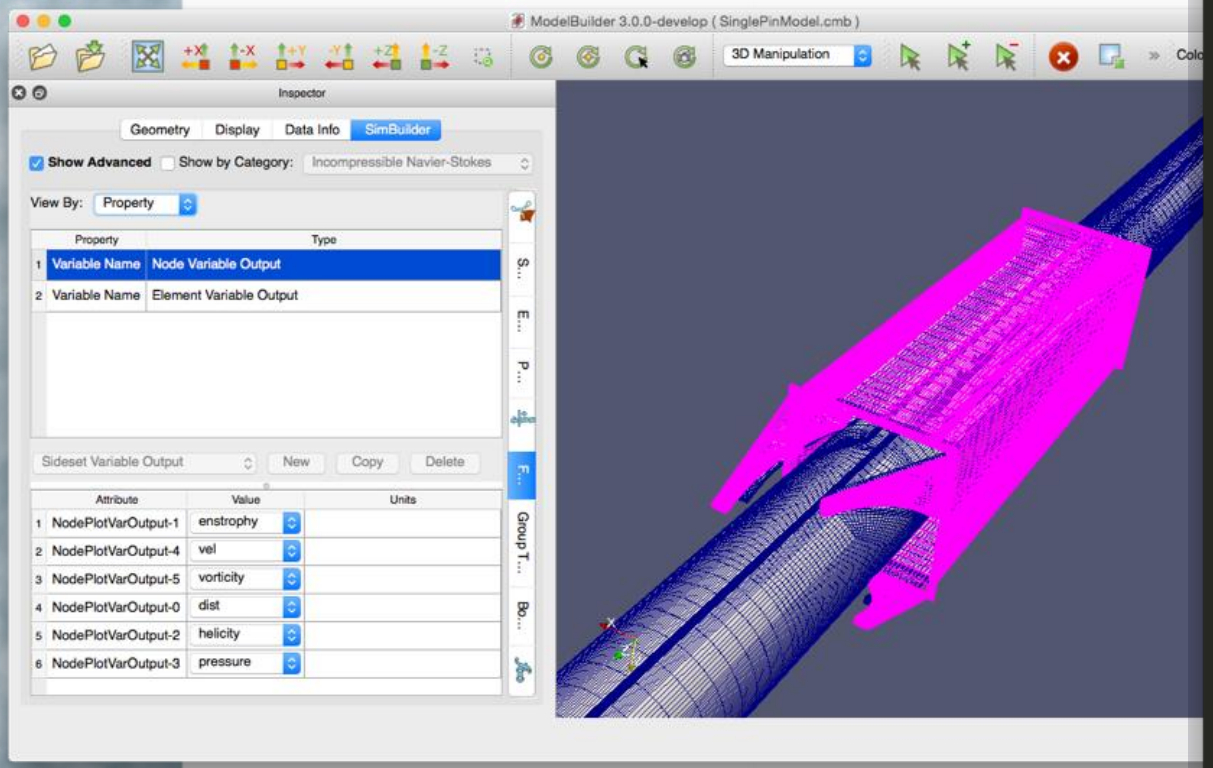


Hydra-TH calculations

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



CMB Hydra-TH support continued



single_pin_v01.cntl

```
# This is a comment
# vi:set ts=8 sw=8 ft=sh:

title
GTRF Elmahdi Spider

cc_navierstokes

  nsteps  10000
  deltat  0.001
  term    10.0

  time_integration
    type    fixed_cfl
    CFLinit 1.0
    CFLmax  4.0
    dtmax   0.05
    dtscale 1.025
    thetaa  0.5
    thetak  0.5
    thetaf  0.5
  end

  # Output options
  pltype exodusii
  filetype serial # distributed
  plti   1000
  ttyi   10
  dump   1000

  # Material model setup & assignment to sets
  material
    id  1
    rho 594.17
    mu  7.2876E-6
  end

  load_balance
```

7 characters selected

Progress and Developments

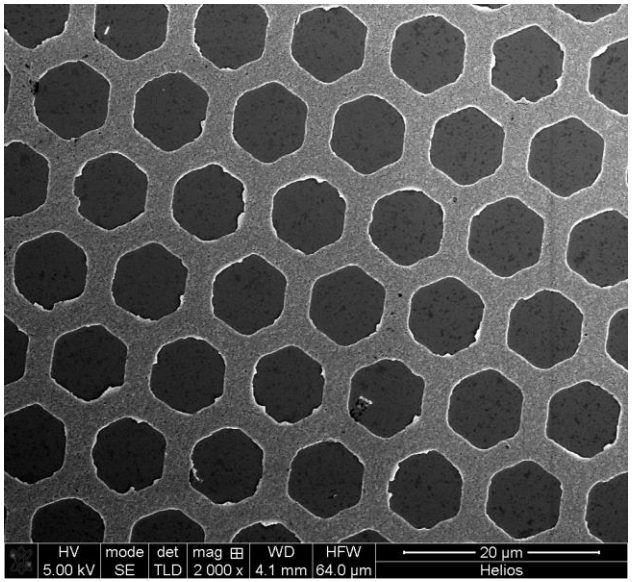
Work is being done to:

1. Optimize the photolithography and electrophoretic deposition methods
2. Couple them together to create a porous network with characteristic boiling chimneys
3. Verify SiO_2 nanoparticle performance

Deadlines:

3/31/15: Completion of manufacturing process with verified characteristics of synthetic CRUD

9/30/15: Completion of flow boiling test matrix and related analysis



Synthetic CRUD

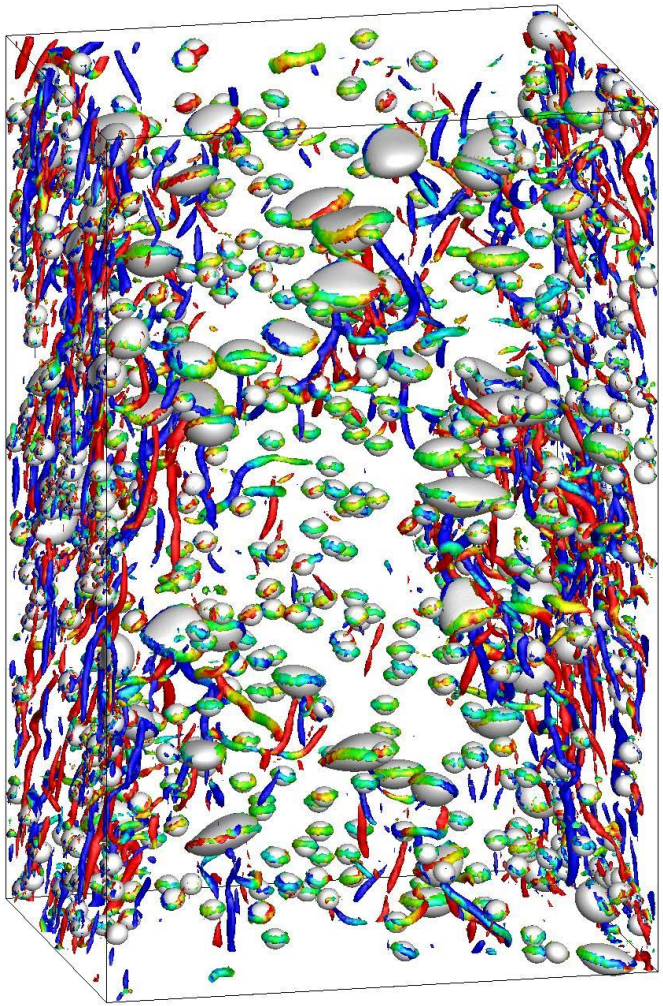
Massachusetts Institute of Technology

Consortium for Advanced Simulation of LWRs

DNS for high volume fraction bubbly flow regimes and machine learning for closure development

- Mining of the results from very large simulations of complex flows to help with the development of two-fluid and LES-like models. Data obtained by averaging over the homogeneous directions and well as local filtering will be collected and we will explore the relations between unknown closure terms and quantities that are evolved in large-eddy and two-fluid simulations, using linear and nonlinear data reduction techniques (such as regression and neural networks, or more advanced techniques).
- Simulations of high void fraction flows where topology changes are an important part of the dynamics, and examination of how to use the results for modeling of such flows. The tasks include obtaining a better understanding of the importance of how the coalescence is modeled, including turbulence, and apply data analysis methods to extract information for modeling of the average or large scale flows.

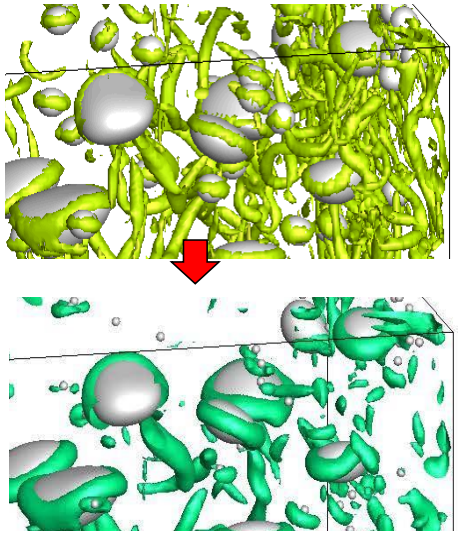
Transient Motion of a Large Number of Bubbles



500 bubbles of different sizes in channel flow with $Re^{+}=500$

"LES-like" filtering

The effect of applying a top hat filter with a size slightly larger than the diameter of the smallest bubbles to both the velocity and the interface. Large bubbles and vortical structures are smoothed and small bubbles become point particles

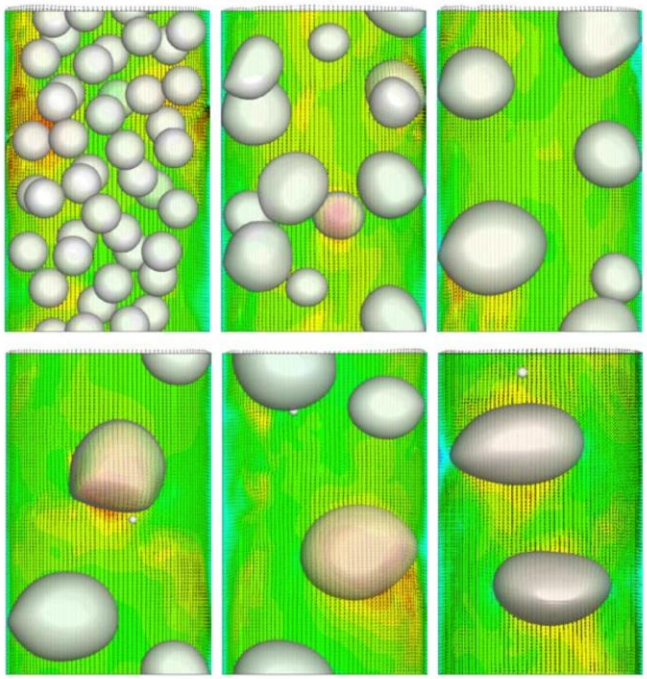


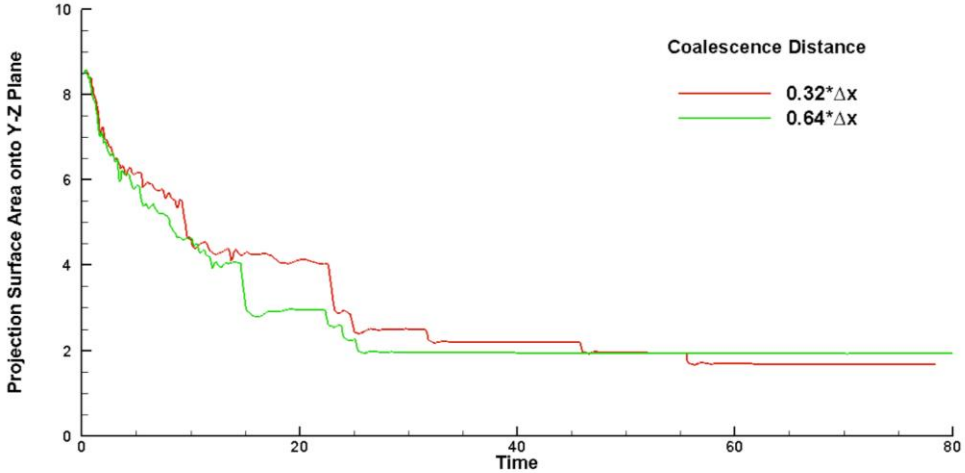
$$\bar{u}(x) = \int G_\Delta(x - x')u(x')dx'$$

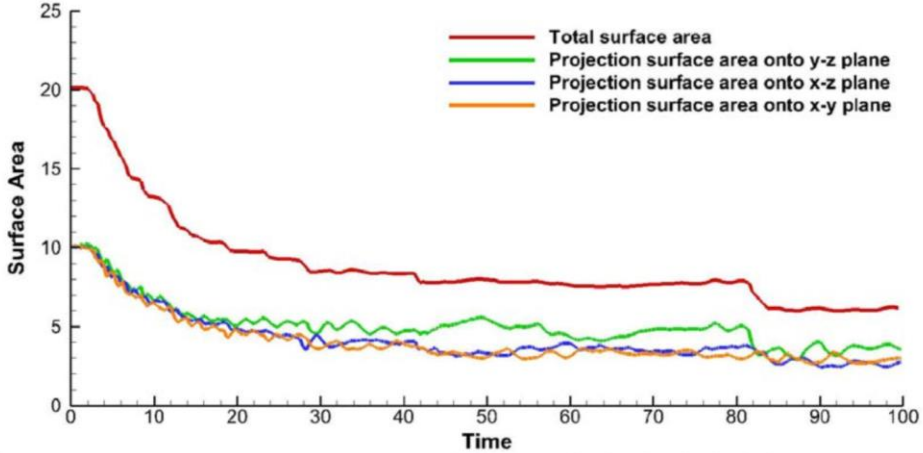
$$\bar{X}(s) = \int G_\Delta(X(s) - X(s'))X(s')ds'$$

$$G_\Delta(x) = \begin{cases} 1 & \text{if } |x| < \Delta; \\ 0 & \text{if } |x| > \Delta. \end{cases}$$

Flow Regime Transitions in High Void Fraction Flows





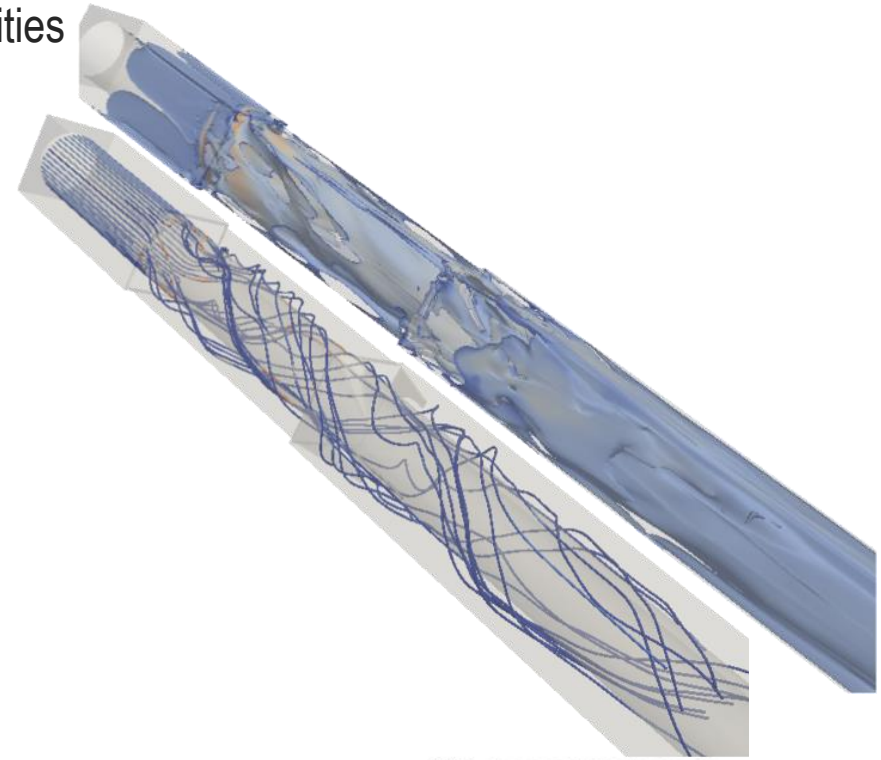


Simulations of bubbly flows undergoing topology changes, resulting in flow regime transitions. The top graph on the right shows the effect of the coalescence criteria.

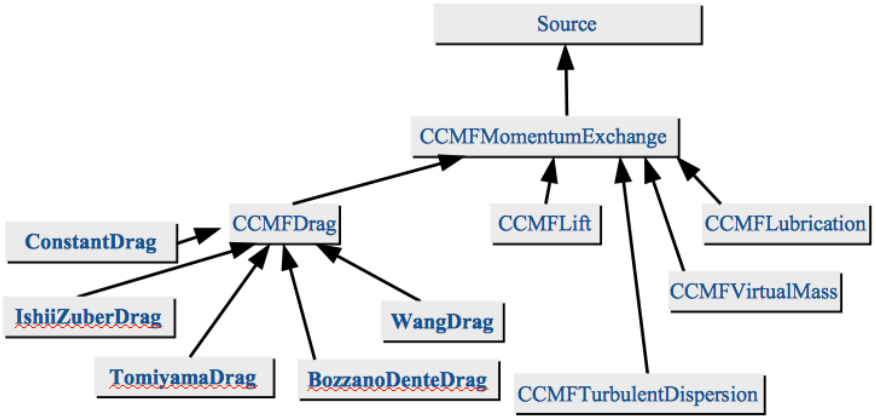
Catalyst In-Situ Analysis and Visualization + Cinema

- Catalyst output requested from Hydra-TH input (.cntl file)
- Specify Python scripts
- Can request specific field information to be output – similar to format for writing out plot, history and dump files
  - Node, element, sideset centered quantities

```
catalyst
   script hydrasinglepin.py
   node vel
   elem div
   node lambda
   node pressure
   node helicity
   elem density
end
```



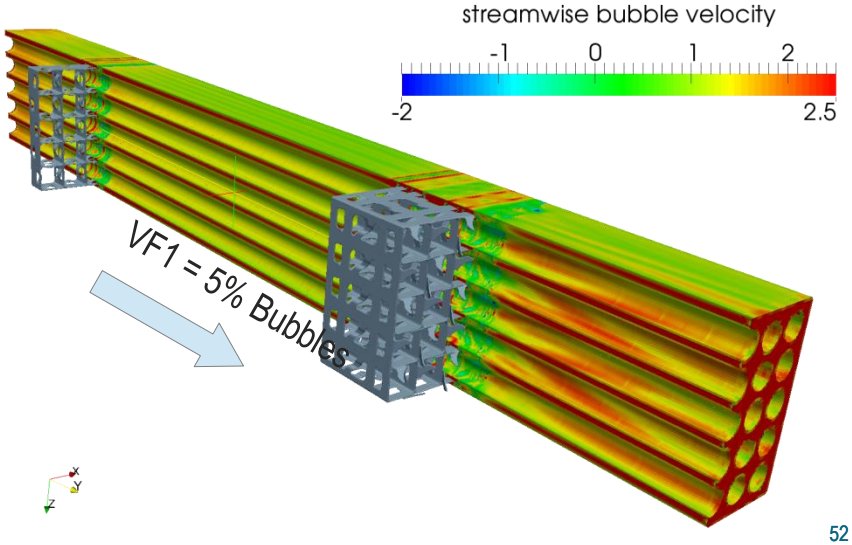
Multiphase Flow in Hydra-TH



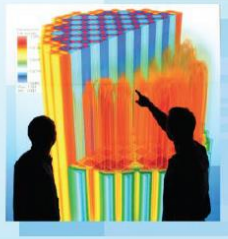
- **Generic *N*-field algorithm:** semi-implicit and fully-implicit, skew-symmetry preserving, predictor-corrector algorithm
- **"Expert-user" multiphase capability:** User can specify different closure for any field-pair
- **Scales:** Tested on Titan with 35K CPU cores
- **Momentum exchange:**
  - drag,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

Example calculation

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

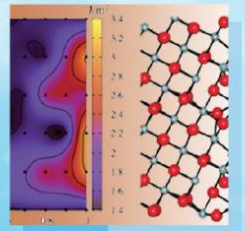


Power uprates and plant life extension



Engineering design and analysis

Science-enabling high performance computing



Fundamental science

Plant operational data

CASL

Consortium for Advanced Simulation of LWRs

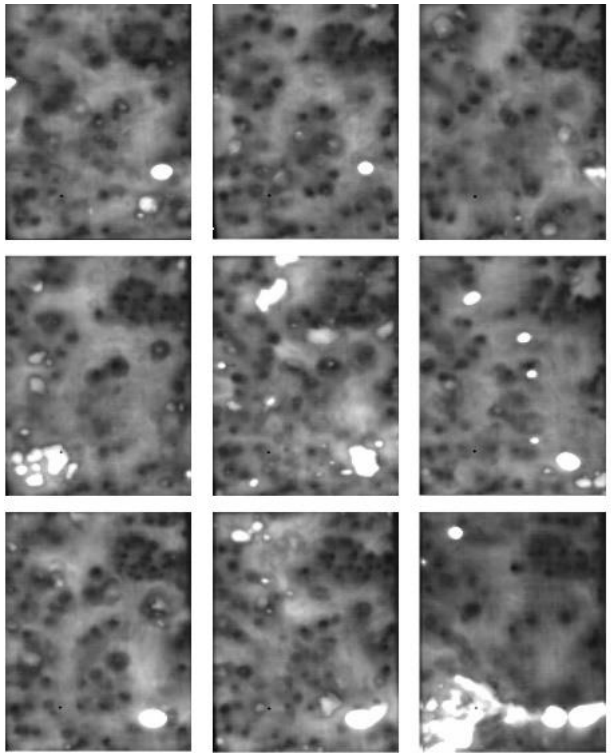
Micro-hydrodynamics in High Heat Flux Boiling and Burnout: Experimental Data and Model Development

Yang Liu
Manu Srivastava
Nam Dinh

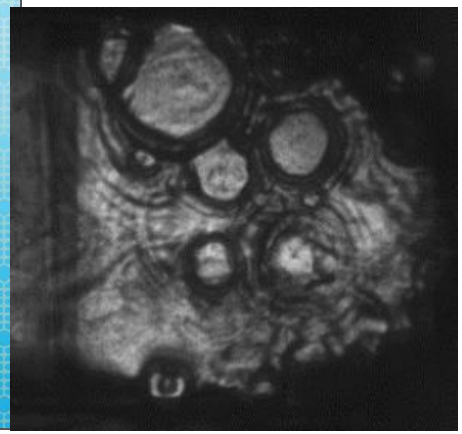
September 2014

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

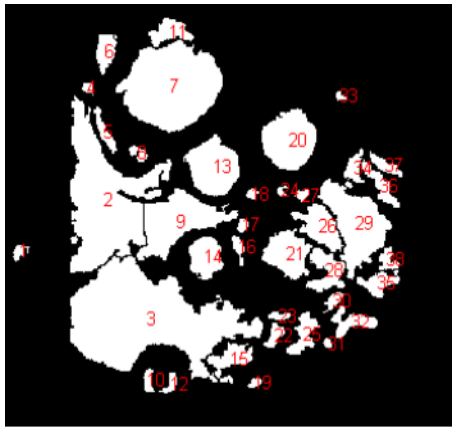
Burnout Caught in Action



Original image



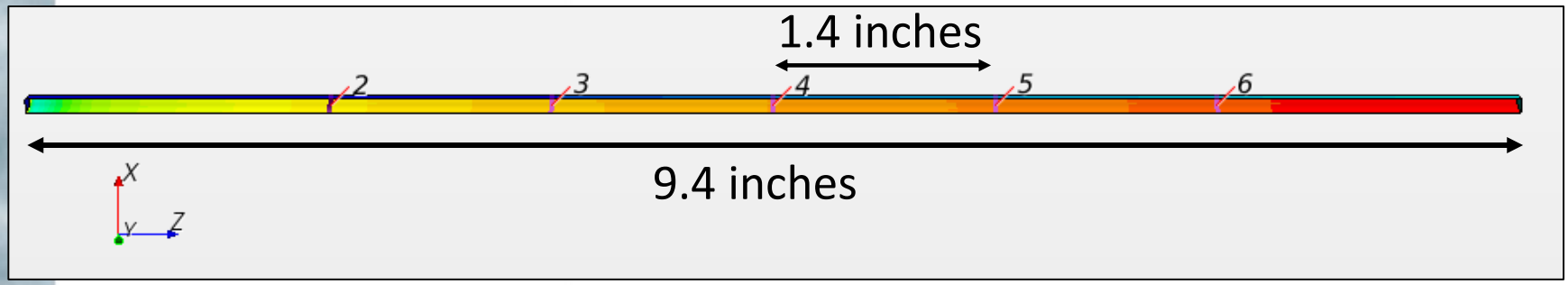
Binary image with separate objects



Rohsenow High Pressure Experiment

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

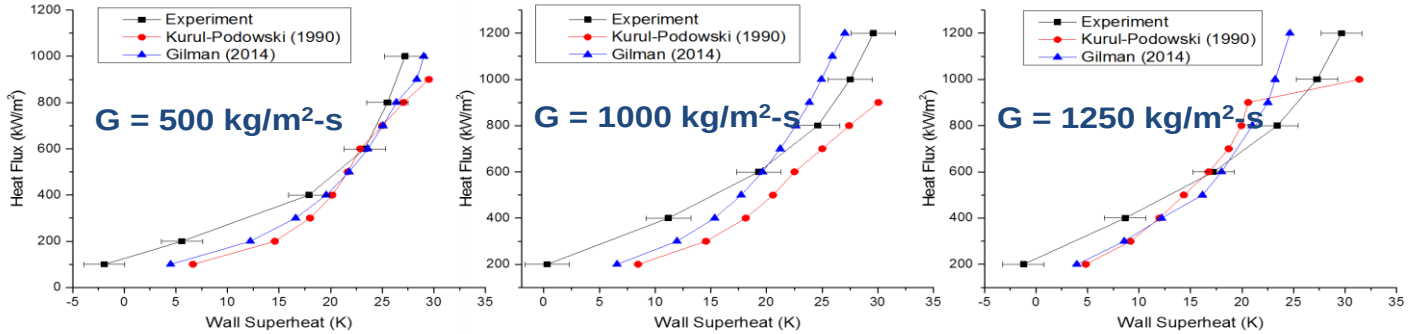
Heat Flux [MW/m2]	Inlet ΔT_{sub} [K]	Thermocouple Positions	Experiment ΔT_{sup} [K]	Experiment Error [K]	Gilman (2014) ΔT_{sup} [K]
3.41	130.7	5, 6	2.58	+/- 1.7	0.98
4.07	130.9	2,3,5,6	2.65	+/- 1.7	1.10
4.61	131.0	2-6	3.92	+/- 1.7	1.02
5.11	136.4	2-6	4.14	+/- 1.7	2.36



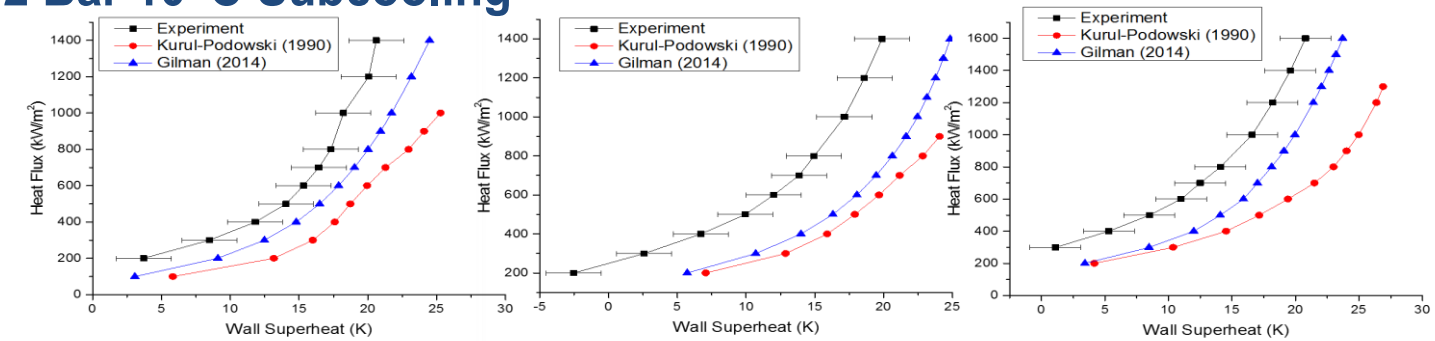
Calibration-free Assessment

extensive small scale CASL database

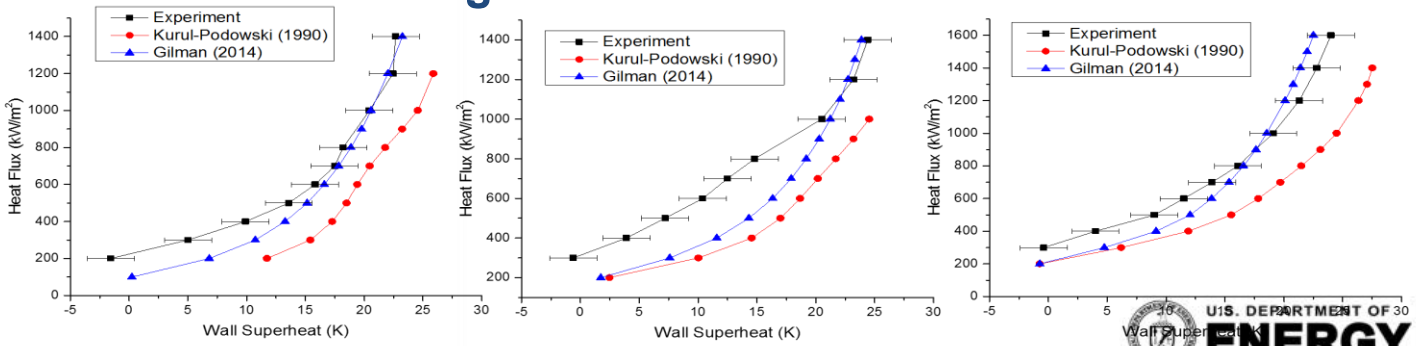
1 Bar 10°C Subcooling



2 Bar 10°C Subcooling



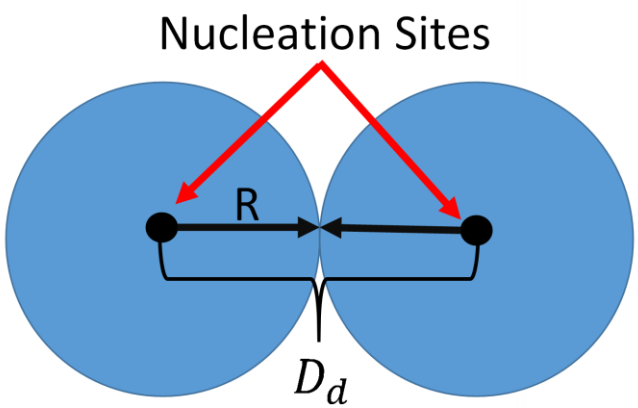
2 Bar 15°C Subcooling



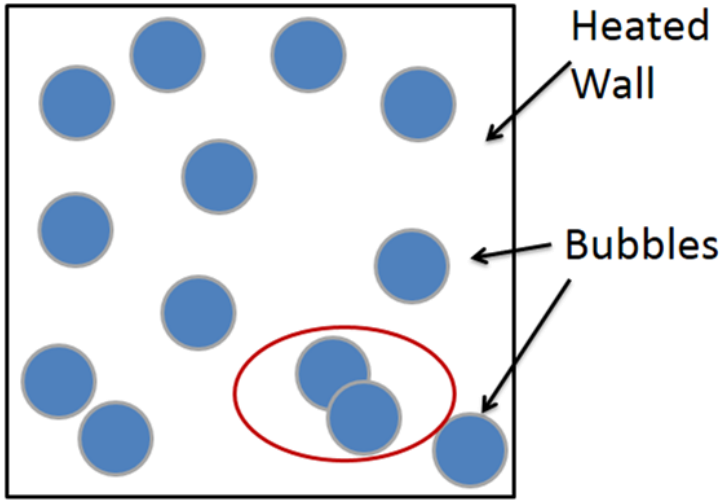
Bubble Merging on the Heater

- Bubbles merge on heater surface prior to departure
  - Indicates size of dry surface patches
- Fraction of nucleation sites ACTIVE at a point in time

$$\rightarrow N_b'' = f t_g N''$$



$$P = 1 - e^{-N_b'' \pi D_d^2}$$



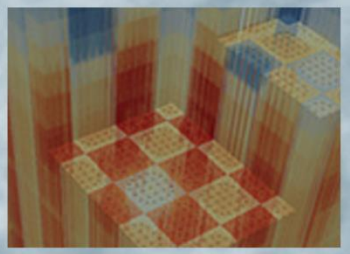
A DOE Energy Innovation Hub

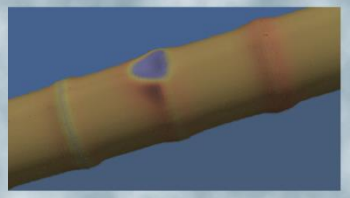
Update on Validation and Modeling Applications (VMA)

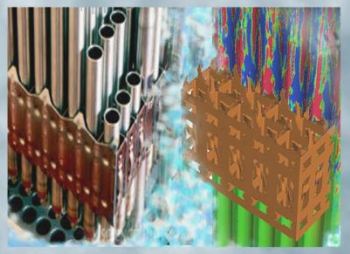
Vince Mousseau

Yixing Sung

Brian Williams







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Outline

- Phase I accomplishments
- VUQ application examples
- Phase 2 strategy and data challenges

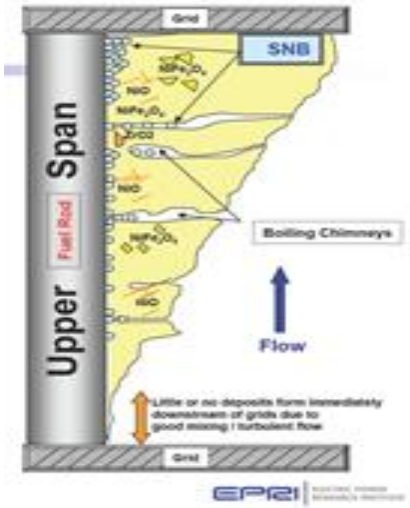
Validation and Modeling Applications (VMA)

Achieving Credible, Science-based Predictive Simulation Capabilities

A DOE Energy Innovation Hub

Objectives and Strategies

- VMA = VUQ + AMA: Validation and Modeling Applications has been formed by combining Validation and Uncertainty Quantification with Advanced Modeling Applications.
- This provides a much tighter coupling between the assessment and application of VERA with its VVUQ.
- This improves technology development and product delivery to address the industrial Challenge Problems.



Requirements Drivers

- Software related to reactor safety analysis must meet quality requirements.
- Provide a clear justifiable case that the software is appropriate for the intended application.
- PCMM, CSAU, SQA, and VVUQ are the key tools to define new standards for software development and application.

Outcomes and Impact

- The DAKOTA software will be delivered as part of VERA and it will introduce modern tools for VVUQ for use by Industry.
- We will help to define VVUQ plans and processes for the CASL challenge problems and for the VERA components.
- These plans and processes when implemented will provide confidence in VERA for industry use by clearly defining value added work.

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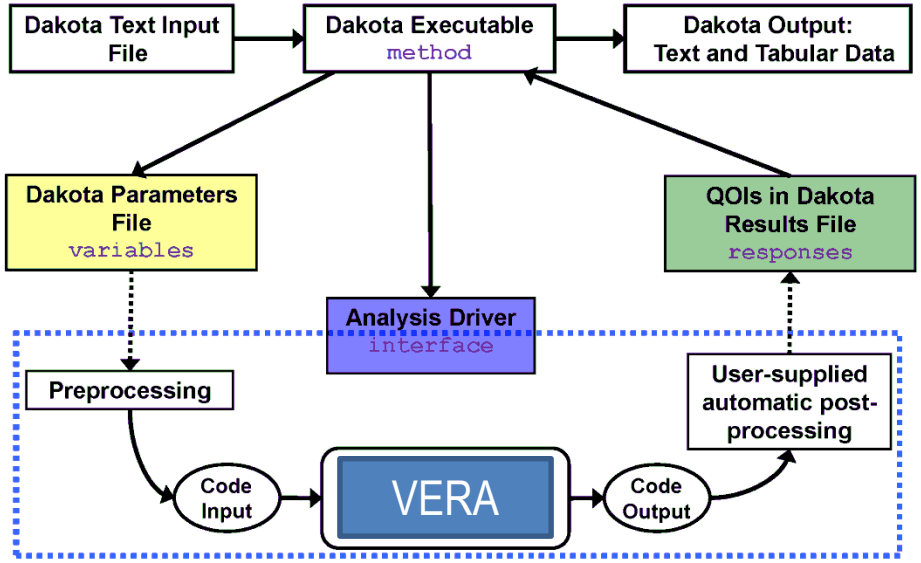
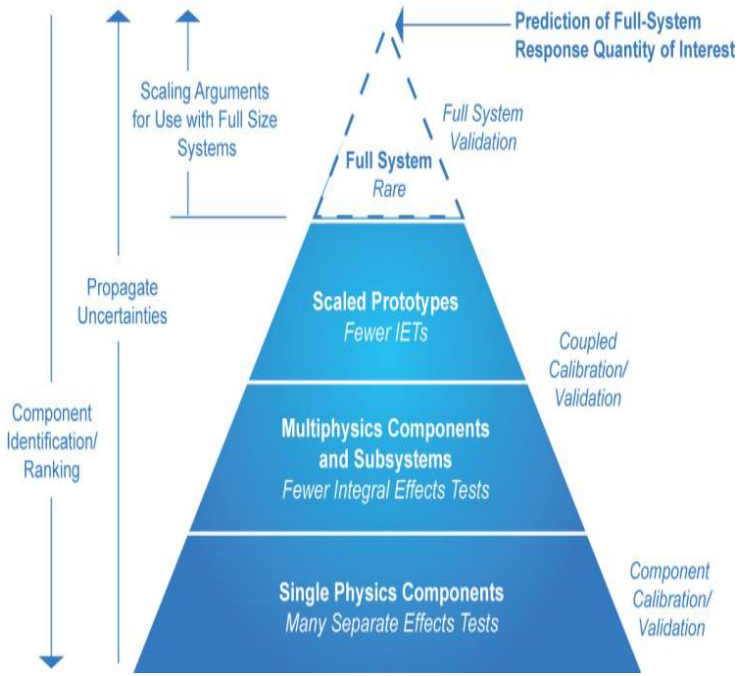
Phase I Accomplishments (1)

- Provided DAKOTA tools and user guidelines to automate and guide VVUQ for code development and challenge problem applications
  - DAKOTA contains tools for optimization, uncertainty quantification, parameter estimation, and sensitivity/variance analysis
- Completed initial VVUQ assessments of CASL tools
  - Revealed simulation and DAKOTA weaknesses have been improved
  - Some of the work has been on "one-off" studies
  - Early work with industry codes



Phase I Accomplishments (2)

- Performed VERA-CS component code VUQ studies
  - Parameter exposure work in subchannel T/H code CTF to improve sensitivity and UQ
  - Initial PCMM analysis of CTF to measure documentation and testing
  - Initial PCMM analysis of neutronic code Insilico to measure documentation and testing
- Worked with CASL partners to collect industry-quality data to address code and model validation needs



Better VUQ engagement in CASL

VUQ Application Examples

- VERA Progressive Problem 6 Study
  - Geometry: Single Westinghouse 17x17 fuel assembly
  - Condition: hot full power (HFP) and Beginning of Life (BOL)
  - Modeling and Simulation: VERA-CS neutronic and subchannel thermal-hydraulic (T/H) code plus DAKOTA

- Turbulent mixing parameter calibration under DNB CP
  - Geometry: 5x5 rod bundle mixing test
  - Condition: Single phase flow and heat transfer for channel exit temperature measurements
  - Modeling and simulation: VERA-CS T/H code CTF plus DAKOTA for calibrating empirical constant

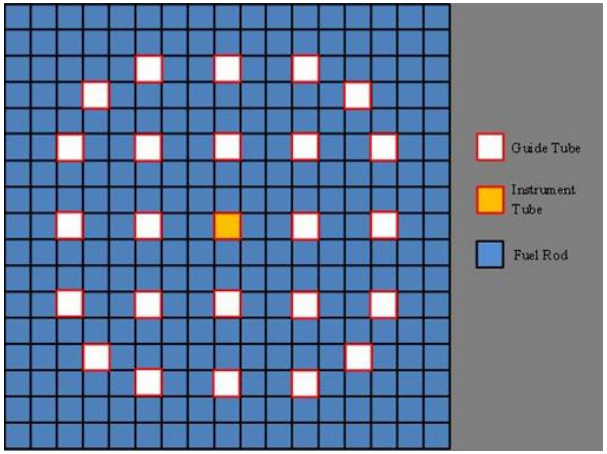
VUQ Example Summary

Initial VERA-CS Problem 6 Multi-scale Multi-physics VUQ

- Phenomenon Identification Ranking Table
  - Define phenomena for fuel, thermal hydraulics, and neutronics
- Quantified Parameter Ranking Table
  - Top down approach (test the trees not branches)
- Low level calibration work with Dittus-Boelter (single phase heat transfer) and McAdams (single phase friction) and neutronics
  - Challenge to get "appropriate" calibration data
  - Key result is the importance of capturing the "joint" distributions between parameters
- Initial Uncertainty Quantification results
  - Problem 6 is single phase liquid: thermal hydraulic uncertainties are small
  - Need to address cross section uncertainties with reduced order modeling and calibration to reduce uncertainties

Problem 6 is a VUQ surrogate for CPs

VUQ Analysis of Cobra-TF for Progression Problem 6

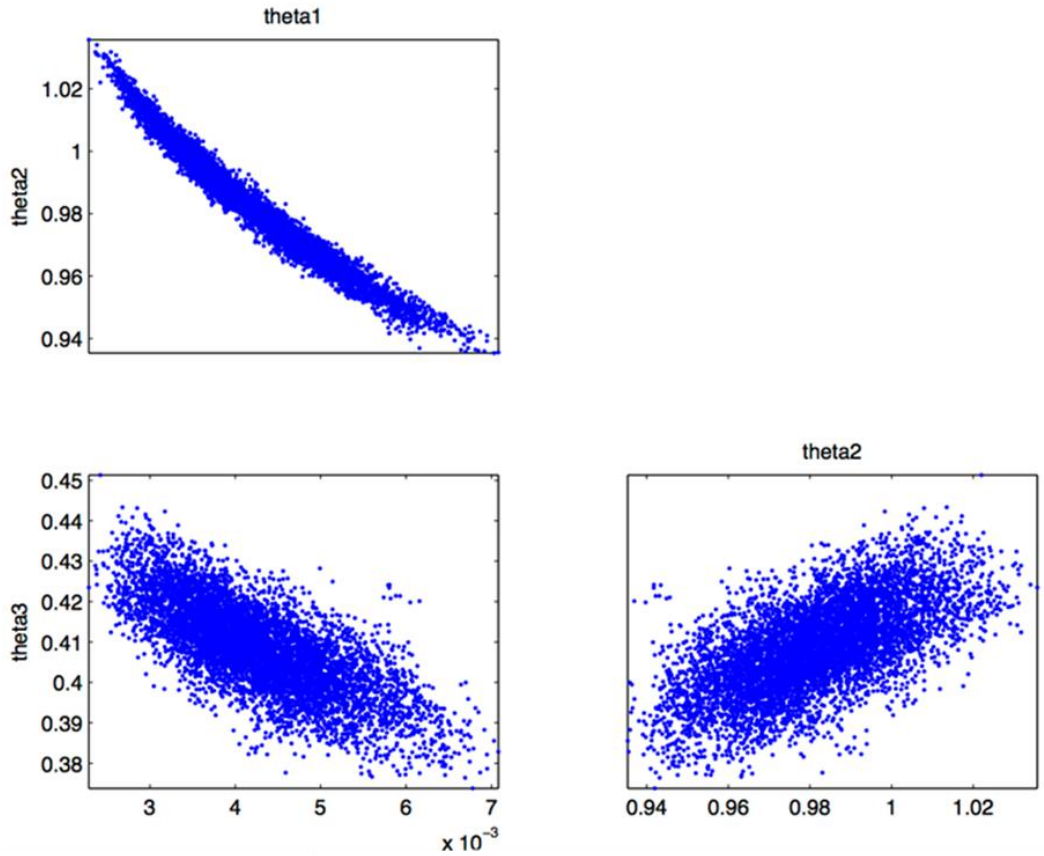


- Simulation of a single PWR assembly
  - Hot Full Power, T/H feedback
  - Boron concentration of 1300 ppm, 100% power
  - Power supplied by neutronics held constant
- Quantity of Interest is maximum fuel temperature
- We have three parameters distributions to construct
  - Expert opinion
  - Marginal (independent)
  - Joint distribution

$$Nu = 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4} = \theta_1\,\mathrm{Re}^{\theta_2}\,\mathrm{Pr}^{\theta_3}$$

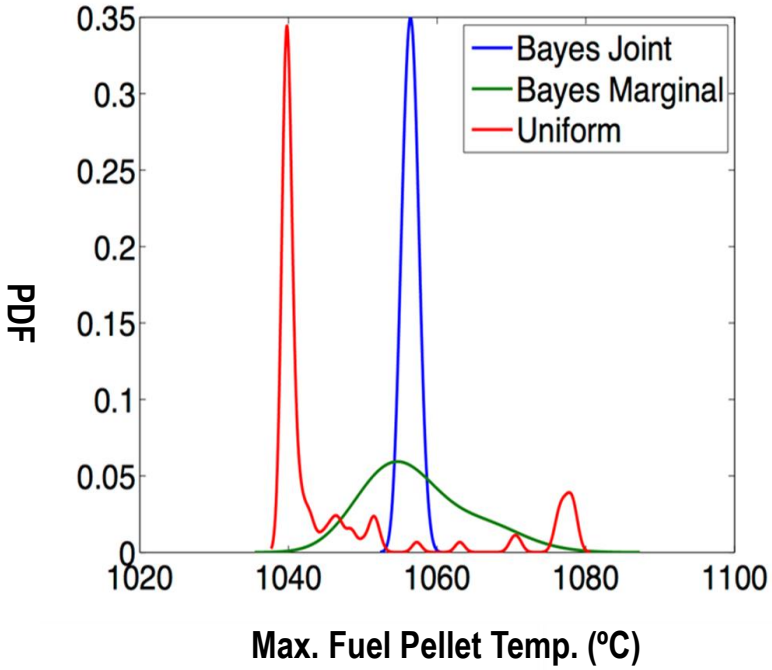
Single phase heat transfer

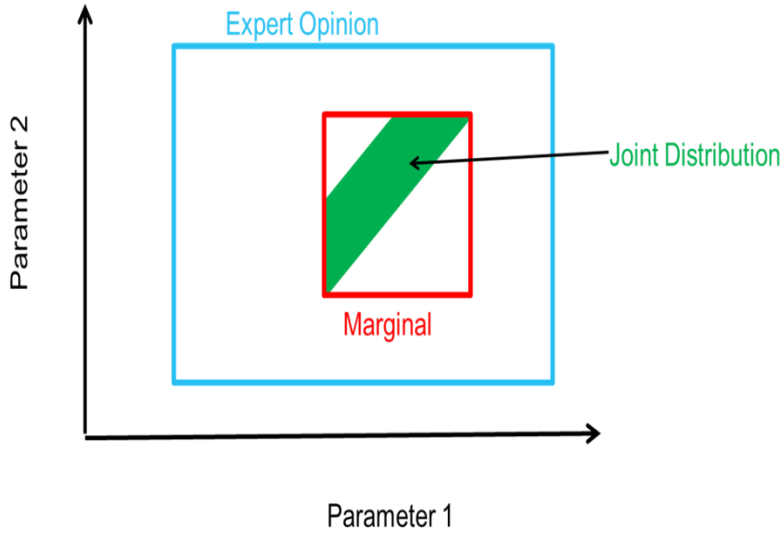
Dittus-Boelter -Bayesian Calibration Reveals Parameter Interactions



Experts assume independent

Dittus-Boelter Calibration





Capturing the joint distribution

Problem 6 UQ Summary

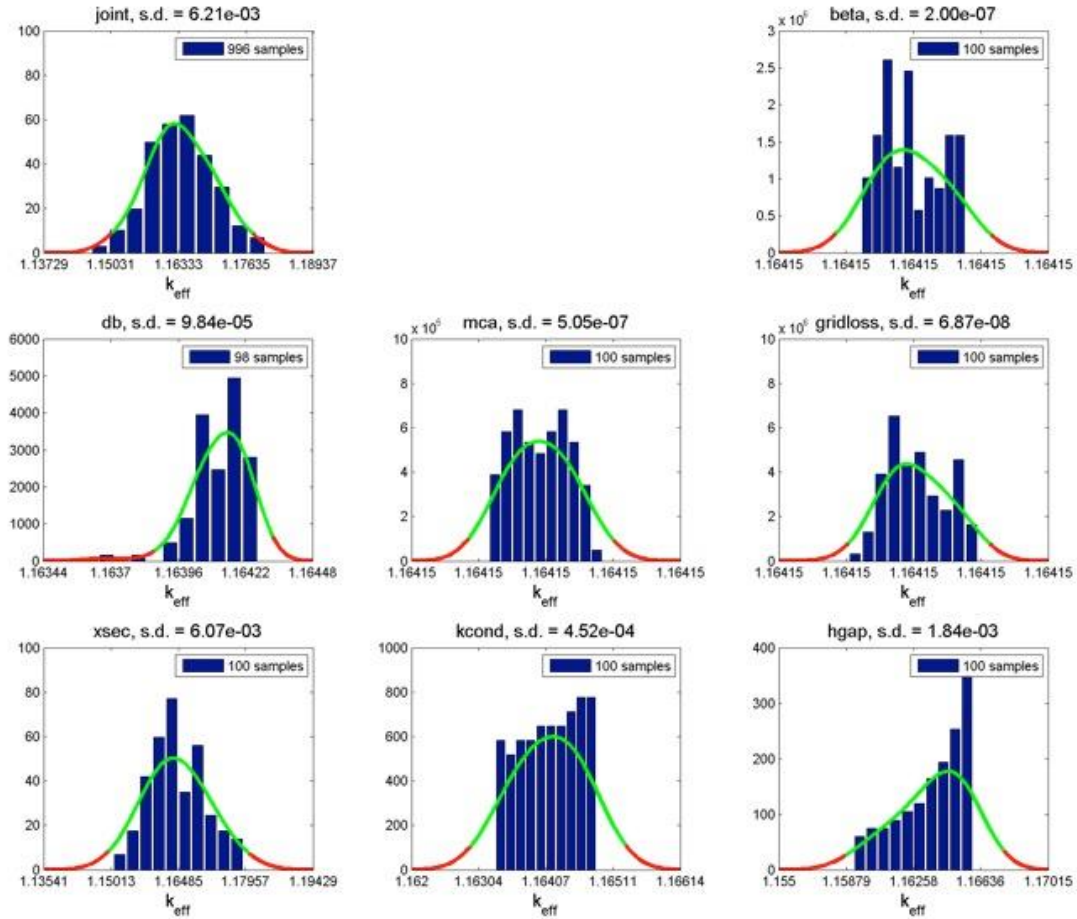
- ***Keff*** – is mainly a function of the cross section uncertainty, and followed by gap conductivity.

- ***Max Pin Temperature*** – Is dominated by gap conductivity, and followed by pellet thermal conductivity. Note we assumed a 10% uncertainty in the thermal conductivity of fresh fuel.

- ***Max Pin Power*** – Is dominated by gap conductivity, and followed by the cross section and fuel pellet thermal conductivity uncertainties

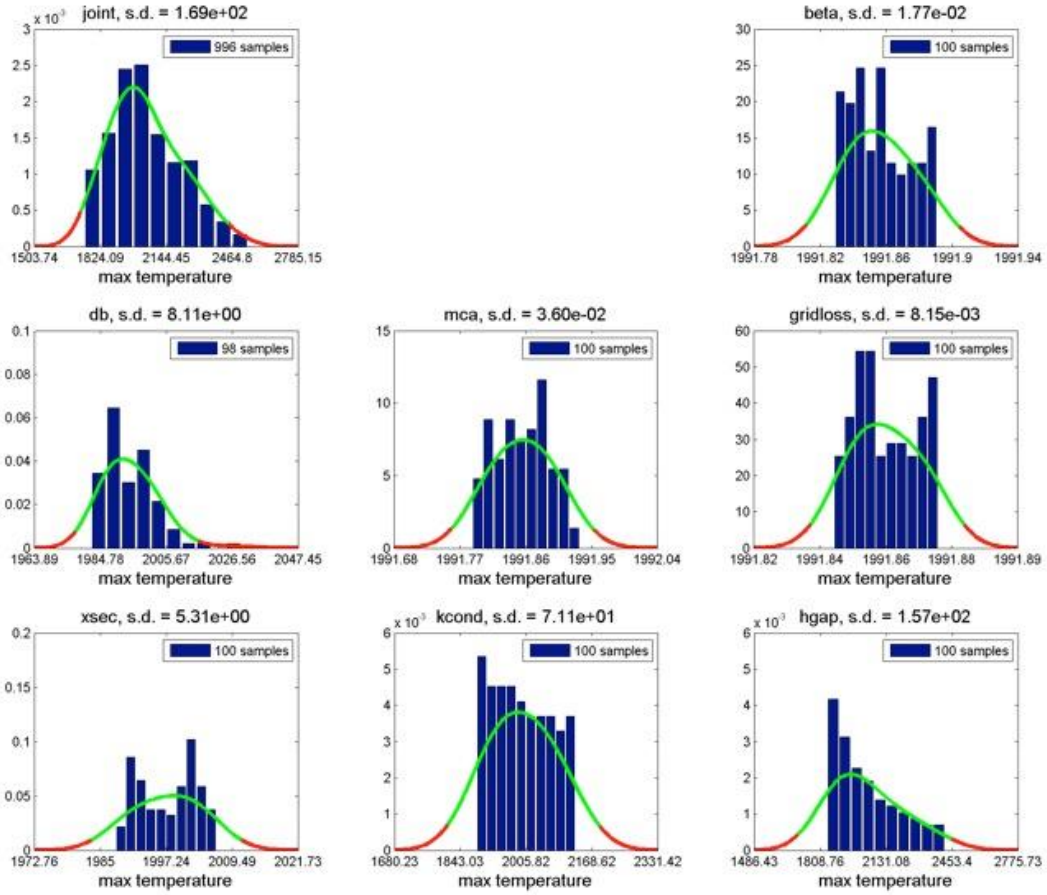
Coupled code BEPU on QoIs

Keff Study



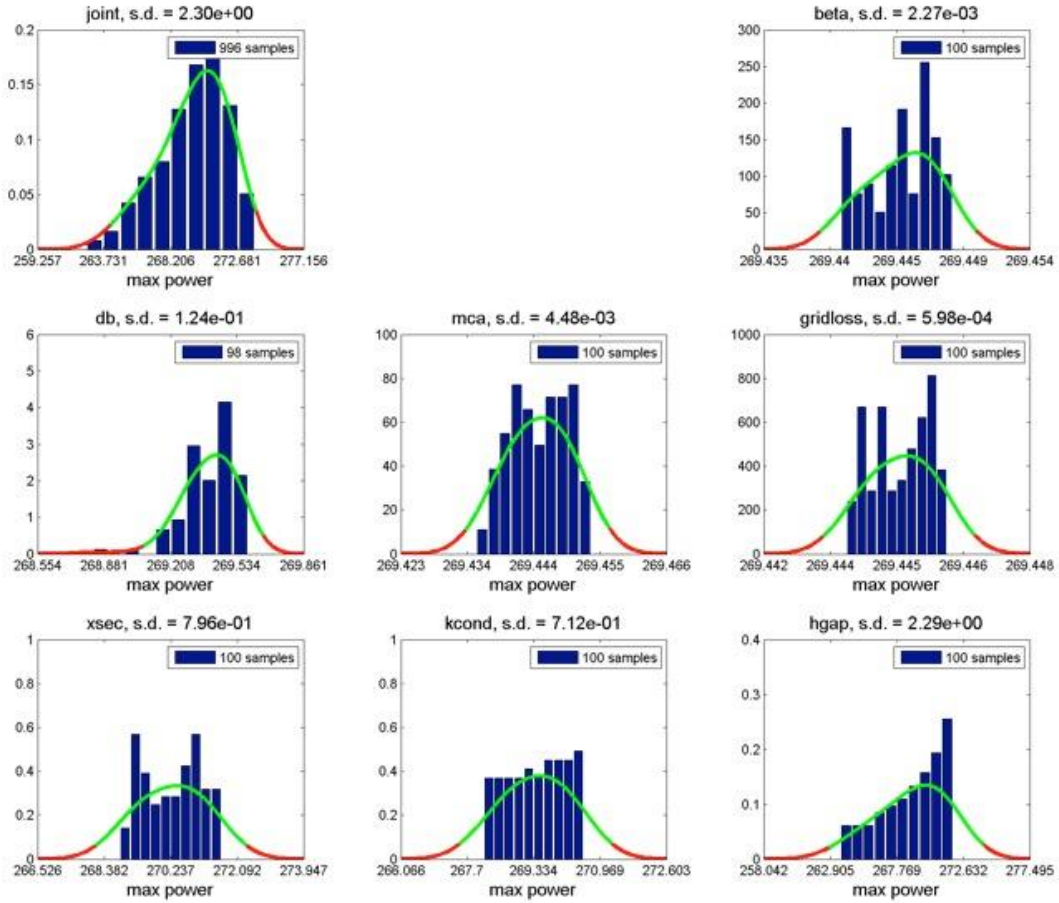
VERA Problem 6 UQ

Max Pin Temperature Study



VERA Problem 6 UQ

Max Pin Power Study



VERA Problem 6 UQ

Initial VUQ DNB CP Study

- T/H solution Verification – quantitatively established that CTF results were mesh converged. Numerical uncertainty approximately zero. Single phase results are almost linear
- Analysis of the experimental data – the code results are symmetric by design. The data are not symmetric
- Initial calibration of turbulent mixing using DAKOTA with data
  - WEC provided proprietary rod bundle mixing and DNB data for CASL validation use
  - This large amount of experimental data allows for both validation and calibration
- Data and calibration are fuel design specific:
  - Initial calibration based on data for non-mixing vane grid spacer

Subchannel Turbulent Mixing Model – Initial DNB Study

The turbulent mixing in subchannels was modeled using the following empirical correlation:

$$\Delta Q = -w' \times \Delta h \times \Delta X \qquad (5\text{-}1)$$

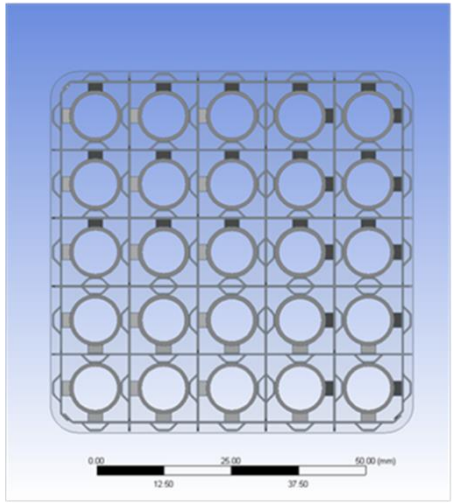
where ΔQ = energy exchange due turbulent mixing (W or Btu/hr)
w' = lateral turbulent flow per unit length (kg/s/m or lbm/hr-ft)
Δh = enthalpy difference between two subchannels (J/kg or Btu/lbm)
ΔX = axial nodal length (m or ft)

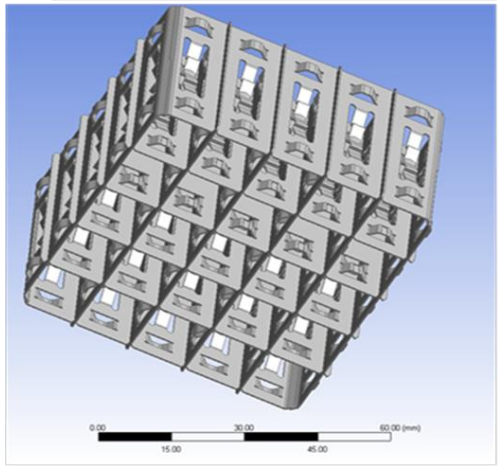
$$w' = ABETA \times G_{AVG} \times S \qquad (5\text{-}2)$$

where $ABETA$ = empirical coefficient,
G_{AVG} = average axial mass flow in the connected channels (kg/s/m^2 or lbm/s/ft^2)
S = rod-to-rod gap width (m or ft)

Mixing Model and Empirical Coefficient

Calibration of CTF Mixing with Rod Bundle data





Eval #	BETA	wRSS
1	0.00600000	17.6802
2	0.00100000	18.566
3	0.00496073	17.57965
4	0.00392327	17.57847
5	0.00408976	17.57021
6	0.00442246	17.56284
7	0.00440553	17.56482
8	0.00442077	17.56318
9	0.00442229	17.56307
10	0.00442244	17.56284
11	0.00442245	17.56284
12	0.00442245	17.56284
13	0.00442246	17.56284

DAKOTA used to calibrate CTF

VVUQ Strategy in Phase II

- PIRT (expert opinion) and QPRT (code sensitivity) “iterated to convergence” (What the experts think are important and what the code thinks is important match) for a challenge problem.
- Validation Data Integrator constructs a validation pyramid that separates low level code validation (bottom) from coupled code validation (top).
- Code VVUQ and Challenge Problem VUQ done in 2 steps
  - Code VVUQ during software development
  - Validation and uncertainty quantification during application
- Initial uncertainty quantifications focus on three CPs; CIPS, PCI, and DNB.
- VUQ requires strong team work in CASL and **support of IC**

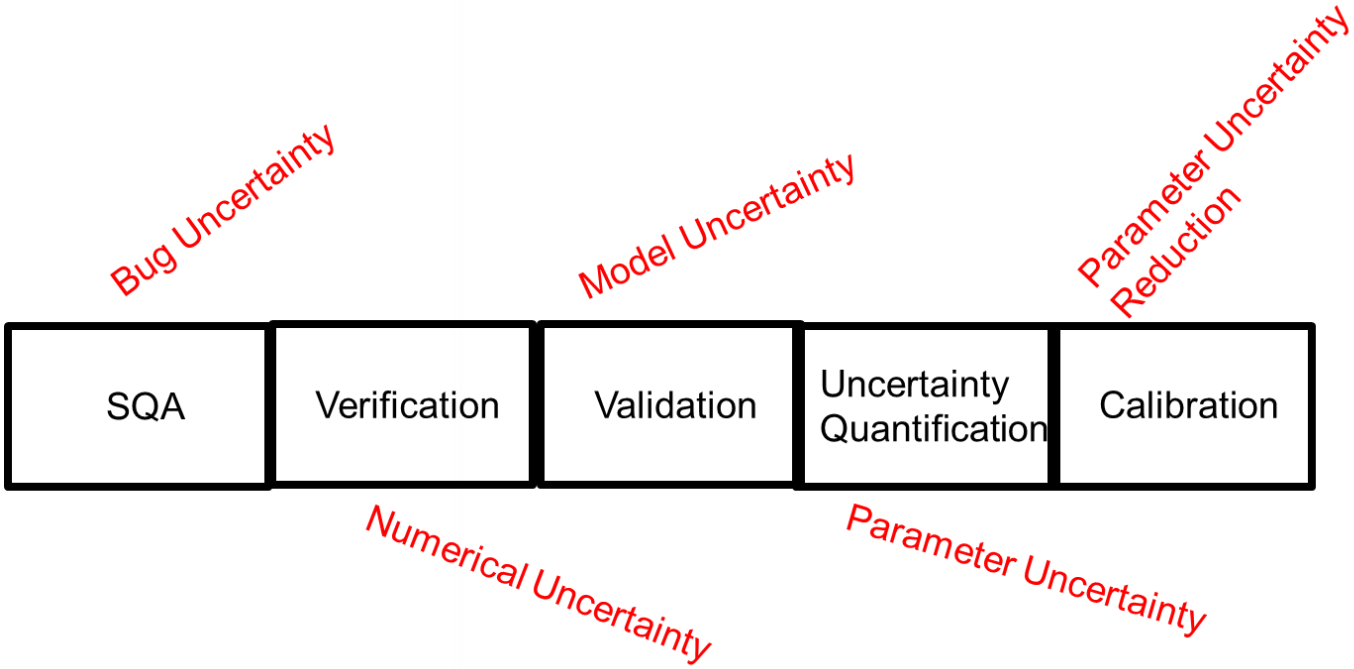
It takes a village to raise a child

Total Uncertainty

- **Verification:** $\left\| QOI_{exact} - QOI_{computed} \right\|$
- **Validation:** $\left\| QOI_{experimental} - QOI_{computed} \right\|$
- **Uncertainty Quantification:** $\left\| QOI_{perturbed} - QOI_{computed} \right\|$
- **Impacts of numerical, model, and parameter uncertainties should be compared and evaluated.**

Holistic view of uncertainty

Predictive Capability Maturity Model (PCMM)



CASL has chosen PCMM which is an iterative process to measure software quality and maturity where one continually works on the lowest score.

The process that connects the tools

CASL VUQ Impacts

- PCMM helps to justify new software application to meet regulatory requirements
  - A “modernized” CSAU.
  - The total uncertainty approach.
  - Improvement of the Wilks formula approach.
- DAKOTA use by CASL
  - Provide better frequentist tools (better statistics).
  - Provide Bayesian tools.
  - Use of HPC when needed for VVUQ (~1000 runs).
- In addition to CASL applications, DAKOTA is coupled to all NRC codes through SNAP (the NRC graphical user interface)

CASL VUQ Benefits Industry

Current Validation Work

- A large amount of validation work being performed for the CASL codes:
  - CTF: PSBT, BFBT, FRIGG, Harwell, GE3x3, CE 5x5, PNNL 2x6, and Westinghouse Mixing Tests.
  - Peregrine: Comparisons with Halden, Studvik SuperRamp, and RIS0.
  - Bison, Abaqus, WEC Vitran: Wear model GTRF data from ORNL.
  - Hydra Validation: TAMU 5x5, MIT subcooled boiling data.
  - Hydra Benchmarks: Erturk, Moser, Prasad, Elmadi, de vahl Davis, and Ghia.
  - Insilico: Validation - Watts Bar; Benchmarks - SHIFT and KENO.
  - MPACT Validation: Watts Bar, SPERT, B&W 1484,1810 and Takahama.
  - MPACT Benchmarks: KENO, Insilico, and Shift.
  - Shift: Watts Bar, B&W 1484,1810.
  - Mamba: Comparison with WALT data and comparison with CRUD pictures and CRUD scrapings from Seabrook.

Large amount of validation work currently underway

Validation Data Hierarchy

- When we do not have the quantity, quality, or relevancy of the validation data we need, we will leverage those who have it or can get it for us.
  - DOE projects, NEUP and the new validation database
  - ***Industrial partners current and new.***
  - "Data mining" of the literature.
- New integral effects experiments designed with CASL software, CPs, and VVUQ in mind from DOE or industry partners.
- New separate effects experiments with CASL in mind from DOE or industry partners.
- The value of validation data increases significantly when the simulation and experiment happen simultaneously.

No rock unturned when looking for validation data

Data from Industry Partners

- Phase I partners provided data critical to CASL software development and CP applications
  - Industry sponsored test and plant data (EPRI)
  - Plant data and measurements (TVA)
  - Fuel design and test data (WEC)
- CASL has well defined process and procedure for data management and control
  - Technology Control Plan (TCP)
  - Protection of proprietary data under nondisclosure agreements (NDA)
- New data continue to be identified and collected in Phase II
  - Separate effects tests to validate individual models.
  - Integral effects tests validate coupled physics and coupled codes.
  - High fidelity test data to validate CFD, fuel, and chemistry codes.

Industry Data Critical to CASL Success

Summary

- Phase I in CASL has been very dynamic and focused on bringing capability of VERA tools to a mature level.
- Advanced VUQ techniques and tools have been applied to code development and challenge problems
- Phase II will move from capability development to production deployment - application driven
- VVUQ tools and methods improve software development and applications to challenge problems
- Data from industry partners are critical to successful application of CASL technology

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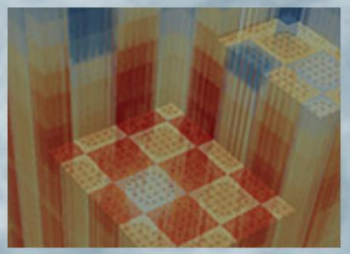
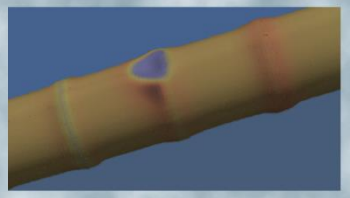
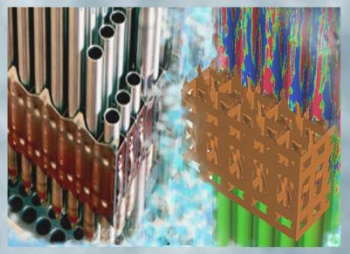
Additional Information on VVUQ Concept and Approach







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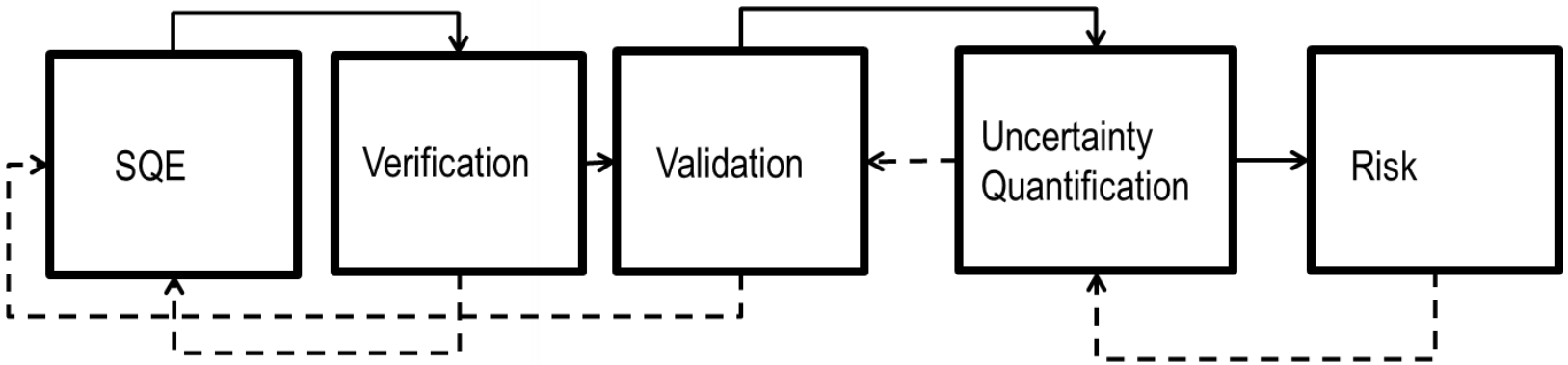
Vocabulary

- It is more important that the work gets done than what it is called.
  - **Software Quality** – Do you know what's in your code?
  - **Verification** – Did you solve the equations correctly?
  - **Validation** – Are you solving the correct equations?
  - **Uncertainty Quantification** – do you know the parameters in your models?
- The names vary form field to field but knowing the answer to these four questions is key.
- These processes depend on each other. Just doing one of these has limited value.

Don't get hung up on names

Dependencies



UQ is an iterative process

Total Uncertainty

This equation is wrong. However, it is better than assuming the first two are zero. We will be happy when new versions of this equation that are better are implemented proving us wrong.

$$\mathrm{UQ}_{\mathrm{total}} = \min \left\{ \begin{array}{l} \left\| \mathrm{QoI} - \mathrm{QoI}_{\Delta x \to 0} \right\|, \\ \left\| \mathrm{QoI} - \mathrm{QoI}_{\mathrm{exp}} \right\|, \\ \left\| \mathrm{QoI} - \mathrm{QoI}_{2\sigma} \right\| \end{array} \right\}$$

Need to account for all modes of uncertainty

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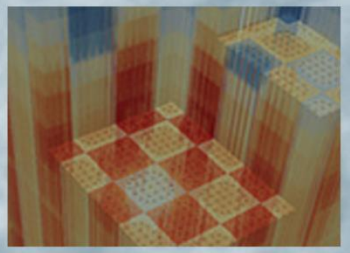
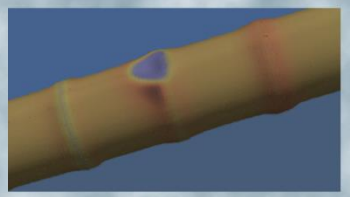
VERA Use Cases

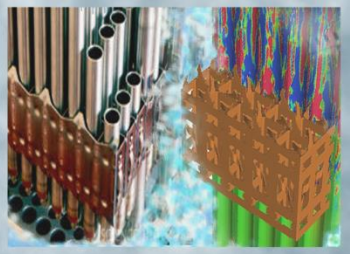
CASL Industry Council

Dennis Hussey, EPRI

March 17-18,2015







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Overview

- Discussion of Use Case Action Items
- Methodology and Assumptions
- Spreadsheet table review

Use Case Action Item

- Action item from September IC meeting (from Chris Lewis)

Develop a table of use cases, needed VERA functionality, resource requirements, value added and timescale (map to specific benchmarks).

Use Case Goals

- Chris Lewis notes
  - Goals will vary from utilities to vendors
  - Utility Value
    - Reduce feed fuel assembly count
    - Improve preventative maintenance needs for LOCA analysis
    - Improve ramp rates
    - Extend equipment life (e.g. fluence analysis)
  - Vendor Value
    - Reduce analysis costs
    - Eliminate testing
    - Reduce likelihood of error in modeling
    - Improved fuel designs

Methodology and Assumptions

- Methodology
  - Review use case document prepared by Rose Montgomery
  - Supplement with IC Value Proposition, discussion with IC members and utilities
  - Assess which VERA resources may be applied to a problem
- Assumptions
  - Many of the use cases are outside current challenge problem scope, applied resources are not well known
  - Value of a use case compared to existing tools will be utility specific
  - Continues to be a work in progress

Placeholder for Spreadsheet

x = required
o = optional

1 = Desktop
2 = Industry HPC (500-1000 Cores)
3 = Titan

VERA Modules Needed

Workflow-Specific Use Cases	*VERA*	*MPACT*	*COBRA-TF*	*HYDRA-TH*	*BISON-CASL 2D*	*BISON-CASL 3D*	*MAMBA*	*INSILICO*	*SHIFT*	*ORIGEN*	*SCALE*	*Rod*	*Assembly*	*Core*	*Resources Required*	*Value Added*	*Timescale*
Normal Conditions of Operation Analysis Workflows													**x**				
Fuel System Changes Workflow	x		x	o	o								x	x	2		
Mixed Core Fuel Transitions Workflow	x	o	x	x	o		x								3		
Burn up Extension Workflow																	
~~Advanced Fuel System Study~~																	
Accident Analysis Workflows																	
Departure from Nucleate Boiling (DNB)	x	x	x	x								x	x	x	2		
Loss of Coolant Accident (LOCA)	x	x	x	x	x	x						x	x	x	2,3		
Reactivity Insertion Accidents (RIA)	x				x	x							x	x	2,3		
~~Combined Events~~																	
Release Source Term																	
Risk Assessments for Known Operational Issues														**x**			
CRUD Deposition, CIPS, and CILC Risk Assessment Workflow														***x***			
CRUD-Induced Power Shift (CIPS)														*x*			
Level 2	x		x											x	1		
Level 3	x		x				x							x	1,2		
Level 4	x	o		x			x								2,3		
CRUD-Induced Local Corrosion (CILC)													*x*	*x*			
Level 3	x		x	x			x								1,2		
Level 4	x	o	x	x			x					x	x	x	2,3		
~~Grid-to-rod Fretting (GTRF)~~																	
~~Fuel Assembly and fuel rod distortion (FAD)~~																	
Pellet-Cladding Interaction (PCI)	x	o	o		x	x						x		x	1,2,3		
Fibrous Debris Flow Study	x		x	x			x								2,3		
Investigate Plenum Flow Anomaly	x	o	x	x									x		3		
Root cause or Apparent Cause investigations of reactor or fuel phenomenon																	
Power uprates and Power Escalation-related Applications																	
Power Uprates	x		x		x	x	x					x		x	2,3		
Power Ramping Study	x	o	x	o	x	x	o					x		x	2,3		
Reactor Integrity and lifetime studies																	
Reactor Vessel Integrity	x	x															
Reactor Internals Integrity	x	x															
Fuel Design	x	x	x	x	x		x					x	x	x	2,3		
Critical Heat Flux Analysis	x		x	x									x		2,3		
Grid Optimization	x		x	x									x		2,3		
Advanced Reactor Designs																	
Uncertainty Studies																	

CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

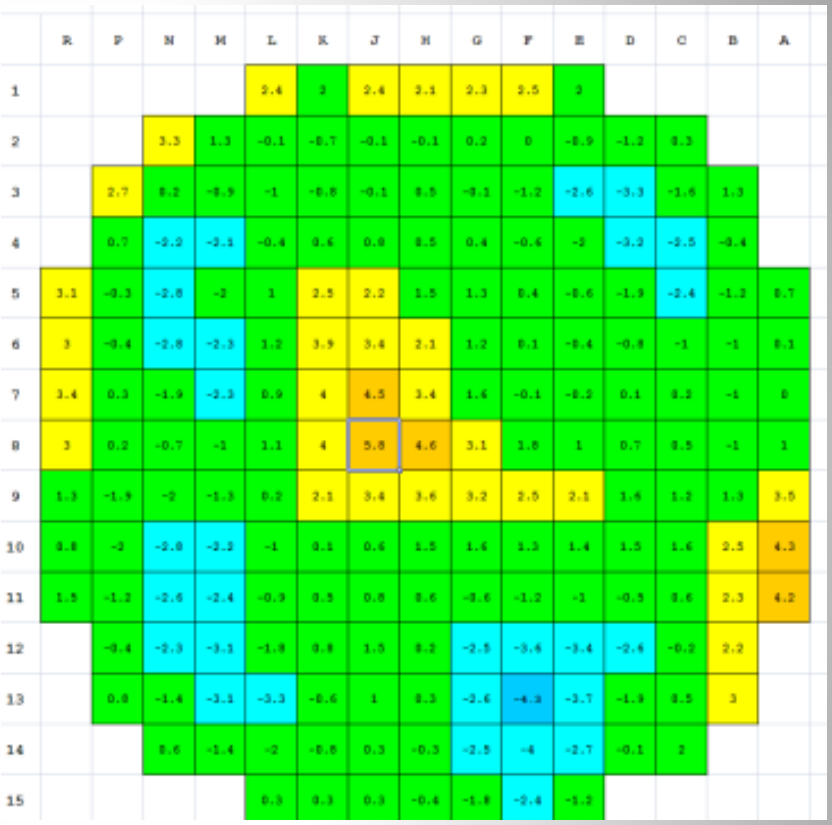
TVA Test Stand
Lower Plenum Flow Anomaly Modeling Using VERA
March 11, 2015

Bill Bird – TVA
Rose Montgomery - TVA

TVA Proprietary Information

Lower Plenum Flow Anomaly (LPFA)

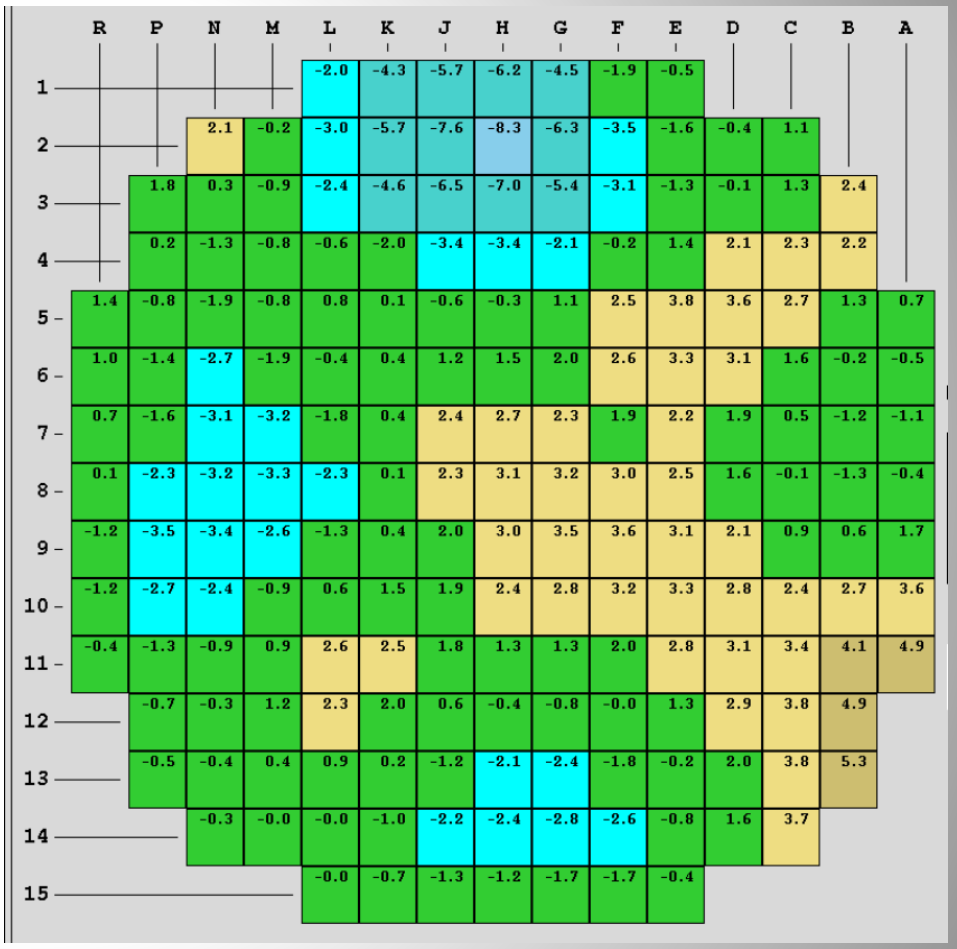
- Many plants (10+) have reported observations associated with LPFA
- Power, flow and temperature measurements deviate from predictions
  - Pattern repeated over many operating cycles
- Postulated root causes
  - Flow vortices within the reactor vessel during operation
    - Standing vortices or periodic
  - Susceptible design and/or as-built geometry, including asymmetry in lower internals and loop inlet/outlet placement
  - Loop flow differentials, including geometric differences in loop geometry
- Possible influencing parameters
  - Reactor Coolant Pump impeller replacement
  - Pump startup sequence



Byron Station, cycle 18

LPFA – Watts Bar Specific

- Watts Bar Nuclear (WBN) Unit 1 has historically experienced core power distributions that differ from design predictions
- The magnitude of the difference of measured versus predicted (M-P) has been as high as 12% in the past at individual core locations
- The pattern persists through the cycle
  - Changes in power don't appear to change the pattern
  - Burnup does appear to change the pattern slightly
  - Steam generator change-out didn't appear to affect the phenomenon
- Consequences
  - WBN-1 is assessed a 3.3% generic DNBR penalty in its safety analysis
  - Reduced FQ & FDH margins
  - CRUD susceptibility



TVA is exploring the flow distribution in Watts Bar unit 1 using VERA's Hydra-TH

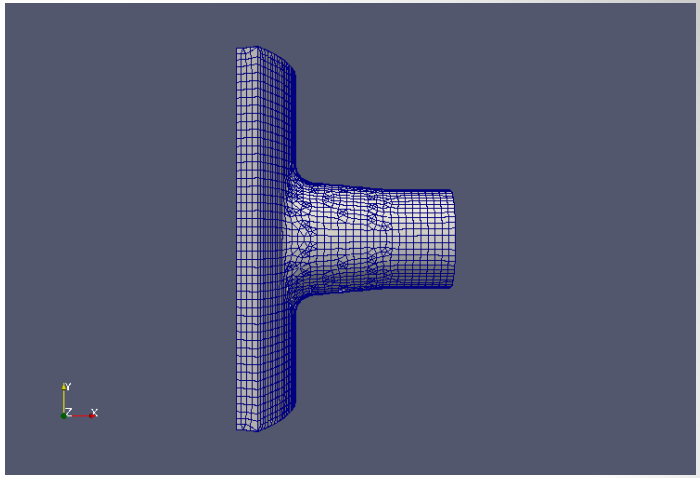
- Work performed by TVA with user support from ORNL/CASL
- Perform steady flow calculation to look for standing flow vortices in lower plenum and downcomer regions
  - Determine impact of identified flow vortices on core inlet flow distributions
- Perform mesh density study
  - Evaluate 3-4 mesh densities to determine density required for calculation fidelity
- Using simplified boundary conditions
  - Intent is to show scalability of Hydra-TH to reactor scale
  - BC's: vessel inlet pressure, flow velocity, temperature/density
  - Currently using Spalart-Allmaras turbulence model
    - Future runs to use k-ε model with implementation of renormalization group theory (RNG k-ε) and/or Shear Stress Transport (SST) k-ω model.

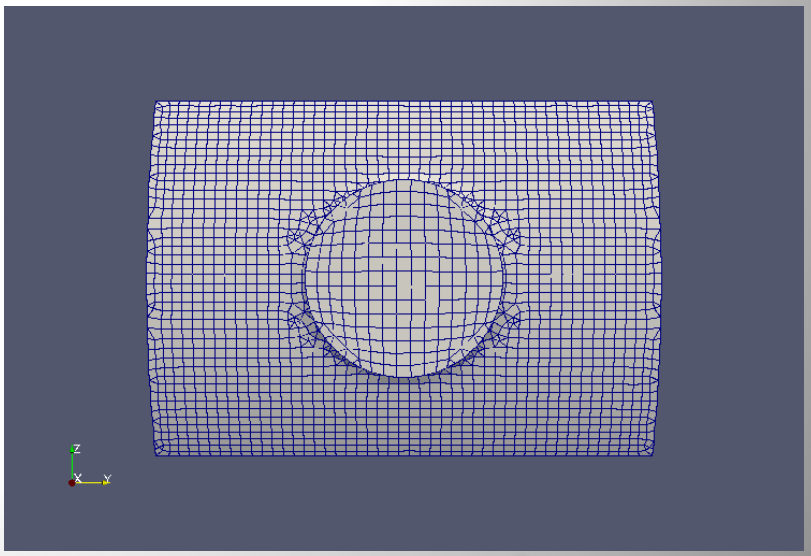
LPFA Expected output and demonstration of capability

- Local flow in downcomer, lower plenum, fuel inlet and exit
- Local coolant temperature at fuel inlet, exit, hot loop, etc.
- Local coolant density within the core region
- Identification of standing vortices
- Indication of influence of pump startup sequence
- Later, with transient simulation, identification of periodic vortices
- Large eddy simulations with submodel of lower internals
- Eventual goal is to use Hydra-TH flow data as an input to VERA-CS to demonstrate the observed power fluctuation.

LPFA – Mesh Studies

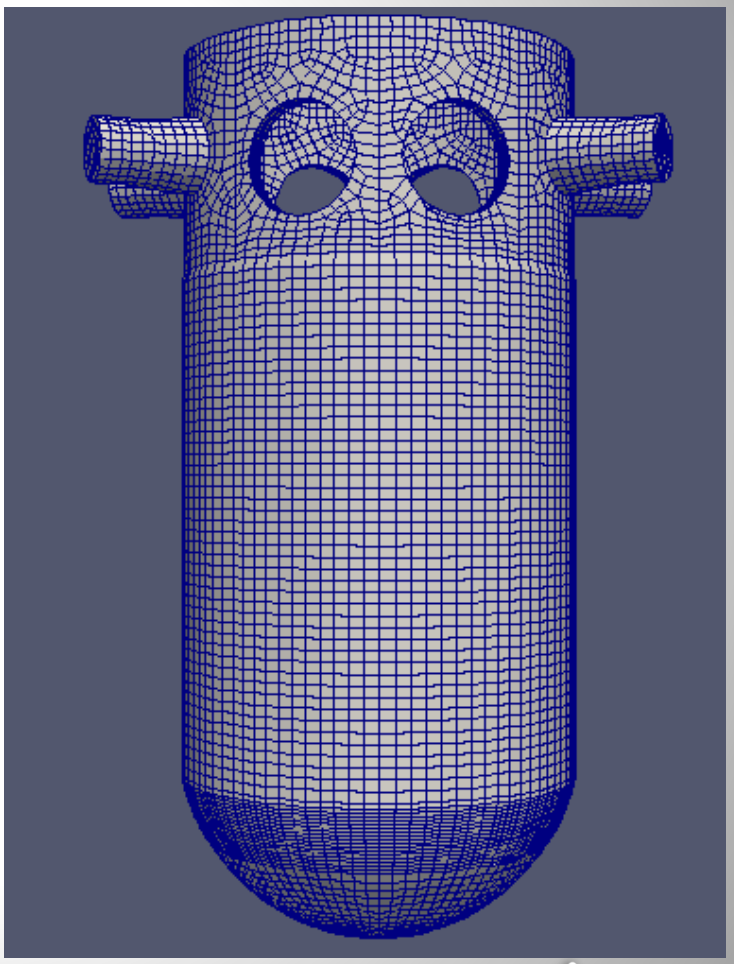
- Initial Hydra-TH runs utilized simplified geometry
  - Inlet nozzle only
  - Varying mesh density
- Two different coarse mesh versions
  - Tet mesh
  - Hex mesh





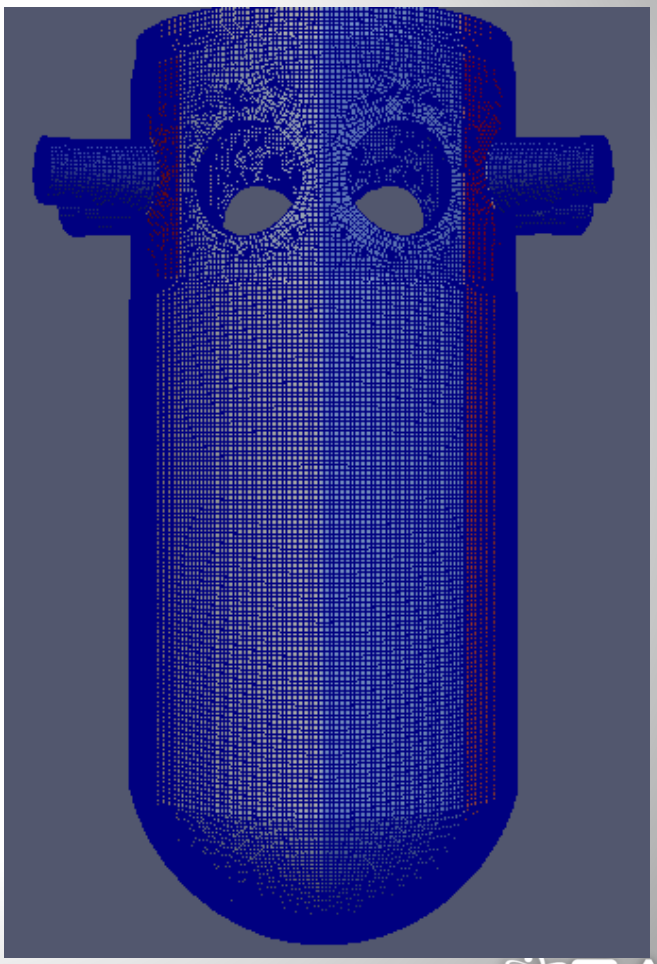
LPFA – Mesh Studies

- Simplified reactor vessel geometry
  - No lower internal structures
  - No modeling of fuel region
  - Flow outlet of model at entrance to fuel region
- Two different coarse mesh versions
  - Tet mesh
  - Hex mesh



LPFA – Mesh Studies

- Simplified reactor vessel geometry
  - No lower internal structures
  - No modeling of fuel region
  - Flow outlet of model at entrance to fuel region
  - Finer Hex mesh



Convergence Study

- Uses simplified reactor vessel geometry
  - No lower internals
  - Finer mesh
- Examine variation in results with changes to convergence criteria
  - eps default value is 1.0e-5
  - eps varied from 1.0e-2 to 1.0e-5 for both the momentumsolver and ppesolver input blocks

TVA

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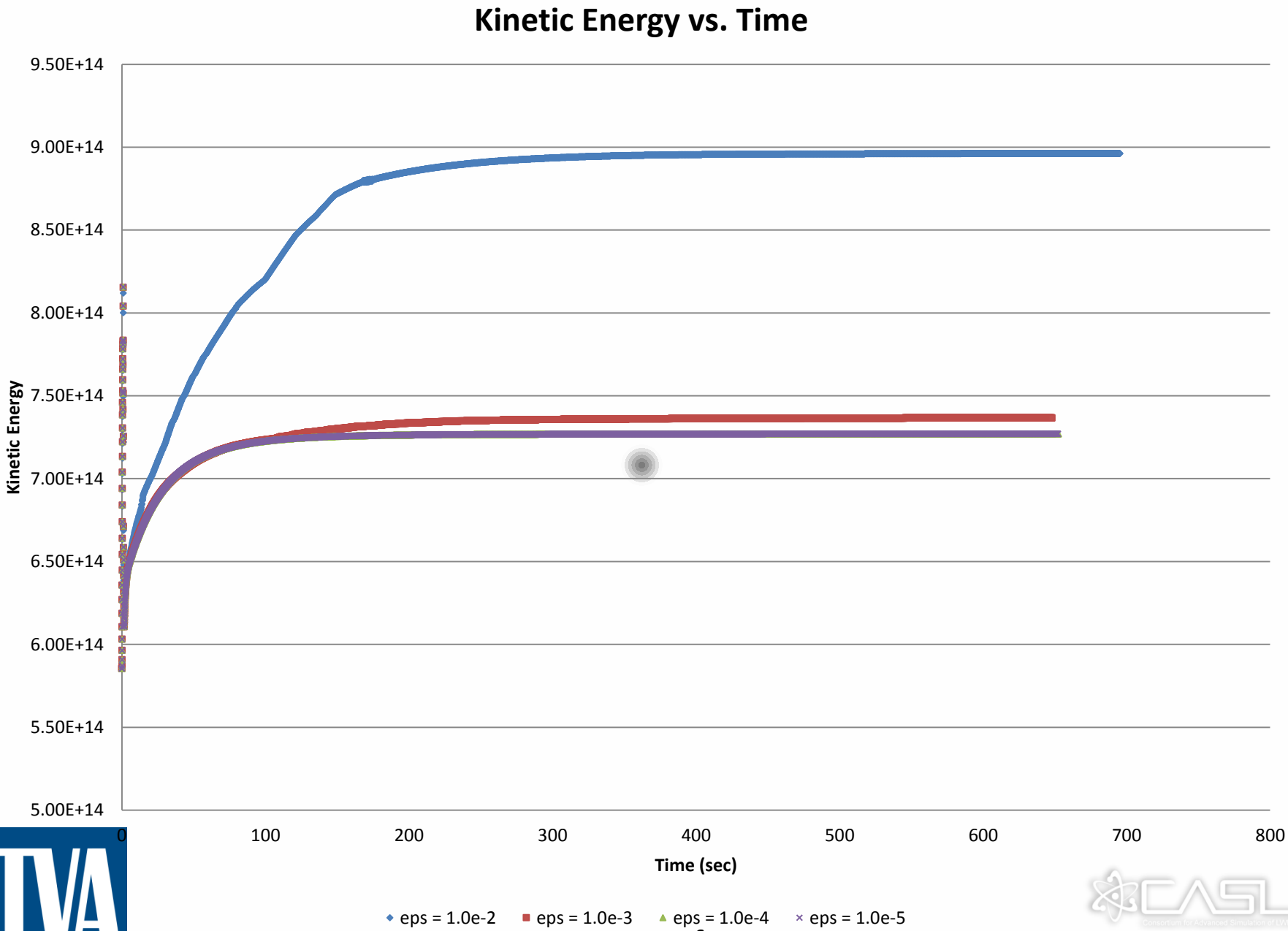
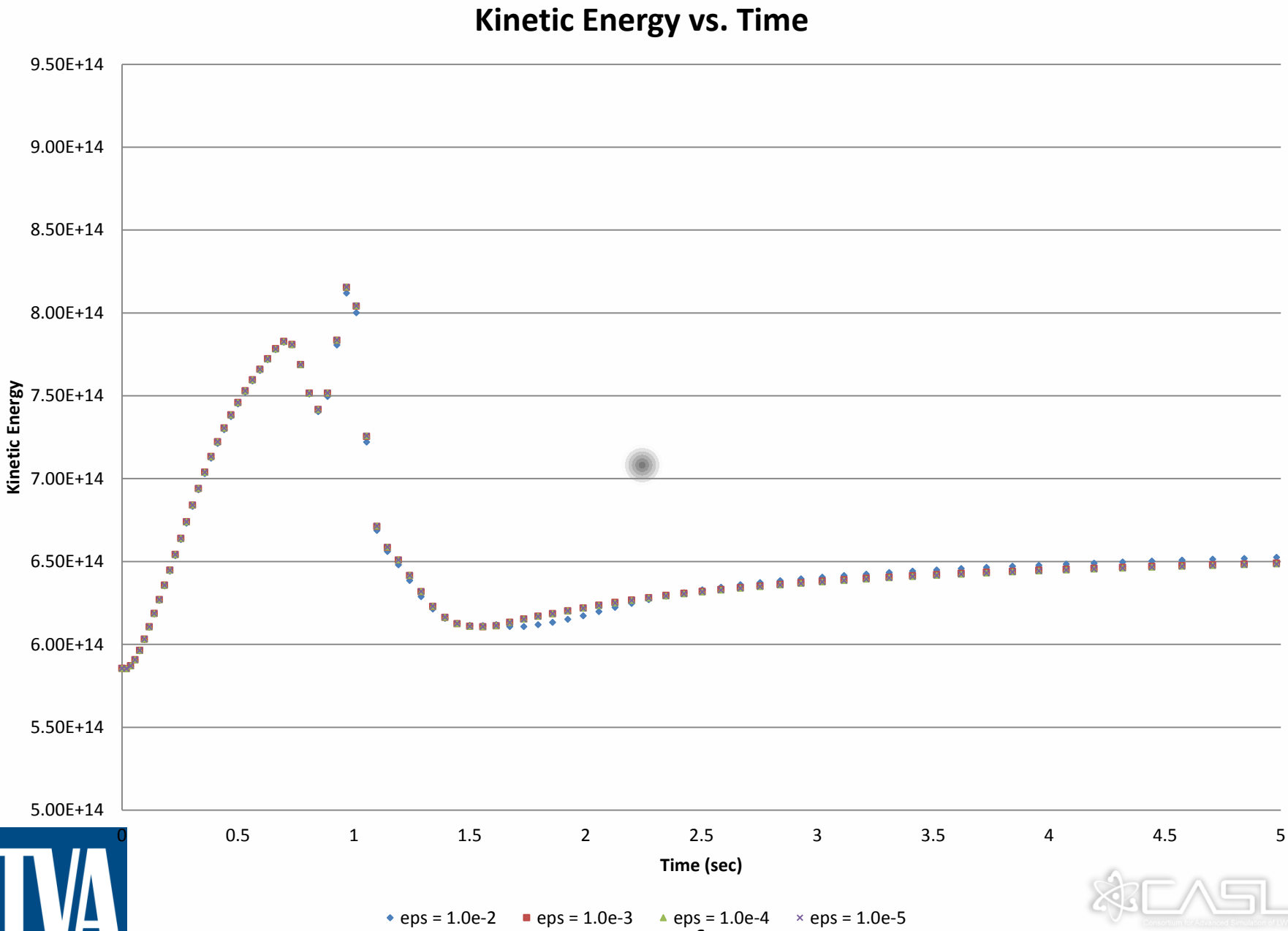
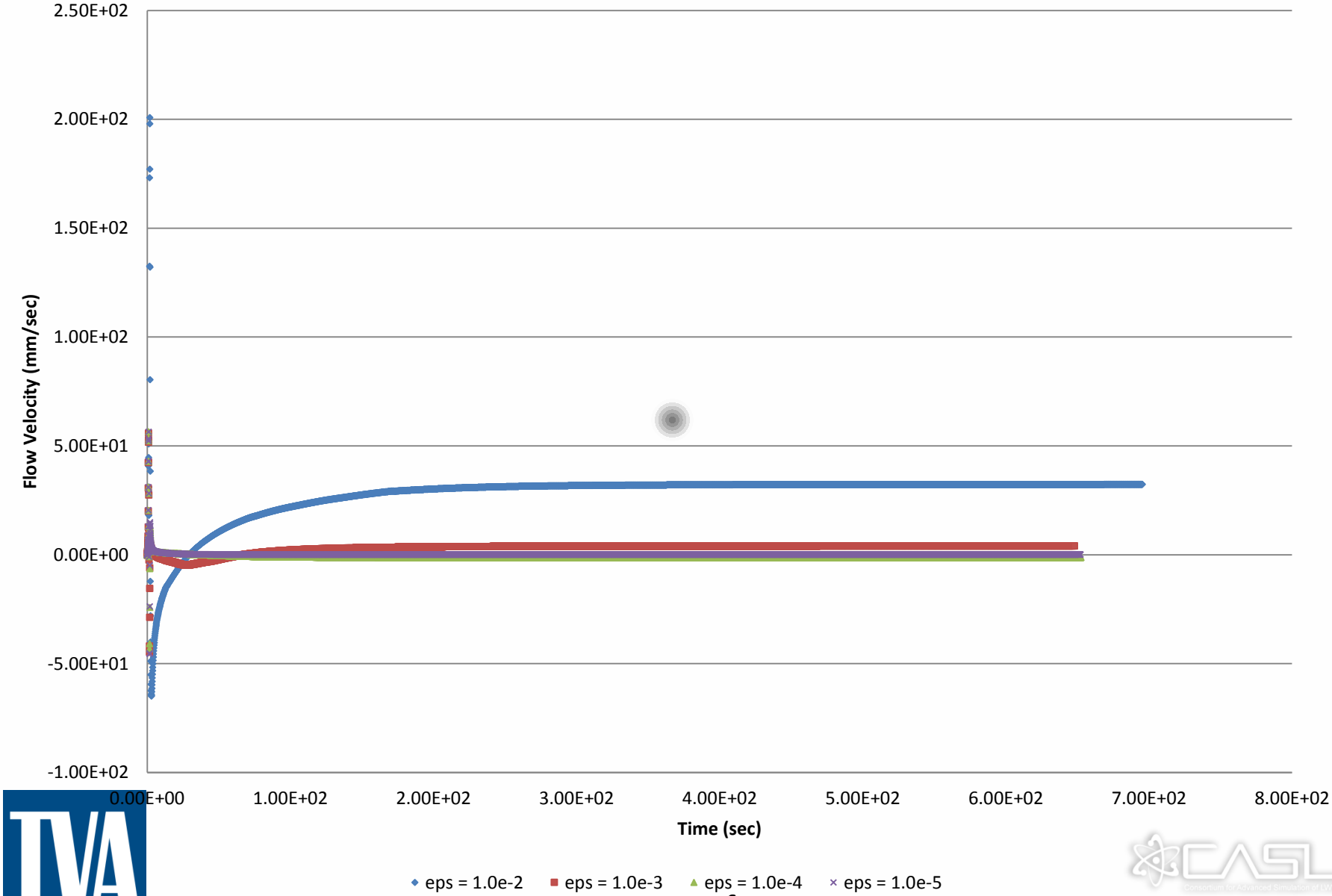


TVA Proprietary Information



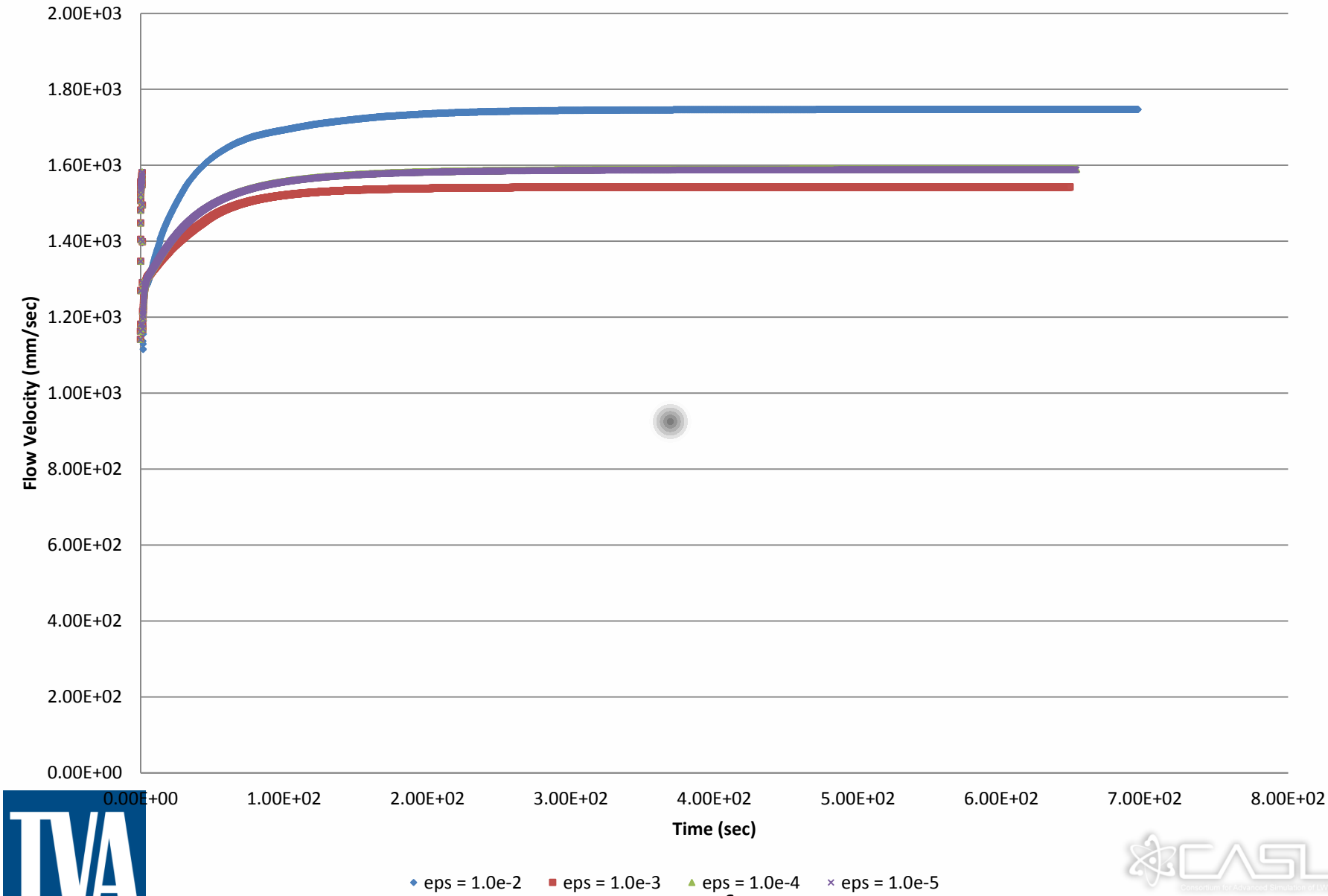
TVA Proprietary Information

Average flow velocity (x-component) at outlet vs. Time



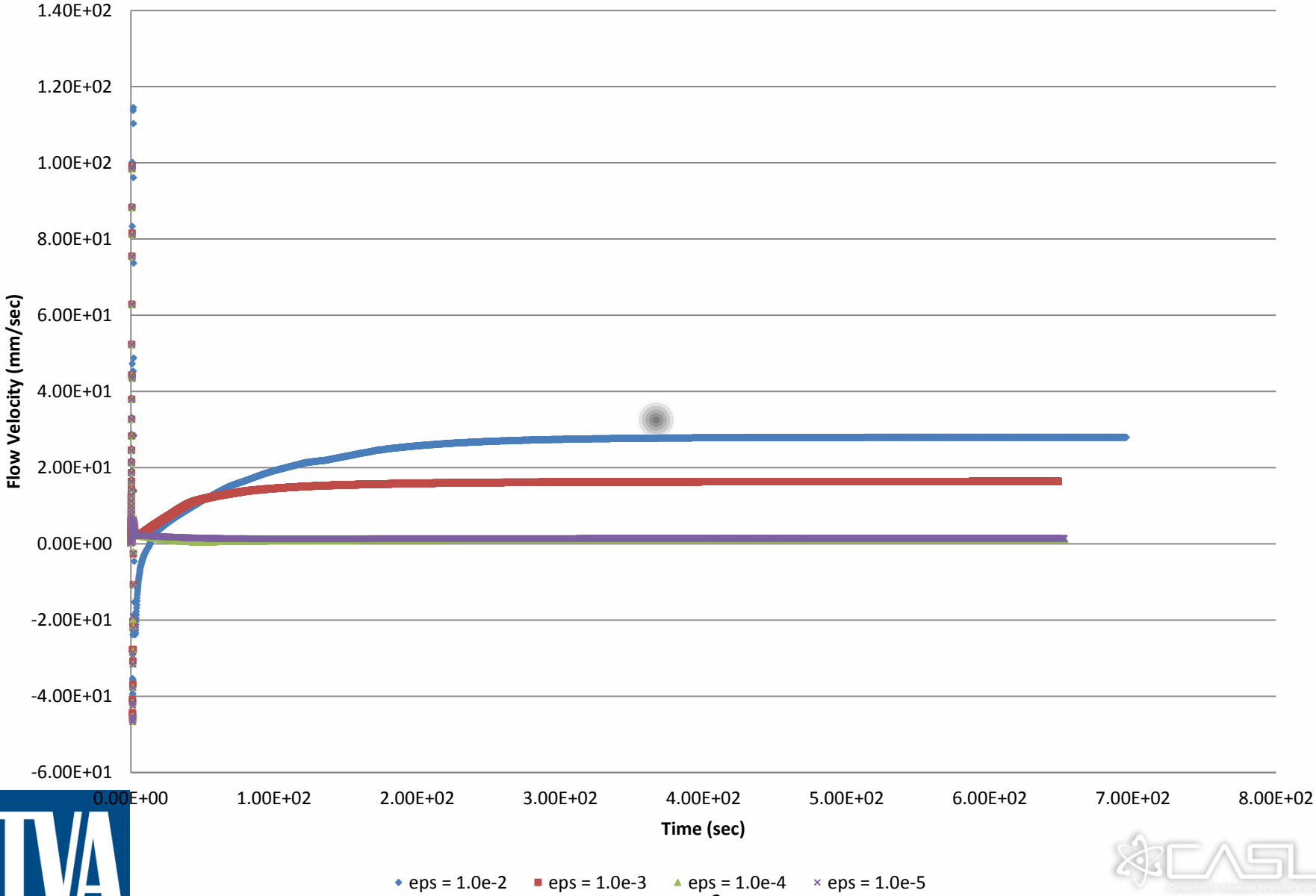
TVA Proprietary Information

Average flow velocity (y-component) at outlet vs. Time



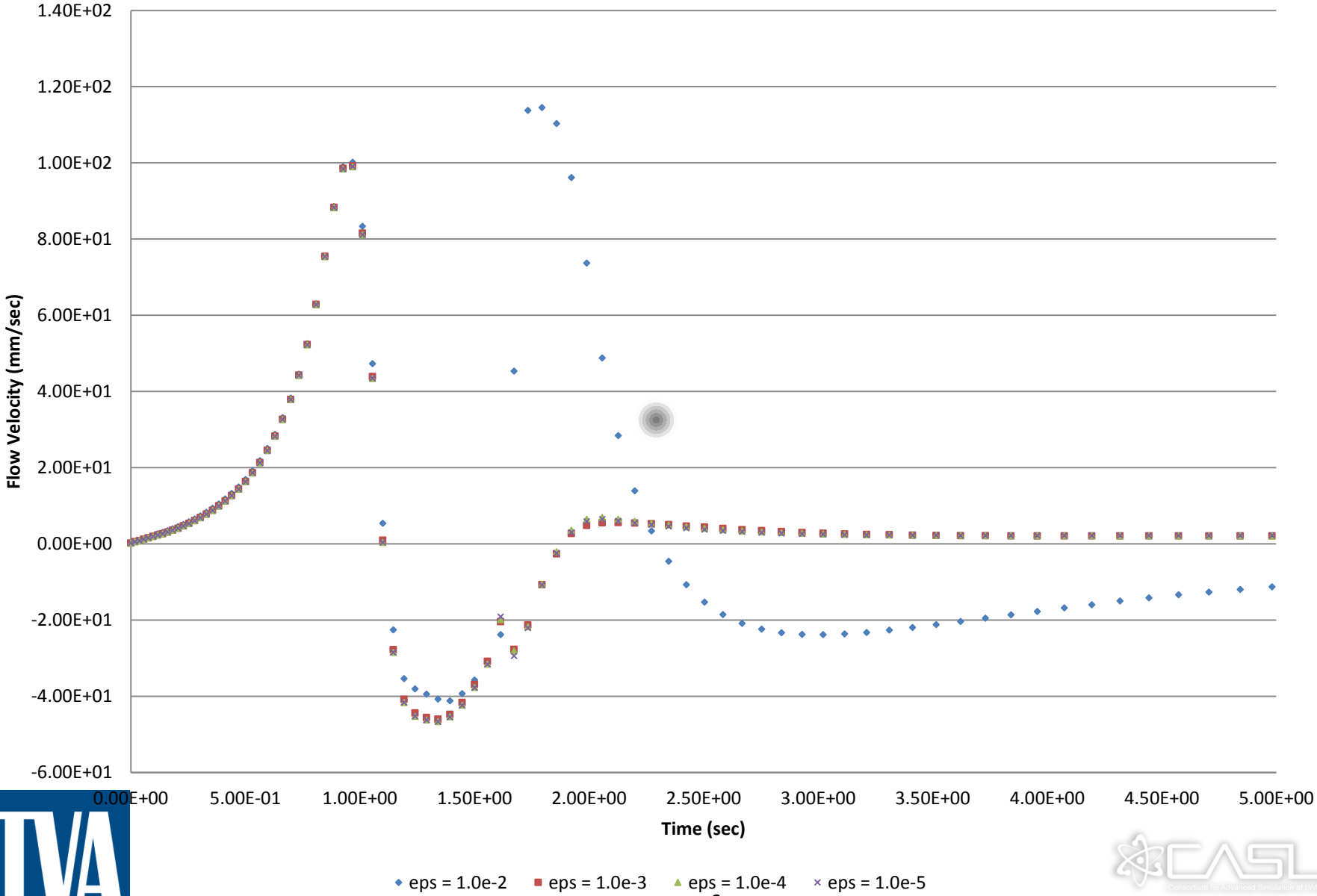
TVA Proprietary Information

Average flow velocity (z-component) at outlet vs. Time



TVA Proprietary Information

Average flow velocity (z-component) at outlet vs. Time



TVA Proprietary Information

Convergence Study results

- As expected, selection of convergence criteria impacts code results
- In general, tighter criteria = increased run time

eps	Solution time (sec)
1.0e-2	7.7400e+3
1.0e-3	7.6048e+3
1.0e-4	1.0408e+04
1.0e-5	1.3831e+4

- For the simplified reactor model, steady state results are practically indistinguishable at 1.0e-4 and 1.0e-5

TVA

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Reactor Coolant Pump Startup Sequence

- Purpose to generate an unsteady flow condition and check method of input of inlet BC
- One pump running at time = 0
- Remaining pumps start at 300, 600, 900 seconds
- eps = 1.0e-5
- Steady state results after 4th pump starts similar to convergence study case with all 4 pumps

Parameter	Convergence Study	Pump startup
eps	1.0e-5	1.0e-5
KE	7.27E+14	7.24E+14
Velx (outlet)	9.78E-2	-1.33E+0
Vely (outlet)	1.59E+3	1.55e+3
Velz (outlet)	1.44E+0	1.21E+0

TVA

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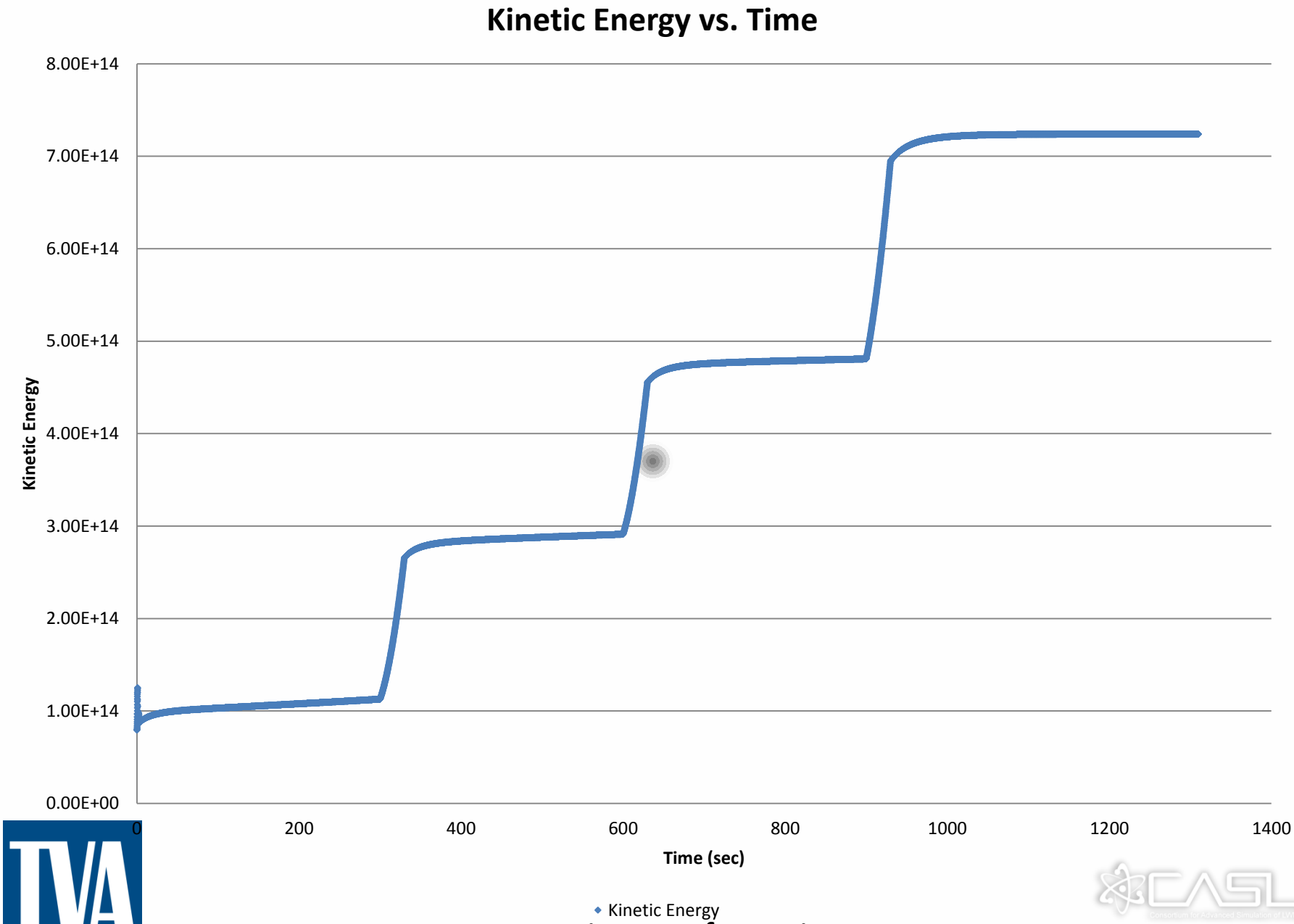

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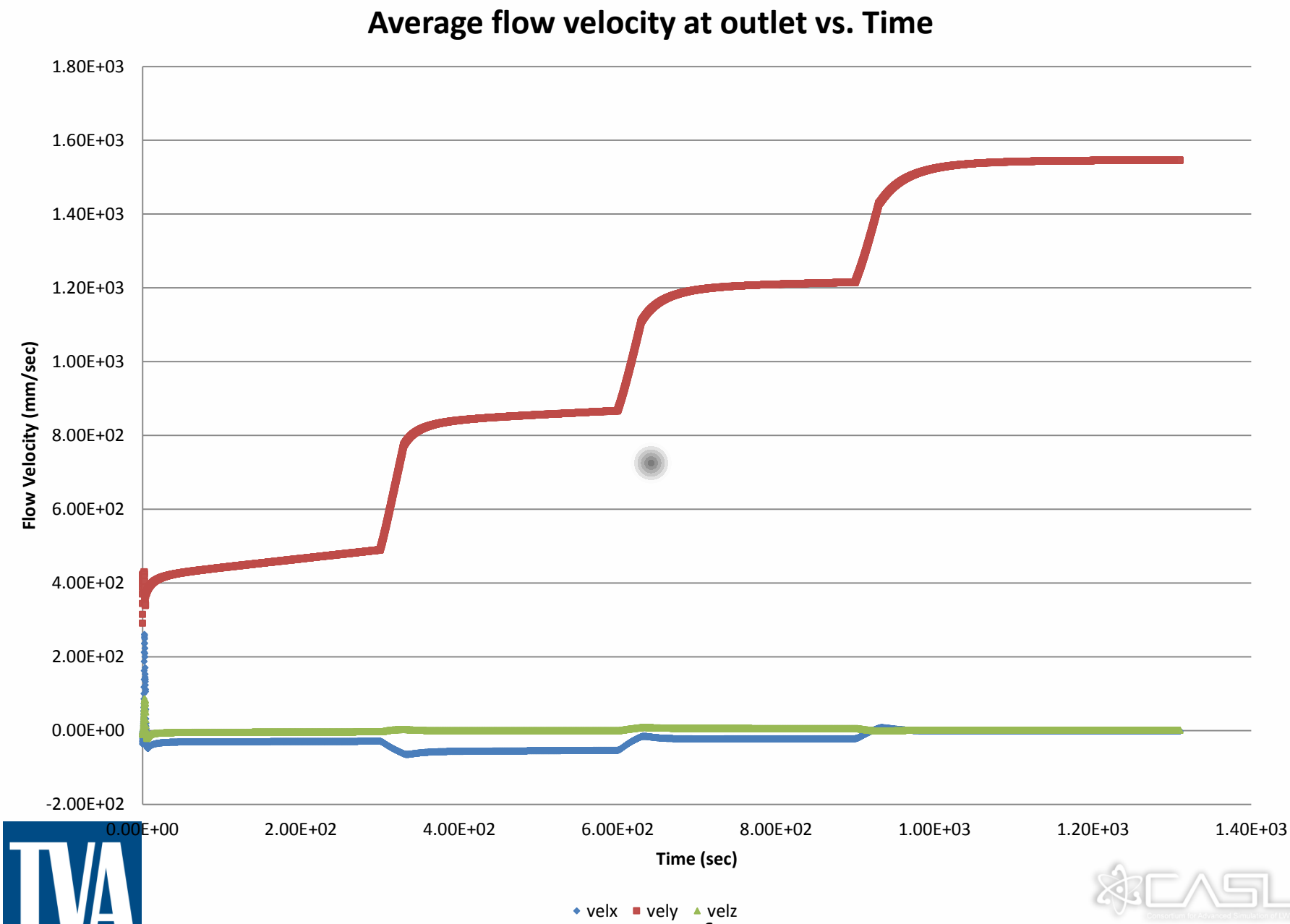
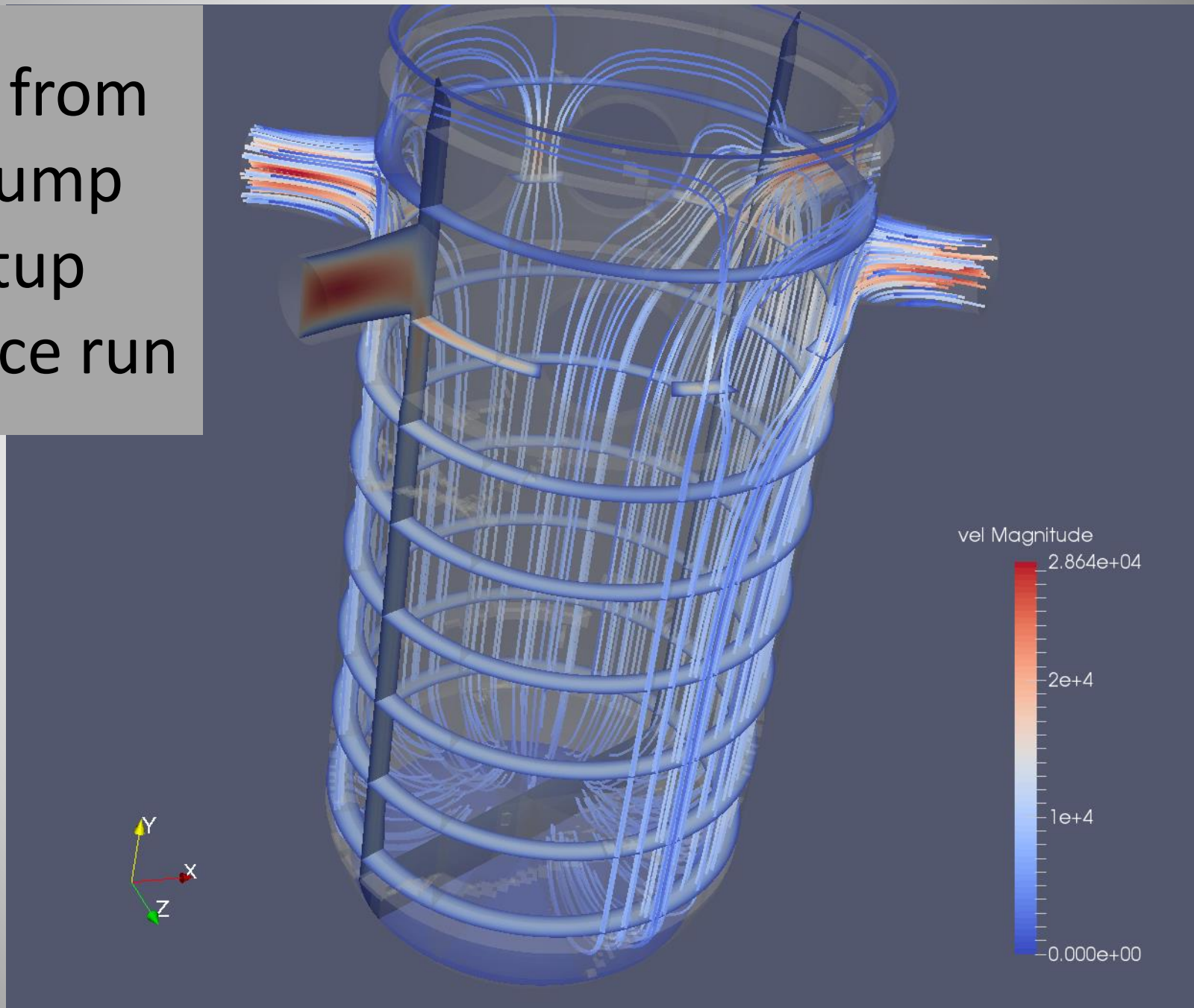


TVA Proprietary Information

Image from the pump startup sequence run



Detailed Reactor Model with Coarse Mesh

- Mesh generated by University of Tennessee – Chattanooga SimCenter
- Includes lower internals but not lower core plate or core support plate
- Used to test various options in Hydra-TH and to grossly visualize flow fields in the lower plenum
- Currently being exercised

TVA

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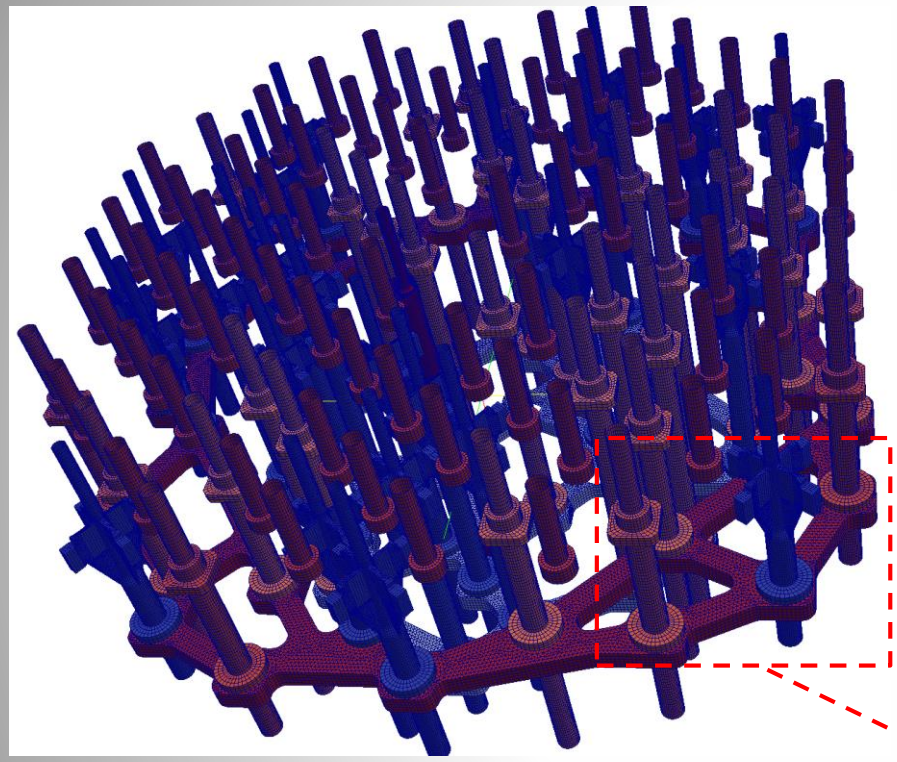
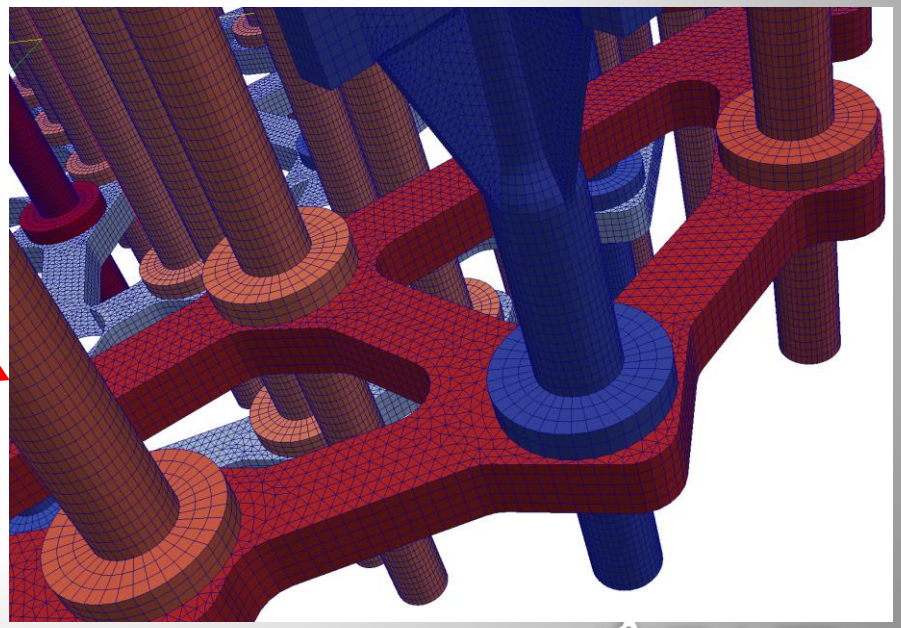
LPFA – Mesh Studies



Mesh created by UT-C SimCenter

Details of lower internal structures shown



Detailed Fine Mesh Model just completed

- Developed by University of Tennessee – Chattanooga SimCenter
  - Includes all details of the lower plenum
  - Includes the core as porous media
  - Includes an upper plenum region with only the CRD housing detail.
  - Doesn’t include the reactor head.

TVA

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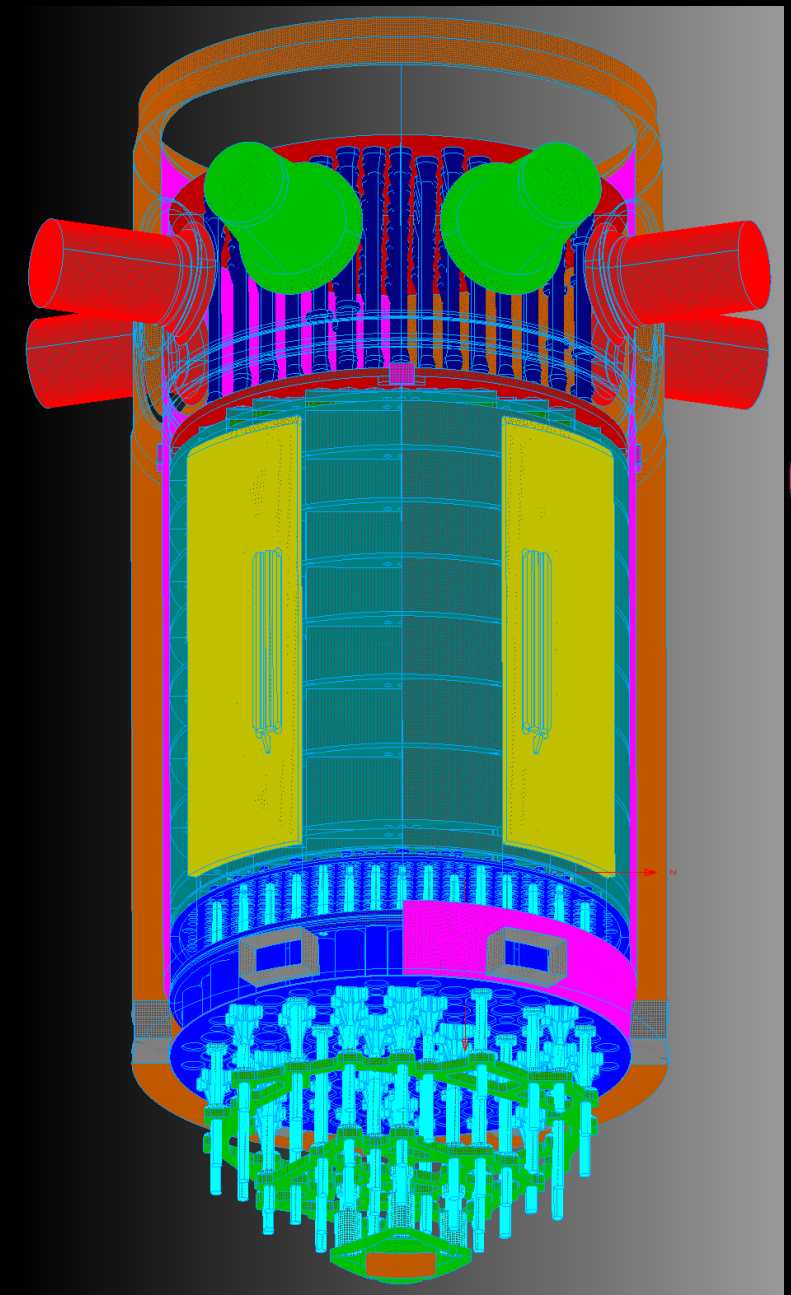
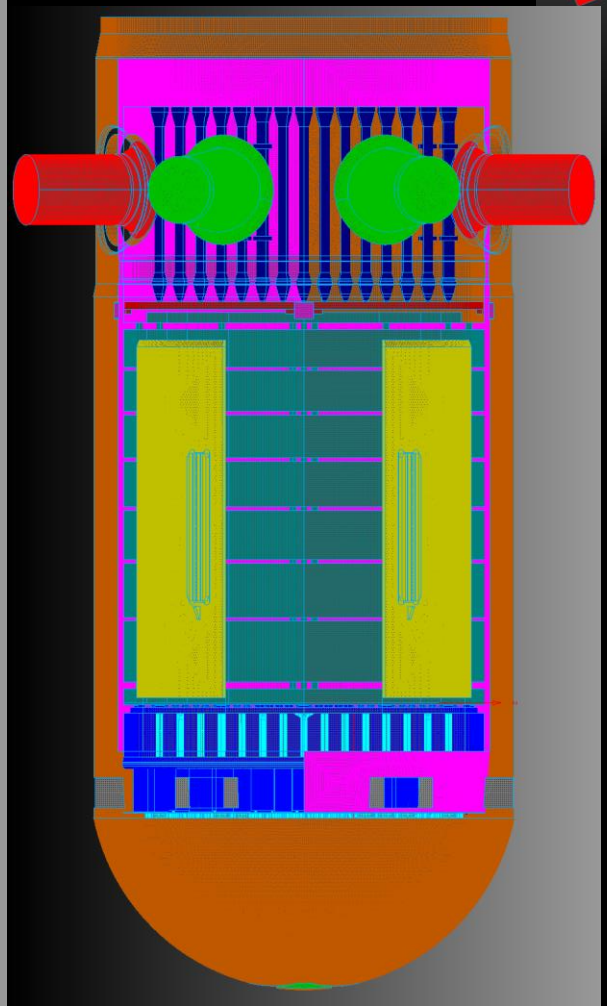
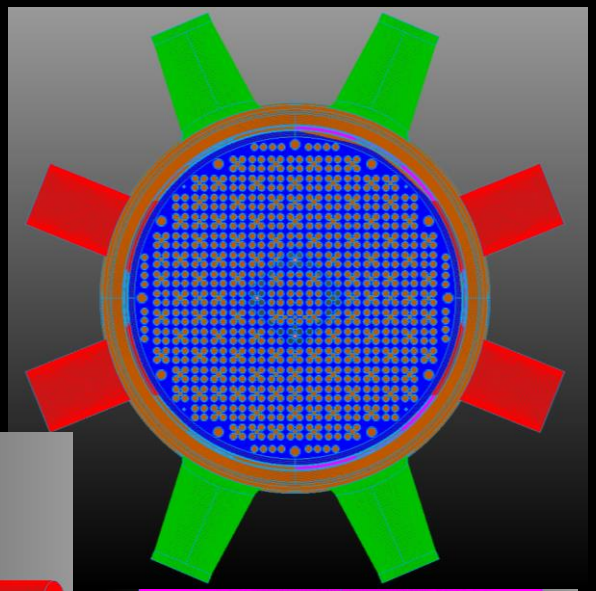
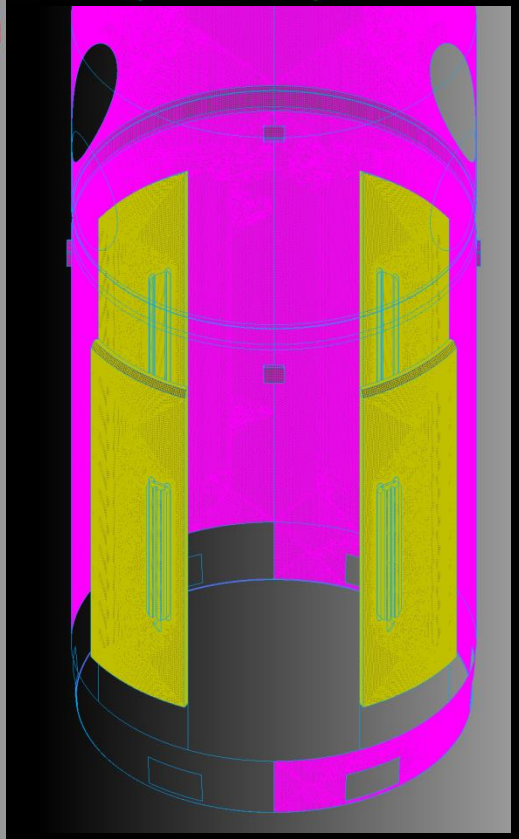
Detailed Fine Mesh Model

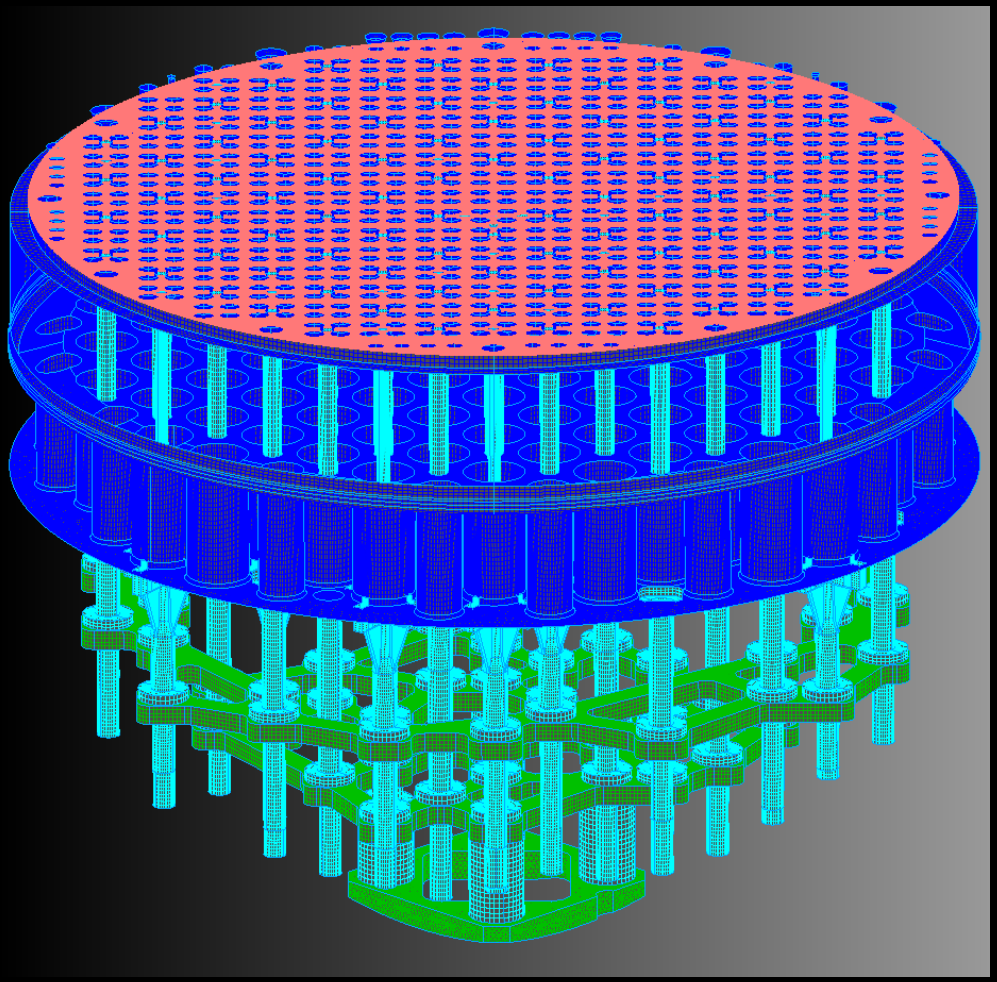


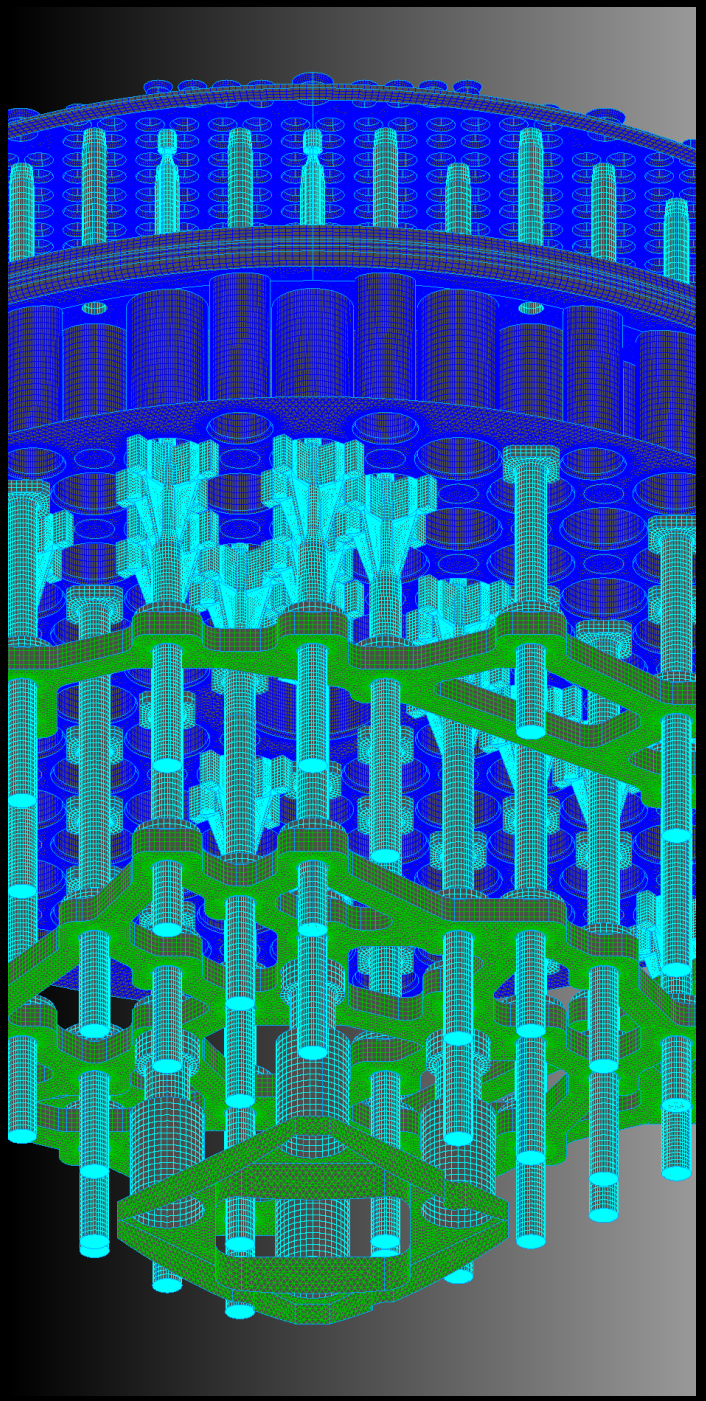




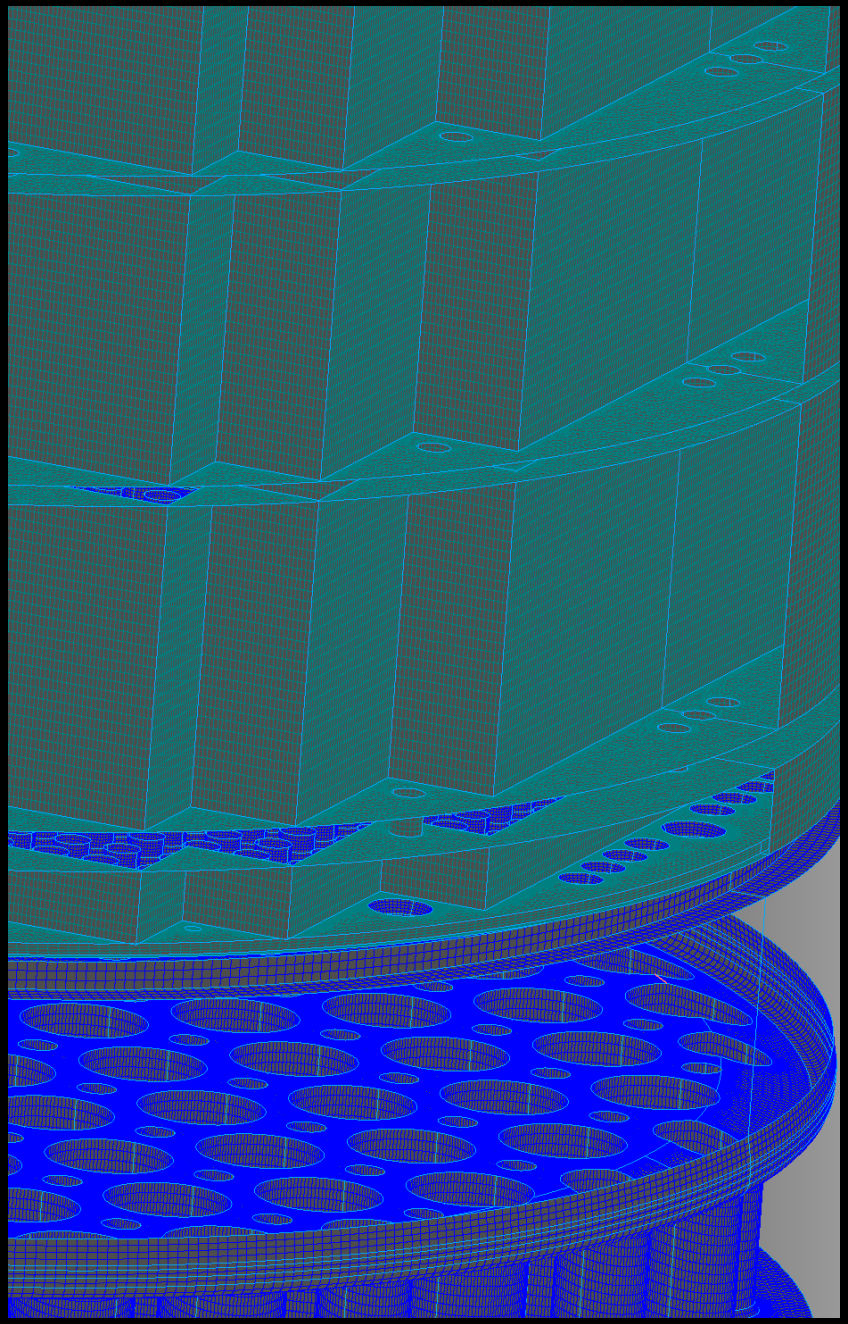


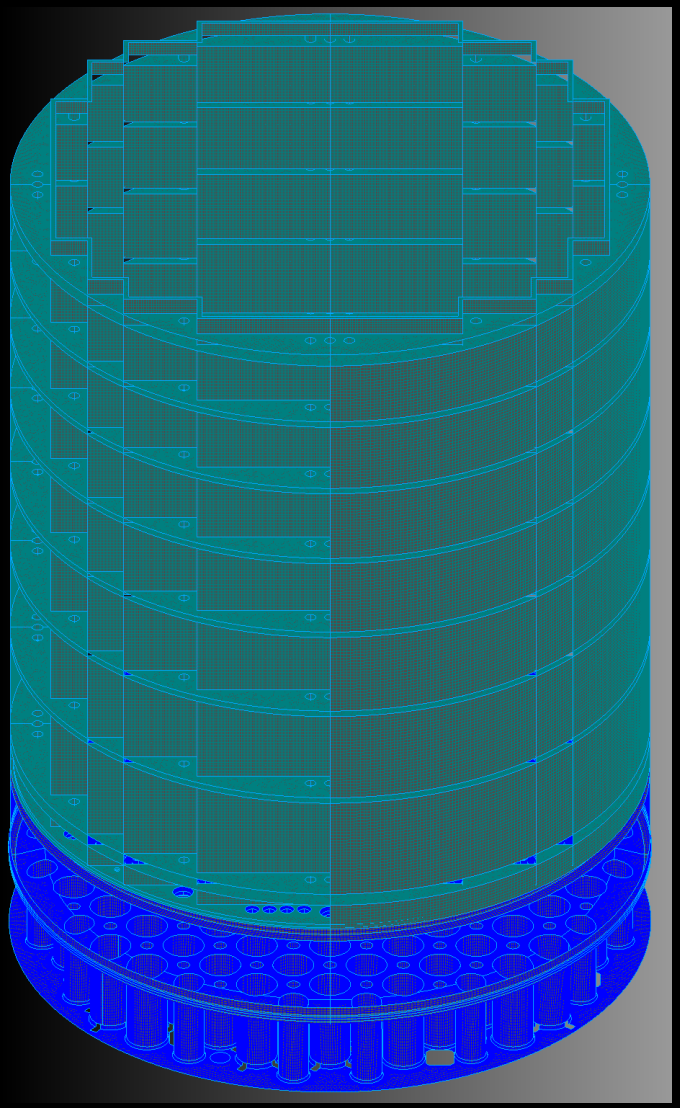
Detailed Fine Mesh Model



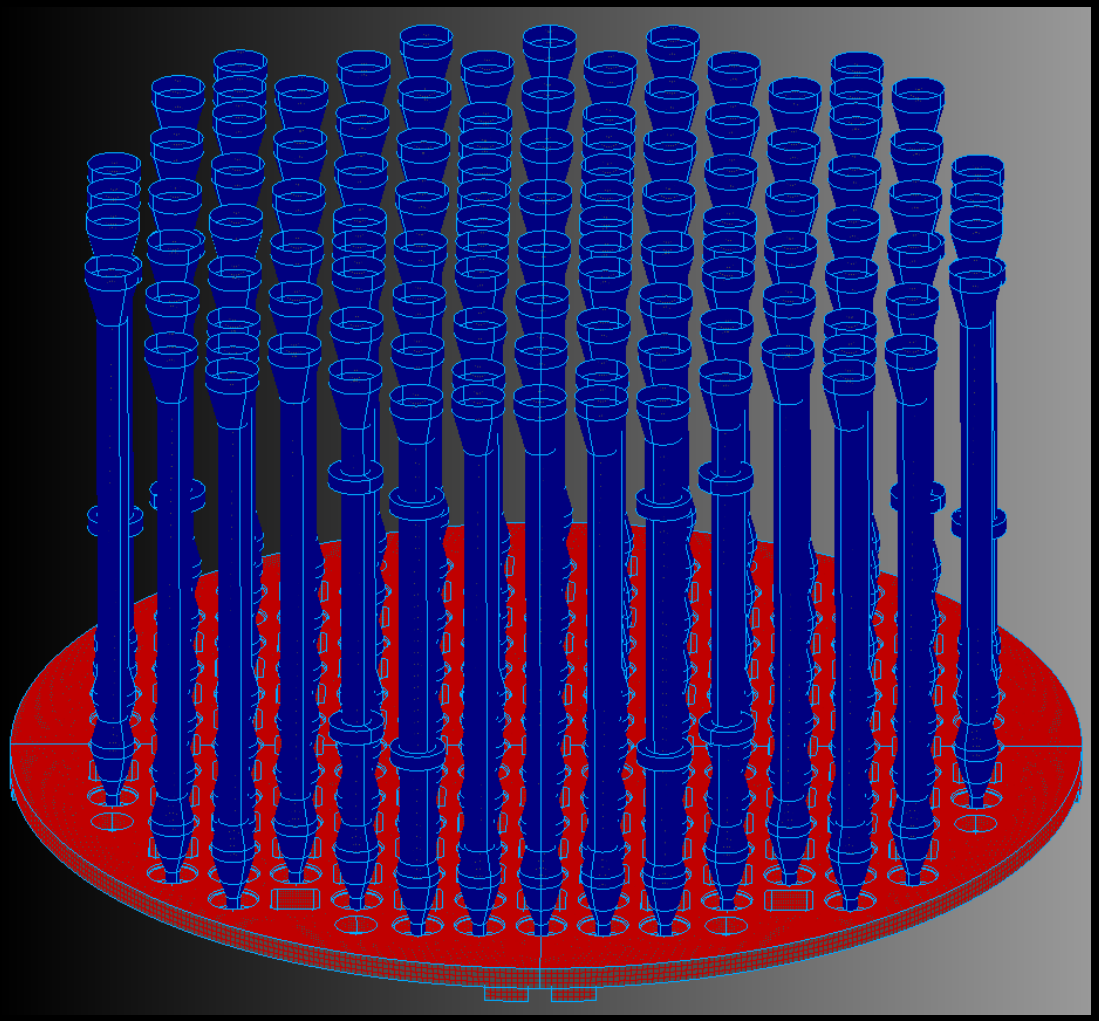


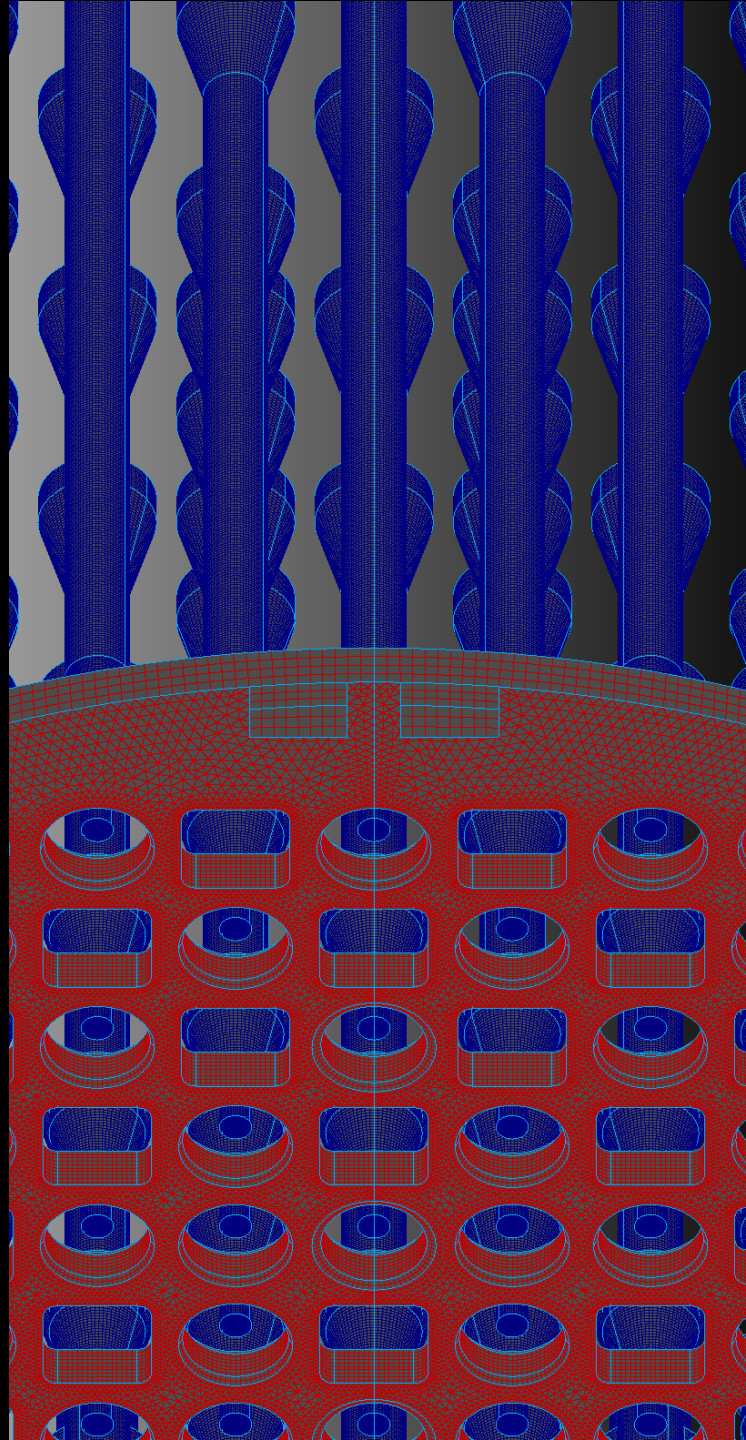
Detailed Fine Mesh Model





Detailed Fine Mesh Model





QUESTIONS?

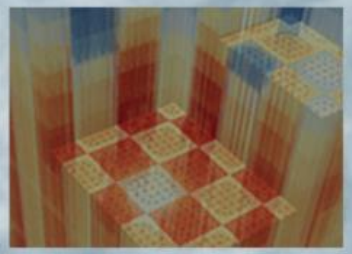
A DOE Energy Innovation Hub

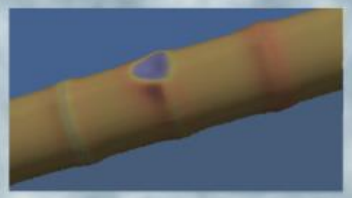
Virtual Reactor Working Group

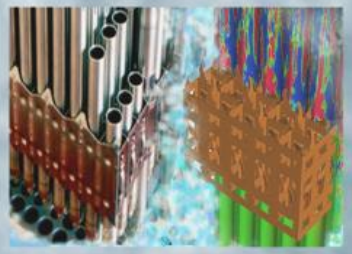
CASL Industry Council Meeting

3/18/2015

Charlotte, NC







U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

Outline

- Basic premise of the Virtual Reactor Working Group
- Interface with the post-CASL entity
- The User portal
- Planned milestones

Basic Premise of the VRWG

- Serves as an administrative body to enable the sustained use and development of VERA
- Finds and supports users
- Facilitates VERA R&D, code upgrades, and distribution
- Funded by the users

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

Basic Premise of the VRWG: Administration

- Manage VERA's business, design, functional, and quality requirements with input from the members
- Manage membership database
- Manage finances
- Interface with others on licensing terms, regulatory licensing, export control requirements

Complex code system with a multitude of touch points that must be meticulously managed

Basic Premise of the VRWG: Find and support users

- Organize user meetings and exchanges
- Create and host VERA tutorials / training
- Provide software support for VERA
- Support VERA's Verification and Validation testing program
- Annual conference, "Roundtable"

Basic Premise of the VRWG: VERA R&D, code upgrades, distribution

- Maintain the official VERA repository
- Facilitate and/or execute VERA R&D as directed by administrative body
- Review and disposition user recommended code enhancements
- Integrate or facilitate integration of code modifications resulting from R&D or user-recommended enhancements
- Fix bugs
- Archive VERA "gold standards"
- Archive user-submitted example simulations
- Distribute VERA
- Maintain connections for community computing resources

Basic Premise of the VRWG: funding

- Post Phase 2, User fees or VERA fees are expected to sustain the VRWG
  - either user-funded or funded collaborative projects
- The VRWG may develop a fee structure that is based on a market analysis
- Phase 2 expects minimal (possibly zero) dues to start
  - CASL funds are budgeted for VERA support so funds from the WG aren't currently needed
  - Fees may or may not include VERA, depending upon the post-CASL entity selection and its approach to VERA marketing

The VRWG is intended to be self-sustaining

Working Group Funding

- The Inter-Institutional Agreement (IIA) is nearly complete by the code authoring institutions
  - Allows for distribution of VERA for Government Use and Test and Evaluation Licenses
  - Terms are still being defined for commercial licenses
  - License terms to be defined in attachment to IIA, which may be periodically modified
- Distribution of VERA via Working Group membership
  - Institutions will join the working group and receive a license to VERA
  - Licenses will be issued to working group members
- Other DOE commercial licenses are under review

KIVA Model License

- KIVA is a LANS combustion model
  - Licensees are allowed access to source code
  - Fees are from 1-5 users for a commercial entity
  - Fee structure varies on nationality and entity class (commercial or non-commercial)

KIVA License Model

Version	License Issue Fee	Annual License Fee Per User
Domestic Licensees		
KIVA-3V	$3,500	$500
KIVA4	$5,000	$1,000
KIVA-4mpi	$15,000	$1,500
Foreign Licensees		
KIVA-3V	$3,500	$1,000
KIVA4	$5,000	$2,000
KIVA-4mpi	$20,000	$2,500
Academic/Not-for-Profit Licensing		
KIVA-3V	$1,500	$250
KIVA4	$3,000	$500
KIVA-4mpi	$7,500	$500

International RELAP5 Working Group

- RELAP5 is a NRC licensed plant-safety nuclear analysis model
- Mature model applied for 30 years to commercial reactors
- Model is accessed via membership in the International RELAP5 Users Group (IRUG)
  - Working Group membership applies a tiered-model that varies with support received by working group, source code access and institutional purpose

International RELAP5 Working Group Pricing

Membership Tier	Annual Domestic License Fee	Annual International License Fee	Benefits/Support
Member (Regular User)	$25,000	$48,000	Multiple copy use is allowed. Source code included 80 hours of support
Member (Super User)	$56,000	$70,000	Same as member except 200 hours of support
Multi-use Participant	$8,400	$15,200	Multiple copy use allowed. Object code only 20 hours staff assistance
Single Use Participant	$5,600	$10,700	Single copy use allowed. Object code only 5 hours staff assistance
University	Free	Free*	Object code only No staff assistance

Interface with the Post-CASL Entity

- Initial TDO post-CASL entity description:
  - Responsible for primary VERA distribution and user support
  - Manage the VERA Working group
  - Facilitate VERA training
  - Coordinate further development of the VERA suite of tools
  - Liaison with other ModSim initiatives
  - Accessible to all potential Users (as limited by export control)
  - Capable of providing support to all Users
  - Able to conduct continued outreach activities

Virtual Reactor.org
CASL VERA User Support Portal

Products and Services | Support | Community | About

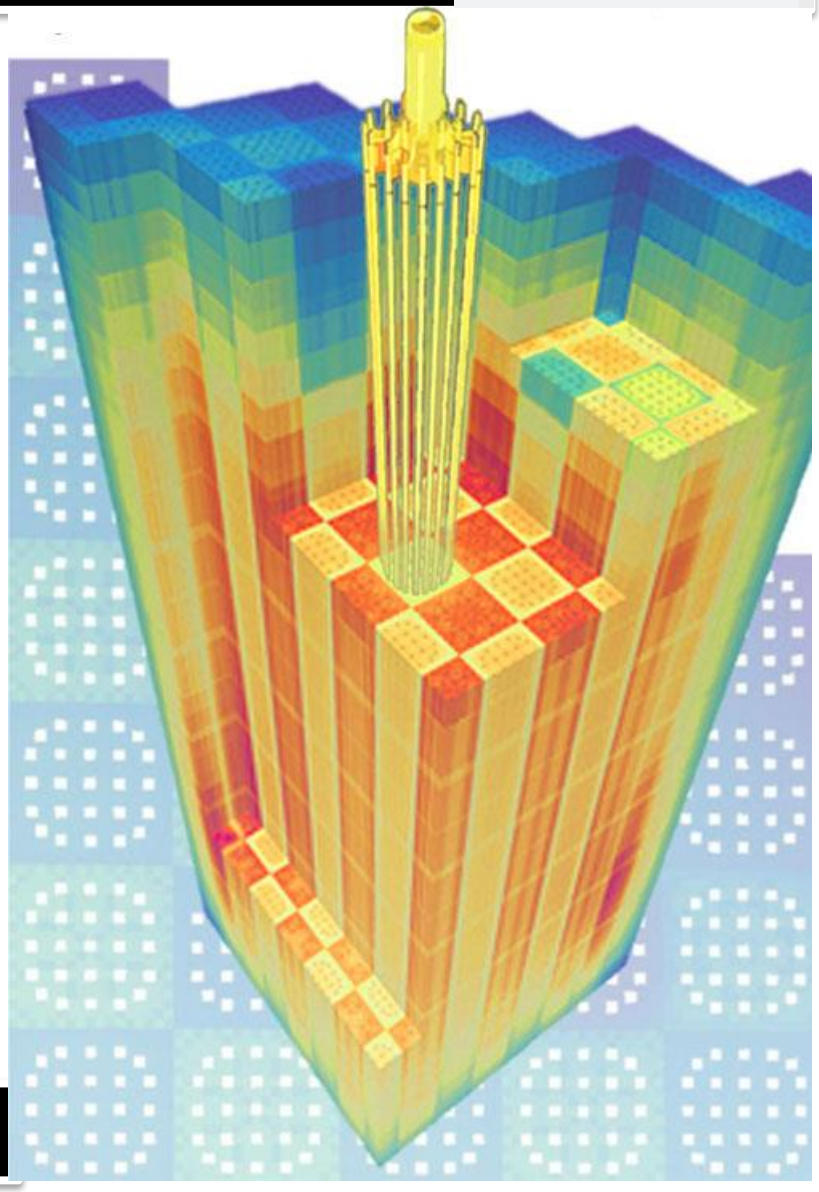
User Name

Password

Login

Forgot password?

- Registered Users
  - ✓ Download software and user manuals
- Access Tutorials
- Interface with the VERA user community
  - ✓ User simulations
  - ✓ Industry whitepapers
  - ✓ Post questions/issues
- Open and track user requests



New to VERA? Find out more about CASL and request a copy of VERA

The VRWG User Portal

- Primary point of contact for new and current users
- Access to documentation, tutorials, software updates for approved users
- The place to discuss VERA applications with the user forum
- Get VERA support
- Submit proposed VERA mods, example simulations, white papers

User Portal

- Portal supplements existing CASL.gov website, but is designed for post-CASL entity
  - Must be able to disengage from lab hosting at the end of Phase 2
- Maintenance will require significant web programming skills and funds to actively moderate it
- Software download from this site must be vetted for cybersecurity and export control concerns

Essential for building a user base, but currently not in CASL's direct line of sight

Planned Milestones

- Post-CASL entity market analysis this year
  - Fees and structure to be recommended based on this study
- Virtual Reactor Working Group kickoff this year
- VERA tutorials established this year
- VERA training workshop pilot this year
- User Portal website established this year

Dependent on VERA releases and available support

Summary

- VRWG will be initiated this year and will utilize a user portal website to effectively serve users and deliver product
- VRWG structure is compatible with the post-CASL entity envisioned to sustain CASL technology and is a candidate
- A detail-oriented highly organized approach is needed to navigate concerns about managing expectations, licensing terms, export control regulations
- The VRWG will need to collect fees to sustain the organization

VRWG is essential to making CASL products 'used and useful' to the nuclear community

Safety Analysis Topics for CASL Meeting 3/17-18/2015

1. Temperature/power distribution in core region following a steam line break

2. Flow distribution in core plenum/core region following a locked rotor

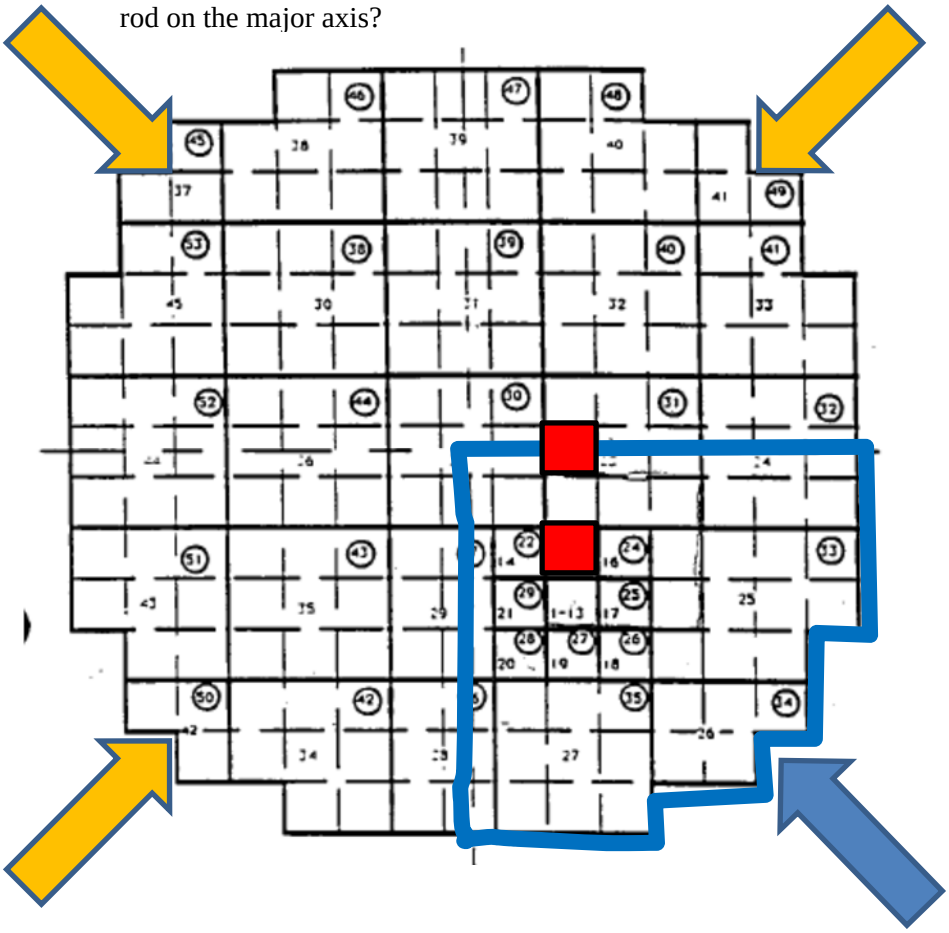
Details:

1. Temperature/power distribution in core region following a steam line break

   The event is a double-ended guillotine break of one steam line in a 4-loop W PWR (i.e., McGuire or Catawba). The reactor is initially at Hot Zero Power with all 4 RCPs operating. A break in one SG will cause the cold leg temperature in that loop to decrease significantly. The colder water will enter the lower reactor vessel plenum and mix some with the relatively hotter fluid from the other 3 loops. The degree of mixing assumed in the current analysis is based on thermal mixing test data obtained in 1989 for McGuire during a test performed in MODE 3 by isolating 3 of the 4 SGs then depressurizing the non-isolated SG by 450 psig over 7 minutes. There is also assumed to be a stuck rod in the core which can either be in the cold quadrant or on the major axis. The cold water combined with EOC reactivity coefficients and a stuck rod leads to a power excursion with an asymmetric peaking distribution. The problems to be solved are:

   A. What is the core wide radial temperature distribution and power distribution vs. time with a stuck rod in the cold quadrant?

   B. What is the core wide radial temperature distribution and power distribution vs. time with a stuck rod on the major axis?



2. Flow distribution in core plenum/core region following a locked rotor

   The event is a locked rotor of 1 of the 4 RCPs from Hot Full Power conditions. The immediate cessation of flow in one loop could cause an asymmetric inlet flow distribution that cannot be approximated without a split core model, which the current system analysis does not have. Consequently, the assumption is that the flow mixes uniformly in the reactor vessel inlet plenum prior to entering the core region. The time frame of interest is the first 5 sec of the transient. The problem to be solved is:

   A. What is the reactor vessel downcomer flow distribution (e.g., are there any azimuthal velocities in the vicinity of the locked rotor loop) and reactor vessel inlet flow/temperature distribution vs. time when one of the RCP rotors locks?

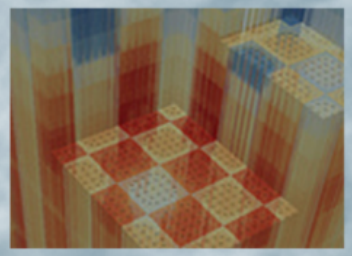
Fuel Performance Modeling in CASL Fuel, Materials and Chemistry (FMC) Focus Area

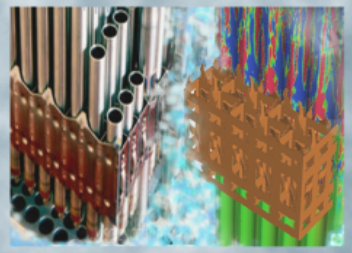
Chris Stanek
Los Alamos National Laboratory

Rich Williamson
Idaho National Laboratory

Brian Wirth
University of Tennessee

On behalf of the FMC team

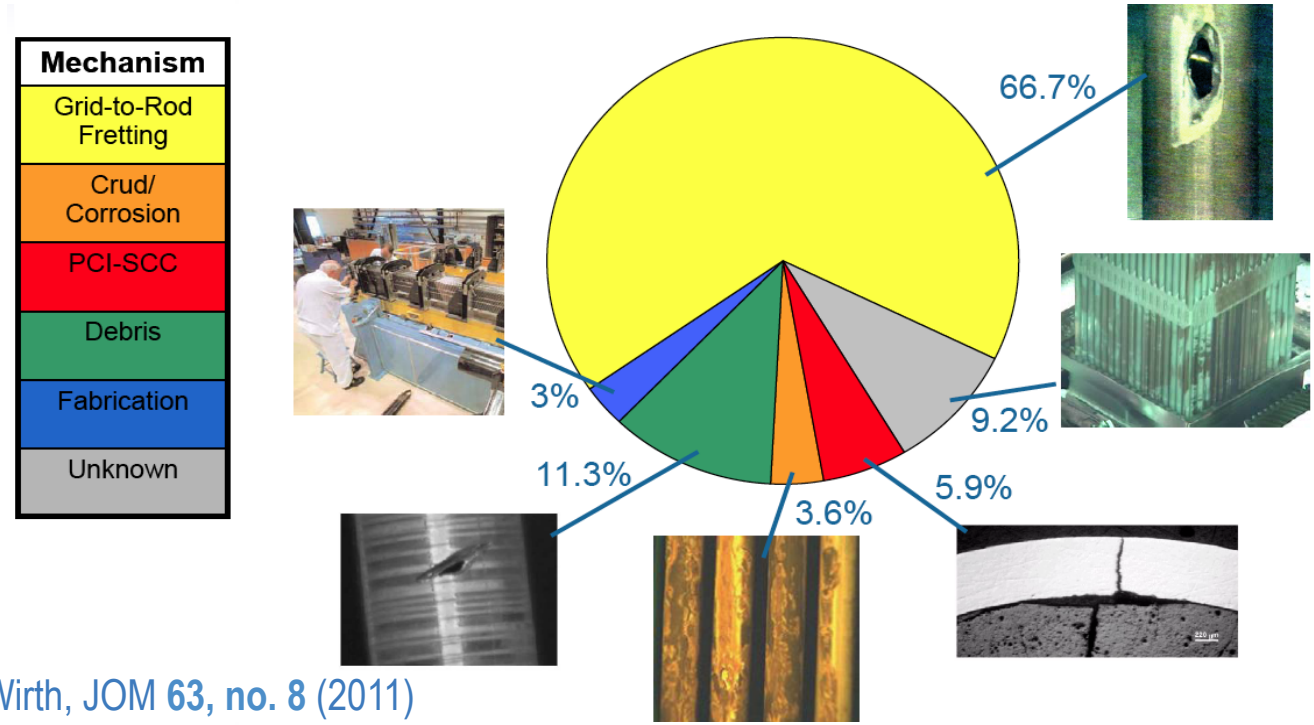




CASL INDUSTRY COUNCTIL MEETING
Charlotte, NC
March 18, 2015

CASL Challenge Problems

Summary of US fuel failure mechanisms (2000-2008)



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

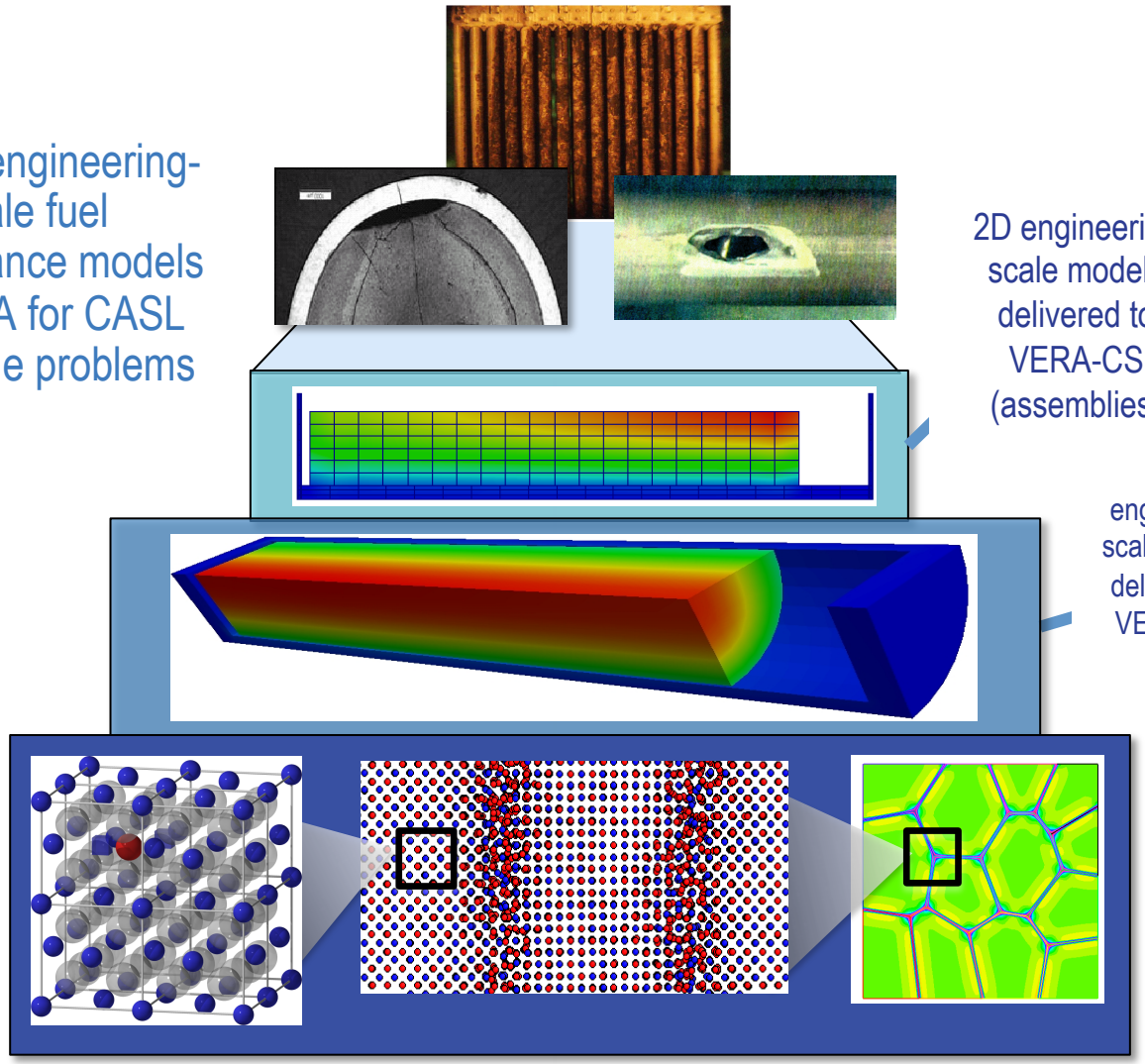
Challenge Problem	Cost to Industry
PCI	~$600M
GTRF	~$650M
CIPS/CILC	~$135M

From CASL Industry Council Value Proposition Study March 2014

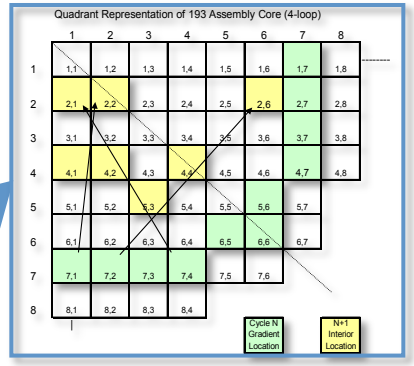
Fuel, Materials and Chemistry (FMC)

Enabling Improved Fuel Performance through Predictive Simulation

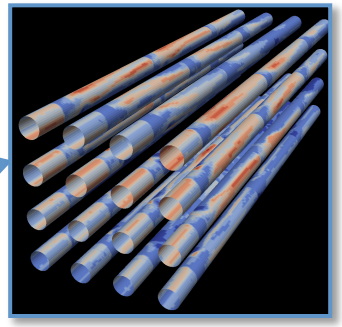
Deliver engineering-scale fuel performance models to VERA for CASL challenge problems



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



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



Challenging, multiscale processes control nuclear fuel performance

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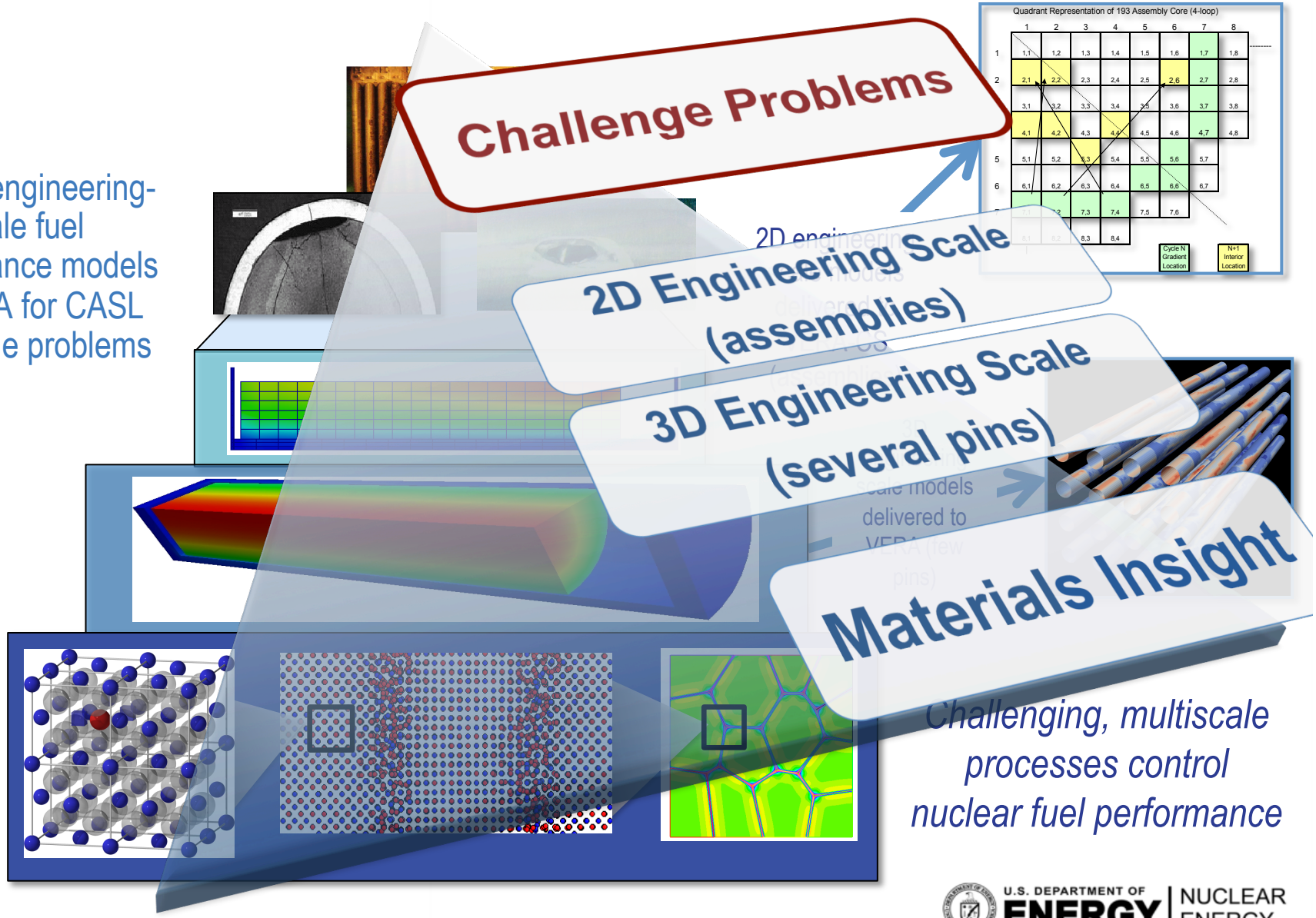
Fuel, Materials and Chemistry (FMC)

Enabling Improved Fuel Performance through Predictive Simulation

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



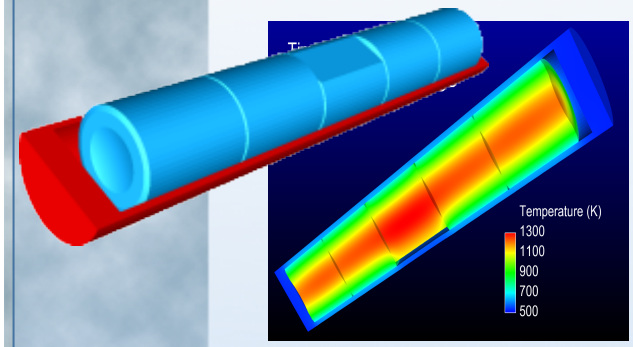
Challenging, multiscale processes control nuclear fuel performance

U.S. DEPARTMENT OF ENERGY | NUCLEAR ENERGY

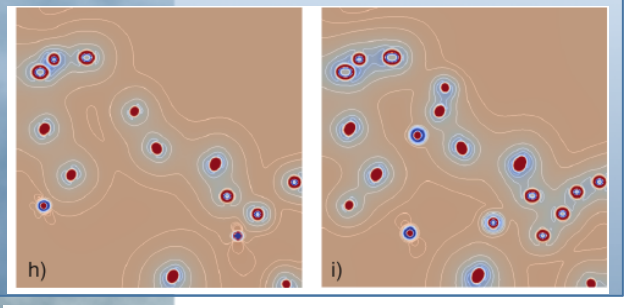
FMC delivers engineering scale fuel performance models and materials physics-based constitutive models for CASL challenge problems

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

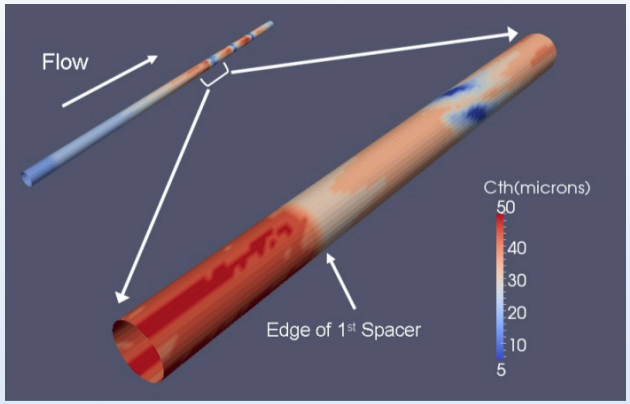
PCI



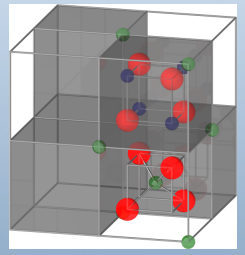
BISON-CASL
(formerly Peregrine)
Fuel Performance

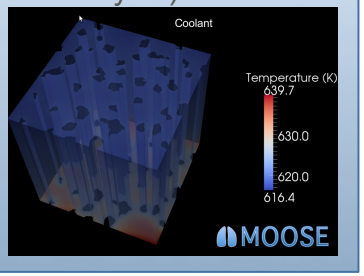


CRUD

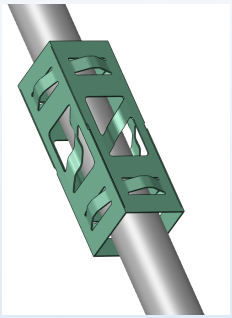


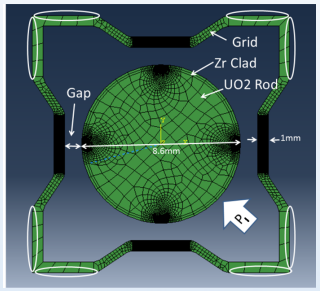
MAMBA
(MPO Advanced Model for Boron Analysis)



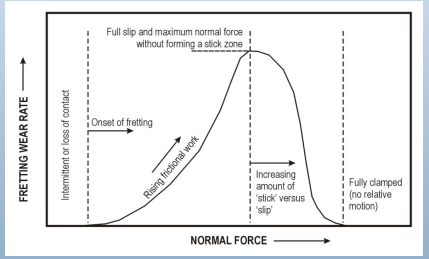


GTRF





Structural Mechanics & WEAR MODELS



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

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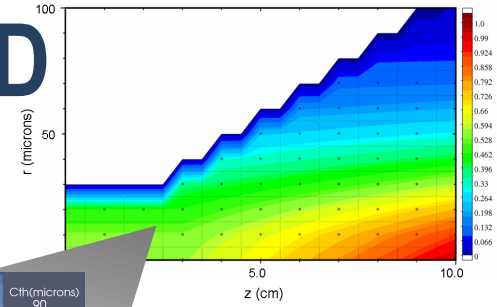
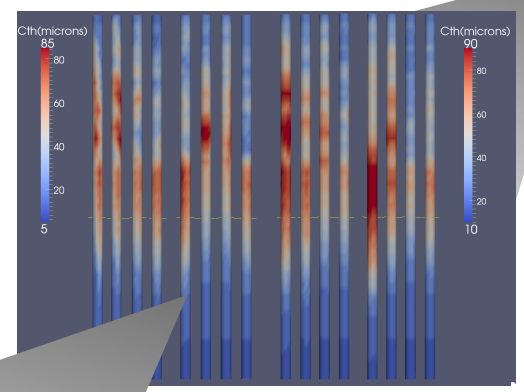
FMC Approach to CRUD

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



1D-2D MAMBA

Pin-scale CRUD formation/growth model, which can be used for VERA-CS CIPS-risk analysis (assemblies), as well as for subgrid capability (CFD, fuels, etc.)

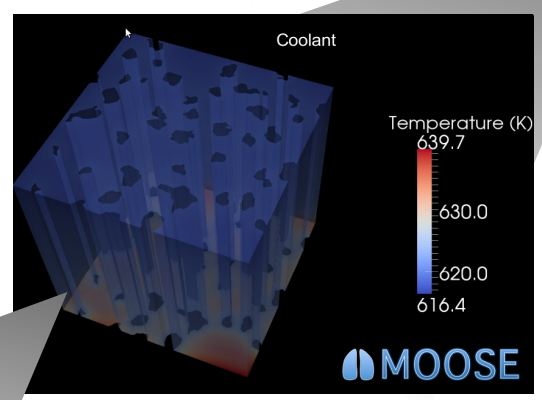


3D MAMBA

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

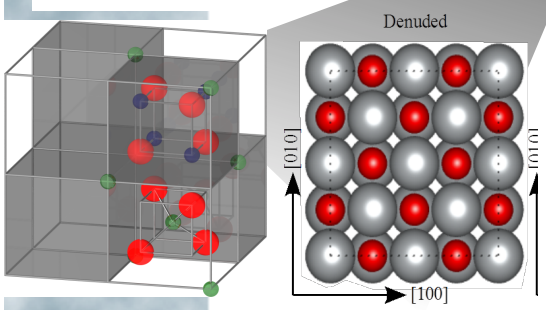
Thermodynamics

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



MAMBA-BDM

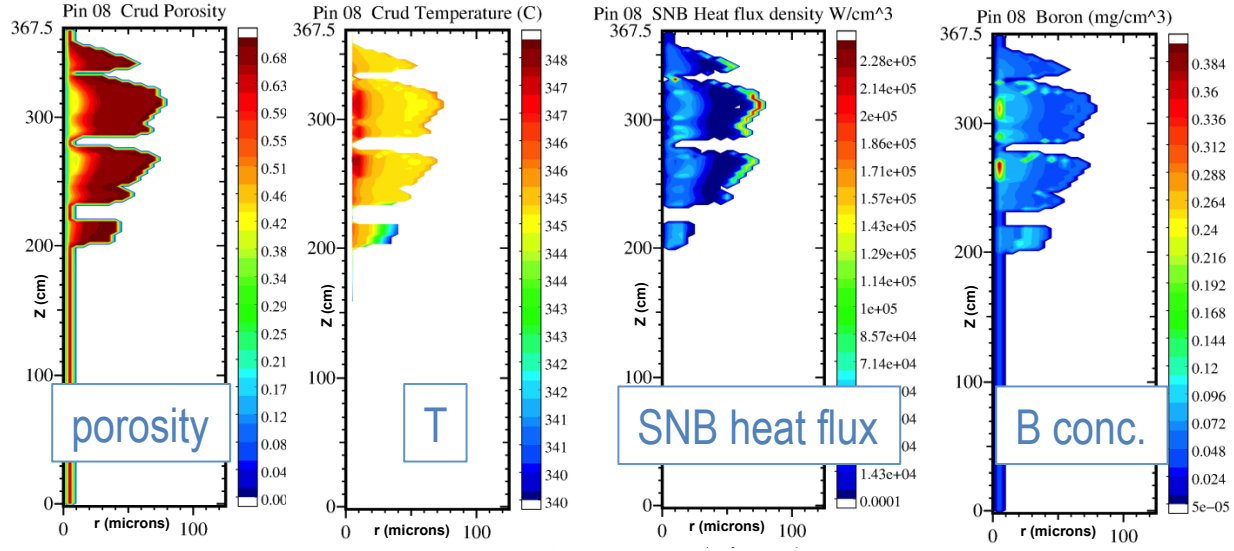
Microscale CRUD formation/growth model, which can be used for CILC-risk analysis

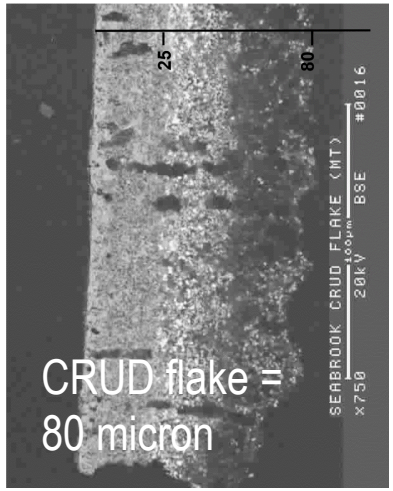


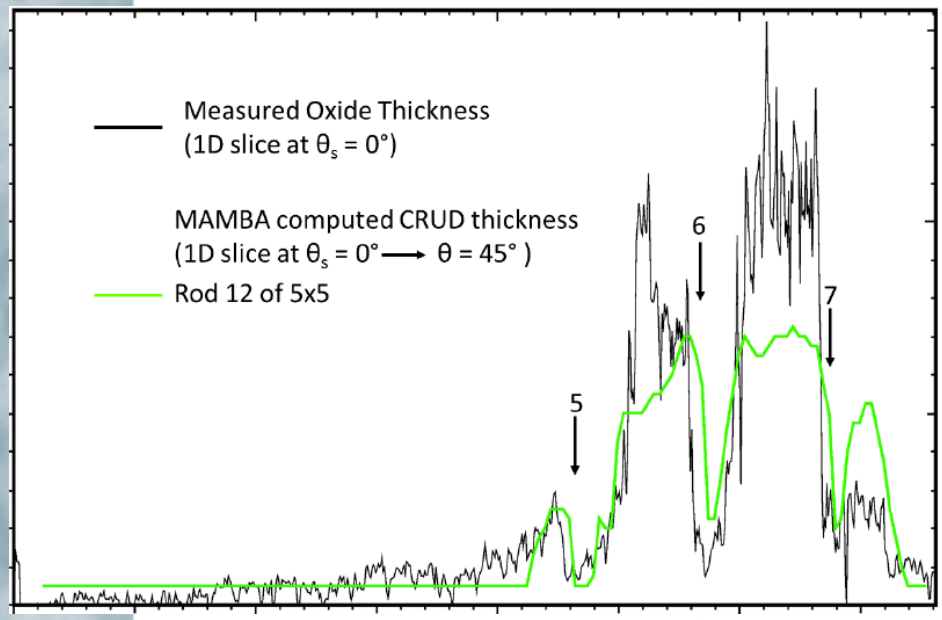
Benefit to Industry:

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

Coupled MAMBA-CFD Comparison to Plant Data



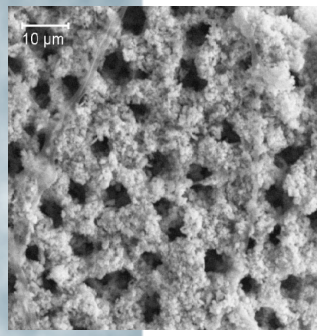




Both axial position and azimuthal thermal hydraulic flow dramatically affect CRUD deposition patterns

Initial comparison to plant oxide thickness data encouraging

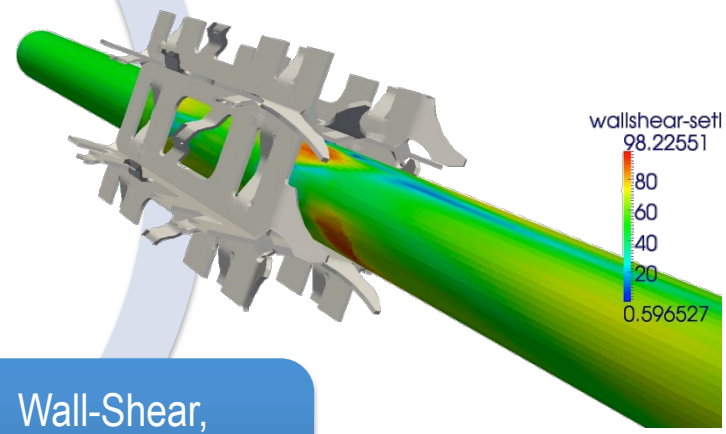
Hydra-TH – MAMBA Coupling (subgrid)



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

Hydra-TH Thermal Hydraulics Simulation

- **CRUD Induced Power Shift**
- **CRUD Induced Localized Corrosion**



Wall-Shear, Temperature, Heat Flux

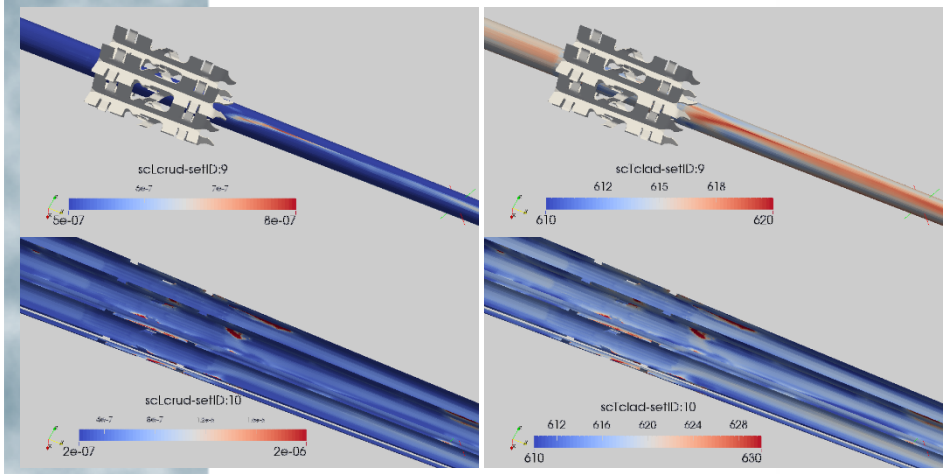
MAMBA Sub-Grid Scale Model

Surface Chemistry Integrated in to Hydra-TH

Milestone Accomplishments

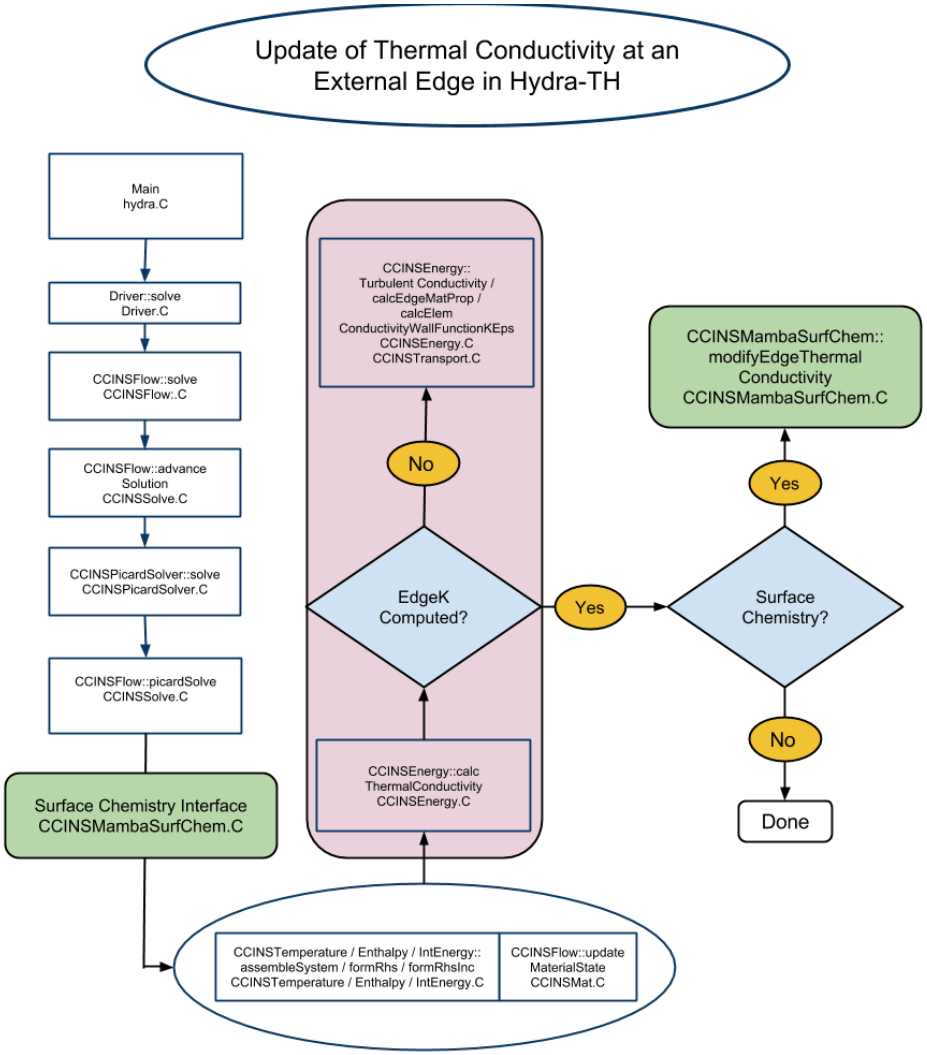
- New 1D version of MAMBA created and incorporated into HYDRA-TH
- HYDRA-MAMBA capability demonstrated for 3x3 rod problem for single grid span
- Models run for 12-70 days to deposit CRUD and feedback of CRUD on thermo-hydraulics demonstrated
- Results summarized in LANL report LA-UR-14-27156

Single Span 3x3 Rod Bundle Case



CRUD thickness (left) and clad temperature (right) at 9 days

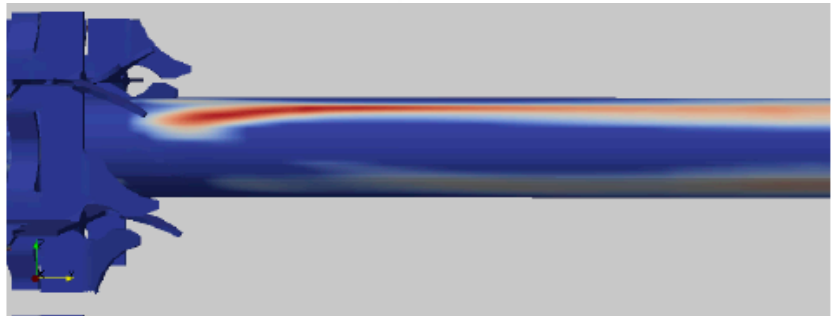
Hydra-TH-Mamba Integration



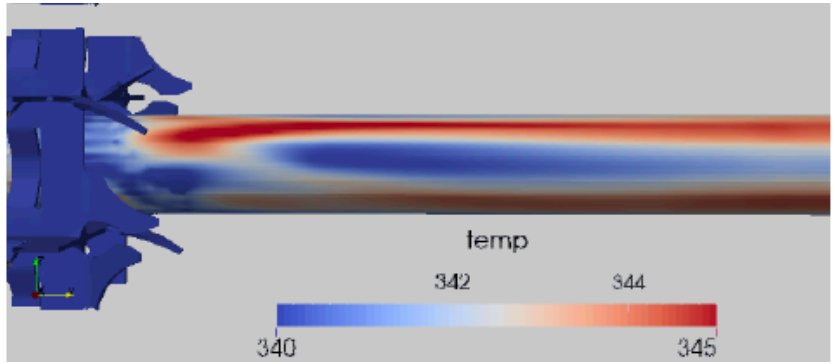
Key personnel: Nadiga, Christon, Berndt and Kendrick (LANL)

CRUD leads to Higher Clad Temperatures

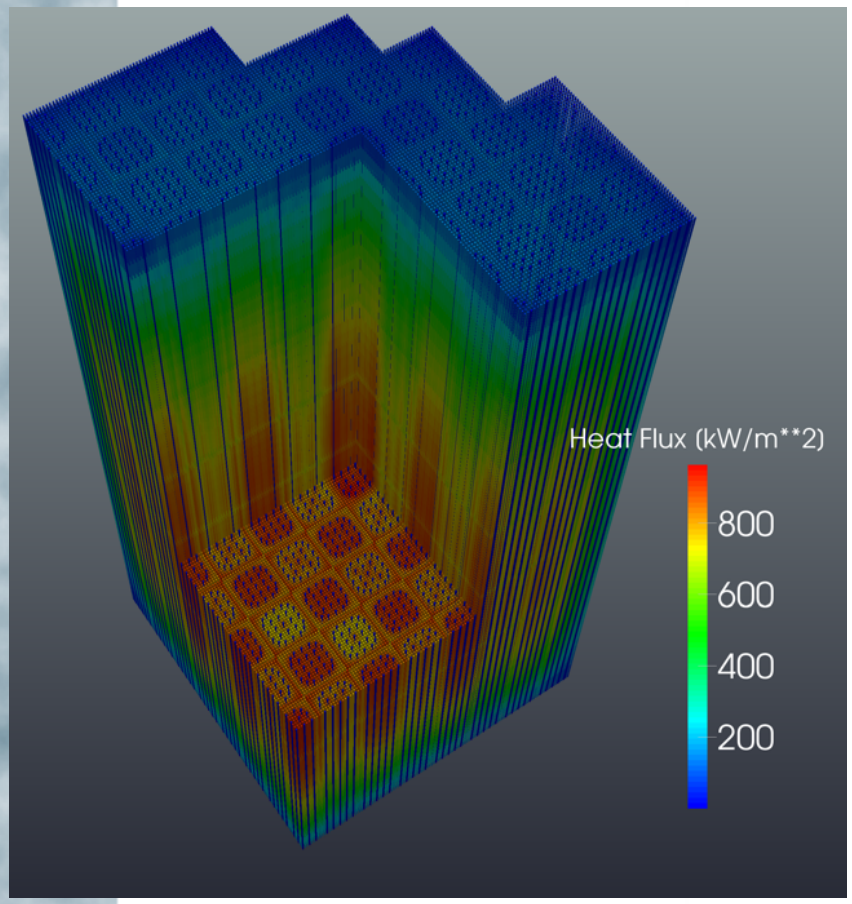
No CRUD

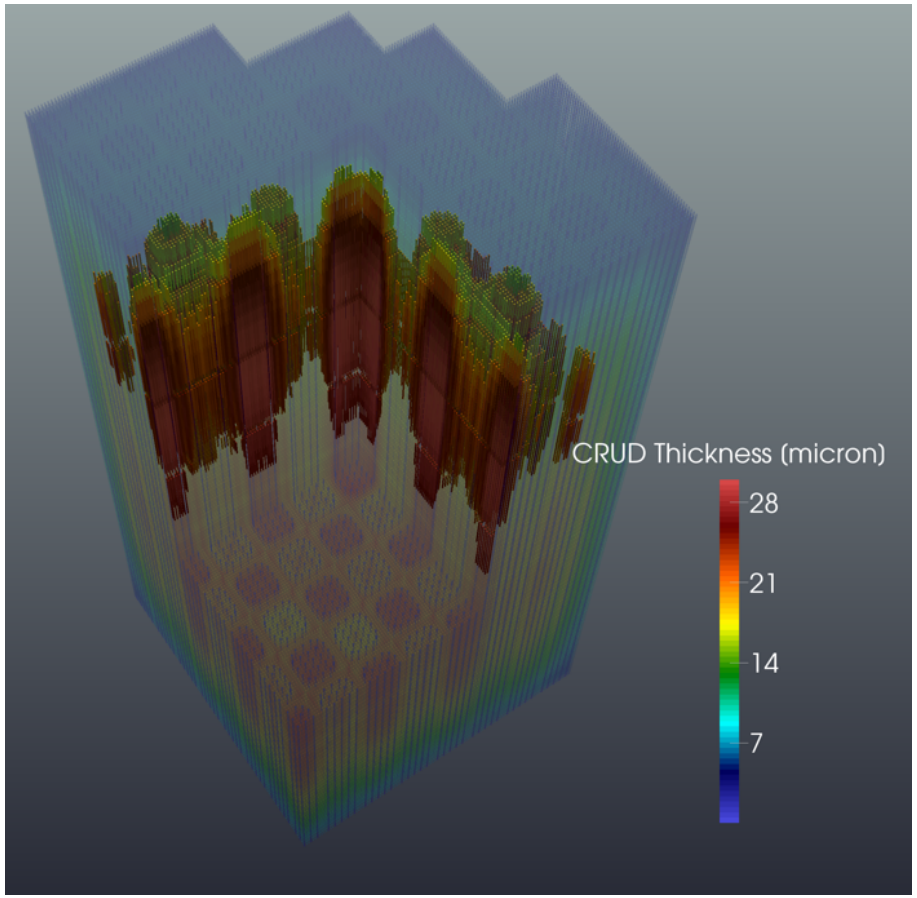


With CRUD



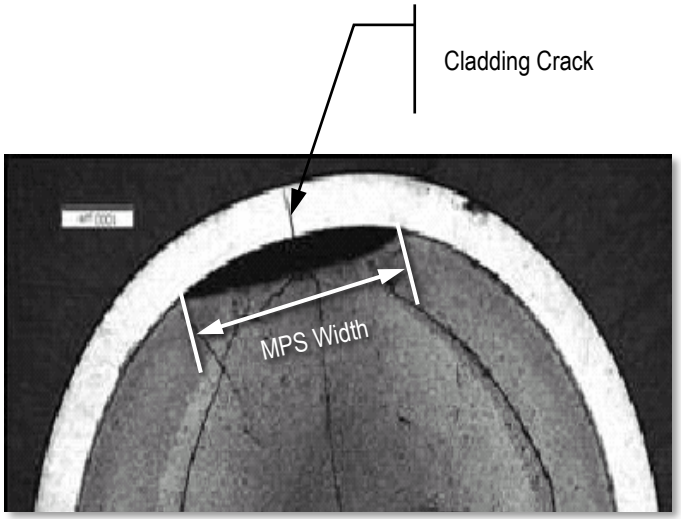
Initial CTF - MAMBA-Subgrid Results (courtesy of Bob Salko)



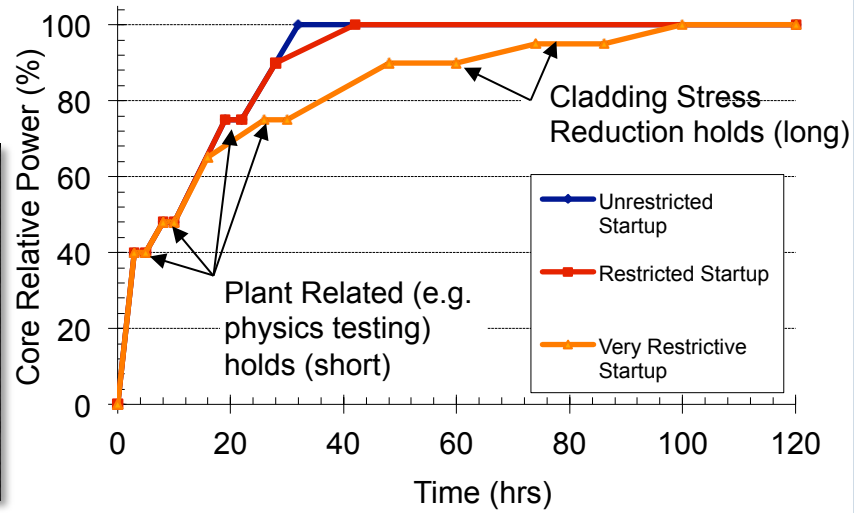


PCI Challenge Problem

Typical MPS Defect in PWR Fuel



Impact of MPS Defect on Power Operation



Question posed by industry:

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

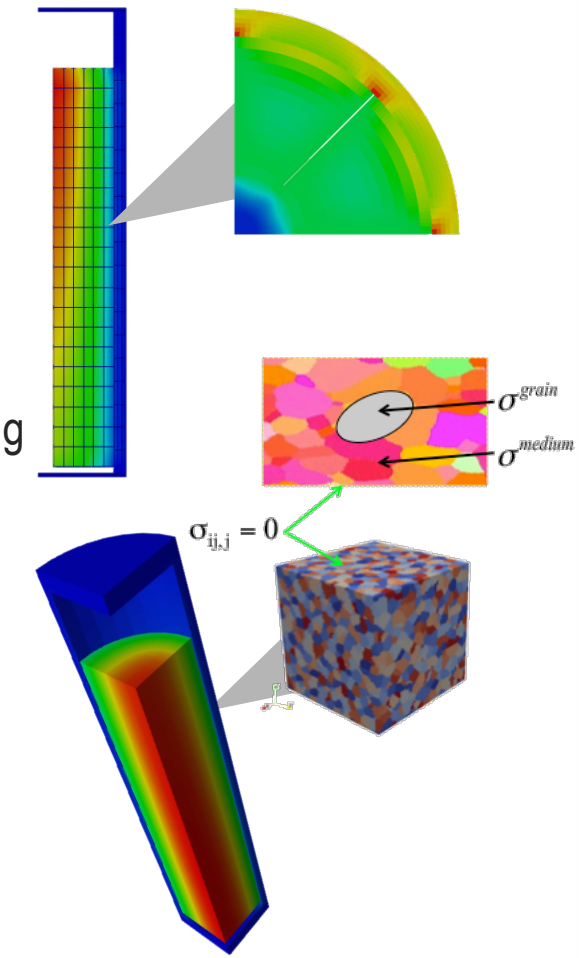
Answers:

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

The above answers combine to reduce uncertainty

BISON-CASL:
Advanced Fuel Rod Modeling Capability for LWRs

- Purpose
  - Enhance the modeling of thermal, mechanical, and chemical behavior of LWR fuel using multi-physics and multi-scale methods to reduce uncertainties in performance and safety margins
- Approach
  - Based on the MOOSE finite element computational framework and leverages the BISON nuclear fuel modeling environment
  - BISON-CASL focuses on specific functionality to model the behavior of LWR fuel
    - advanced material properties and constitutive relationships
    - Challenge problem specific analysis methodologies
  - Designed to leverage results from lower length scale models/methods
  - Benchmark and validation efforts working in parallel with development activities



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3-D Modeling of Fuel Crack and MPS Defects With BISON-CASL: *L1:CASL.P9.01*

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TEAM:

Robert Montgomery
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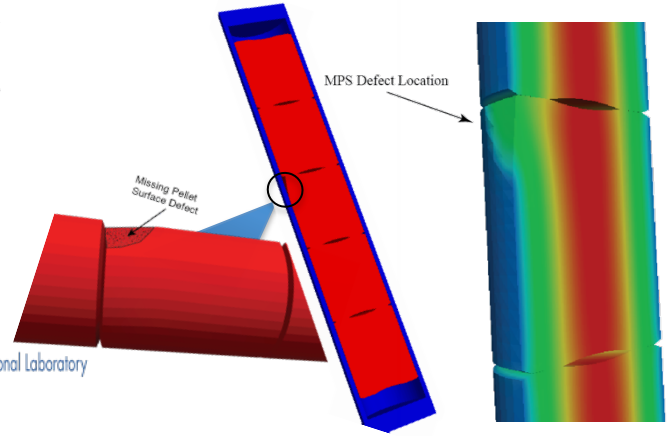
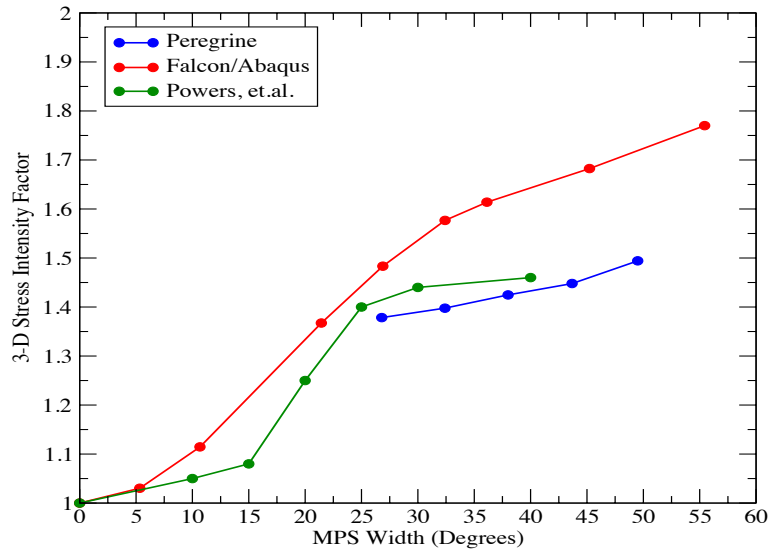
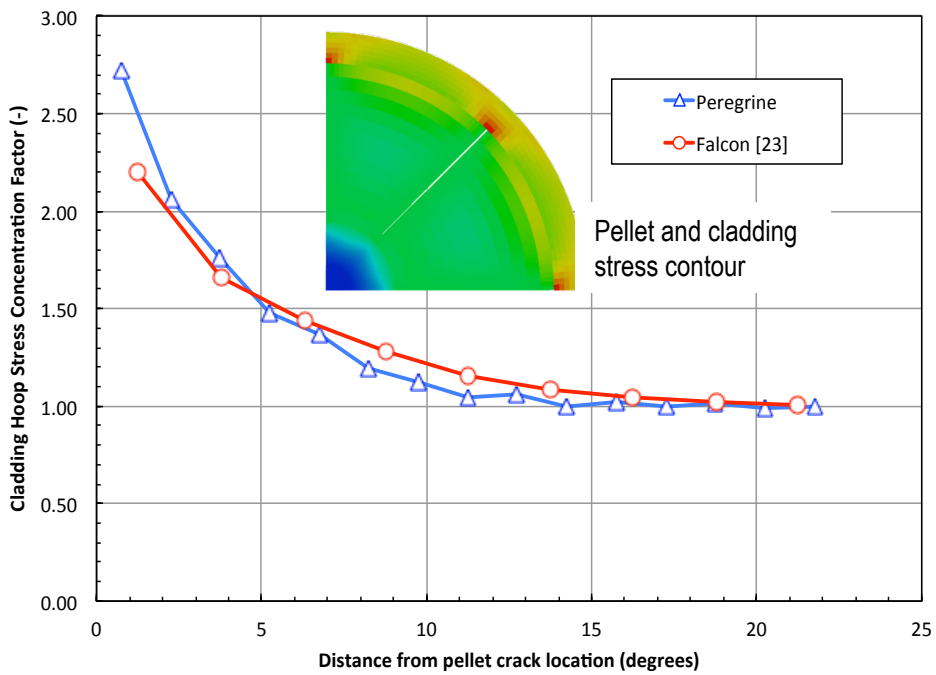
Wenfeng Liu
Mohammed Zikry
Rich Williamson
Jason Hales
Ben Spencer

Pacific Northwest NATIONAL LABORATORY
ANATECH CORP.
NC STATE UNIVERSITY
Idaho National Laboratory



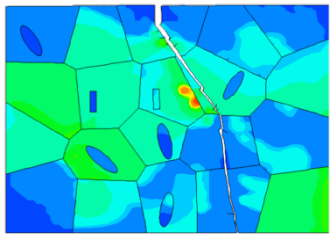




* 2-D PCMI modeling is consistent with current state of the art in fuel behavior modeling for PCI

* Impact of MPS defect size on stress concentration factors similar to Falcon and general-purpose structural analysis codes

* Dislocation-density crystal plasticity model coupled with microstructural features was able to characterize crack growth evolution unique to Zr-alloys



Dislocation density contour

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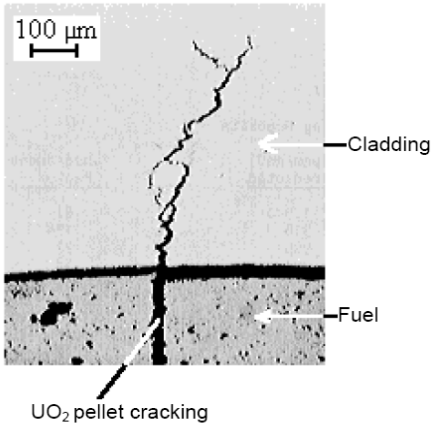
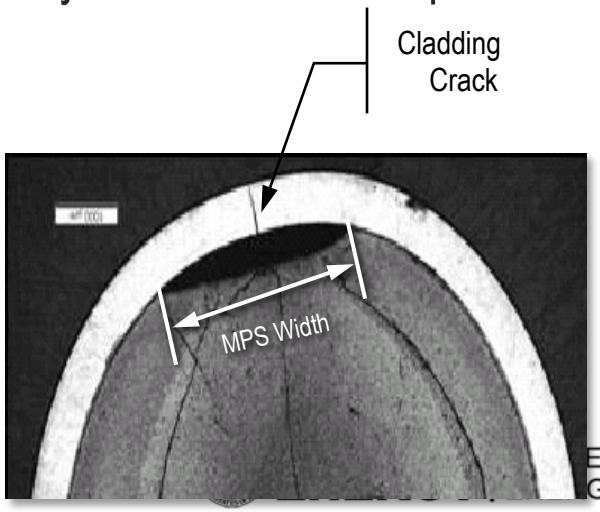
Classical and Non-Classical PCI

- Classical PCI is when a fractured pellet comes into contact with the cladding
  - Driven by the localized strains in the vicinity of a pellet crack as well as the presence of a chemical species, such as iodine, that drive corrosion-induced cracking of the cladding

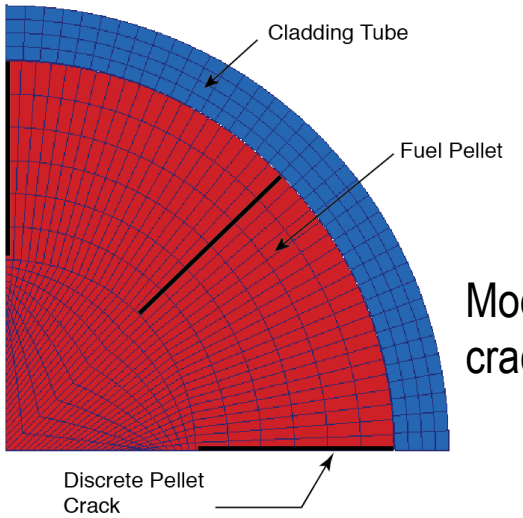
- Non-classical PCI failure is associated with the presence of a missing pellet surface (MPS) defect
  - MPS defects occur as a result of pellet mishandling or upsets in the manufacturing process
  - The presence of an MPS defect during a localized power ramp can cause severe bending moments in the clad in the vicinity of the MPS once pellet-cladding mechanical contact is present





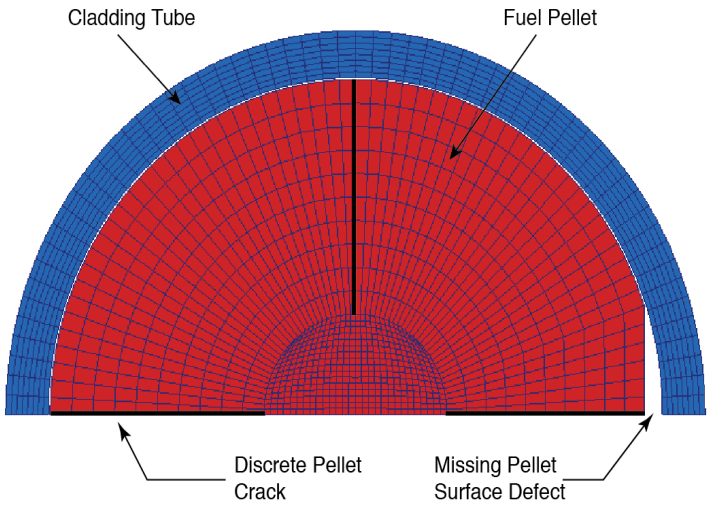
Modeling Approach: 2-D Boundary Conditions

- Classical PCI



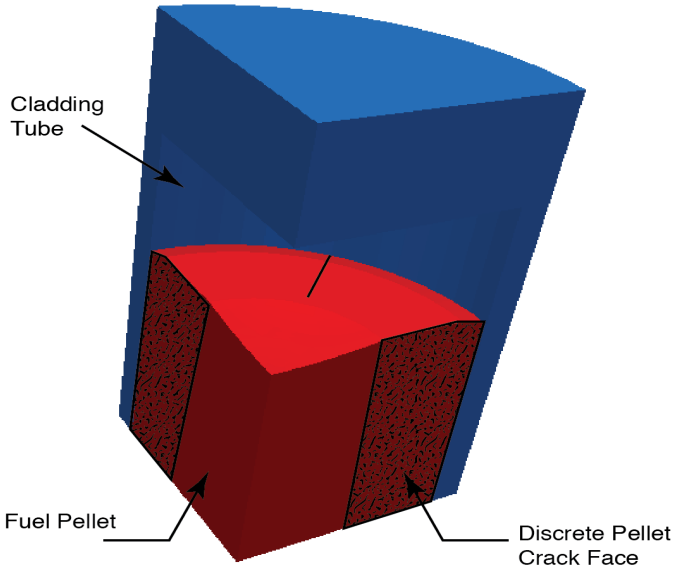
Model corresponds to 8 radial cracks in the fuel

- Missing Pellet Surface

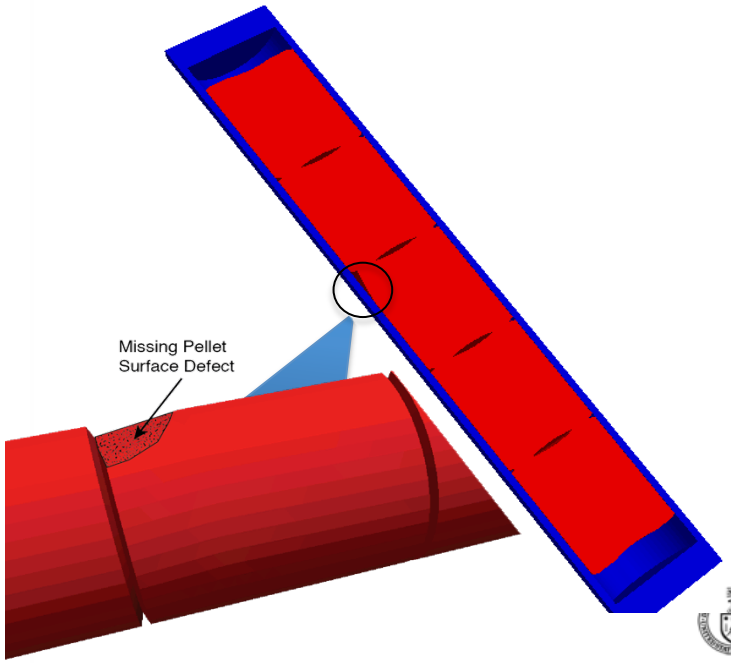


Modeling Approach: 3-D Boundary Conditions

- Classical PCI



- Missing Pellet Surface



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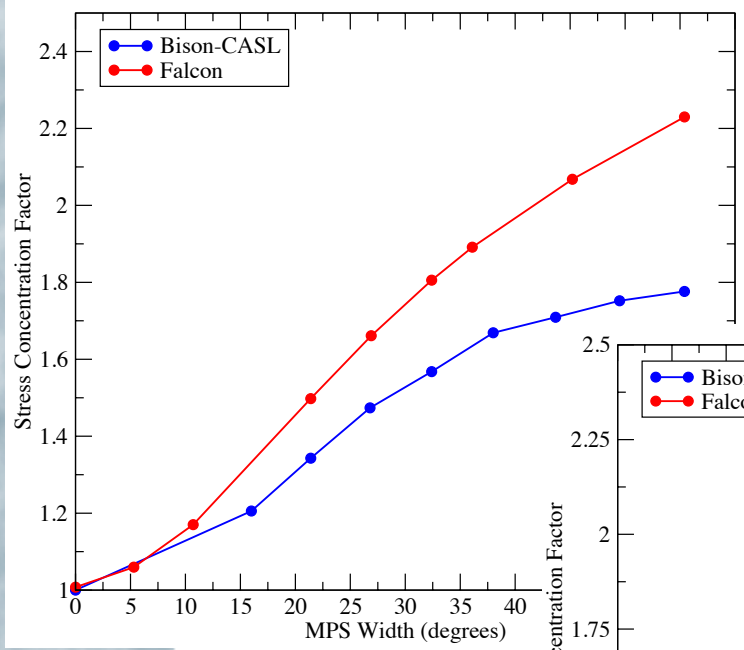
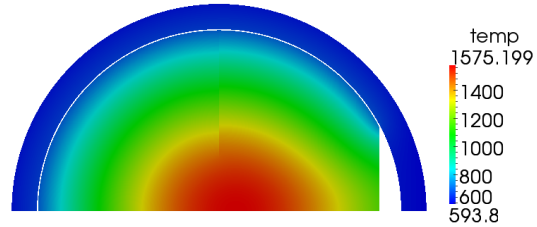
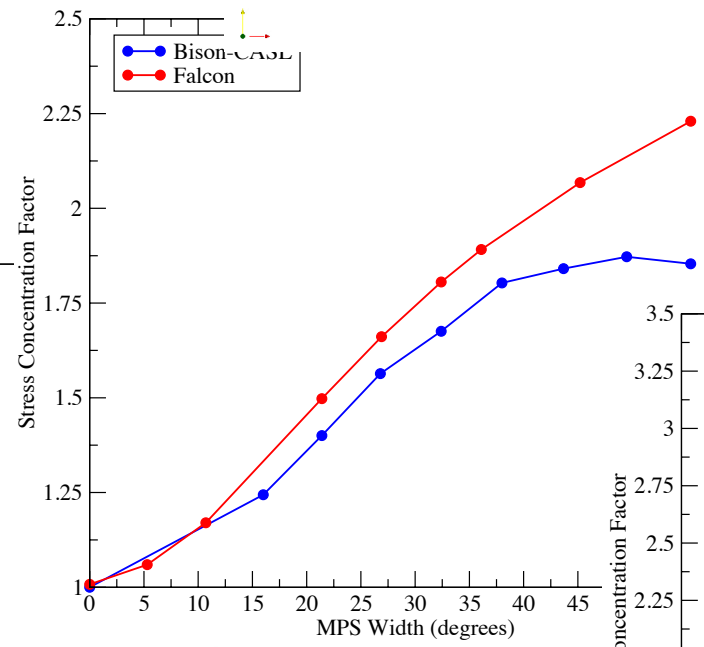
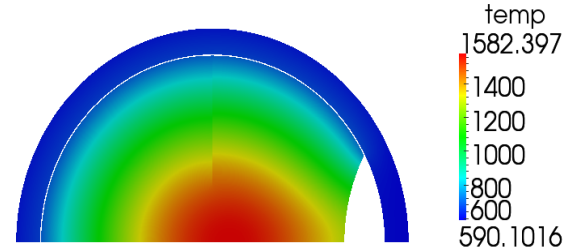
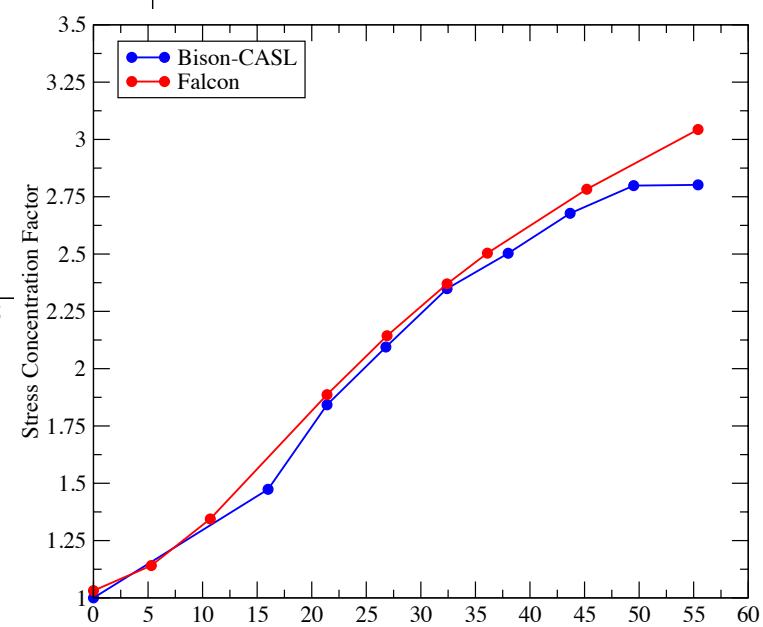
2D MPS Results:
Comparison of BISON-CASL to Falcon





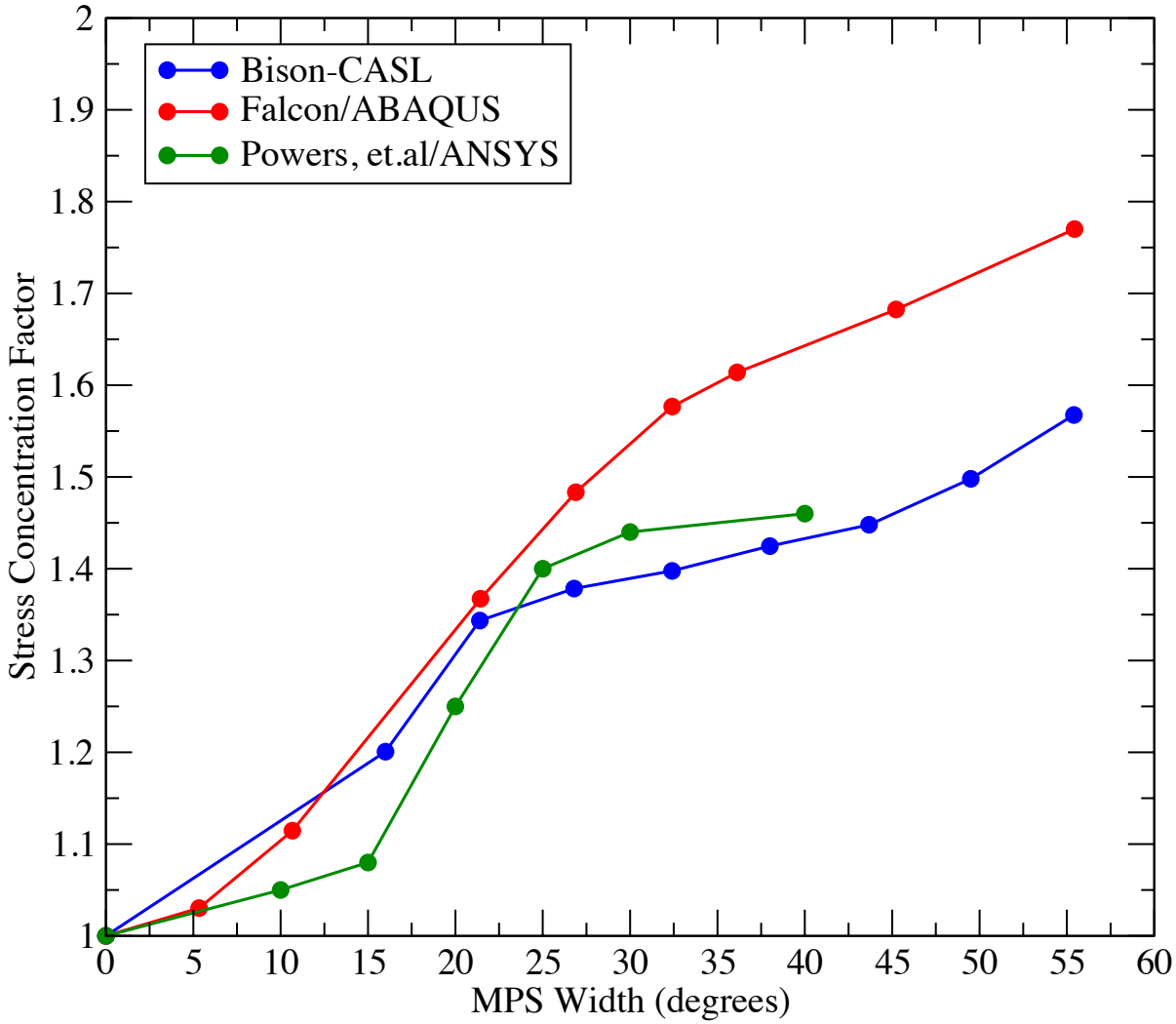


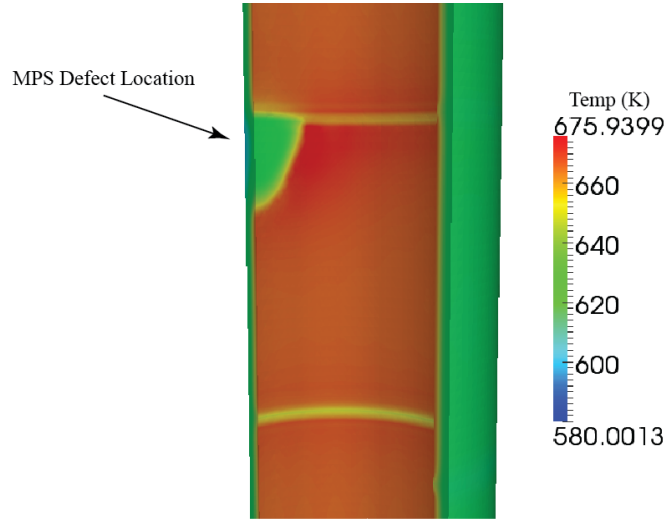


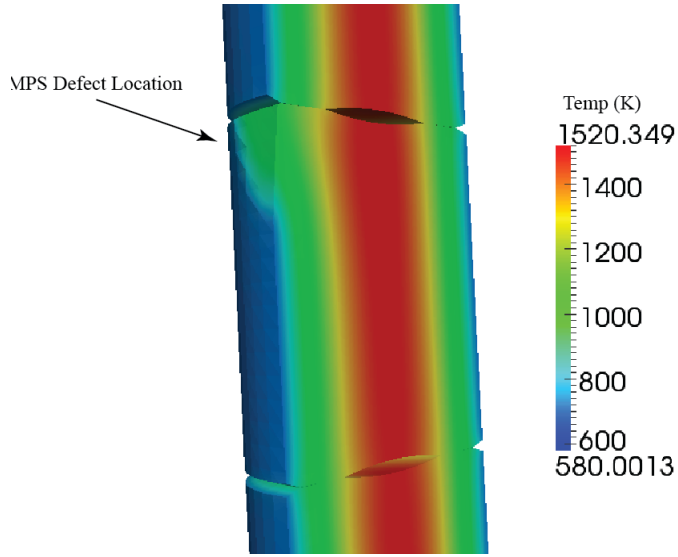


- Falcon used 50% radial cracks and assumed a 90 degree model
- With the curved MPS and the crack correction the results agree

3D MPS Results:
Comparison of BISON-CASL to Falcon







Operating PWR PCI Analysis

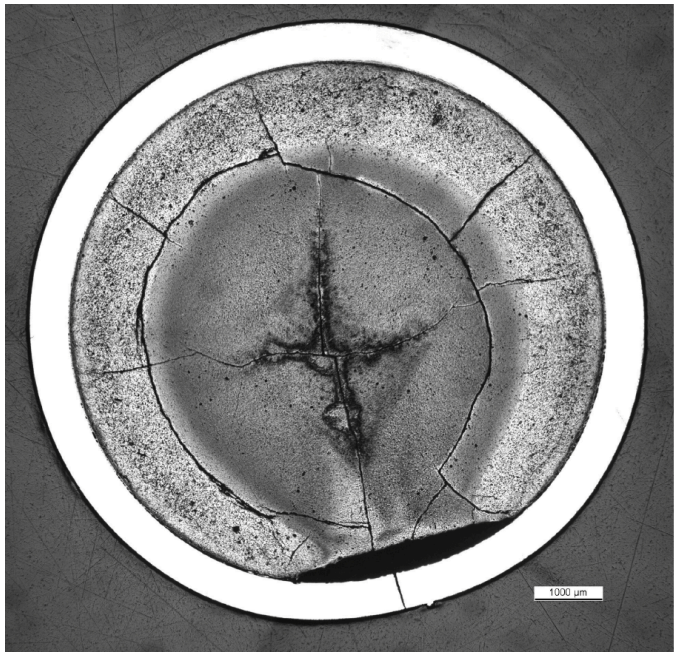
During 2003, Exelon PWRs experienced fuel rod failure indications in three of their PWRs. Most of the fuel rod failures occurred during reactor startup following a refueling outage shortly after the unit had achieved full power operation.

A root cause analysis (RCA) concluded that the leakers were likely due to flaw assisted PCI, most likely a missing pellet surface (MPS).

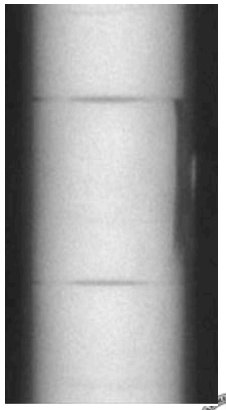
Data request made by CASL for: fuel design, dimension and properties; power history (including startup and shutdown).

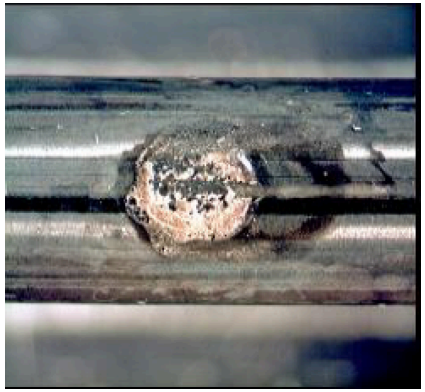
Exelon approved CASL data request. Data expected May 1, 2015.

BISON-CASL will be used to analyze fuel failures.



Y. Aleshin, et al. "The Effect of Pellet and Local Power Variations on PCI Margin " Top Fuel 2010, Paper 041.





Improved Mechanistic Models of Cladding Deformation

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

Improved models for clad deformation required for PCI and safety assessments

TEAM:
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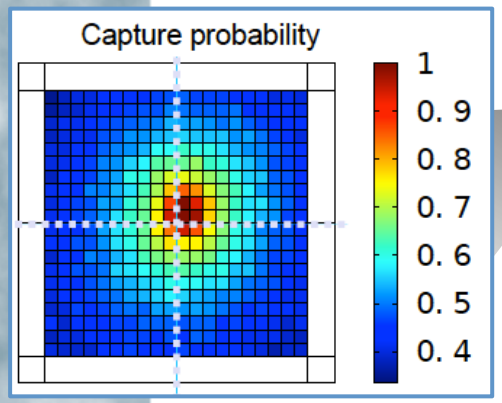
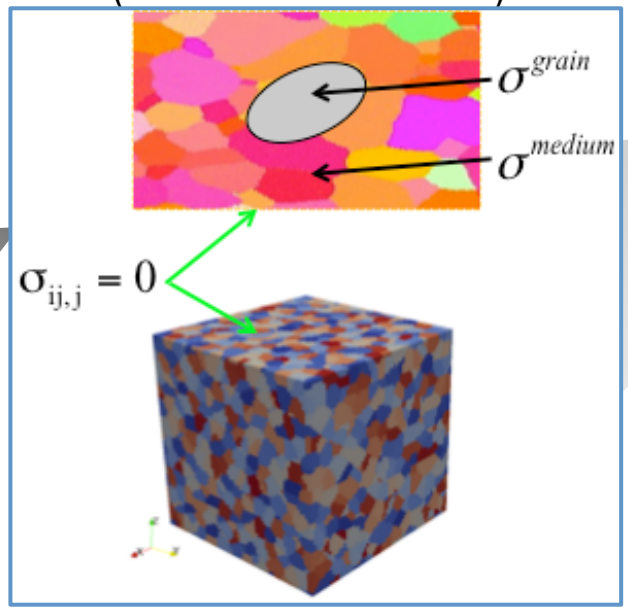
Robert Montgomery
Jason Hales

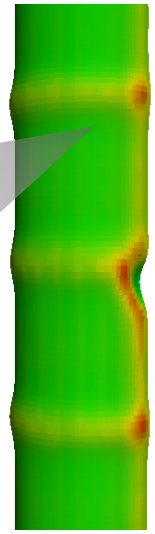
Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)

BISON-CASL engineering scale fuel performance

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





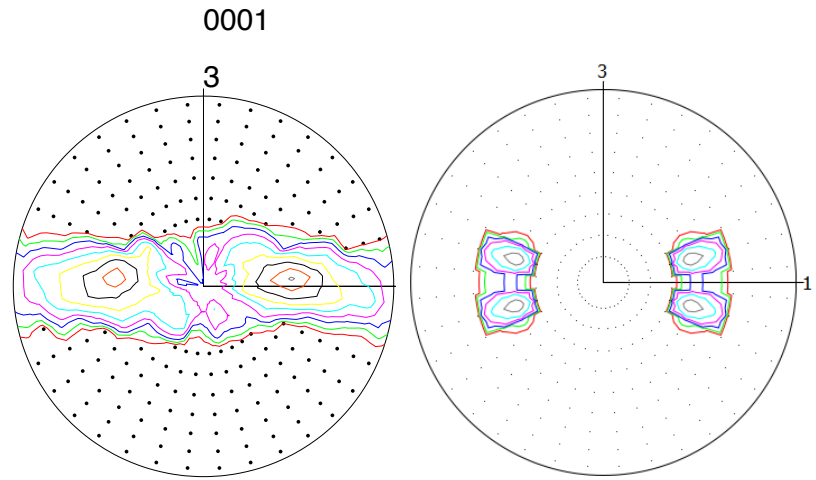


Using BISON-CASL - VPSC (Vulture) to Model Plastic Deformation

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

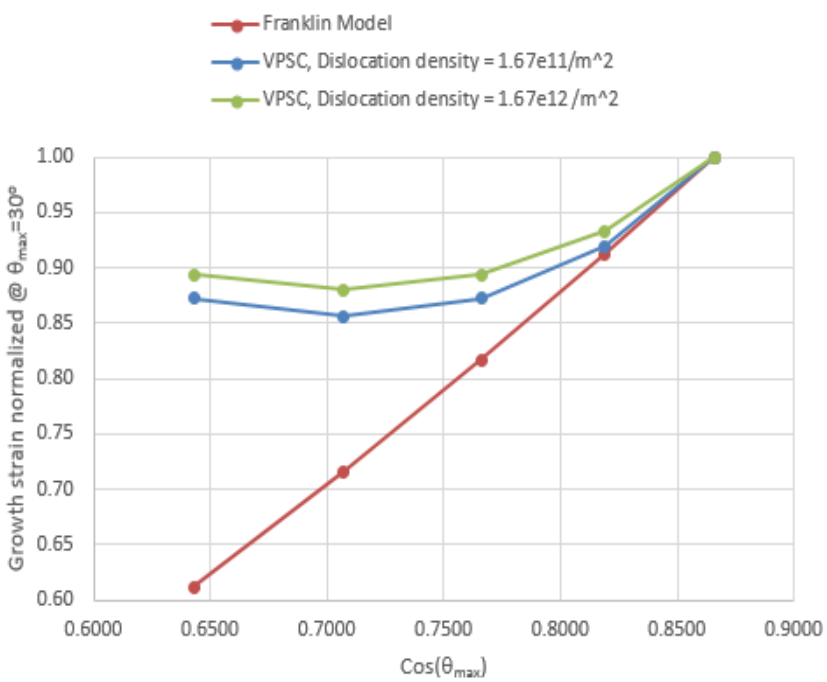
A 4 grain texture is constructed from full texture of cladding tube by imposing the same Kern factors (projection of c-axes along tube main directions)

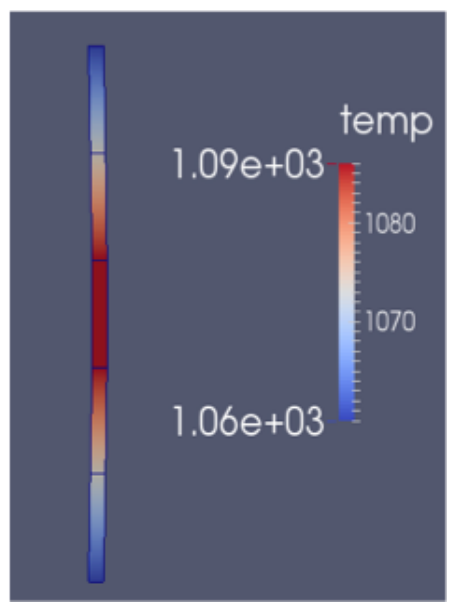
Predictions are within 10% of those obtained using the 1944 grain texture



1944 grains

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





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

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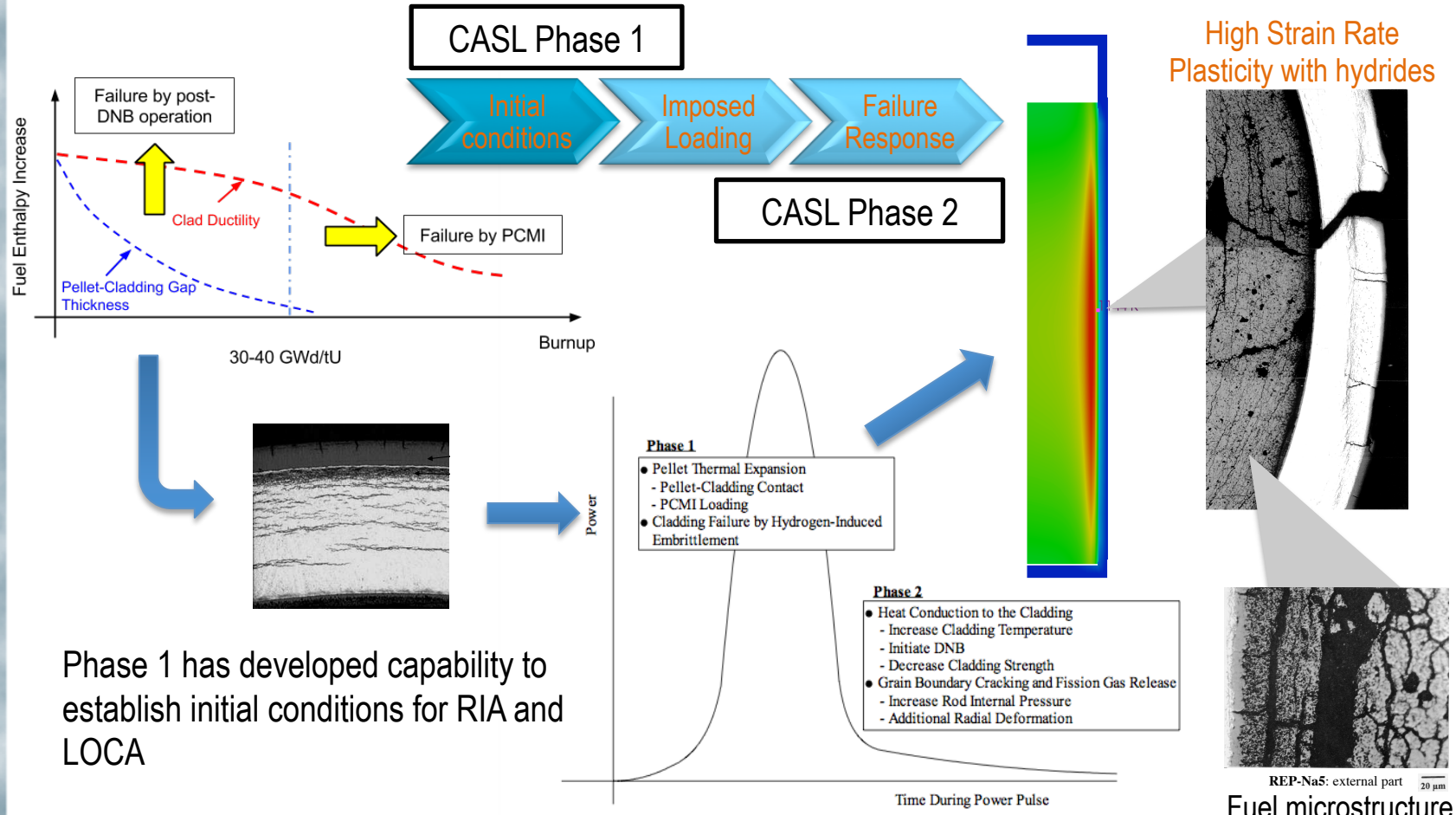
Modeling PCI is prerequisite to modeling RIA and LOCA



Fuel microstructure behavior

Phase 1 has developed capability to establish initial conditions for RIA and LOCA

Phase 2 will develop capability to respond to RIA and LOCA loads

Summary

For PCI, ultimate goal is to improve ability to predict cladding failure

- Material Properties and Behavior
  - Fuel Pellet
    - Thermal Expansion, Fuel Swelling, and Relocation – affects gap thickness
  - Cladding
    - Thermal and Irradiation Creep – affects gap thickness and induced plastic deformation
  - Fission Gas
    - Production and Release – presents of reactive species for SCC
  - Coolant
    - Hydriding and Oxidation – corrosion of the clad
- Impact of MPS Defect on Power Operation

Quantitative analysis of PCI failures for operating PWR using BISON-CASL an important step toward providing 3D fuel performance analysis tool and improved materials models (Sept 2015)