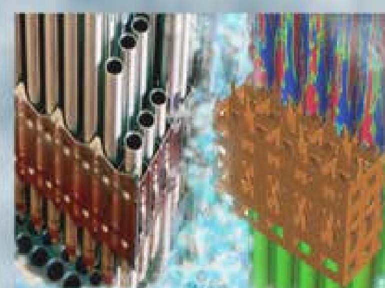
CASL-U-2015-0061-000

CASL: A DOE Energy Innovation Hub – RPI Lahey Seminar, Troy, New York



Douglas B. Kothe, CASL Director
Oak Ridge National Laboratory

February 20, 2013

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2015-0061-000

CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub

Douglas B. Kothe
Oak Ridge National Laboratory
Director, CASL

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CASL

A DOE Energy Innovation Hub in the Office of Nuclear Energy

- First Introduced by Secretary in the President's FY2010 Budget

- A Different Approach
  - "Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges" – *Steven Chu*
  - "Create a research atmosphere with a fierce sense of urgency to deliver solutions." – *Kristina Johnson*
  - Characteristics
    - Leadership – Outstanding, independent, scientific leadership
    - Management – "Light" federal touch
    - Focus – Deliver technologies that can change the U.S. "energy game"

Mission

Provide leading edge modeling and simulation capabilities to improve the performance of currently operating Light Water Reactors

Vision

Predict, with confidence, the performance and assured safety of nuclear reactors, through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly within the U.S. nuclear energy industry

Goals

1. Develop and Effectively Apply Modern Virtual Reactor Technology
2. Provide More Understanding of Safety Margins While Addressing Operational and Design Challenges
3. Engage the Nuclear Energy Community Through Modeling and Simulation
4. Deploy New Partnership and Collaboration Paradigms`

CASL Key Elements

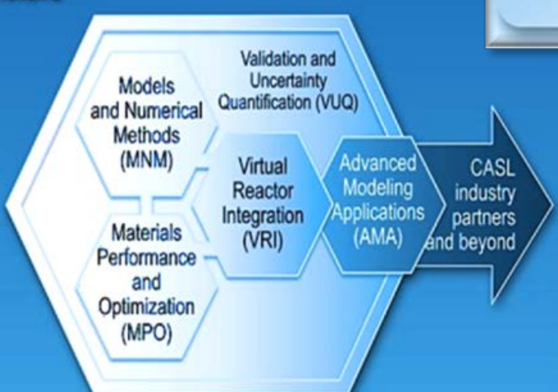
Outstanding team, industry challenges, compelling plan

U.S. team with a remarkable set of assets

- Key nuclear energy vendor, utility, R&D institute
- Leading DOE labs in science, nuclear energy, national security
- Preeminent university nuclear engineering programs
- World leaders in high-performance computing (HPC) and computational science

Executing a compelling and urgent plan

- Predictive simulation with a new virtual reactor
- High-fidelity models for power core phenomena
- A modern and extensible software system
- Validated against Westinghouse-TVA reactors
- Deployed through industry test stands



Tackling tough industry challenges that matter

- Power uprates
- Lifetime extension
- Reduced waste
- Advanced fuels
- Advancing LWR design while assuring safety

DOE Energy Innovation Hubs

Large, highly integrated & collaborative creative teams working to solve problems in areas presenting the most critical barriers to achieving national climate & energy goals

CASL Key Elements

Creative collaboration, fostering innovation, predictive simulation solutions

CASL
Consortium for Advanced Simulation of LWRs

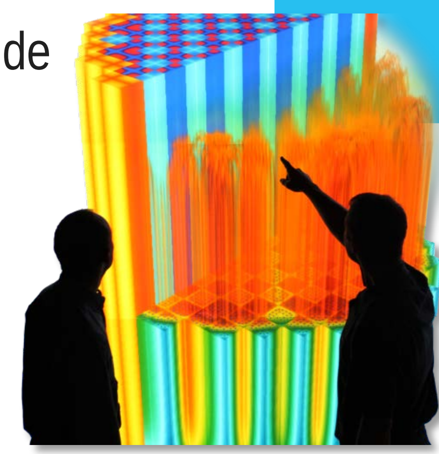
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL is addressing industry needs

- Driven by 3 key issues for nuclear energy:
  - Reducing cost
  - Reducing amount of used nuclear fuel
  - Enhancing safety
- Applying and developing advanced M&S capabilities to create a usable Virtual Reactor environment for predictive simulation of LWRs
- Focused on performance of pressurized water reactor (PWR) core, vessel, and in-vessel components to provide greatest impact within 5 years

CASL advisory groups

Industry Council	• Reviews plans, specifications, and products • Advises on gaps and critical needs • Advises on incremental technology deployment
Science Council	• Provides independent assessments of alignment between scientific work, as planned and executed, and overall goals



Creating a Virtual Reactor

Enable assessment of fuel design, operation, and safety criteria

CASL
Consortium for Advanced Simulation of LWRs

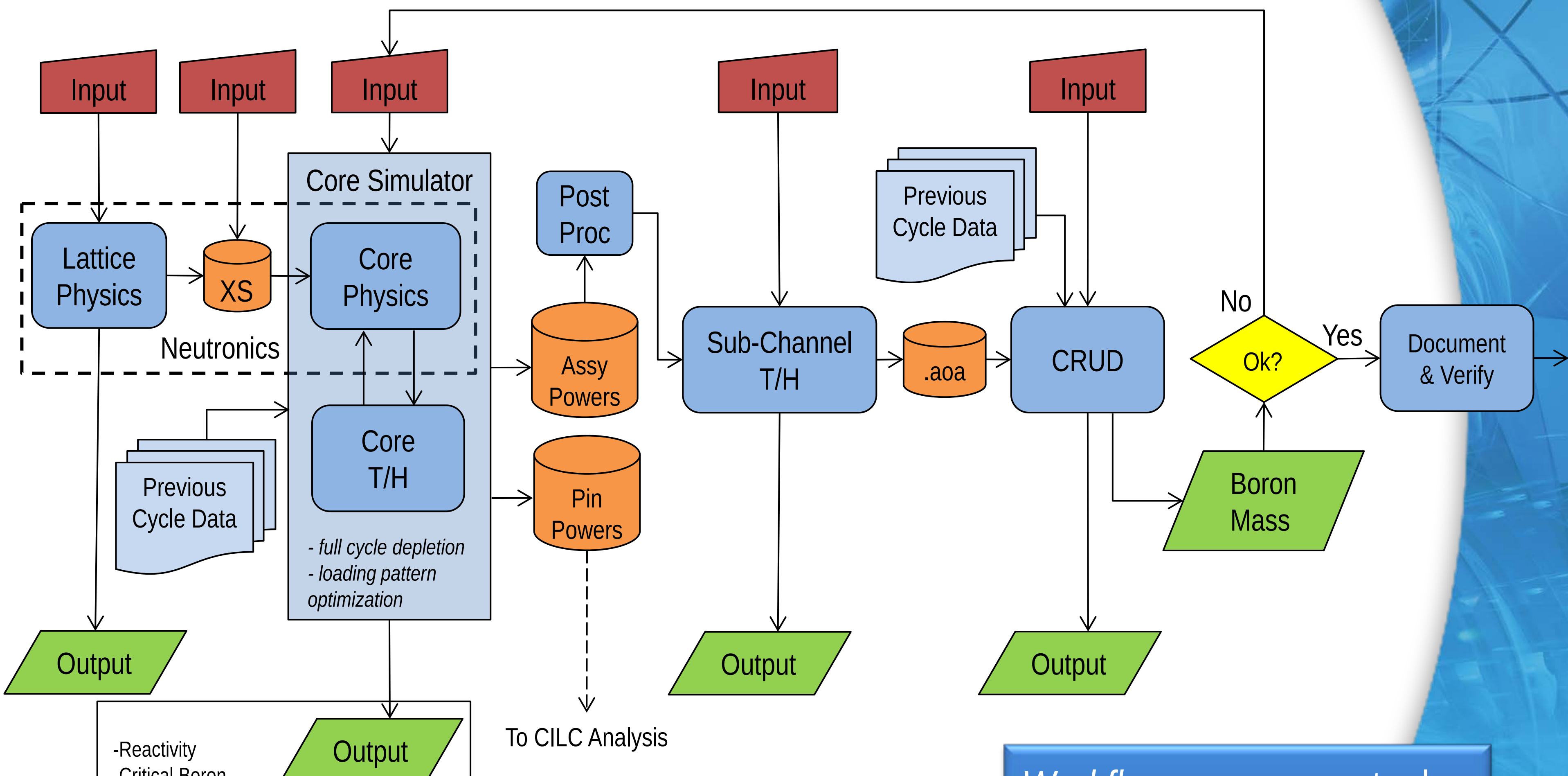
Deliver improved predictive simulation of PWR core, internals, and vessel	• Couple Virtual Reactor (VR) to evolving out-of-vessel simulation capability • Maintain applicability to other nuclear power plant (NPP) types
Execute work in 6 technical focus areas	• Equip VR with necessary physical models and multiphysics integrators • Build VR with a comprehensive, usable, and extensible software system • Validate and assess the VR models with self-consistent quantified uncertainties

MPO	RTM	THM	VUQ	VRI	AMA
Materials performance and optimization	Radiation transport methods	Thermal hydraulics methods	Validation and uncertainty quantification	Virtual reactor integration	Advanced modeling applications

Integrated and interdependent projects span the range from basic science to application

An Example Nuclear Industry M&S Workflow

Crud Induced Power Shift Risk Evaluation



-Reactivity
-Critical Boron
-Critical Control Rod Positions
-Assembly and Rod Powers
-Assembly and Rod Exposures
-Core Coolant Density Distribution
-Core Axial Offset
-Instrument Response
-Neutron Fluence

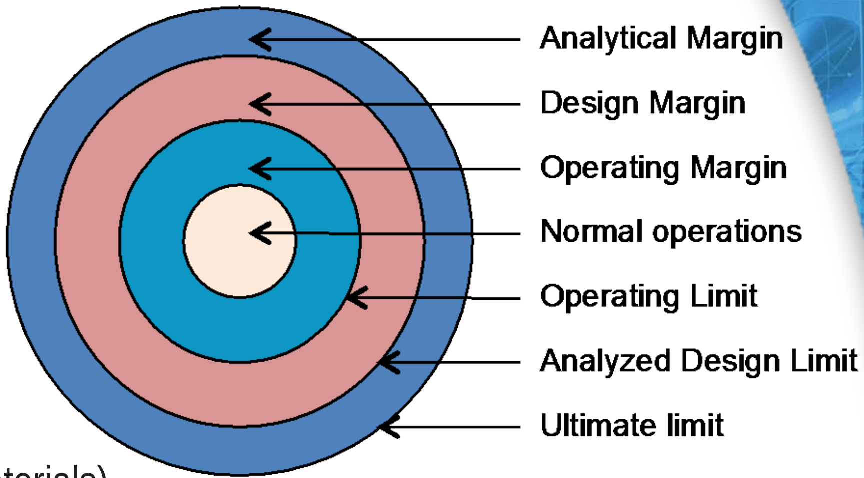
Criteria

Compare calculated Boron mass over entire cycle to a 'low risk' threshold = X lbm Boron

Workflow: processes, tools, and technologies used to take a problem to a solution or a concept to a design

Margin Management

Validated M&S tools can play a key role here



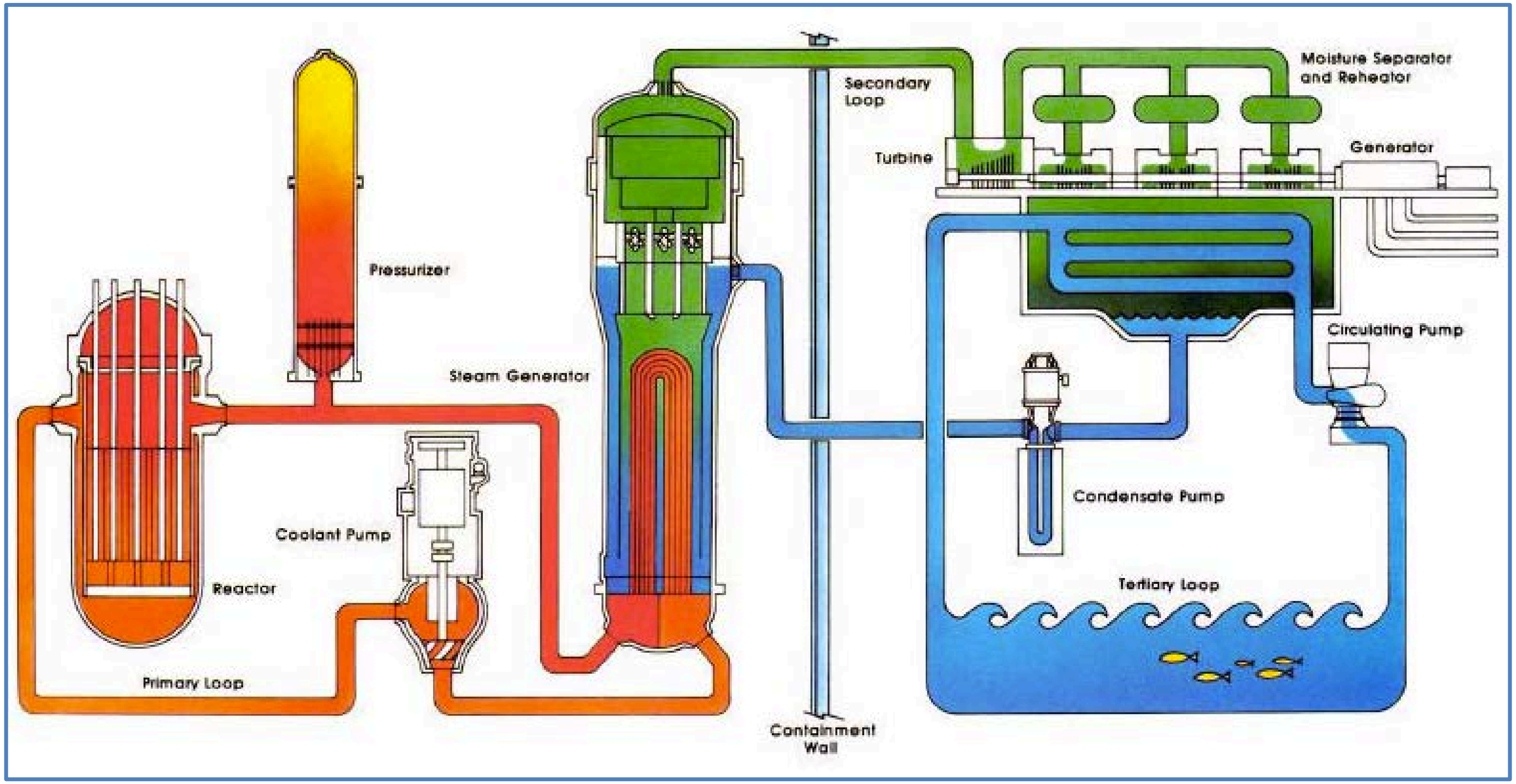
- Requires a strategic approach
  - How much is needed? How to allocate?
  - How can margin be transferred from one bucket to another?
- Key considerations
  - Plant operating parameters & assumptions (plant optimization & flexibility, load follow)
  - Fuel hardware (advanced product features & materials)
  - Design software and methodology (advanced technologies)
  - Core monitoring, In-core fuel management
  - Margins for the unknown or uncertain
  - Reload flexibility
  - Regulatory changes
- Margins can be "recovered"
  - Change in design or operation or testing, reduced safety factor
  - Reduced calculational conservatism (possibly employing advanced analytic tools)
  - Changes to design characteristics of a limiting variable
  - Decrease in the margin of one parameter to increase the margin in another
  - Modification of system or component

Margin trade-offs and evaluation of risks require involvement of many stakeholders within the Utility (Fuels and Plant Operations) and suppliers (BOP, NSSS, T/G, etc.)

One of the strategic targets for the CASL VERA toolkit is to provide enhanced insights in the area of critical reactor margins

Anatomy of a Nuclear Reactor

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)



Power: ~1170 MWe (~3400 MWth)

Core: 11.1' diameter x 12' high, 193 fuel assemblies, 107.7 tons of UO_2

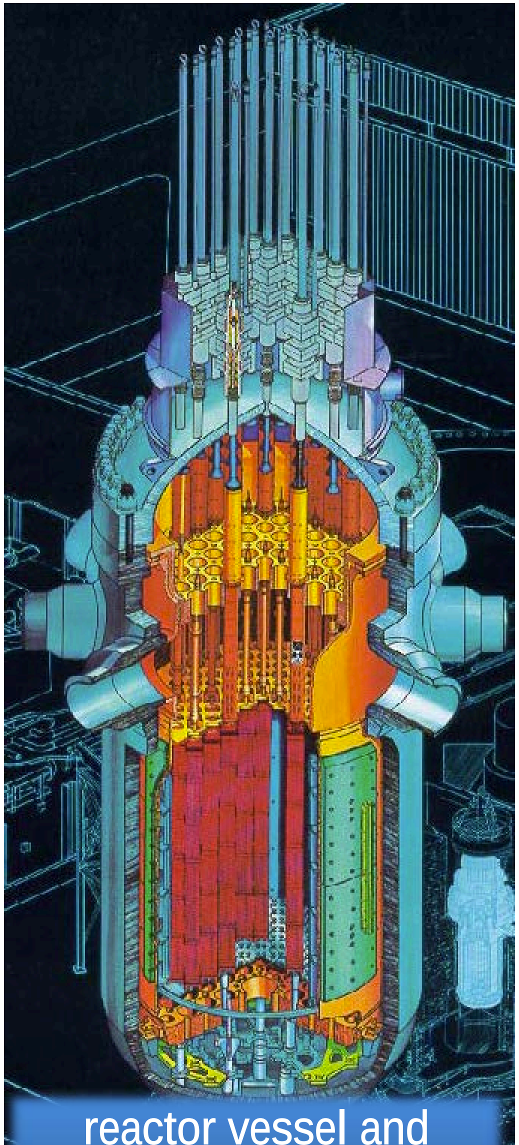
Coolant: pressurized water (2250 psia), T_{in} ~ 545°F, T_{out} ~ 610°F, 134M lb/h (4 pumps)

Pressure Vessel: 14.4' diameter x 41.3' high x 0.72' thick alloy steel

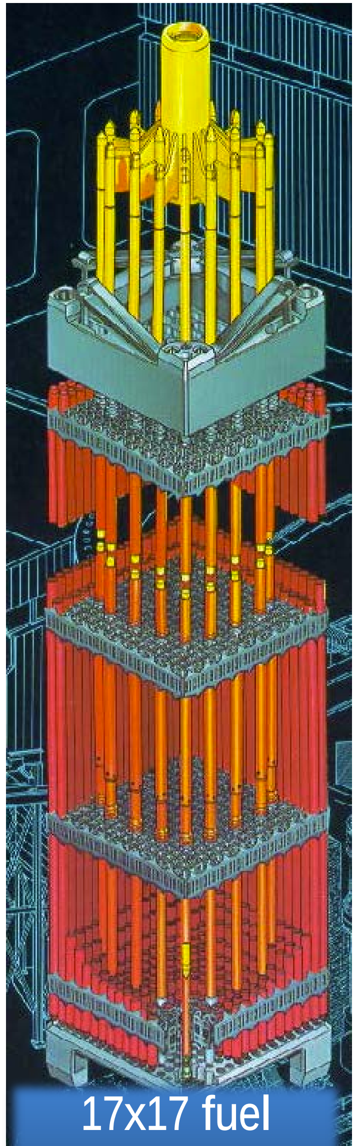
Containment Building: 115' diameter x 156' high steel / concrete

Anatomy of a Nuclear Reactor

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)



reactor vessel and internals



17x17 fuel assembly

Core
- 11.1’ diameter x 12’ high
- 193 fuel assemblies
- 107.7 tons of UO_2 (~3-5% U_{235})

Fuel Assemblies
- 17x17 pin lattice (14.3 mm pitch)
- 204 pins per assembly

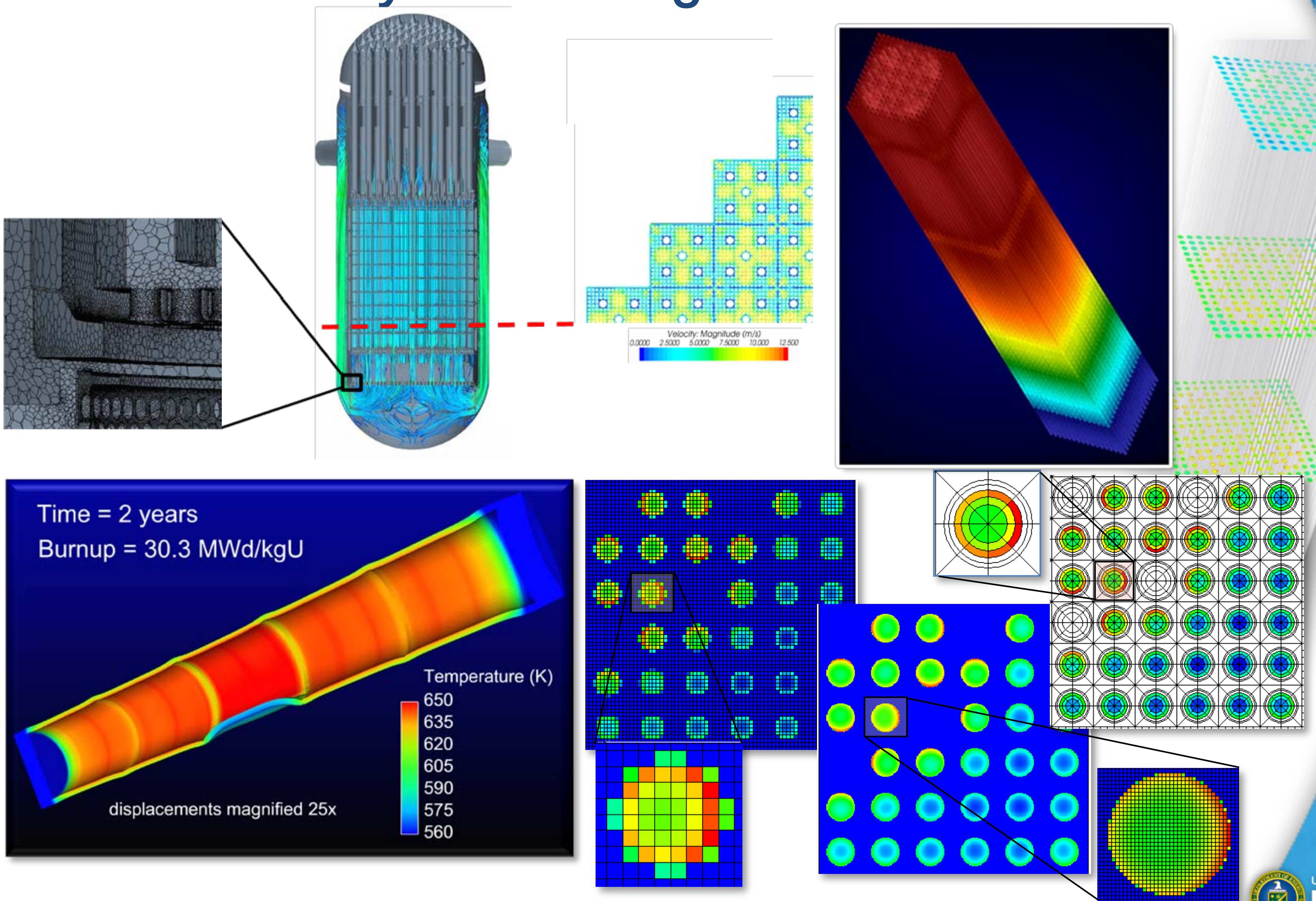
Fuel Pins
- ~300-400 pellets stacked within 12’ high x 0.61 mm thick Zr-4 cladding tube

Fuel Pellets
- 9.29 mm diameter x ~10.0 mm high

Fuel Temperatures
- 4140° F (max centerline)
- 657° F (max clad surface)

~51,000 fuel pins and over 16M fuel pellets in the core of a PWR!

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



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

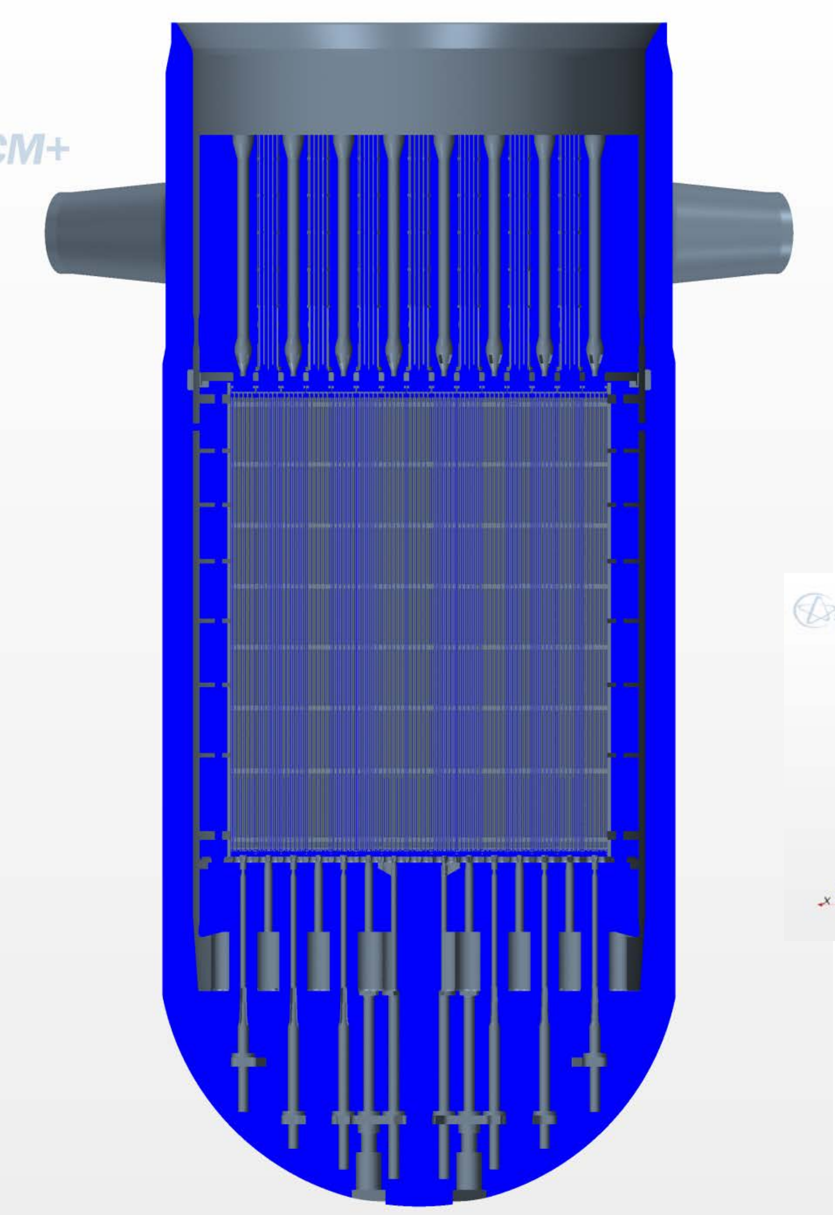
Nuclear Applications Must Support a Wide Range of Spatial and Temporal Scales

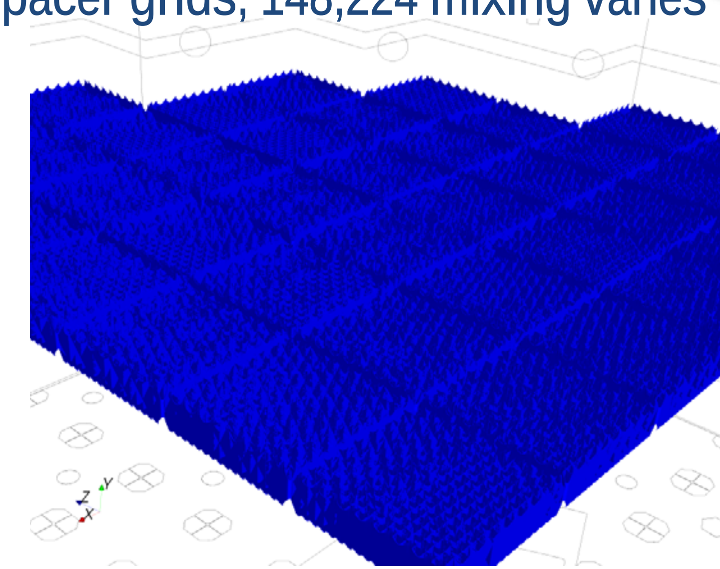
- Nuclear fuel behavior and performance
  - Spatial scale: fuel pellet to fuel pin to fuel sub-assembly (3x3 pins)
    - From dislocations/voids/cracks (< 1 μm) to grains (<100 μm) to clad (<1 mm) to pellet (<5 cm) to pins (<4 m)
- Single-phase thermal hydraulics
  - Spatial scale: fuel sub-assembly (3x3 pins) to fuel assembly (17x17 pins)
    - From mixing vanes (<1 mm) to boundary layers (<1 cm) to turbulent structures (<10 cm) to assemblies (5 m)
- Multi-phase thermal hydraulics
  - Spatial scale: fuel assembly (17x17 pins) to full core (193 assemblies or >51K pins)
    - Same as single phase except now add bubbles (<1 mm to 1 cm) and full core (<10 m)
- Neutron transport
  - Spatial scale: fuel pellet to fuel pin to fuel assembly to full core; also 2D lattice
    - From burnable absorber layers (<1 mm) to pellet (< 1 cm) to lattice (<1 m) to full core (< 10 m)
- Coolant chemistry and CRUD deposition/buildup
  - Spatial scale: fuel pellet to fuel pin to fuel subassembly(?)
    - From oxide/hydride layers (<10 μm) to CRUD layers (< 0.1 mm) to pellets (<5 cm) to pins (<4 m)

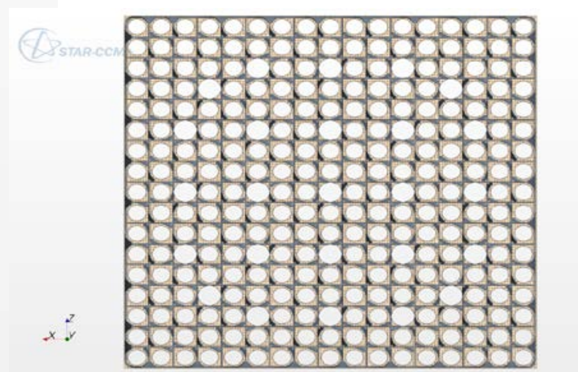
Operational time scales: hours to days to years to decades
Safety time scales: sec to min to hours to days

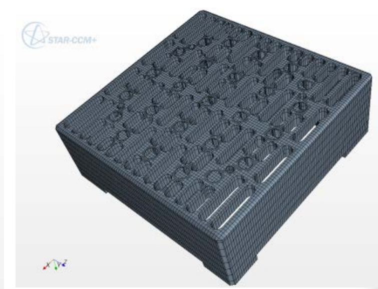
Computational Model of a Quarter Core

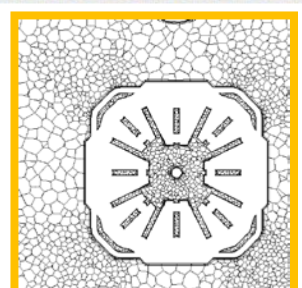
48 fuel assemblies, 13,944 fuel rods, 434 spacer grids, 148,224 mixing vanes



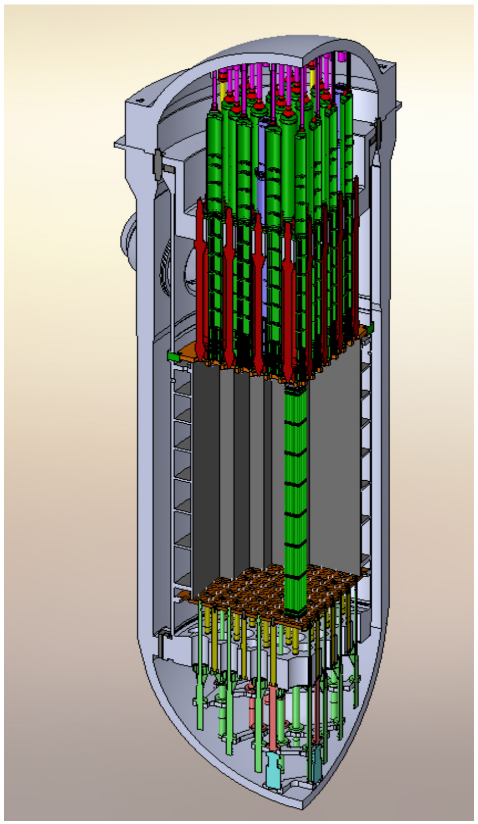




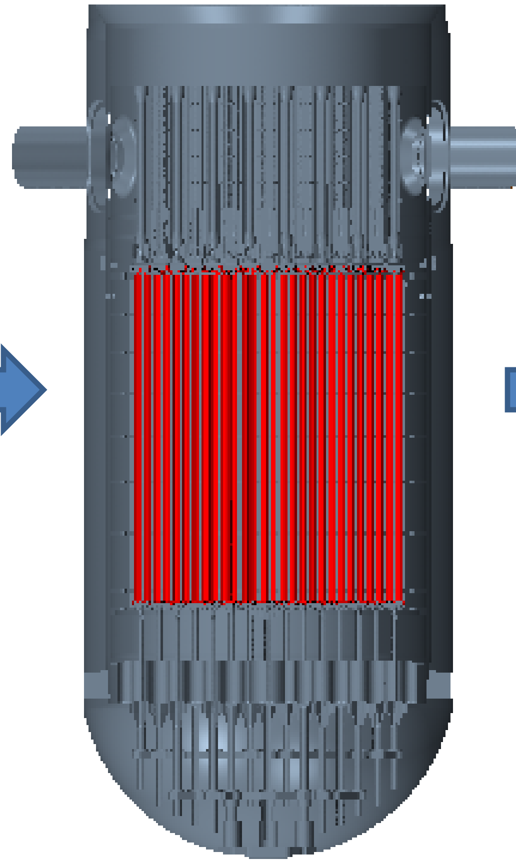




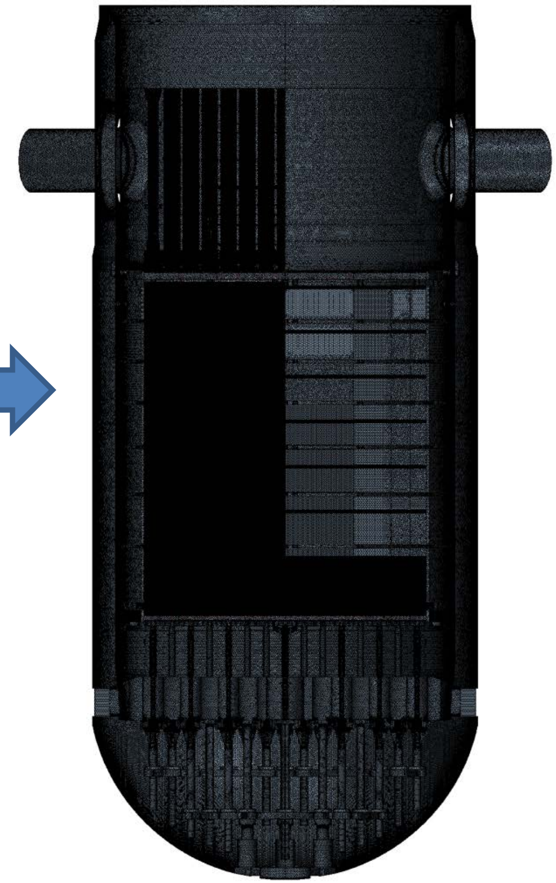
Quarter Core Geometry & Mesh



CAD Model



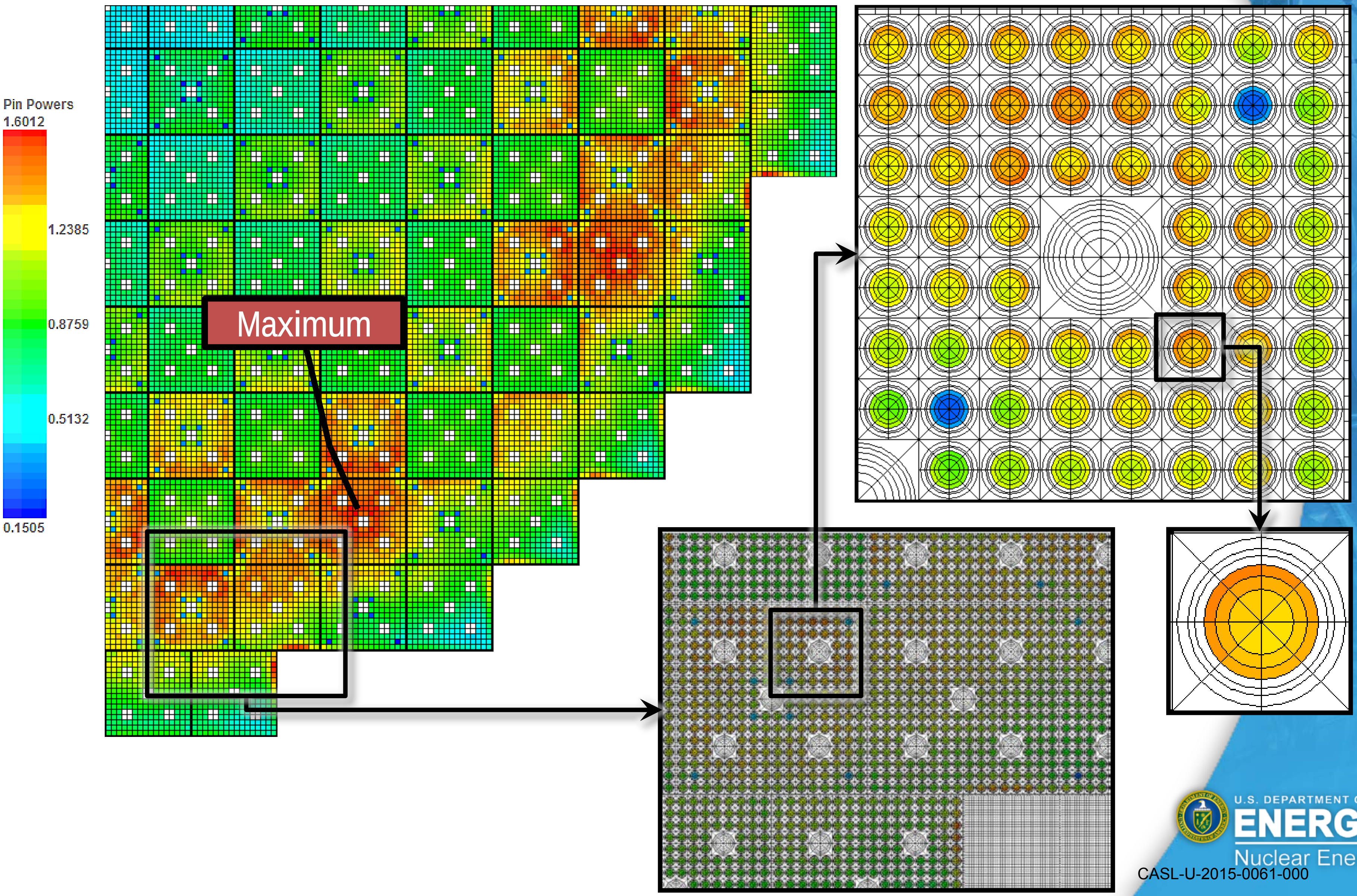
CFD Model



Mesh: 333M cells

Pin-Resolution of Neutron Behavior is Required

Current practice is to construct 3D power distributions with 1D/2D/nodal



CASL Organization

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Nuclear Science and Engineering Directorate
Jeff Binder, Associate Laboratory Director

Science Council
Bill Oberkampf, Chair

Industry Council
John Gaertner, Chair

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Partnerships
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Project Management
Jeff Banta
Finance
Victoria Shope
Legal
Jud Hightower

Technical Focus Areas

MPO
Materials Performance & Optimization
Lead Chris Stanek
Deputy Lead Brian Wirth

VUQ
Validation & Uncertainty Quantification
Lead Jim Stewart
Deputy Lead Mike Pernice

AMA
Advanced Modeling Applications
Lead Jess Gehin
Deputy Lead Zeses Karoutas
Deputy Lead Steve Hess

RTM
Radiation Transport Methods
Lead Bill Martin
Deputy Lead Tom Evans

THM
Thermal Hydraulics Methods
Lead Mark Christon
Deputy Lead Emilio Baglietto

VRI
Virtual Reactor Integration
Lead John Turner
Deputy Lead Randy Summers

Operations Support
Technology Control
Sam Howard
Contracting Authority
Jo Ann Fitzpatrick
Justin Keck
Virtual Office, Community, and Computing (VOCC)
Teresa Robison, A.J. Iurelli, Jamison Daniel
Safety Officer
Jeff Banta
Web Design
Cindy Latham
Information Technology
Ken Barker, Jennifer Tippens
Administrative
Linda Weltman (executive)
Tatia Harris

Stable yet evolving as required

CASL Science Council

Atomic Scientists, 4th Anniversary Reunion, 1946

Guess who at age 4?

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CASL Industry Council

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

Objectives

- 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 FAs

John Gaertner, Chair

Membership and Meetings

- Membership from fuel vendors, design engineering companies, engineering service providers, computer technology companies, and owner/operators of nuclear plants. DOE NE and CASL BOD.
- Meetings are well-attended, spirited, candid, and result in activities that benefit both CASL and members.
- Next meetings: Webcast – February 14, 2013
  Meeting – March 26-27, 2013
  Westinghouse, Cranberry, PA

Recent and Current Activities

- Review VERA Requirements Doc and subsequent revisions –*done*
- Define industry "Analysis Workflow" for VERA compatibility – *done*
- Enhance Website Tech Transfer and information access – *done*
- Identify new utility and SMR members -- *underway*
- Advise on current and future Pilot Studies of VERA.
  - Post-LOCA flow of fibrous material in reactor – *underway*
  - Benchmark of VERA vs current method and data -- *planned*
- Plan for "Test Stands" and applications – *underway*
- Investigate compatibility of VERA with key commercial and proprietary analysis modules – *underway or planned*
- *Investigate documentation, verification and VUQ of VERA --underway*

Membership

AREVA
Global Nuclear Fuels
Westinghouse

mPower*
NuScale*

Dominion*
Duke Energy
Exelon*
EDF
TVA

Bettis
GSE Systems
Rolls Royce
Studsvik Scandpower

ANSYS
IBM
NVIDIA
Cray Computers

EPRI
Battelle

DOE and BOD (ex-officio)

** New members: IC desires SMR vendors and more active nuclear plant owner/operators*

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CASL is in its 6th Plan of Record (PoR-6)

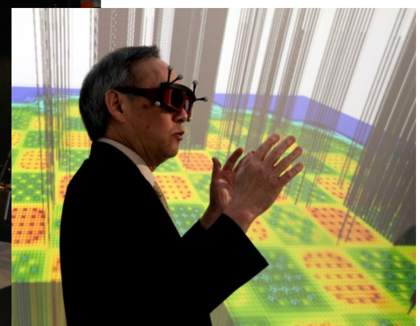
Distinct 6-month periods of planning and execution

Milestone	Oct 2012	Nov 2012	Dec 2012	Jan 2013	Feb 2013	Mar 2013
DOE Reportable Owner: CASL Number:3	CASL.001		CASL.012			CASL.002
L1 Owner: CASL Number: 1			L1:CASL.P5.02			
L2 Owner: FAs Number: 7			L2:VRI.P6.01	L2:VRI.P6.02	L2:CI.P2.05 L2:VRI.P6.03	L2:AMA.P6.01 L2:VRI.P6.04 L2:VUQ.P6.01
L3 Owner: Projects Number: 60	L3:RTM.MCH.P6.04 L3:CI.VOCC.P5.01 L3:THM.CFD.P5.02 L3:THM.CFD.P5.03	L3:VRI.CM.P5.03 L3:VRI.PSS.P6.01	L3:AMA.CHLNG.P5.02 L3:VRI.PSS.P6.02 L3:AMA.VDT.P6.01 L3:MPO.CRUD.P6.01 L3:RTM.PRT.P6.01 L3:PA.P5.03 L3:PA.P5.04 L3:PA.P5.05 L3:VUQ.SAUQ.P5.03 L3:CI.VOCC.P5.04	L3:PM.Metrics.P6.01 L3:EC.P6.01 L3:AMA.APP.P6.01 L3:AMA.VDT.P6.02 L3:EC.P6.02 L3:EC.P6.03 L3:MPO.CLAD.P7.01 L3:PAC.P6.03 L3:THM.CFD.P6.01	L3:VRI.CM.P6.01 L3:VRI.VERA.P6.06 L3:AMA.VDT.P6.03 L3:MPO.FUEL.P6.01 L3:PAC.P6.02 L3:VUQ.VVDA.P5.06	L3:MPO.CLAD.P6.01 L3:MPO.FUEL.P6.03 L3:MPO.GTRF.P6.01 L3:VRI.PSS.P6.03 L3:EC.P6.04 L3:MPO.CLAD.P6.02 L3:RTM.PRT.P6.02 L3:RTM.PRT.P6.03 L3.CI.VOCC.P6.03 L3:AMA.APP.P6.02 L3:AMA.VDT.P6.04 L3:AMA.VDT.P6.05 L3:CI.VOCC.P6.01 L3:CI.VOCC.P6.02 L3:MPO.CORROSION.P6.01 L3:MPO.CRUD.P6.02 L3:MPO.CRUD.P7.02 L3:MPO.FUEL.P6.02 L3:MPO.GTRF.P6.02 L3:THM.CFD.P6.02 L3:THM.CFD.P6.03 L3:THM.CLS.P6.01 L3:THM.CLS.P6.02 L3:THM.CLS.P6.03 L3:THM.CLS.P6.04 L3:PAC.P6.05 L3:VUQ.SAUQ.P6.01 L3:VUQ.SAUQ.P6.02 L3:VUQ.VVDA.P6.01 L3:SLT.SP.P6.01 L3:SLT.MP.P6.01

59 total milestones in PoR-6: 1 Level 1, 7 Level 2, and 51 Level 3 milestones

CASL HQ Visual Venue Overview

The Virtual Office, Community, and Computing (VOCC) laboratory



F-5 Flex System, 3D Immersive Environment with Active Stereo and Tracking

WALDO - 3D, Passive Stereo. Large Object Display Area

3D Mobile Immersive Environment With Active Stereo and Tracking

VOCC Immersion Room

VOCC NET

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How do we all work together?

- CASL's Virtual Office, Community, and Computing (VOCC) Project successfully connected 98 conference attendees from 28 distinct geographic locations, diverse virtual endpoints for the CASL four day science conference. Zero data dropouts or technical difficulties were experienced during this event.
  - IMPACT: Significant cost savings for CASL travel budget. A single virtual event like this can save the program a sizable amount of funds

Roundtable 2012

VOCC NET

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CASL Challenge Problems

Key safety-relevant reactor phenomena that limit performance

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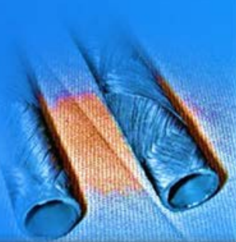
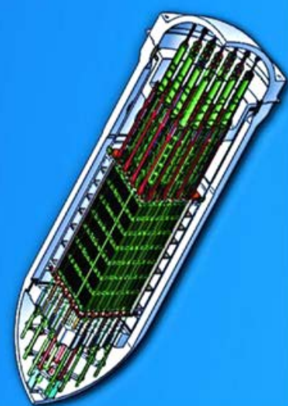
Departure from Nucleate Boiling

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

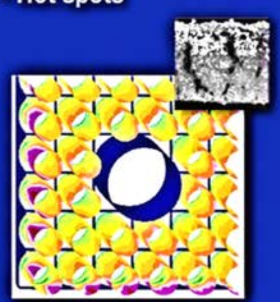


Reactor Vessel and Internals Integrity

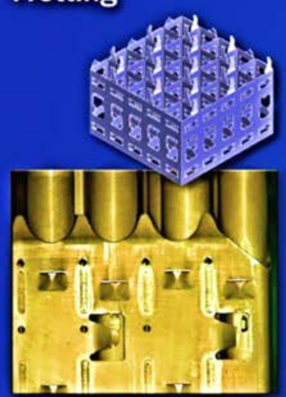


CASL is committed to delivering simulation capabilities for
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

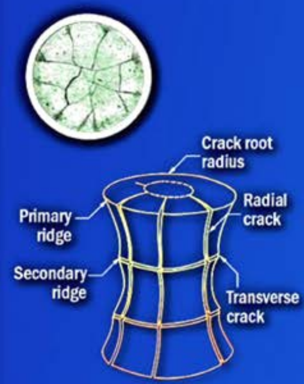
Crud
- Deposition
- Axial offset anomaly
- Hot spots



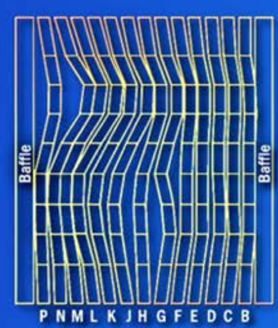
Grid-to-Rod Fretting



Pellet-Clad Interaction



Fuel Assembly Distortion



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Nuclear Energy

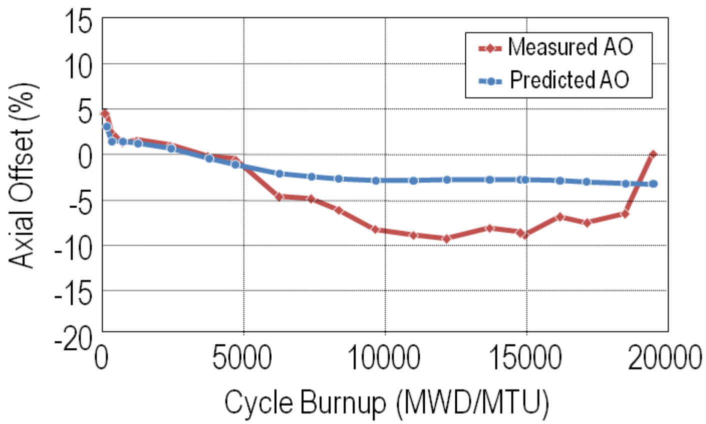
Challenge Problems Directly Support Key Nuclear Industry Drivers

Industry Driver	Industry Driver Performance Measures	Supporting CASL Challenge Problems	Success Metrics for Tangible CASL Support
Power Uprates	• Augment planned U.S. reactor fleet power uprates beyond current value of 2694 MW_e thru 2016 • Increase proportion of stretch (>2%) and extended (>7%) power uprates in U.S reactor fleet	• CRUD, PCI, FAD, GTRF • Cladding Integrity (DNB, LOCA, RIA) • Reactor Integrity (vessel, internals) • Advanced Fuels	• Reduce or eliminate restrictions to uprates associated with current challenge problem • Contribute capability to support one or more license uprate applications
Lifetime Extension	• License remaining ~30% of U.S. reactor fleet to 60 years where appropriate before 2015 • Safely extend lifetimes of U.S. reactor fleet to 80 years where appropriate before 2020	• Reactor Integrity (vessel, internals) • Advanced Fuels	• Provide reliable estimates of reactor environment experienced over lifetime • Contribute capability to support one or more lifetime extension applications
Higher Fuel Burnup	• Increase maximum fuel assembly burnup of 55 GWd/MTU in U.S. reactor fleet • Increase allowable peak fuel rod burnup of 62 GWd/MTU in U.S. reactor fleet	• CRUD, PCI, FAD, DNB, GTRF • Cladding Integrity (LOCA, RIA) • Advanced Fuels	• Provide capability to support increase of average fuel cycle length • Provide capability to support increase NRC fuel burnup limits • Facilitate advanced fuel design
Improved Safety	• Maintain coolable fuel geometry and minimize fuel hydrogen production during/after LOCA • Minimize fuel damage and fission gas release during accidents • Maintain fission product barriers during anticipated accidents	• CRUD, PCI, FAD, DNB, GTRF • Cladding Integrity (LOCA, RIA) • Reactor Integrity (vessel, internals) • Advanced Fuels	• Facilitate advanced fuel design • Improve understanding and quantification of margins

CRUD-induced power shift (CIPS)

Definition of Problem

- High uncertainty in predicting CIPS due to uncertainty in crud source and boiling surface area
- High uncertainty affects fuel management and thermal margin in many plants



Need for Advanced Simulation

- Current tools do not account for crud impact on neutronics and more accurate models needed to evaluate boiling surface area and crud deposits
- ➢ Predict boron feedback in neutronics
- ➢ Predict boiling surface area for each rod in core
- ➢ Predict higher fidelity with improved multi-physics models to predict CIPS

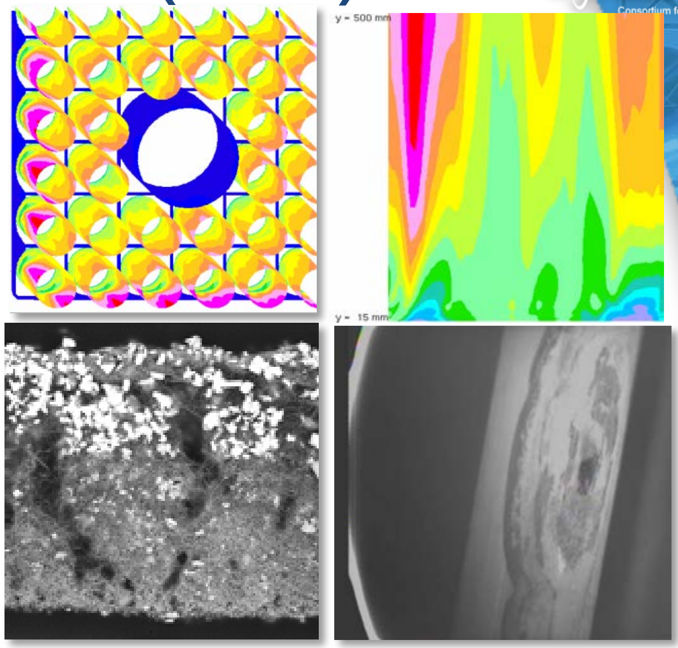
Success Targets

- Develop CASL tools which reduce CIPS prediction uncertainty
- Validate using plants/cycles data
- Provide capability to increase flexibility in incore fuel management

VERA Tools

- Full or quarter core
- MPACT- COBRA - MAMBA (light)

CRUD-induced localized corrosion (CILC)



Definition of Problem

- Hot spots and excessive boiling with high CRUD concentration in coolant can lead to thick CRUD deposits, CRUD Induced Localized Corrosion and fuel leaker
- Not understanding real margin to CILC fuel leakers, limits fuel management for power uprates

Need for Advanced Simulation

- Current tools do not accurately model boiling surface area for all rods in core and crud deposits
- ➢ Predict boiling surface area for each rod in core
- ➢ Utilize CFD to accurately model thermal hydraulic conditions around fuel rods
- ➢ Predict cladding oxidation rate
- ➢ Predict higher fidelity with improved multi-physics models to predict CILC

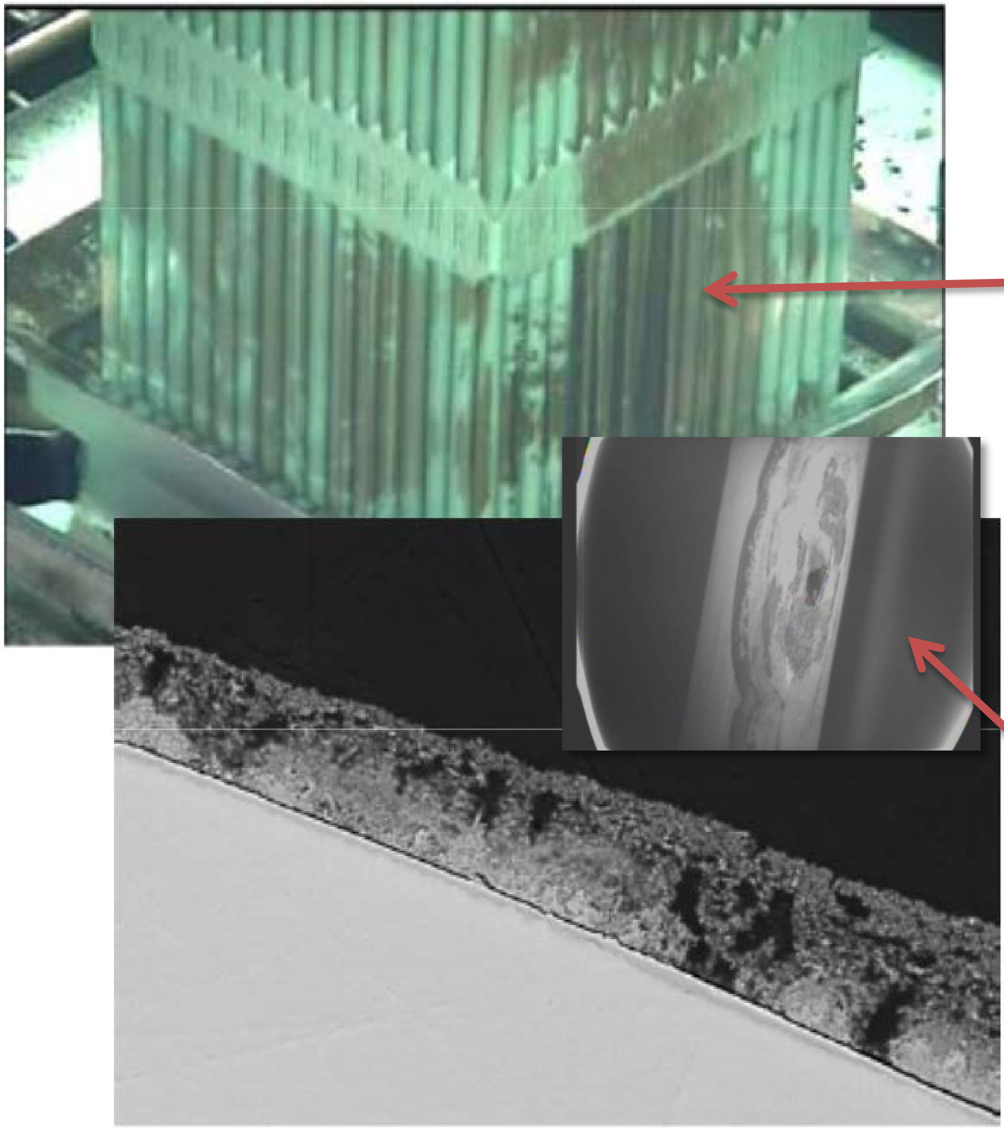
Success Targets

- Develop advanced CRUD tools which reduce CILC prediction uncertainty
- Validate using WALT loop crud test data and plants/cycles with CRUD and CILC leakers
- Provide capability to increase flexibility in incore fuel management

VERA Tools

- Sub-region of core
- MPACT/Denova – Hydra - Peregrine - MAMBA

CRUD: Porous Corrosion Product Deposition



Problem Definition

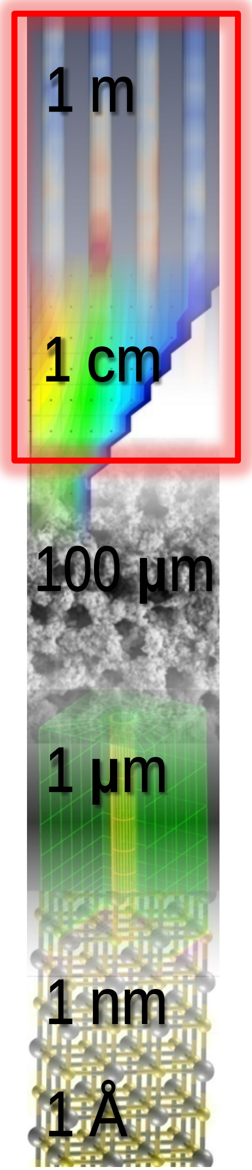
- Reactor internals corrode, releasing products into coolant
- Sub-cooled boiling creates porous deposits
- Boric acid in coolant hides out in CRUD pores

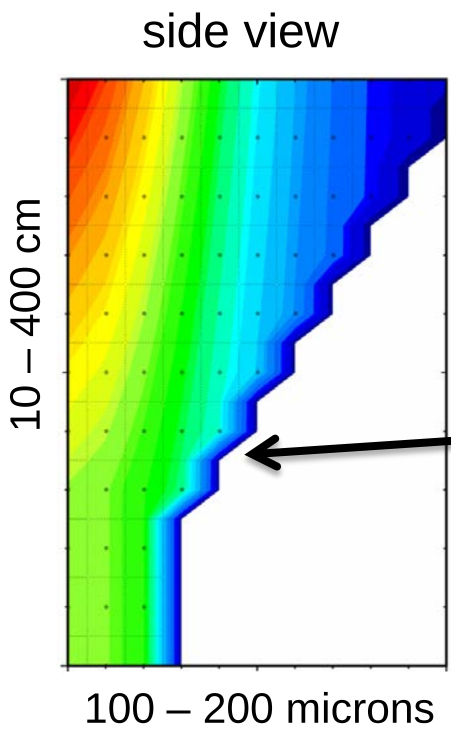
Effects on Plant

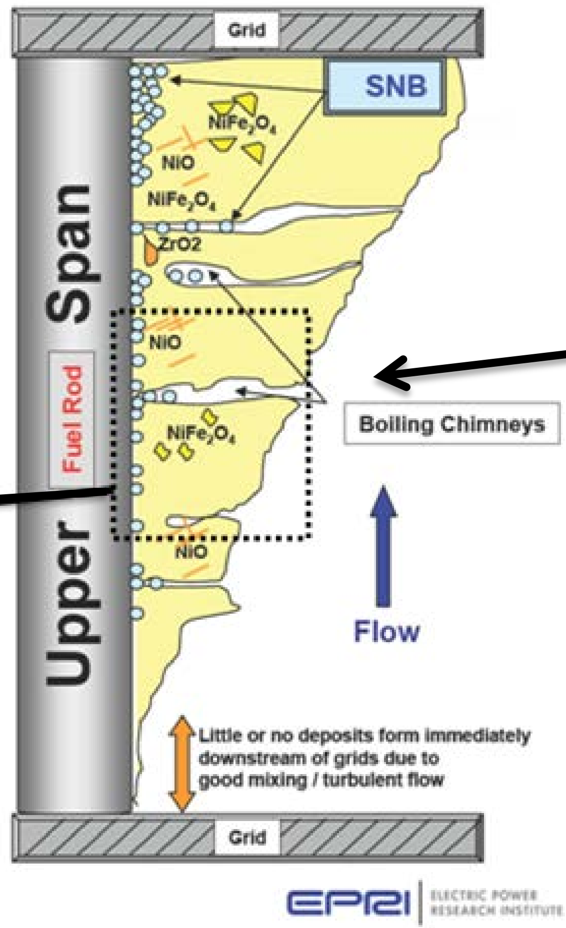
- CRUD-Induced <u>Power Shift</u> (CIPS) due to boron
- CRUD-Induced <u>Localized Corrosion</u> (CILC) due to degraded heat transfer
- <u>Increased worker dose</u> due to CRUD activation

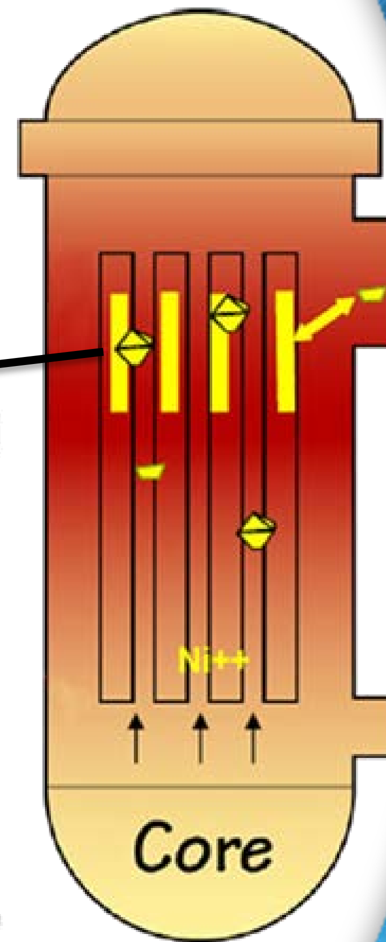
<u>Images:</u> D. Wells. "EPRI Chemistry and Radiation Management PWR Primary Water Chemistry Guidelines Revision Project Updates – Optimized Fuel Crud and SRMP Revision." EPRI P-TAC Summer Meeting, Atlanta, GA, 8/29/2012.

Engineering Scale: MAMBA Framework









– MPO Advanced Materials/Boron Analyzer

– Examines CRUD buildup on upper spans of core

- Node size: ~1cm x ~10µm (pancake shaped)

Coolant Chemistry and CRUD Growth

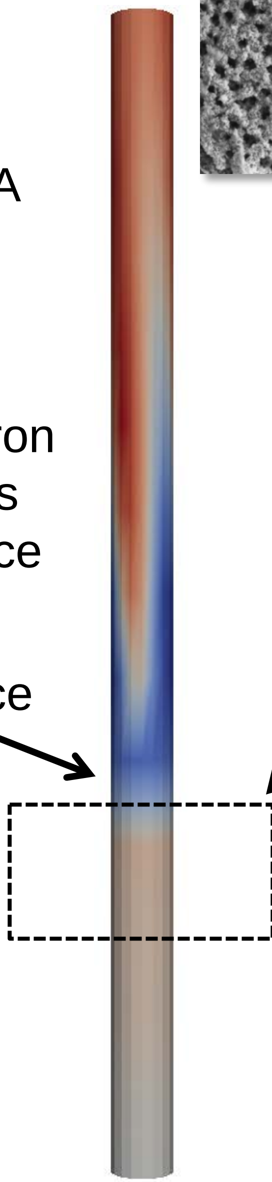
Thermal hydraulics + transport + fuel performance + chemistry + structural mechanics

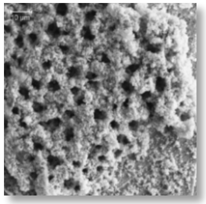
Boron concentration within crud layer (colored contours) grown within MAMBA over 60 days of operation

Variations in crud thickness and boron due to T variations on cladding surface

Reduced crud and boron due to turbulence behind mixing vanes

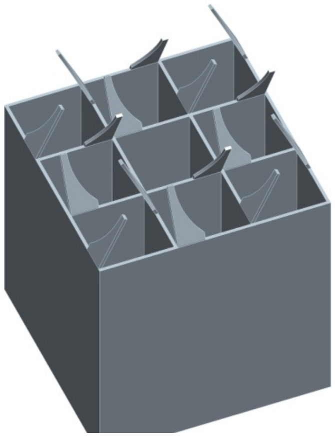
80 cm section of fuel rod

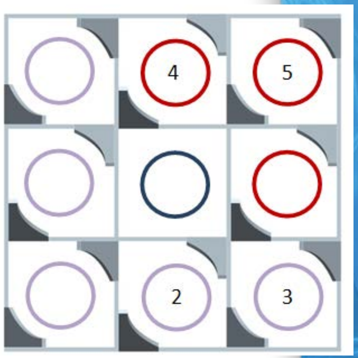




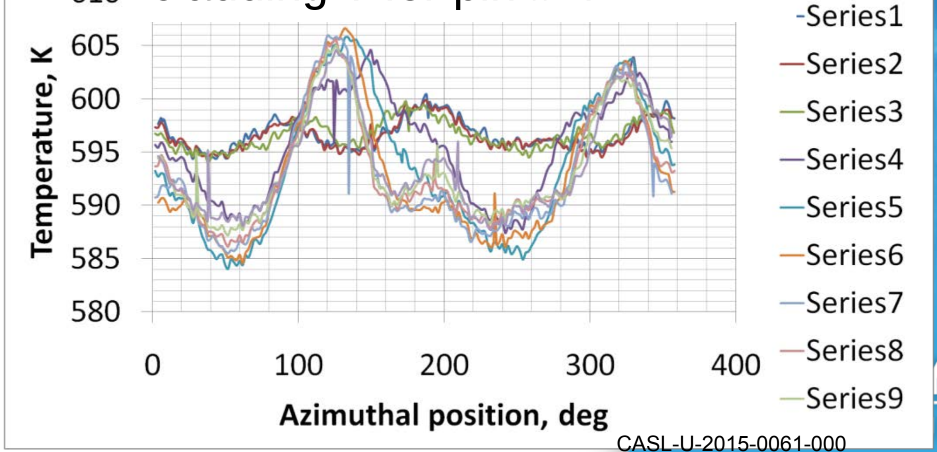
Large azimuthal variation in fluid/cladding temperature computed

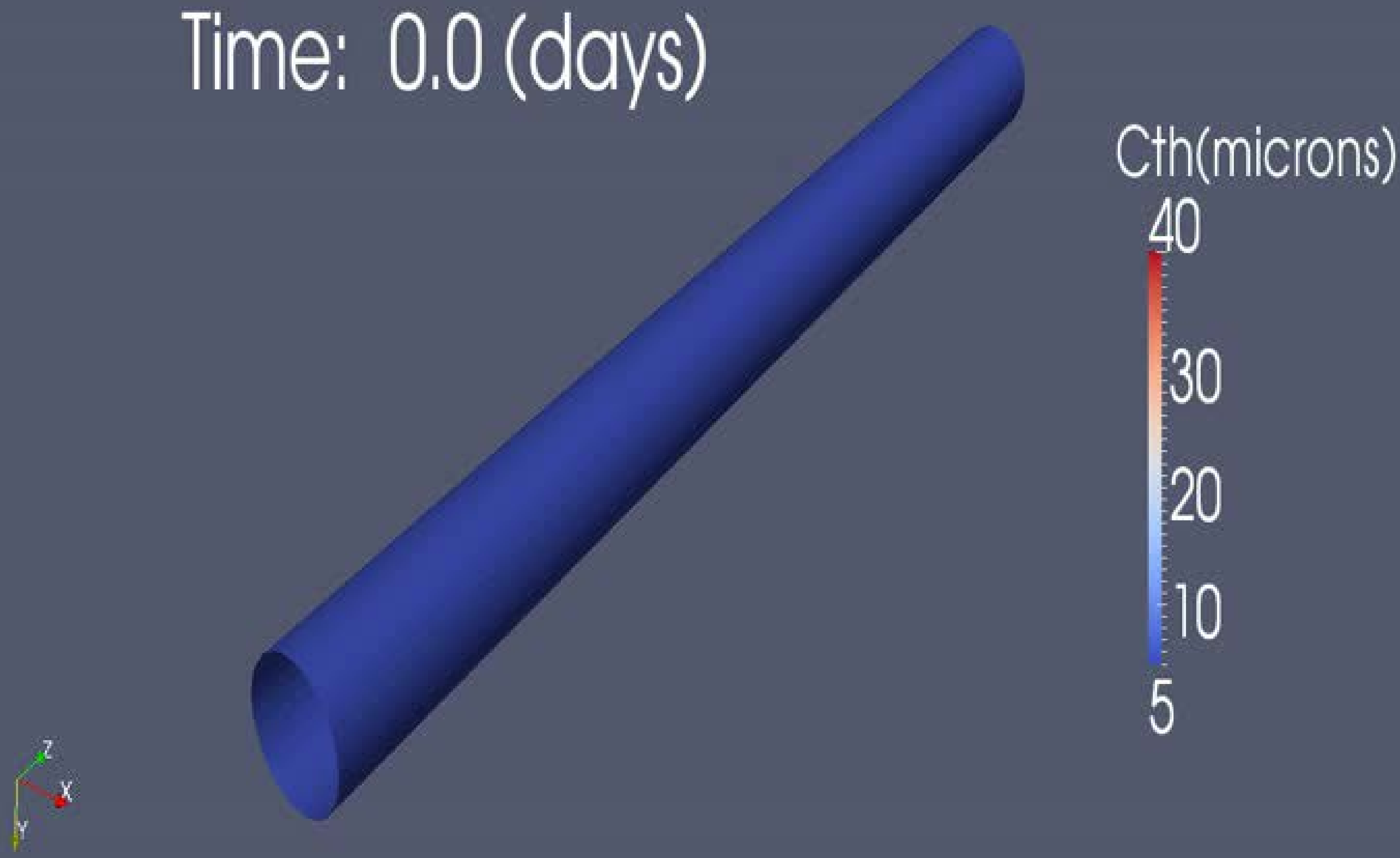
Spacer with mixing vanes





CFD computed cladding T for pin # 4



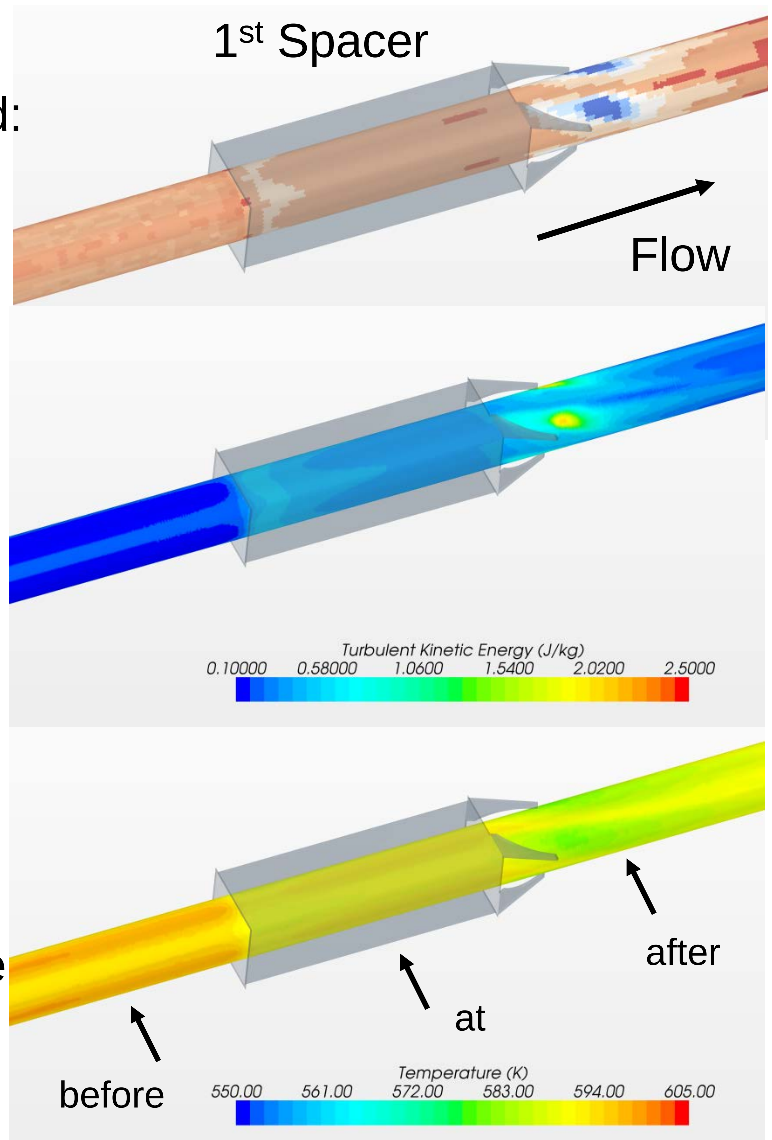

Time: 0.0 (days)
Cth(microns)
40
30
20
10
5
Z
X
Y

Positive Feedback between CRUD growth and CFD

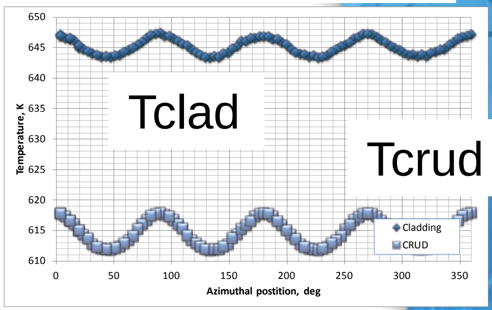
Chemistry computed:
Crud Thermal
Resistance

CFD computed:
Turbulent Kinetic
Energy

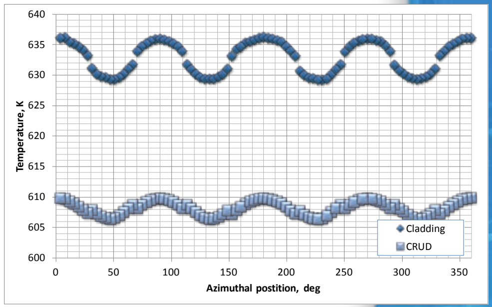
Fuel computed:
Cladding Temperature



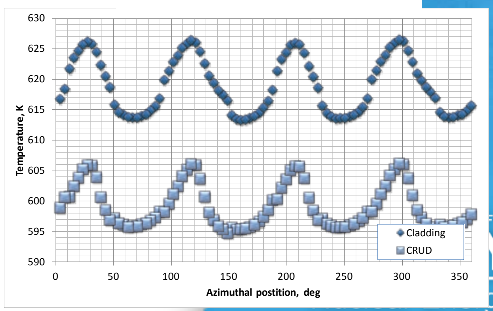
Before Spacer



At Spacer

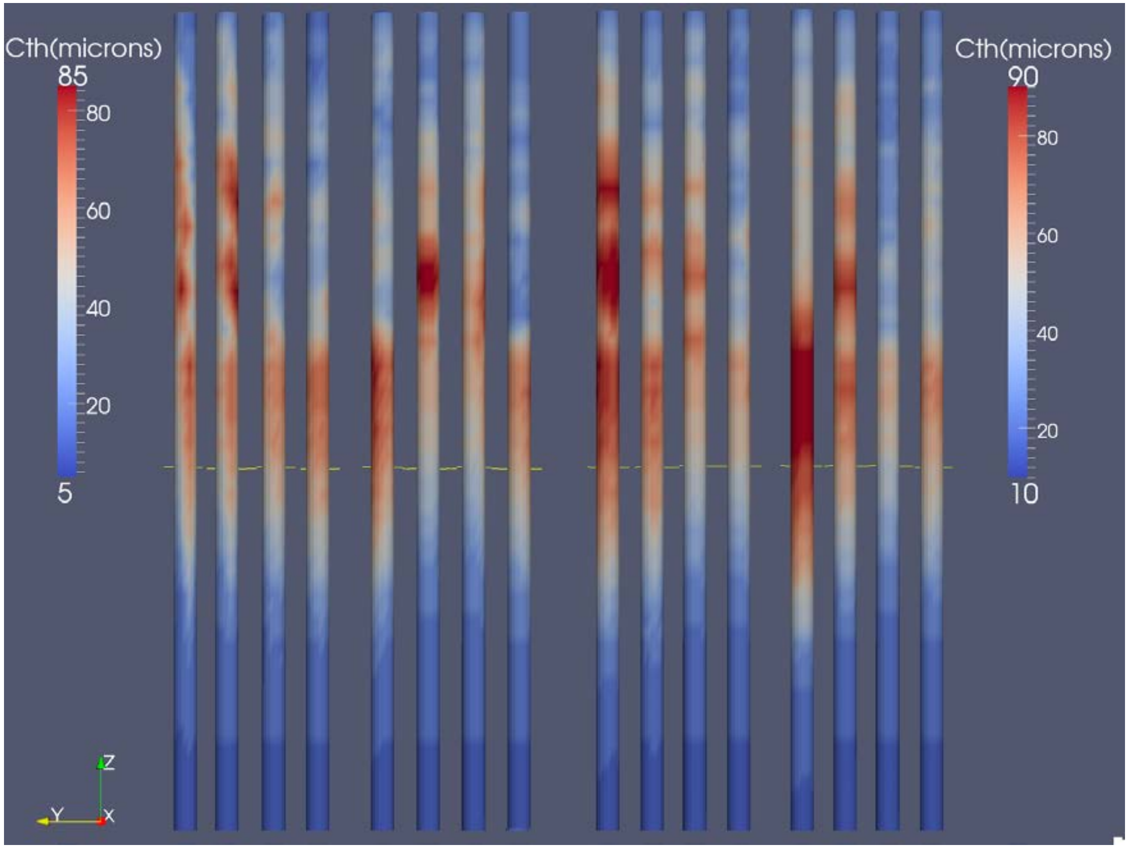


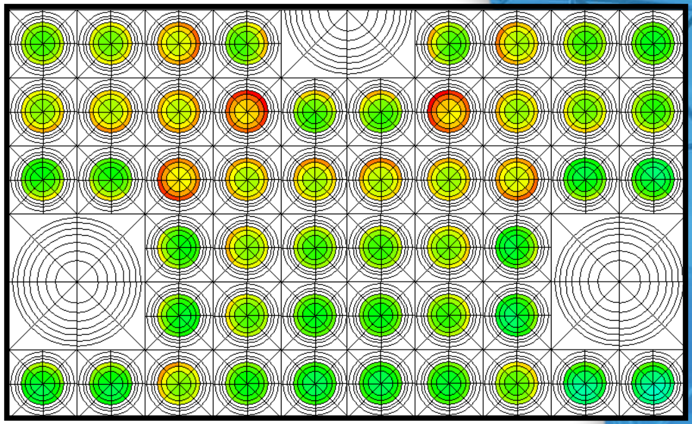
After Spacer

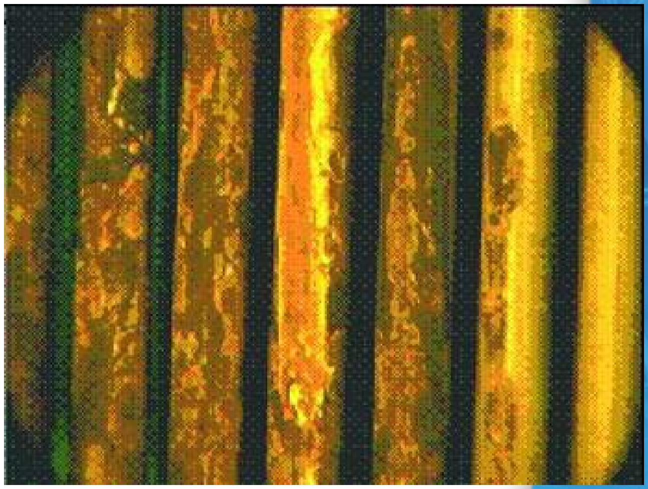


Extension to 4x4 Subassembly:

Qualitative Comparison to CRUD Formations





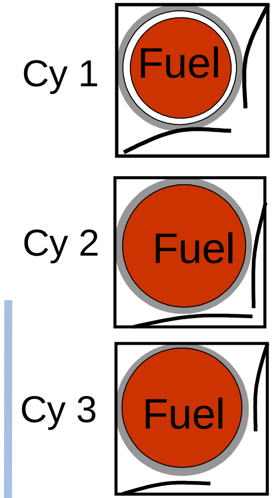


Quantitative benchmarking to industry code benchmarks and experimental data currently underway

Grid To Rod Fretting (GTRF)

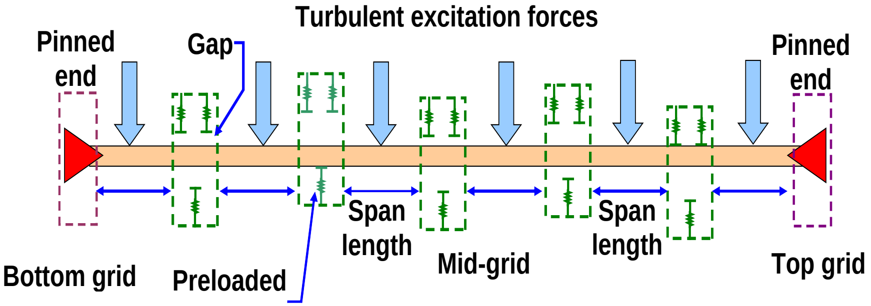
Definition of Problem

- Clad failure can occur as a result or rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation
- Good progress made in improving grid designs; however, rod vibration & wear still occurs next to core shroud in some plants
- Power uprates and burnup increase potential for grid to rod fretting



Need for Advanced Simulation

- Current tools do not predict rod wear margin in core
- ➢ Predict grid to rod gap
- ➢ Predict turbulent flow excitation by CFD
- ➢ Predict rod vibration & wear at any location in core



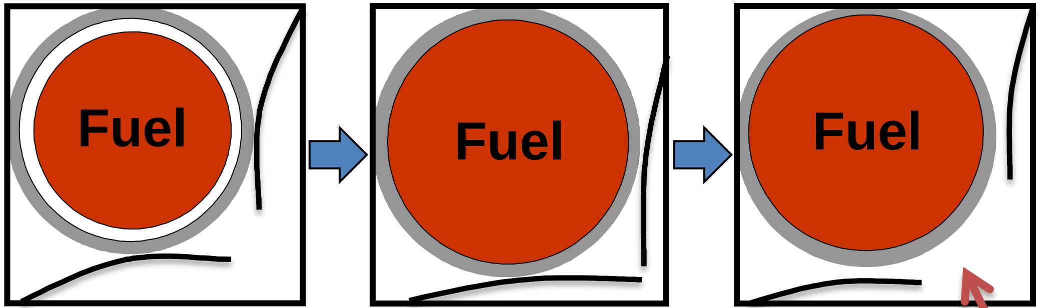
Success Targets

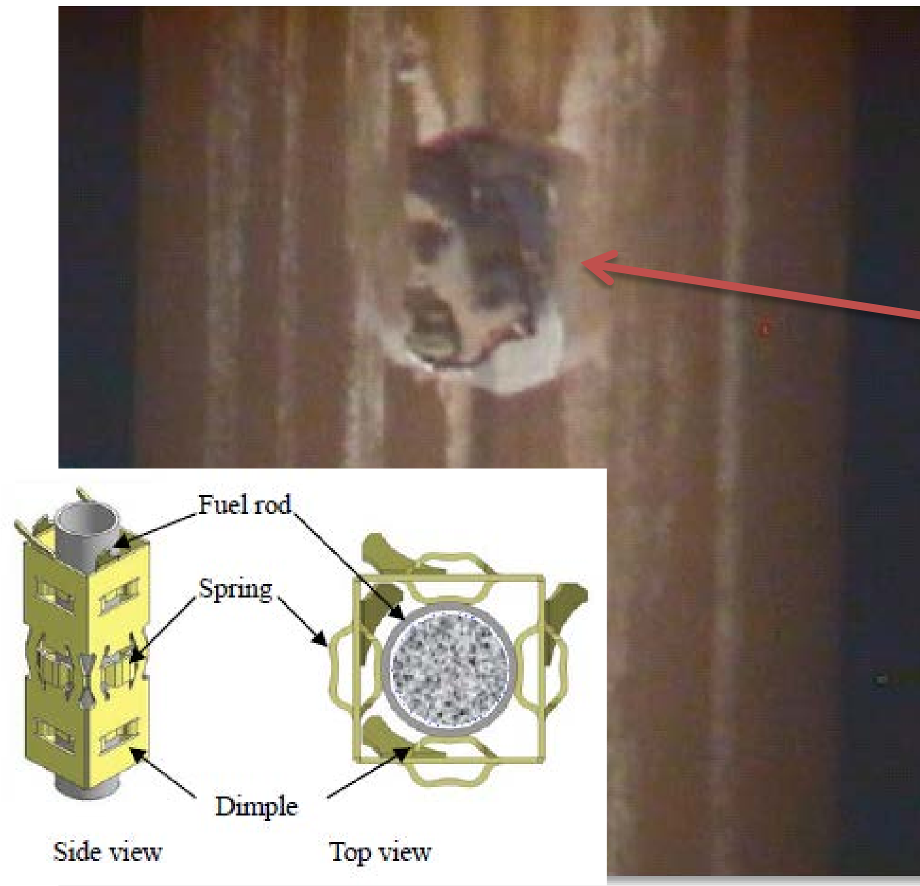
- Develop CASL capability to predict rod wear for any rod in core
- Validate tools using experimental data and plant data
- Provide capability to evaluate impact of spacer grid design features effect on GTRF

VERA Tools

- Sub-assembly of core
- Methodology still evolving
- MPACT - Hydra – Peregrine – Salinas? - ???

GTRF: Grid-to-Rod Fretting





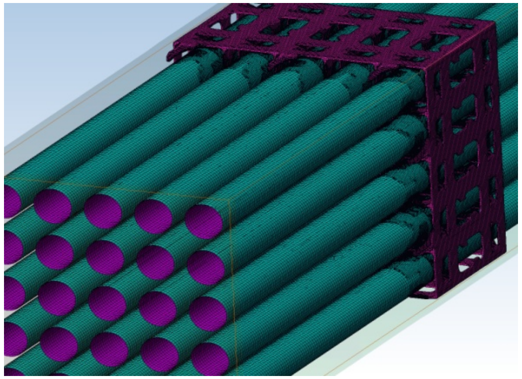
Problem Definition

- Flow turbulence induces fuel rod vibrations
- Radiation & creep cause fuel & spacer to separate
- Vibrations cause rapid wear on fuel rods
- Grid springs relax over time

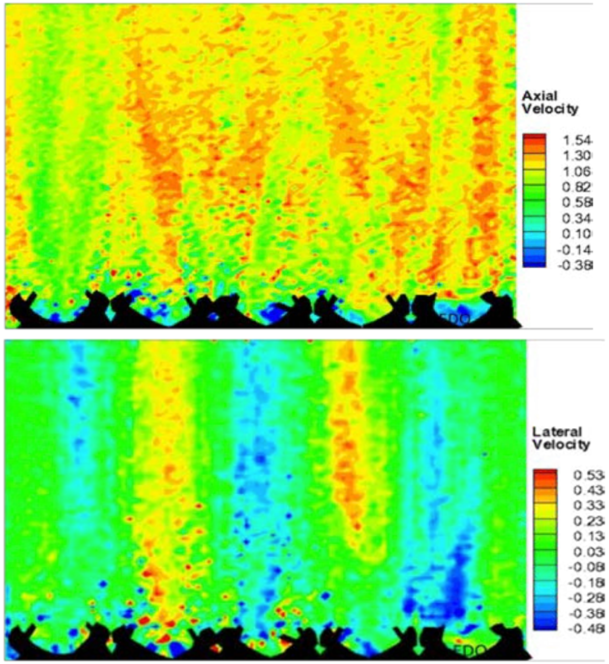
Effects on Plant

- Rapid fuel failure at fretting contact point
- Release of wear debris into coolant
- Sets limits on coolant flow rate
- Requires more grid spacers, can increase core pressure drop

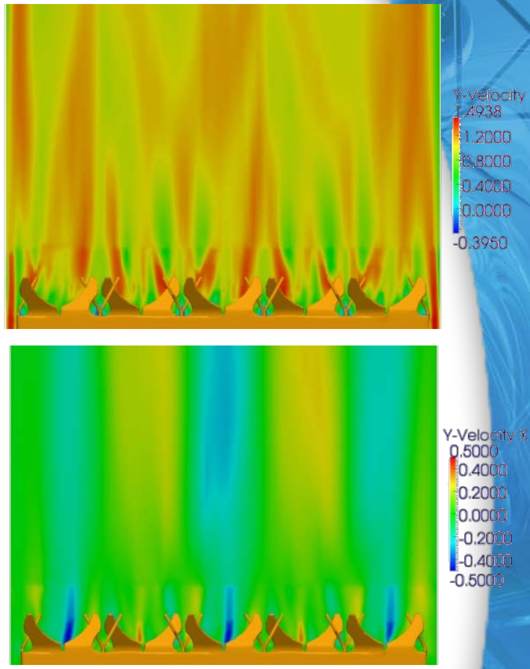
5x5 V5H study shows good agreement with experimental data



- Re = 28,000
- Predicted mean peak velocities within 5% of experiments

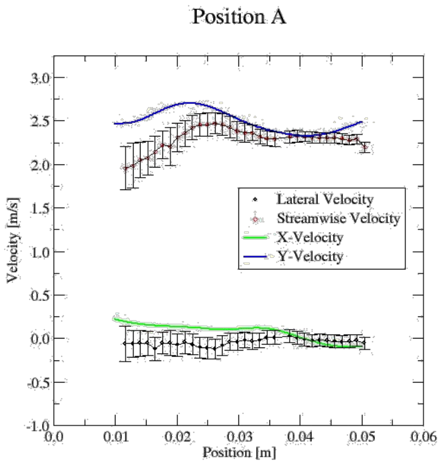


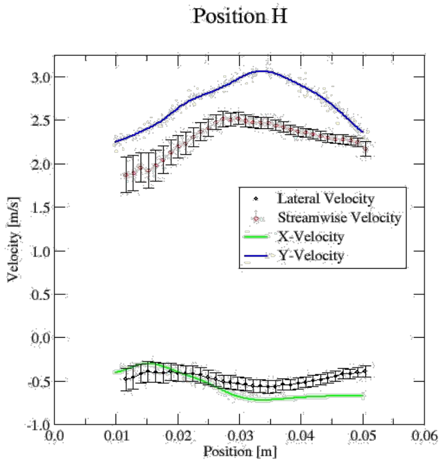
Texas A&M experiments

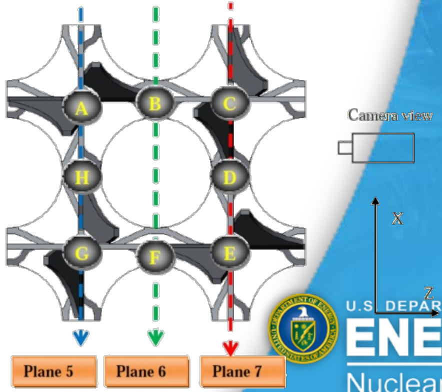


Hydra-TH calculations

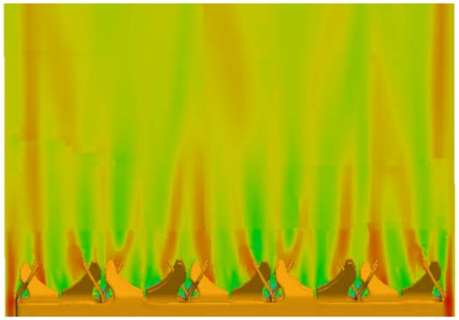
- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)



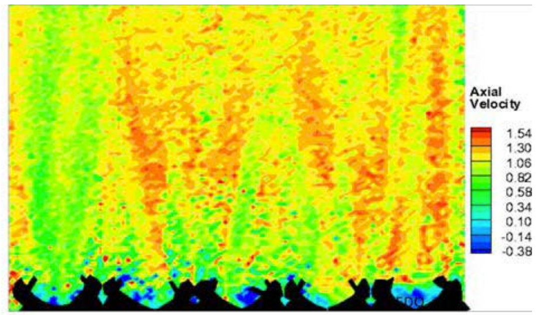




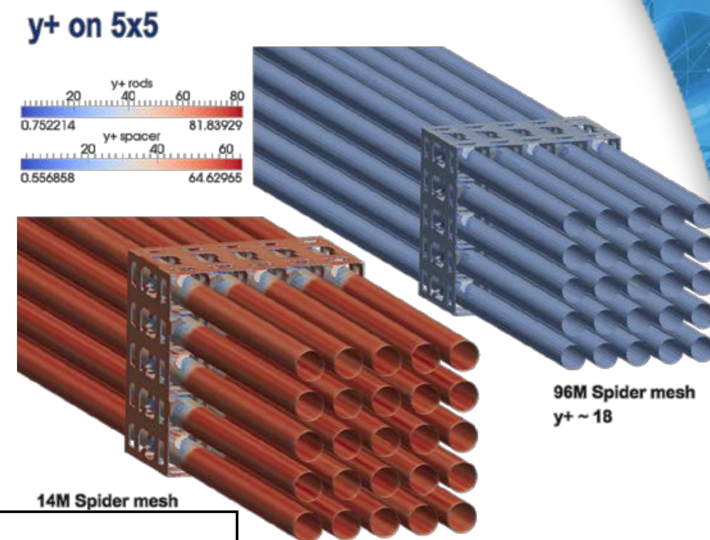
Turbulent Flow in a 5x5 Rod Bundle



Hydra-TH

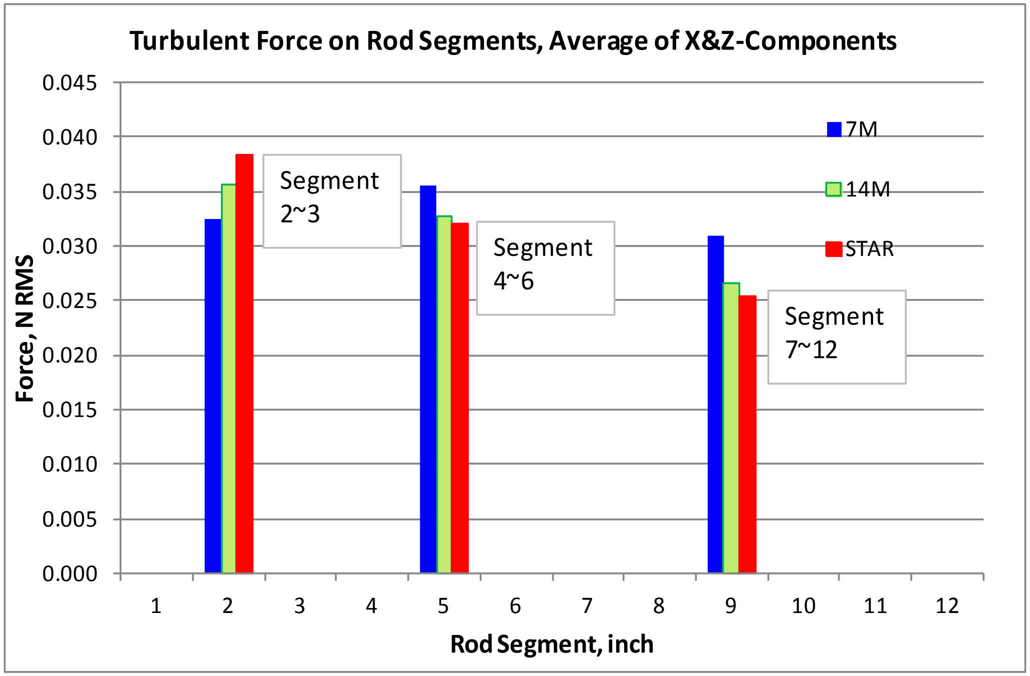


TAMU Experiment

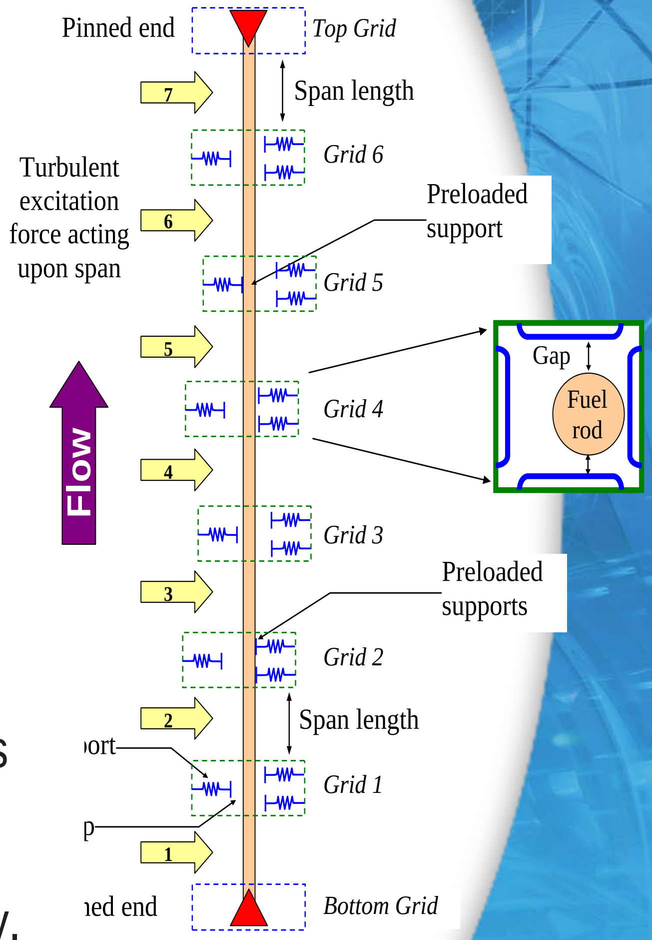


Helicity Contours

Coupling Computed Fluid Turbulent Forces to Fuel Rod Vibration Model



- Three lumped forces are used to replace the forces calculated at every one inch segment along each span. It is assumed that the lumped forces are not correlated to each other in the time domain.
- VITRAN (Westinghouse tool) is used in this feasibility study. The fuel rod model has six support grids . For each span, the three lumped RMS forces are applied. The magnitude of each RMS lumped force is the average lumped force of the X and Z-components.

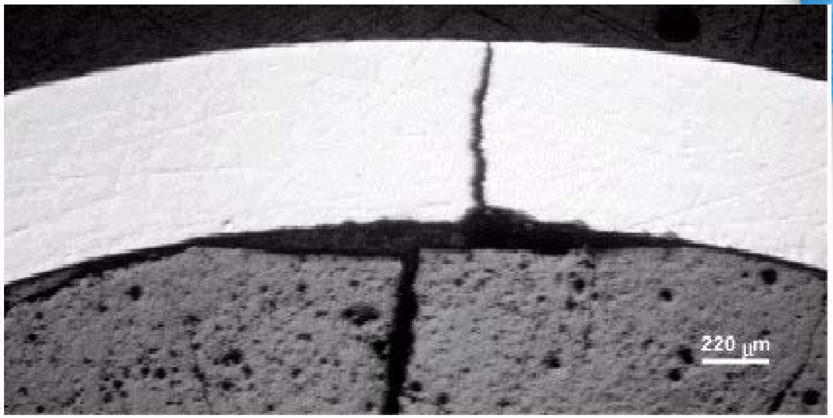


CASL-U-2015-0061-000

Pellet Clad Interaction (PCI)

Definition of Problem

- Cladding "creeps down onto pellets after about one cycle of operation. During power maneuvers, pellet expands and creates stresses against cladding
- Pellet imperfections such as Missing Pellet Surface (MPS) increase local stresses resulting in clad failure



Need for Advanced Simulation

- Current fuel rod performance tools do not model fuel rod in sufficient detail and are not linked to neutronics and TH
  - ➢ Develop 3D FEA advanced fuel rod tool to properly model PCI (Peregrine)
  - ➢ Couple fuel rod tool to neutronics & TH and apply for core wide analyses to evaluate PCI margin

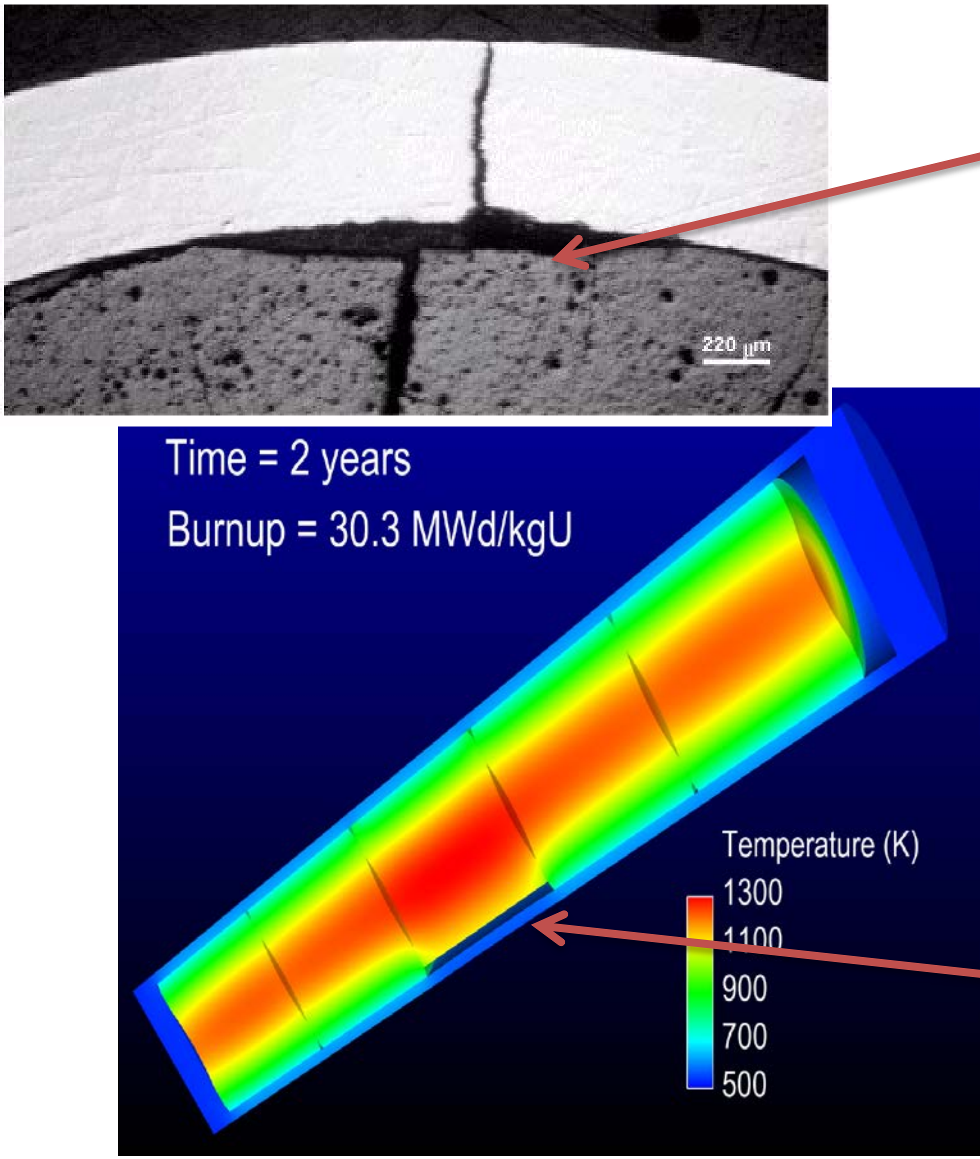
Success Targets

- Develop CASL capability to model 3D fuel rod performance and PCI margin
- Validate tools using available fuel rod performance data and plant data with PCI failures
- Provide capability to increase flexibility of power maneuvering of the plant

VERA Tools

- Sub-region of core
- MPACT/Denovo - Hydra - Peregrine

PCI: Pellet-Clad Interaction



Problem Definition

- Missing pellet surfaces sometimes exist on fuel
- Corrosive fission products generated during operation
- Fuel-clad contact causes localized temperature changes

Effects on Plant

- Missing pellet surface induces localized clad stresses, causing cracks
- Iodine stress corrosion cracking (SCC) of clad
- Clad can form brittle hydrides under temperature gradients

Departure from Nucleate Boiling (DNB)

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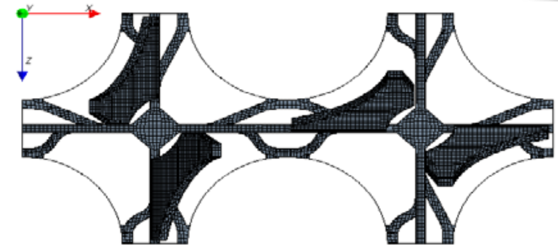
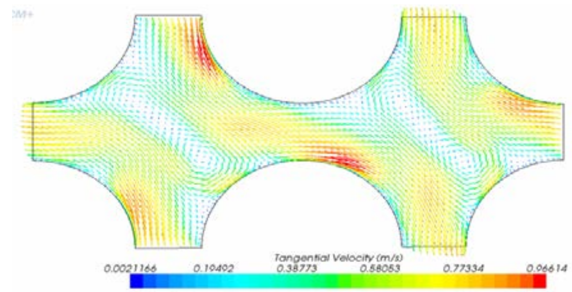
Definition of Problem

- Local clad surface dryout causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures
- Detailed flow patterns and mixing not explicitly modeled in single & two-phase flow downstream of spacer grids
- Simplified pin modeling and steady-state developed DNB correlations used in DNB transients result in loss of DNB margin
- Power uprates require improved quantification and increased margins for DNB





Need for Advanced Simulation

- Current tools do not model detailed flow patterns and mixing downstream of mixing grids and simplified models used in DNB transients

➢ Develop improved mixing method downstream of mixing grids using CFD tools for single and two-phase flow.

➢ Develop detailed coupled pin-resolved radiation transport models for application to DNB transients

Success Targets

- Develop CASL capability to predict DNB utilizing more advanced methods to reduce margin and enhance understanding
- Validate tools to available mixing and DNB data
- Provide capability to evaluate impact of spacer grid design features effect on DNB

VERA Tools

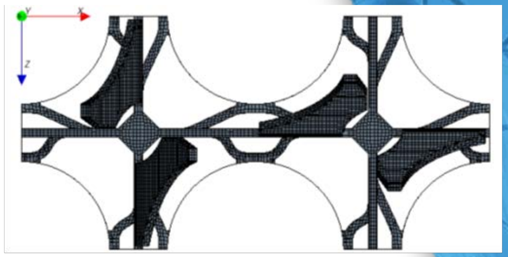
- Plan just being initiated
- MPACT – COBRA/Hydra – Peregrine - RELAP

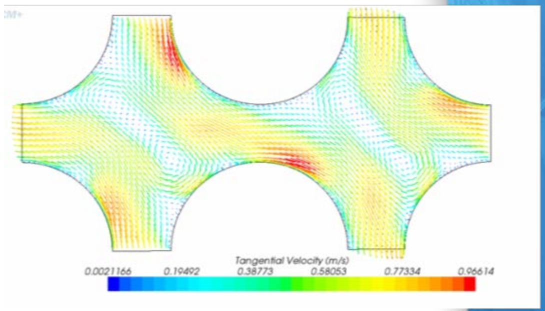
DNB Relevant Experimental Data Collection & Modeling

Description, Linkages, Completion Criteria

- Collect rod bundle DNB test data for CASL and develop models using CASL thermal-hydraulic codes for DNB-related predictions by March 29, 2013

- Milestone Linkages
  - COBRA-TF Integration
  - Hydra Demonstration and Testing
- Completion Criteria
  - Report documenting zero power physics testing to support model development and comparisons of calculated and measured results





Technical Approach

- DNB and mixing 5x5 bundle data selection/collection (12/15/2012)
- Installation of COBRA-TF on WEC computer platform (12/15/2012)
- Preparation of selected 5x5 bundle configuration for CFD input (01/15/2013)
- Data modeling with VIPRE-W and COBRA-TF (03/01/2013)
- Report preparation and review (03/15/2013)
- Stretching activities:
  - Mixing and DNB simulation using STAR-CCM+
  - HYDRA software installation on WEC computer platform
  - HYDRA simulation of single-phase mixing in 5x5 rod array

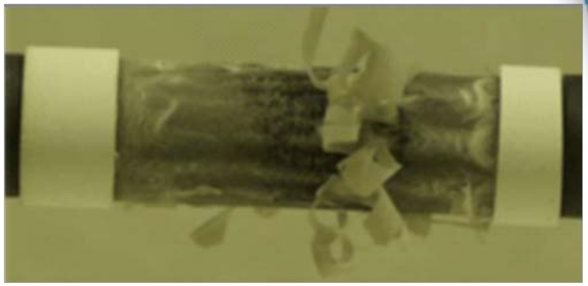
Personnel, Costs, Potential Issu

- Yixing Sung, Lead
- Test Data: Dinh, Buongiorno
- Sub Channel: Palmtag, Popov Zhang
- CFD: Nourgaliev, Christon, Yan
- Cost Estimate (person-months, dollars)
  - 8 PMs

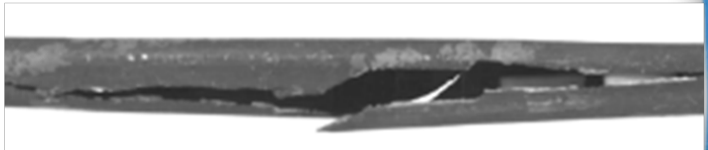
Clad Integrity during RIA & LOCA

Definition of Problem

- Current LOCA & RIA analyses use relatively simplistic fuel rod models to account for physical changes during the transient (e.g., swelling and burst, oxidation mechanics) that are largely based on unirradiated material performance
- Proposed revisions to acceptance criteria due to high burnup effects (e.g., hydrogen uptake) could require margin recovery for some plants
- Clad failure followed by fuel dispersal concern for both RIA & LOCA
- Understanding fuel performance during Post-DNB heat transfer is required for both RIA and LOCA



Breakaway Oxidation During LOCA



Clad Failure in RIA test with Fuel Dispersal

Need for Advanced Simulation

- Current analyses use simplistic fuel rod models
  - ➢ Validate and improve Peregrine predictive capability for normal operations to obtain fuel initial conditions at initiation of accident simulation
  - ➢ Validate and improve Peregrine predictive capability for analyzing unirradiated and high burnup fuel under LOCA and RIA conditions
  - ➢ Investigate benefits of Accident Tolerant Fuel with Peregrine

Success Targets

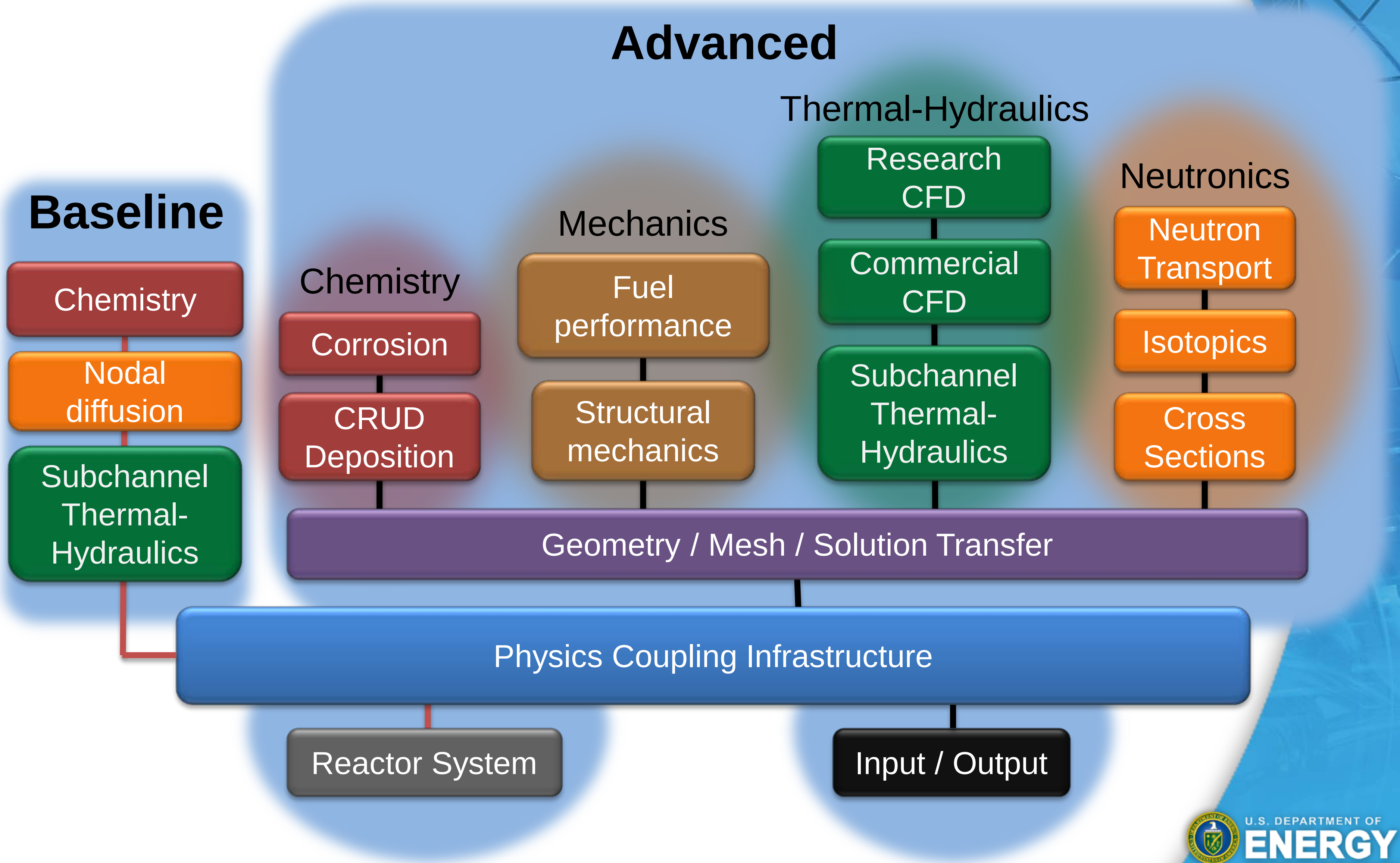
- Develop and implement modeling improvements to more accurately access fuel performance during RIA and LOCA
- Validate Peregrine using available data for LOCA , RIA and ATF
- Provide capability to evaluate impact of ATF features effects on RIA & LOCA

VERA Tools

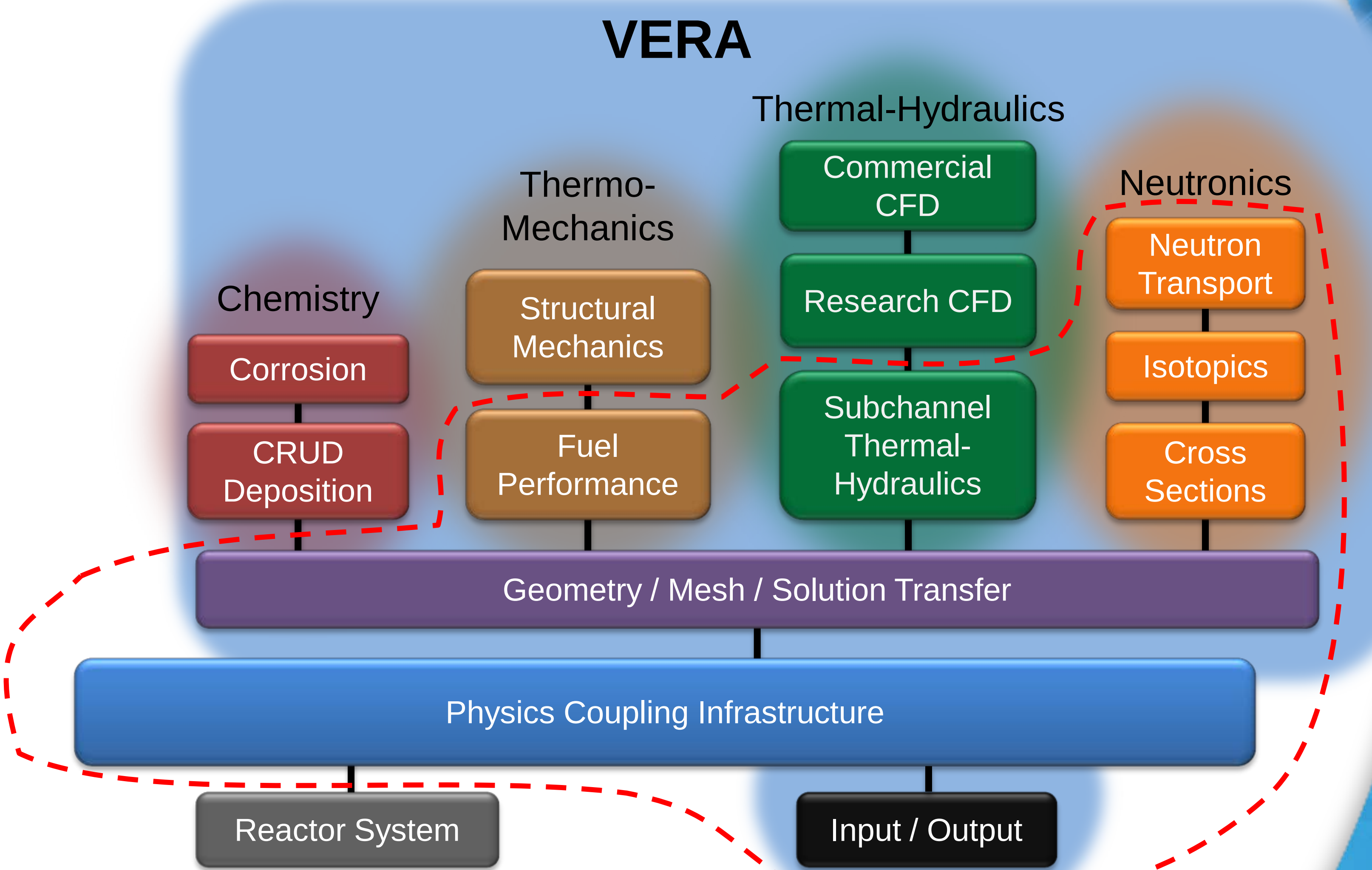
- Plan just being initiated
- RIA: MPACT – Hydra – Peregrine
- LOCA: Peregrine (B.C. from WEC)

Virtual Environment for Reactor Applications (VERA)

CASL's virtual reactor for in-vessel LWR phenomena



Some of our VERA components comprise a new type of "Core Simulator" (VERA-CS)



The Core Simulator facet of VERA (VERA-CS) is a code system for modeling steady-state LWR conditions and depletion, providing reactor conditions and distributions *needed to solve our Challenge Problems.* VERA-CS includes components for neutron transport, cross sections, thermal-hydraulics, fuel temperature, & depletion.

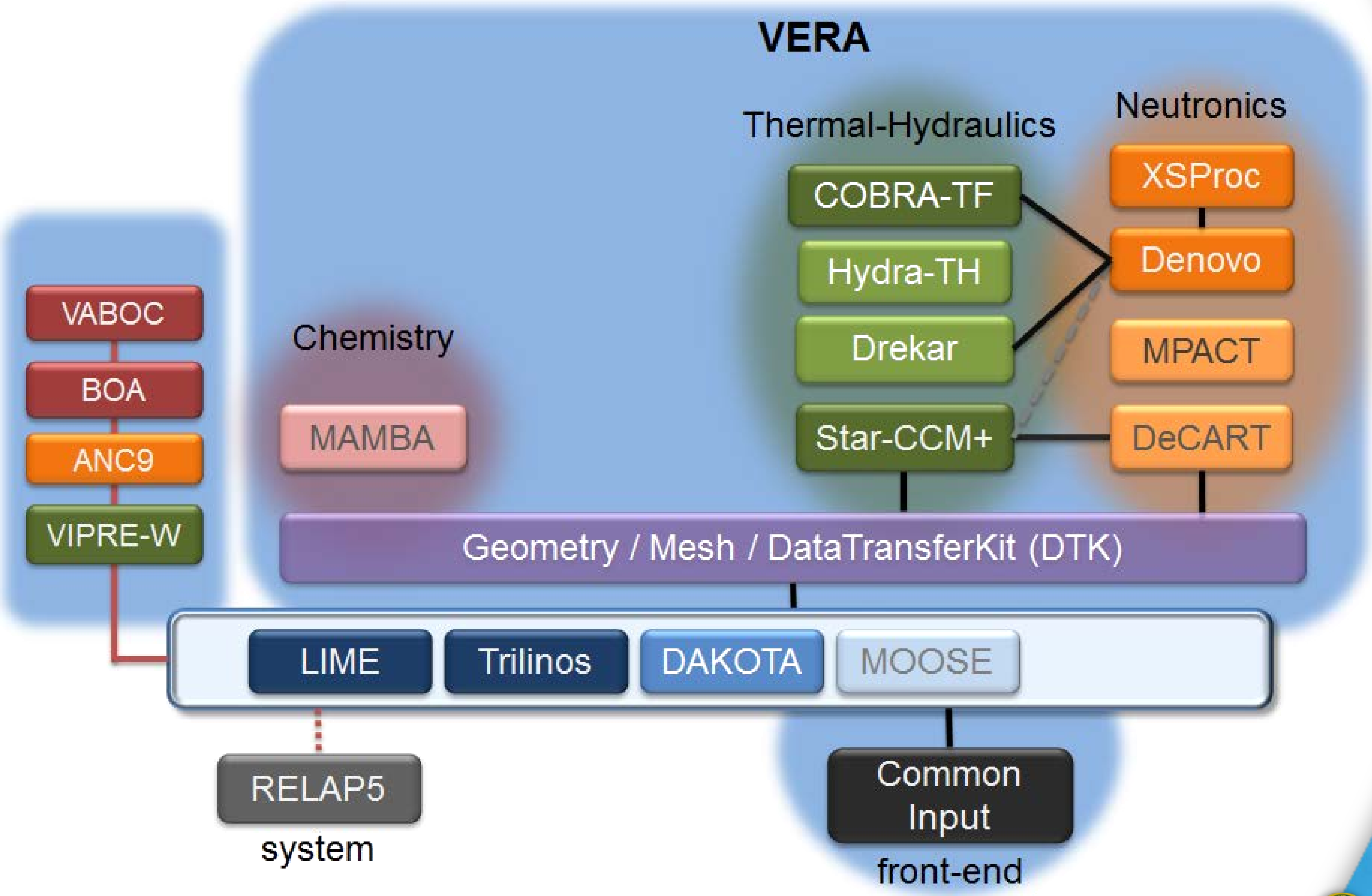
VERA-CS vs. Industry Core Simulators

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

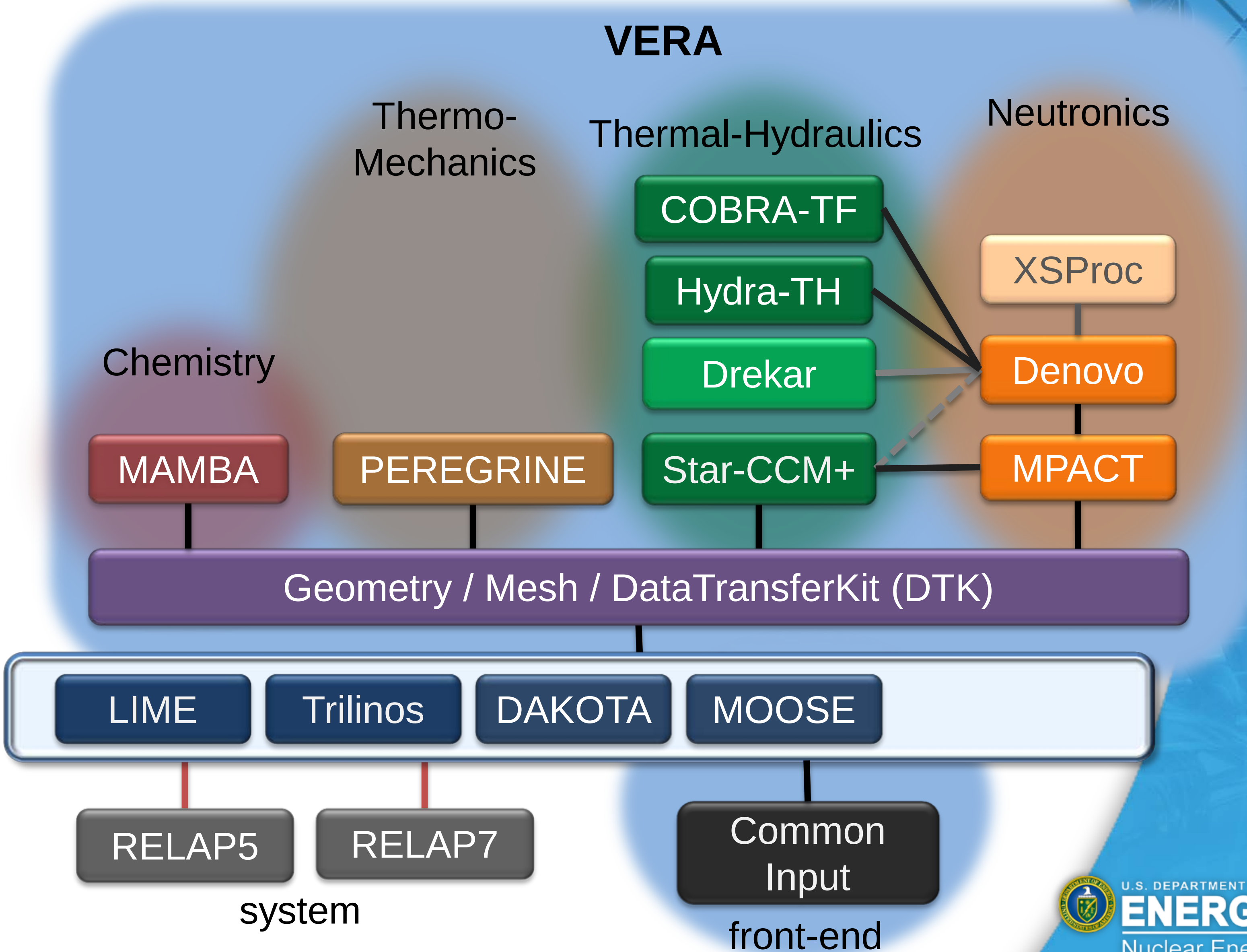
(*) pin-homogenized or pin-resolved depending on application

- What's "good enough"? Quantified margins and uncertainties will guide us

VERA 2.3 (12/2012)



VERA 5.0 snapshot (03/2015)



CASL
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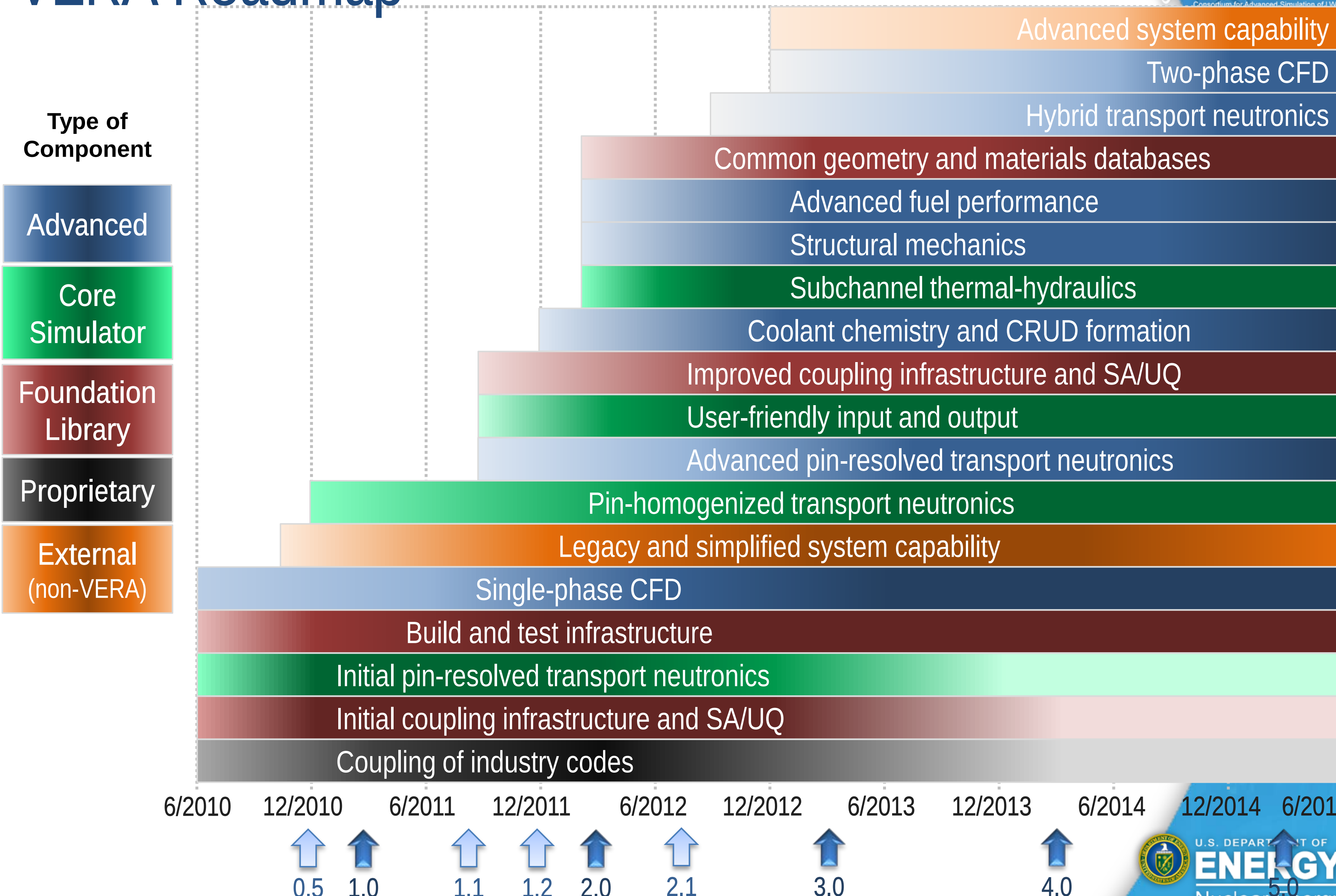
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

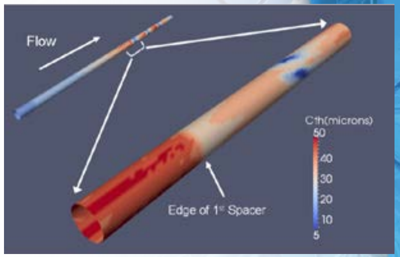
CASL-U-2015-0061-000

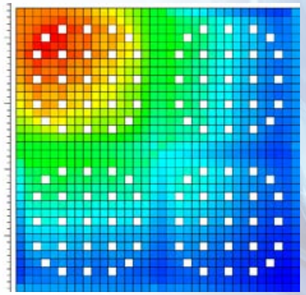
VERA Roadmap

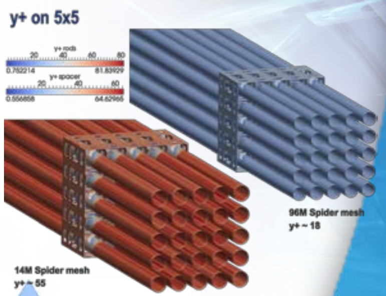


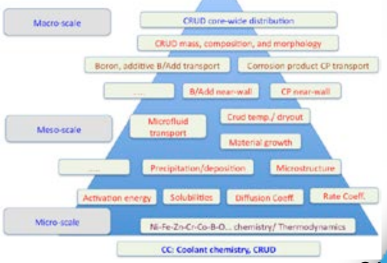
Enabling R&D Objectives

- Materials Performance and Optimization (MPO)
  - Mature 3D fuel performance capability with full assessment against CRUD/PCI/GTRF problems. Validated fuel performance models inform assessments of safety margin (PCI) and best operational practices (CRUD, GTRF). Functional capability and partial assessment for RIA- and LOCA-based transient problems.
- Radiation Transport Methods (RTM)
  - Robust 3D pin-resolved transport and prototype hybrid Monte Carlo transport with modern cross section/shielding treatments and coupling to T-H, fuel, and corrosion chemistry capabilities
- Thermal Hydraulics Methods (THM)
  - Robust 3D steady-state/transient turbulent multi-phase capability with subcooled boiling models, an initial assessment of DNB, and complementary with a modern subchannel capability
- Validation and Uncertainty Quantification (VUQ)
  - Mathematical tools and methodologies integrated and accessible to enable quantifying sensitivities and uncertainties in full-scale multi physics PWR simulations

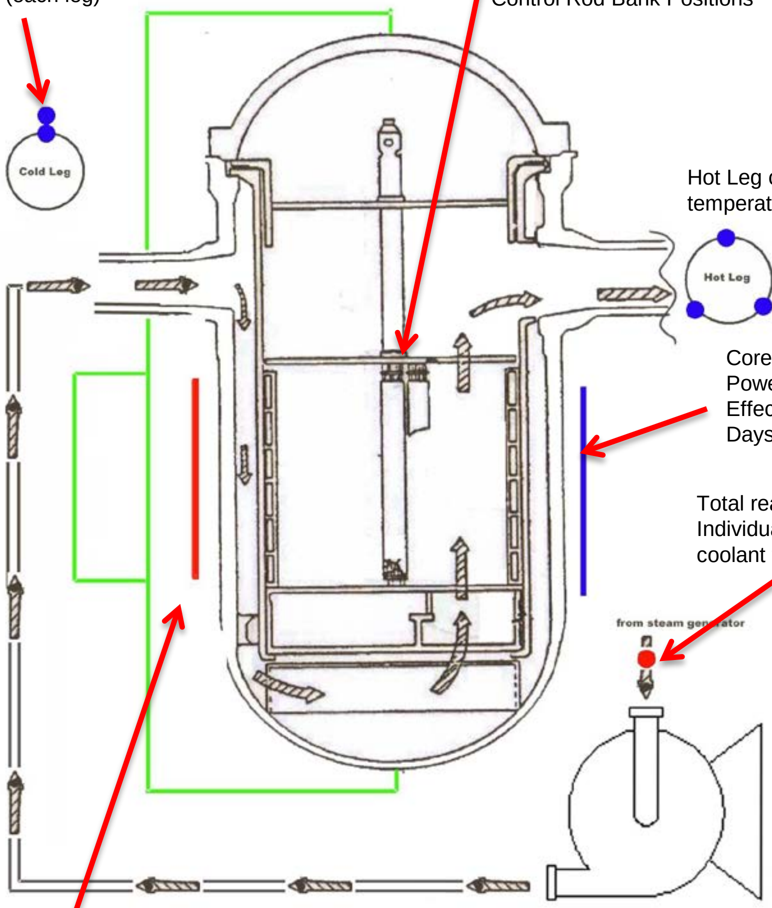








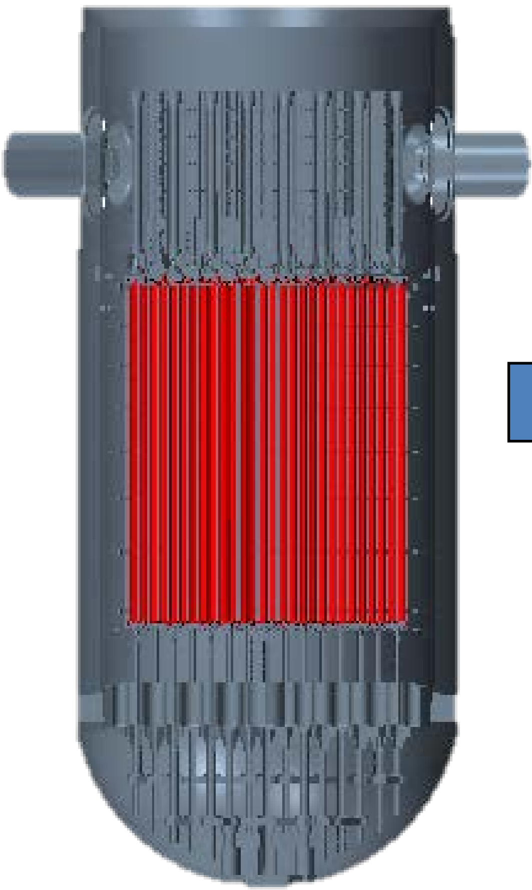
Extensive commercial PWR data covering 15 years of operation provided to CASL by TVA



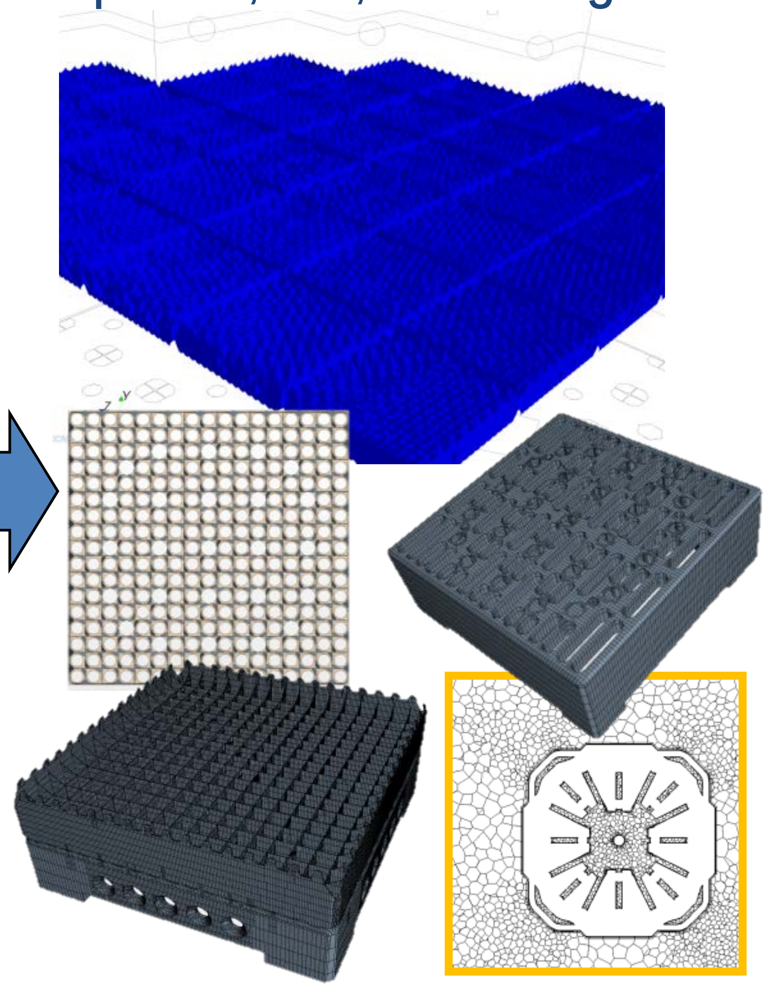
- TVA provided detailed information on Watts Bar Unit 1 Cycles 1 through 10
  - Core cycle design
  - Core performance observations
  - Measured operating data from various instrumented locations (see graphic) on a 5-day average basis for the complete cycle
  - Cycle 1 startup testing information
  - Applicable coolant chemistry information
- Zero power physics testing for all cycles to be provided in FY13, along with other supplementary data as needed

4-Loop Westinghouse PWR Multi-Physics Model Development

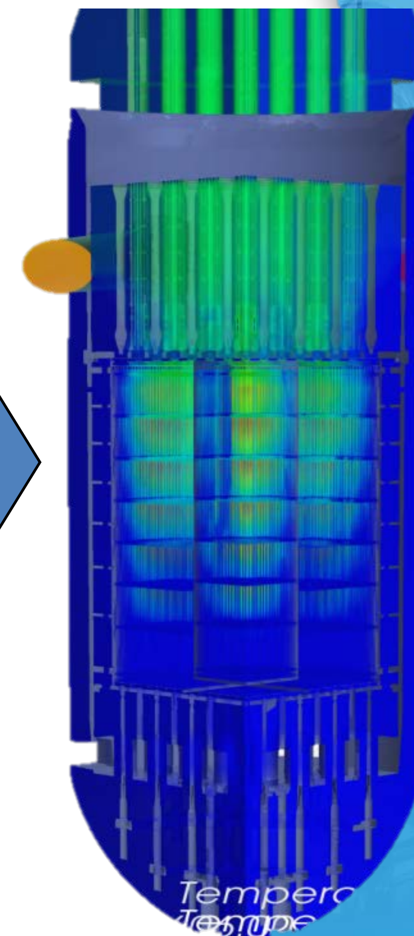
- RPV ID 173”, 193/4 Fuel Assemblies,13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; 1.2 billion cells



CFD Model



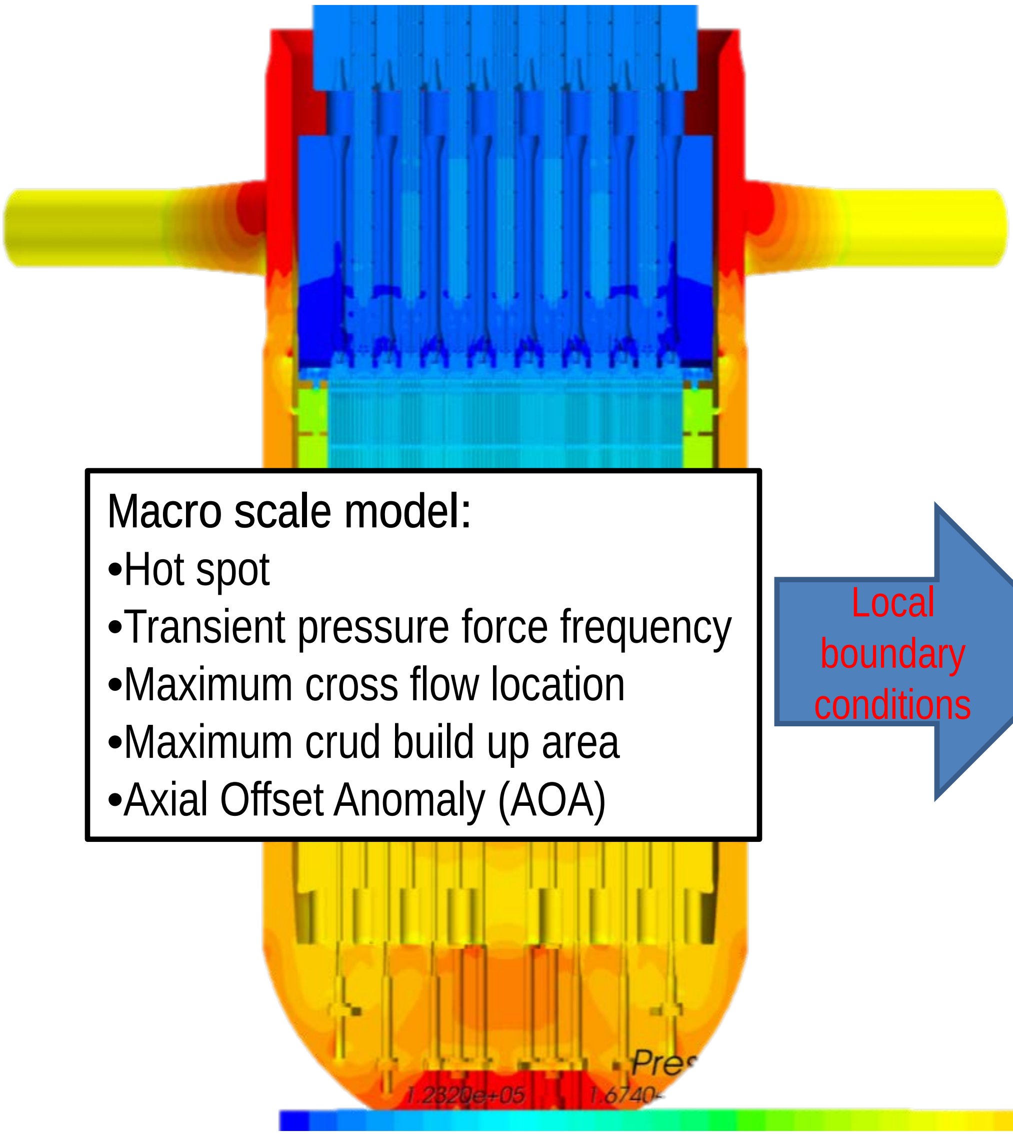
Mesh

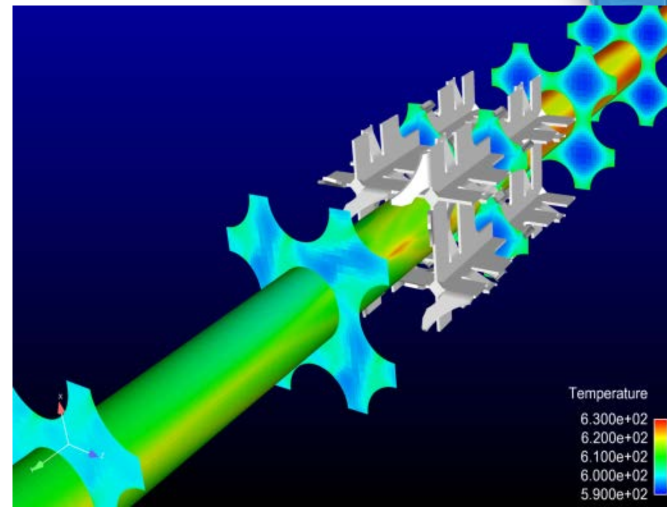


Results

We Strive to Build a Computational Microscope

Actively steered by SA, UQ, DA





Macro scale model:
- Hot spot
- Transient pressure force frequency
- Maximum cross flow location
- Maximum crud build up area
- Axial Offset Anomaly (AOA)

Local boundary conditions →

Micro scale model:
- Peak cladding temperature
- Transient pressure force frequency
- Maximum cross flow
- Maximum crud build up area

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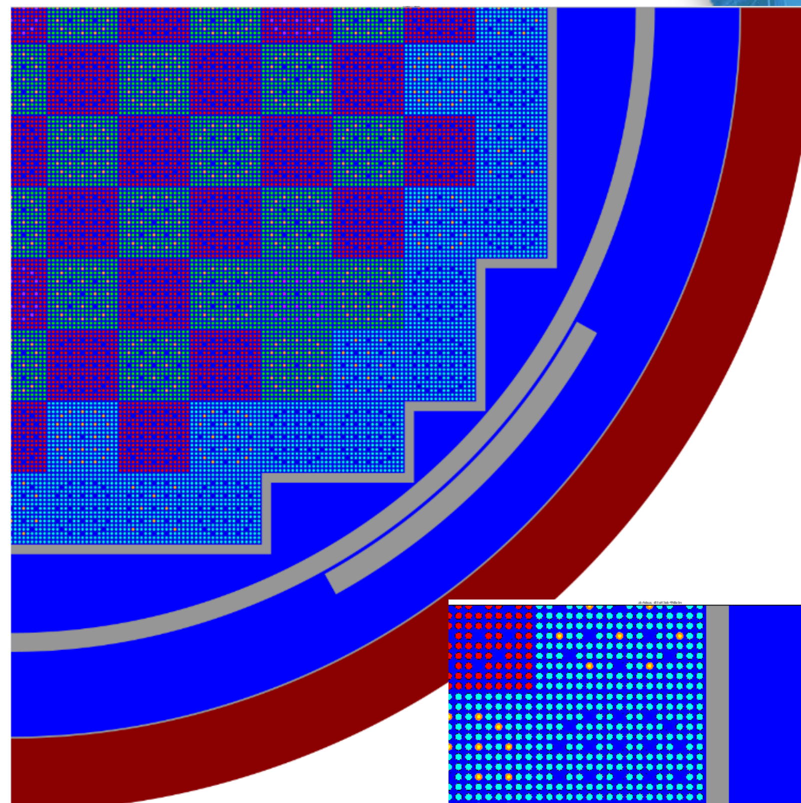
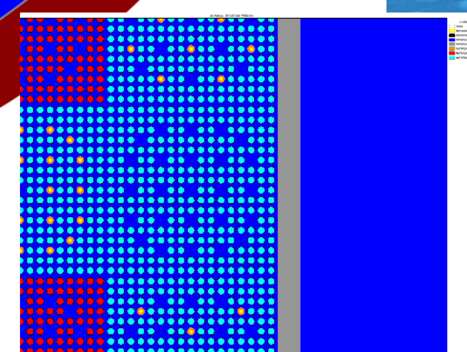
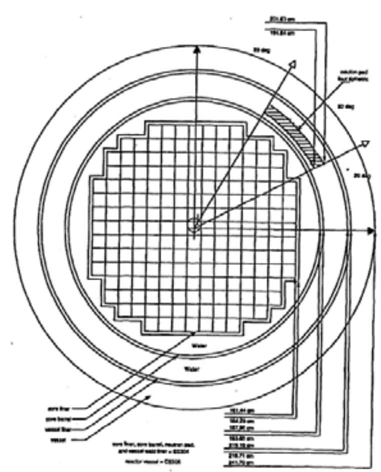
Problem Specifications - CASL-U-2012-0131-001

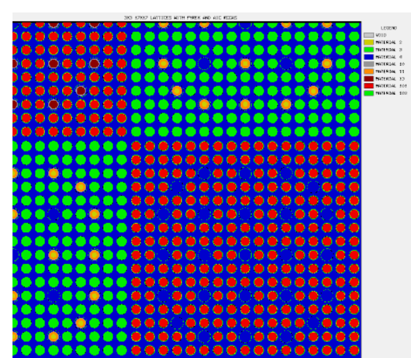
- AMA problem specs revised and augmented. Some revisions are:
  - Added Problem 1E (IFBA pin cell)
  - Added Problems 2K-2P (radially-zoned enrichment, IFBA, WABA, and Gadolinia)
  - Added new 2D problems for 3x3, quarter core, and a simple reflector case (new section “Miscellaneous Benchmarks”)
  - Switched to development version of CE KENO-VI (SCALE 6.2 dev) for parallelization and recent fixes for reference solutions





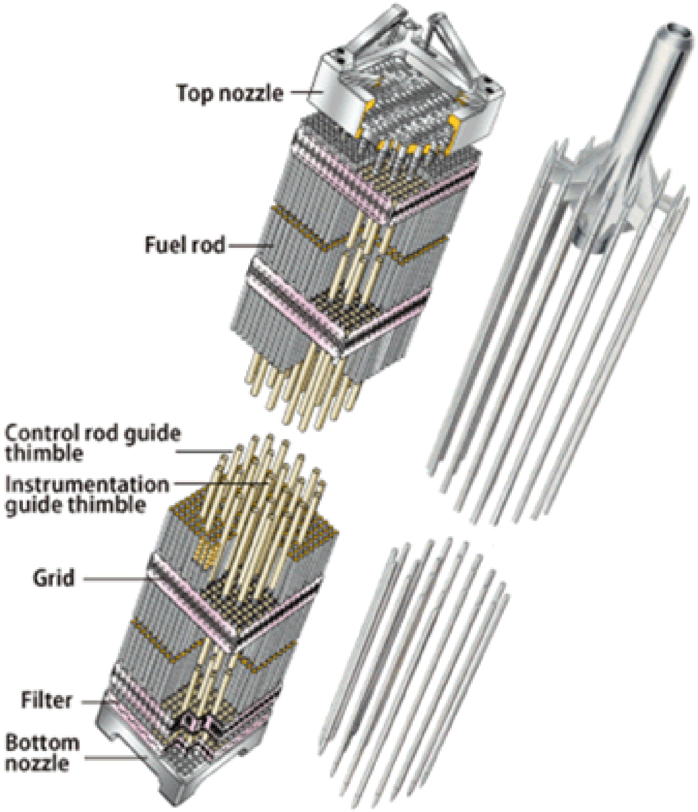
	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1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





Problem 2 Cases

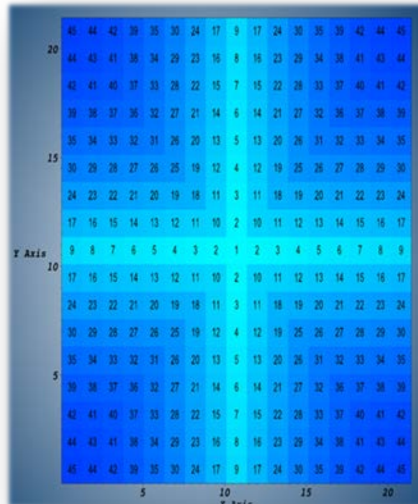
- Westinghouse 17x17 assembly 2D lattices based on Watts Bar 1 Cycle 1
  - 3.1% enriched UO_2
  - Beginning of life fresh fuel only
  - 565K-600K moderator temperature
  - Three variations in fuel temperature
  - Two pyrex patterns
  - Two control rod types
  - Two instrumentation patterns
  - One radially-zoned enrichment
  - Three IFBA patterns
  - Two Gadolinia patterns

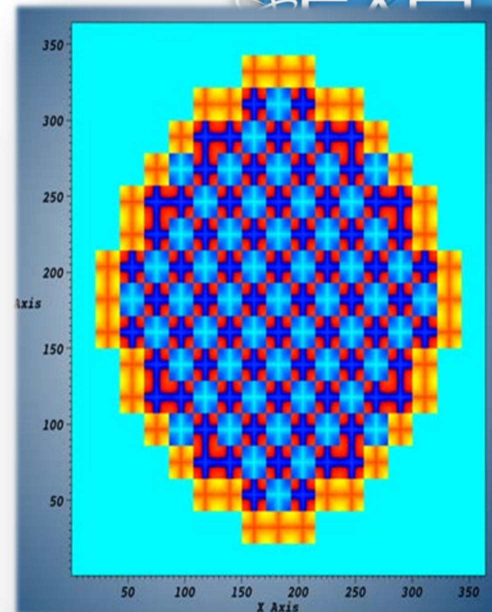


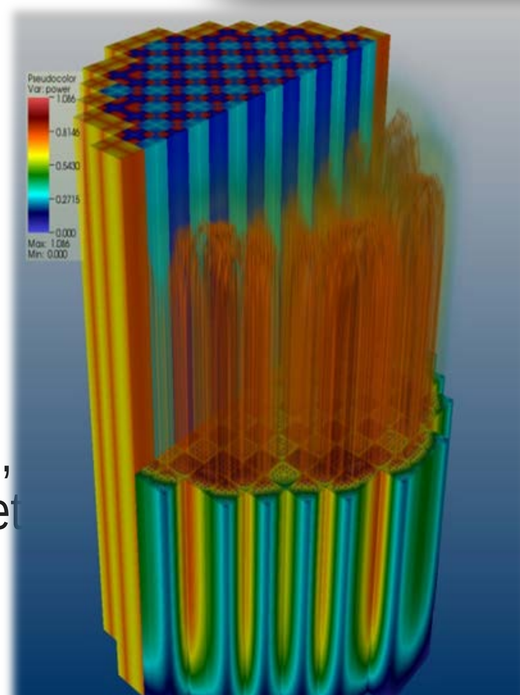
Not exhaustive benchmark, but covers many of possible PWR cases

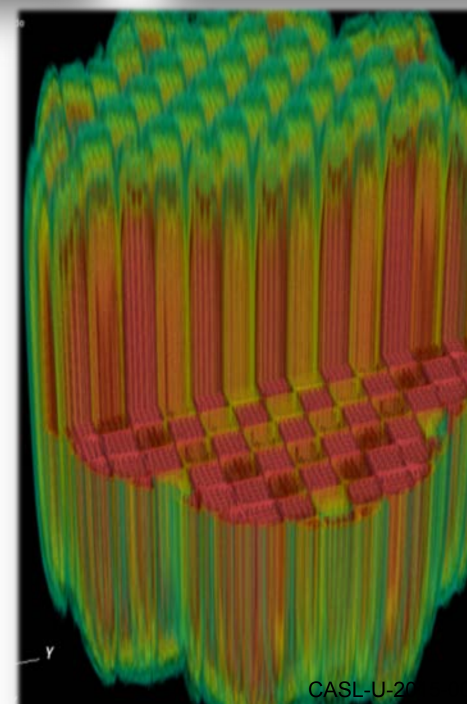
What about neutron transport?

- PWR-900 full-core reactor test problem
- 2 and 44-group, homogenized fuel pins
- 2×2 spatial discretization per fuel pin
- 17×17 fuel pins per assembly
- 289 assemblies
  - 157 fuel, 132 reflector
  - high, med, low enrichments
- Space-angle unknowns:
  - 233,858,800 cells
  - 128 angles (1 moment)
  - 1 spatial unknown per cell
- This example does include grids, control rods, burnable poisons, et









What does this mean for a reactor core simulator?

Where we want to be…

- reproduce fidelity of 2D calculations using consistent 3D methods
- produce all state-points for an 18-month depletion cycle in O(8 hours)
- O(72) state points per cycle (1 week steps)
- steady-state, coupled neutronics simulation with T-H feedback = $O(10^{19})$ unknowns

Where we are…

- assuming 2% peak, we can solve 1.7×10^{13} unknowns/hour (XT5)
- we can solve a reduced 3D problem ($O(10^{15})$ unknowns) in 175 hours
  - assumes status quo on a 1 PF/s XT5 machine

So…

- to reach 2D fidelity at 3D we need to solve $\sim 10^4$x more unknowns
- to run all state points in one day at this fidelity using existing code and methods would require ~140 EF/s

THM targets and approach

We use experiments and ITM simulations to improve multiphase models in VERA-CFD

- Deliver next-generation T-H simulation tools to VERA, interfaced with the latest VUQ technologies, and accommodate tight coupling with other physics
- Computational Fluid Dynamics (CFD) Project: Deliver to VERA non-proprietary, scalable, verified and validated component-scale CFD tools

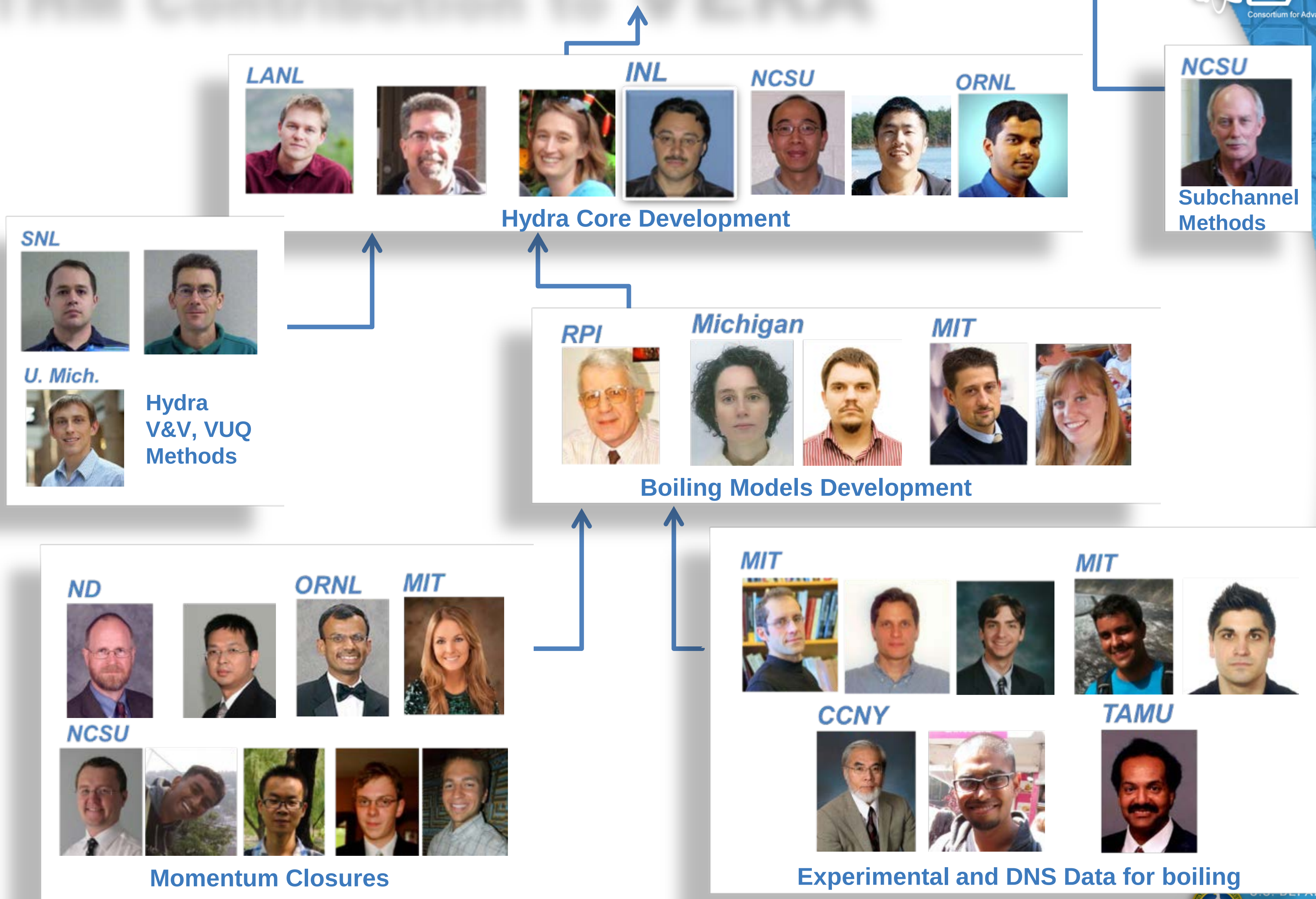
Interface Tracking Methods (ITM)

- Generate microscale simulation results data for CFD closure models and validation

Experiments

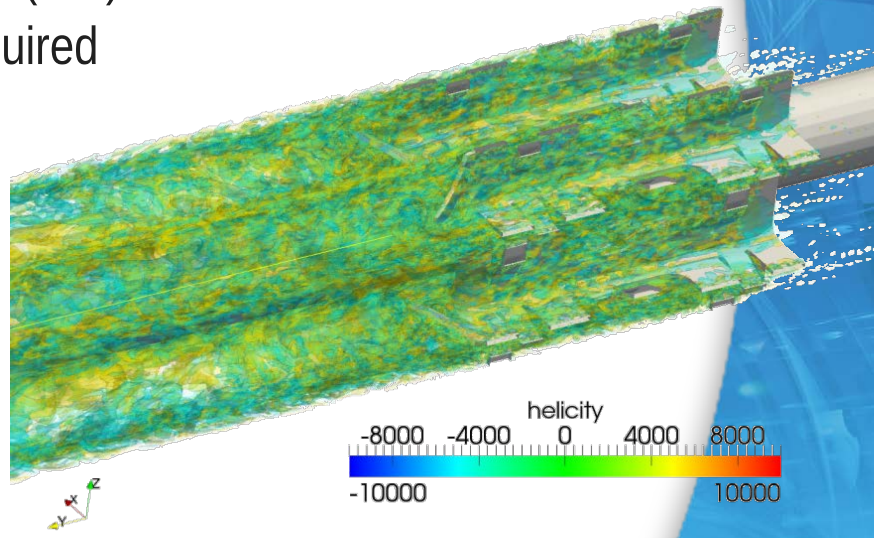
- Provide validation data for CFD/ITM and fundamental understanding

THM Contribution to VERA



CASL Challenge Problems with major THM focus

1. **Grid-to-rod fretting (GTRF)**
   - Analysis thus far single phase, with LES, to compute turbulent excitation forces
   - Determine level of fluid-structure interaction (FSI)
   - Determine level of turbulence modeling required
2. **CRUD formation (CIPS/CILC)**
   - Subcooled boiling models
   - Coupling CFD with CRUD growth
3. **DNB**
   - By 2015, assessment of our CFD tools
   - Longer term, develop CFD-based DNB predictive model



Hydra-TH: model formulation

(5*N*)-equation (in 3D), *N*-field formulation

- **Mechanical & thermal non-equilibrium**
- **Pressure equilibrium**
- **Multiple-bulk-pressure**
- **Hyperbolic (provable when *N*=2)**
- **EOS: generic; for water – IAPWS-IF97, IAPWS-95 (SNL)**
- **Closures: from NPHASE (RPI) data base**
- [Turbulence: ($\kappa-\varepsilon$) model]
- [Interfacial area transport (IAT) in the future]

Application Focus

1. **Subcooled boiling**
2. Departure from nucleate boiling (DNB)
3. Loss-of-coolant accidents (LOCA)
4. Reactivity-Initiated Accidents (RIA)
5. Reflooding

In the future (items 2–5)

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Hydra-TH: governing equations

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Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot (\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k) = \boxed{\Gamma_k}$$

Strong non-linearity

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k]) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \boxed{\mathbf{M}'_k} + \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}^m_{ki}} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot (\alpha_k [\bar{\rho}_k \tilde{e}_k + \bar{p}_k] \tilde{\mathbf{v}}_k) = \boxed{\mathbf{M}'_k} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k + \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}^{Re}_k}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}^{Re}_k}\right]\right) + \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v^e_{ki}}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W'_k}$$

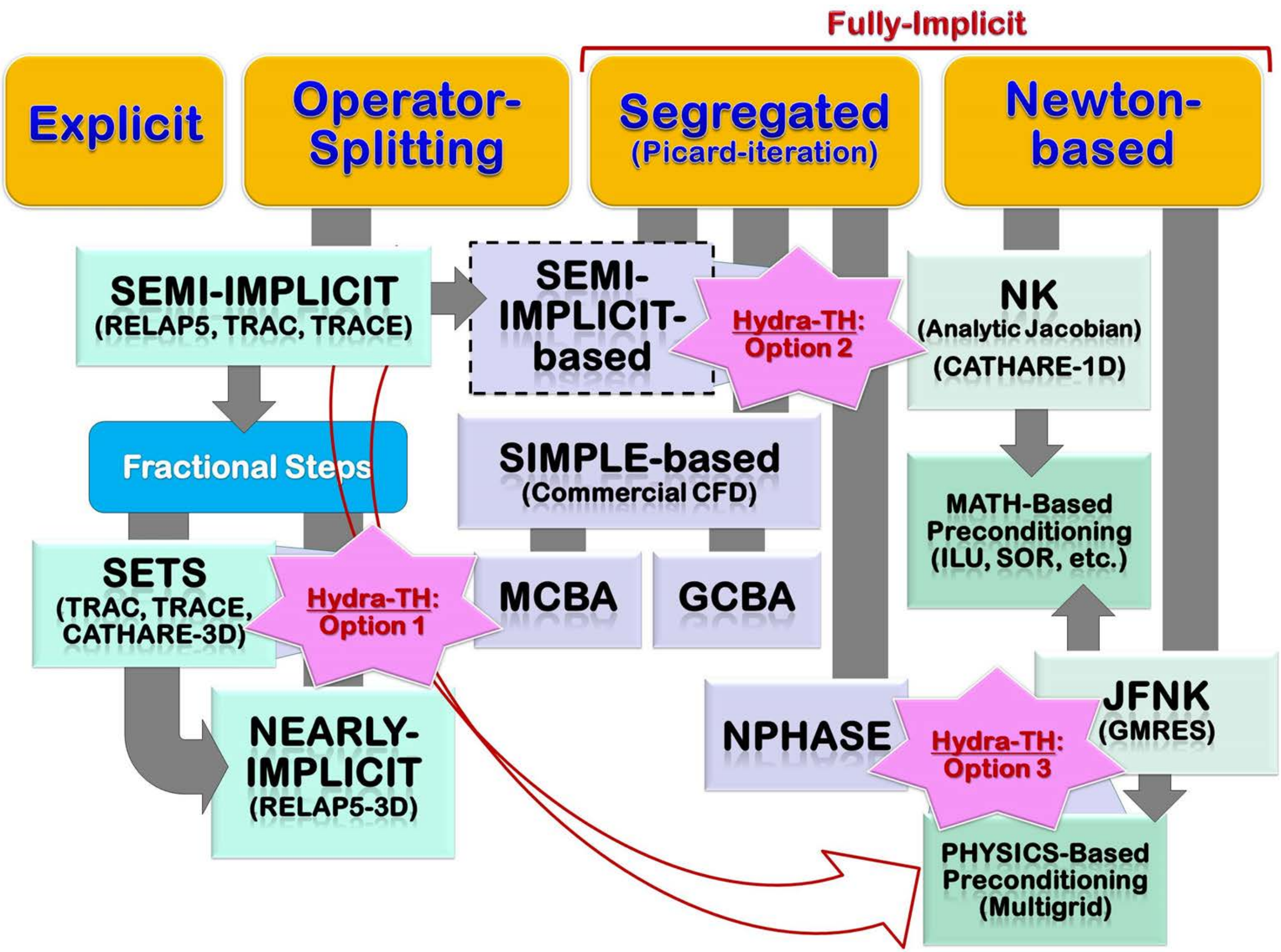
+ Turbulence equations

To close:

+ N equations of state, $\bar{p}(\bar{\rho}_k, \tilde{u}_k)$
+ Constitutive physics (for terms in boxes, $\boxed{\Psi}$)
+ Compatibility condition, $\sum_k \alpha_k = 1$
+ Bulk pressure difference models, $\Delta \bar{p}_{(ij)}(\mathbf{U}),\ i \neq j,\ (i,j) = 0, \ldots, N-1$

U.S. DEPARTMENT OF ENERGY Nuclear Energy

Hydra-TH Multi-Phase Flow Strategy/Roadmap



- "Option 1" (without inter-phase transfer) exercised
- "Option 2" - Picard (for single field) exercised

Fully-Implicit Picard Time Marching

- Extended semi-implicit projection algorithm to fully-implicit time-stepping
- Projection is a preconditioner to each Picard iteration
- Removes any time step size restrictions, second-order accurate in time

Iterative procedure: outer loop around projection:

$$n \rightarrow \text{Picard}(\diamond \rightarrow \diamond\diamond) \rightarrow n+1$$

1. Momentum prediction: $\overline{\mathbf{v}}^{\diamond} \rightarrow \overline{\mathbf{v}}^{*\diamond\diamond}$

$$[M - \theta\Delta t(K^{\diamond} - A^{\diamond})]\overline{\mathbf{v}}^{*\diamond\diamond} = [M + (1-\theta)\Delta t(K^{n} - A^{n})]\overline{\mathbf{v}}^{n} - \Delta t \mathbf{B} p^{n} - \Delta t \theta \delta A^{\diamond}\overline{\mathbf{v}}^{\diamond}$$

2. Pressure update: $p^{n} \rightarrow p^{\diamond\diamond}$

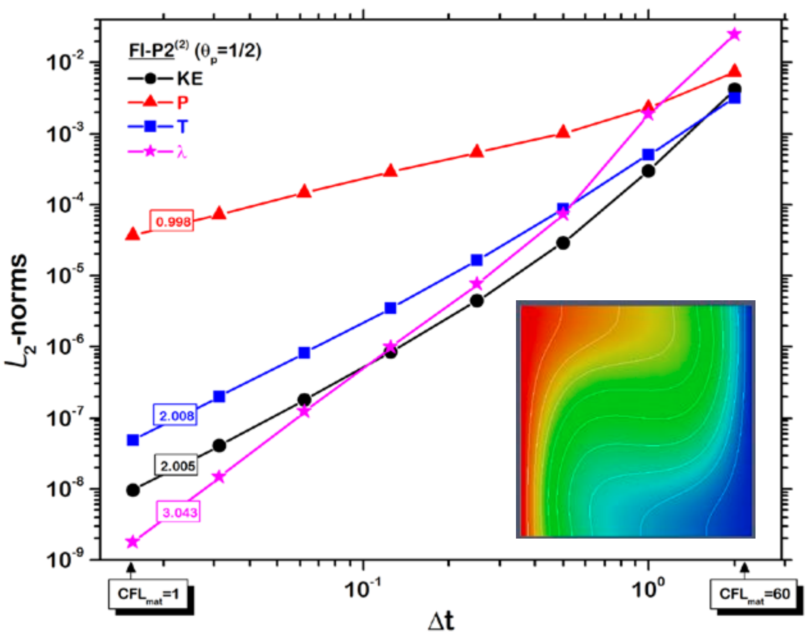
$$\nabla^2 (p^{\diamond\diamond} - p^{n}) = \nabla \cdot (\rho \overline{\mathbf{v}}^{*\diamond\diamond})/\Delta t$$

3. Velocity projection: $\overline{\mathbf{v}}^{*\diamond\diamond} \rightarrow \overline{\mathbf{v}}^{\diamond\diamond}$

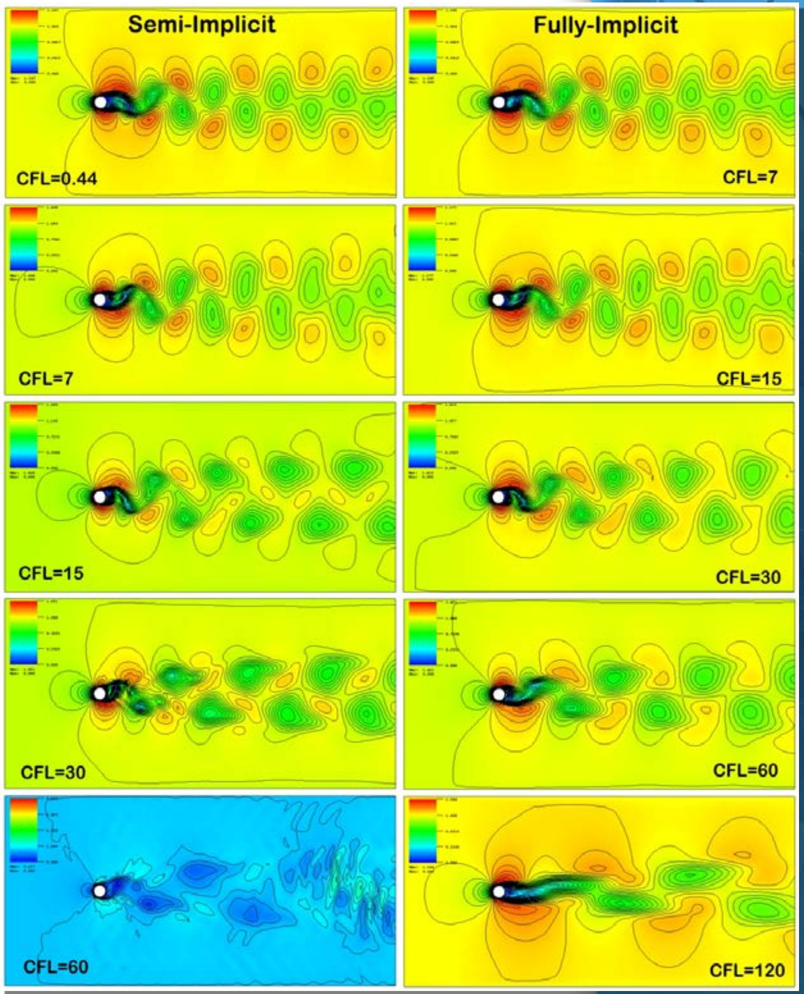
$$\overline{\mathbf{v}}^{\diamond\diamond} = \overline{\mathbf{v}}^{*\diamond\diamond} - \Delta t \nabla p^{\diamond\diamond}/\rho$$

Fully-Implicit and Scalable Algorithms

- Provides stability for long-time events
- Removes any time step size restrictions
  (required for stiff inter-phase coupling)
- Second-order accurate in time

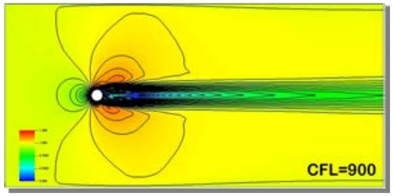


CFL



CFL=900

Oversteps vortex dynamics, but remains stable



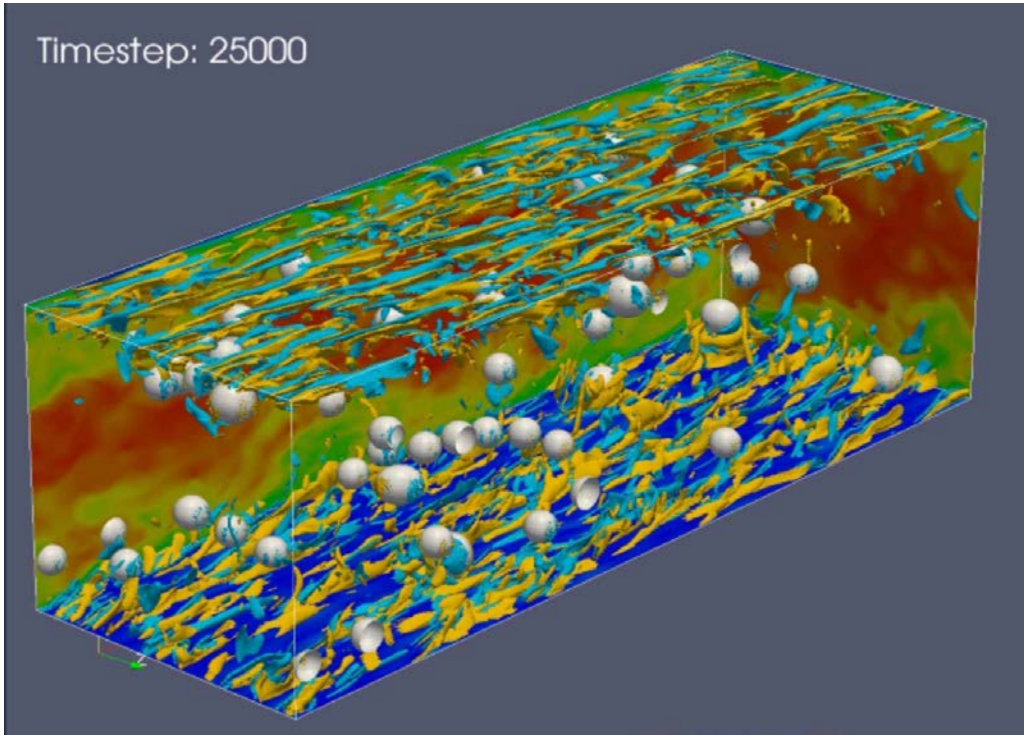
Remains stable when semi-implicit has failed

Now let's add multiphase: Track every bubble?

"ITM-Informed" Closure Models

- Improved closure models for deformed bubbles/crowding effect
- Provide information on near wall turbulent viscosity behavior

PHASTA (I. Bolotnov, NCSU)

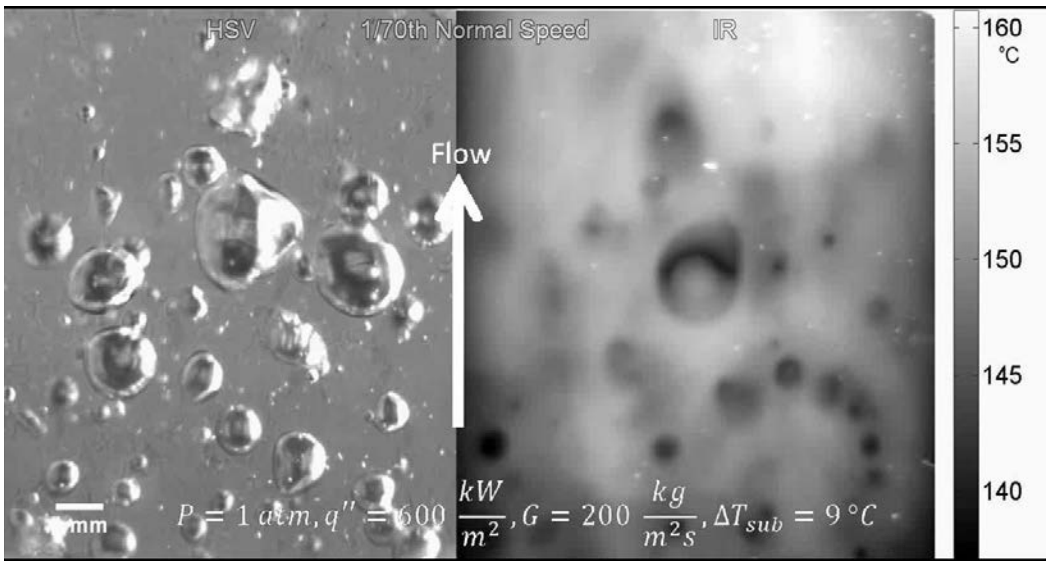


FTC3D (G. Trygvason, ND)

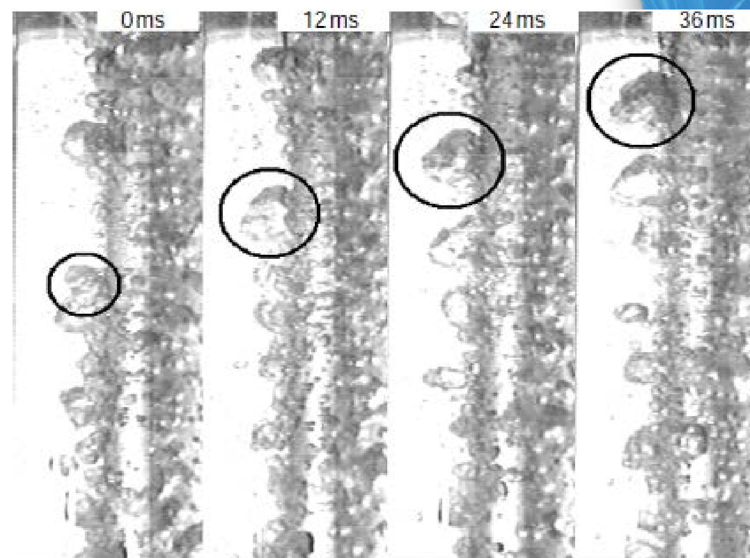
Advanced Wall Boiling Closures
Leveraging new physical Understanding

- A two-headed approach:
  - Advanced heat partitioning approach (Podowski, RPI)
  - Newly Formulated Flow Boiling Partitioning (NURETH15 preview)

High-speed video from above the boiling surface - IR thermography from below the boiling surface



Post processing gives nucleation site density, bubble departure frequency, local heat transfer coefficient (J. Buongiorno, MIT)



Significant bubble coalescence near the heated wall of an annular flow channel as indicated by the increasing bubble mushroom region (Tu et al., 2005).

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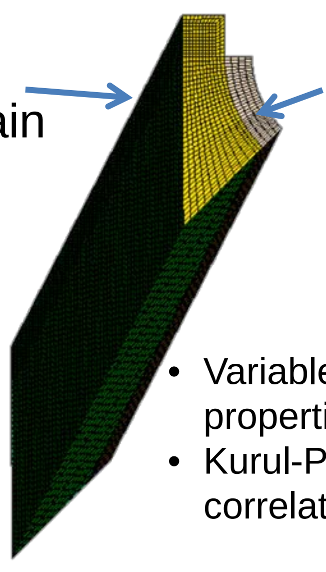
Advanced Wall Boiling Closures (Cont.)

Leveraging new physical Understanding

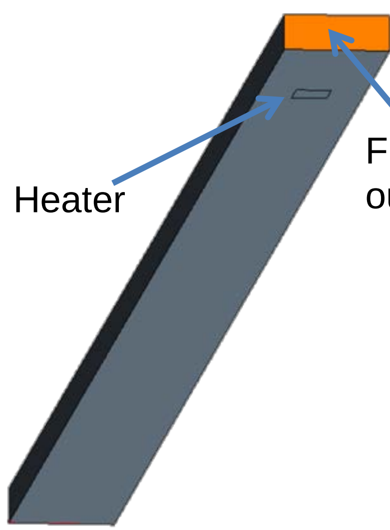
- Mechanistic sub-cooled boiling model applicable to simulate flow and heat transfer in PWR fuel assemblies (Podowski, RPI)
- Implementation, testing and validation of models for heat partitioning and bubble density transport (Manera, U. Michigan)
  - Validation using MIT Experimental data

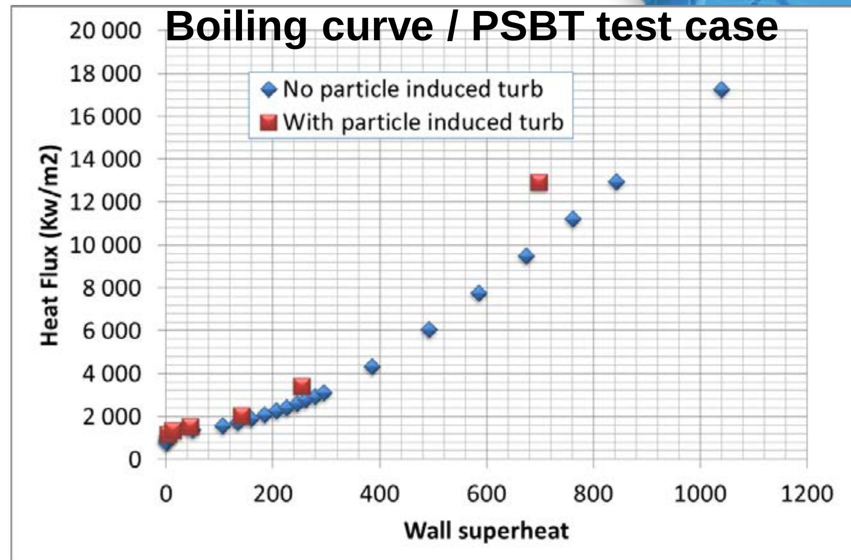
PSBT Geometry

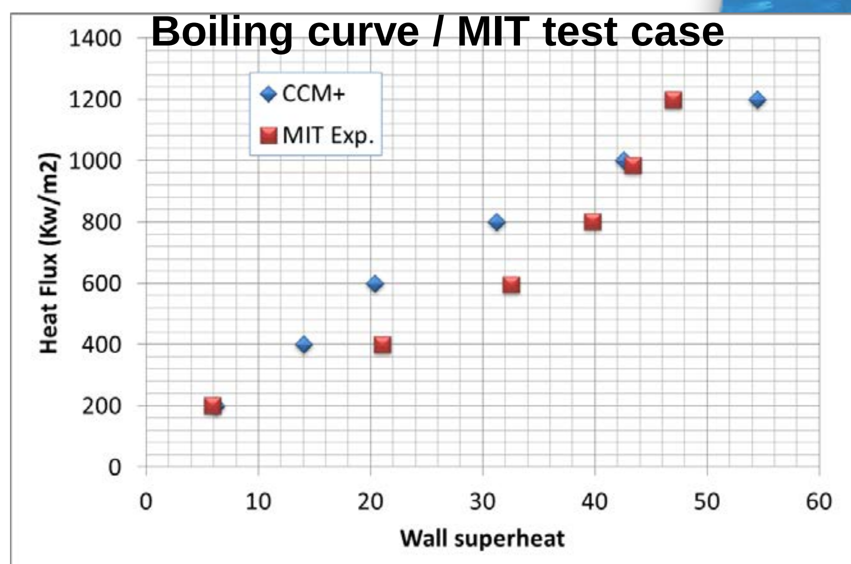


- Variable liquid properties
- Kurul-Podowski correlation

MIT Test Case



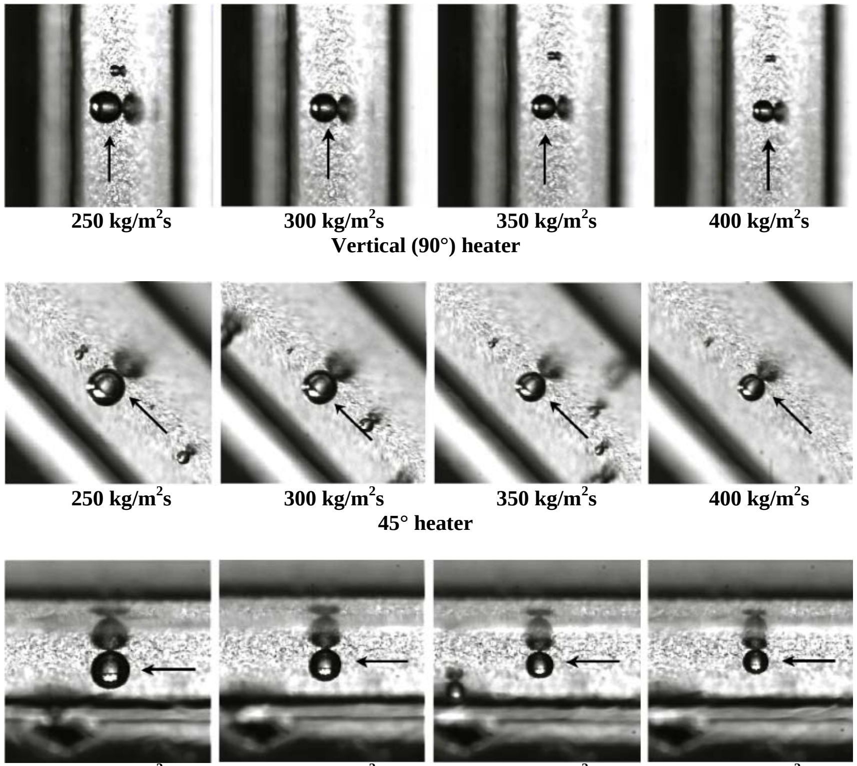




Flow Boiling Tests

Buongiorno, MIT

Generated database for bubble departure diameter in subcooled flow boiling as a function of mass flux, heat flux, subcooling, orientation angle, pressure



250 kg/m^{2}s 300 kg/m^{2}s 350 kg/m^{2}s 400 kg/m^{2}s
Vertical (90°) heater

250 kg/m^{2}s 300 kg/m^{2}s 350 kg/m^{2}s 400 kg/m^{2}s
45° heater

250 kg/m^{2}s 300 kg/m^{2}s 350 kg/m^{2}s 400 kg/m^{2}s
Downward-facing horizontal (0°) heater

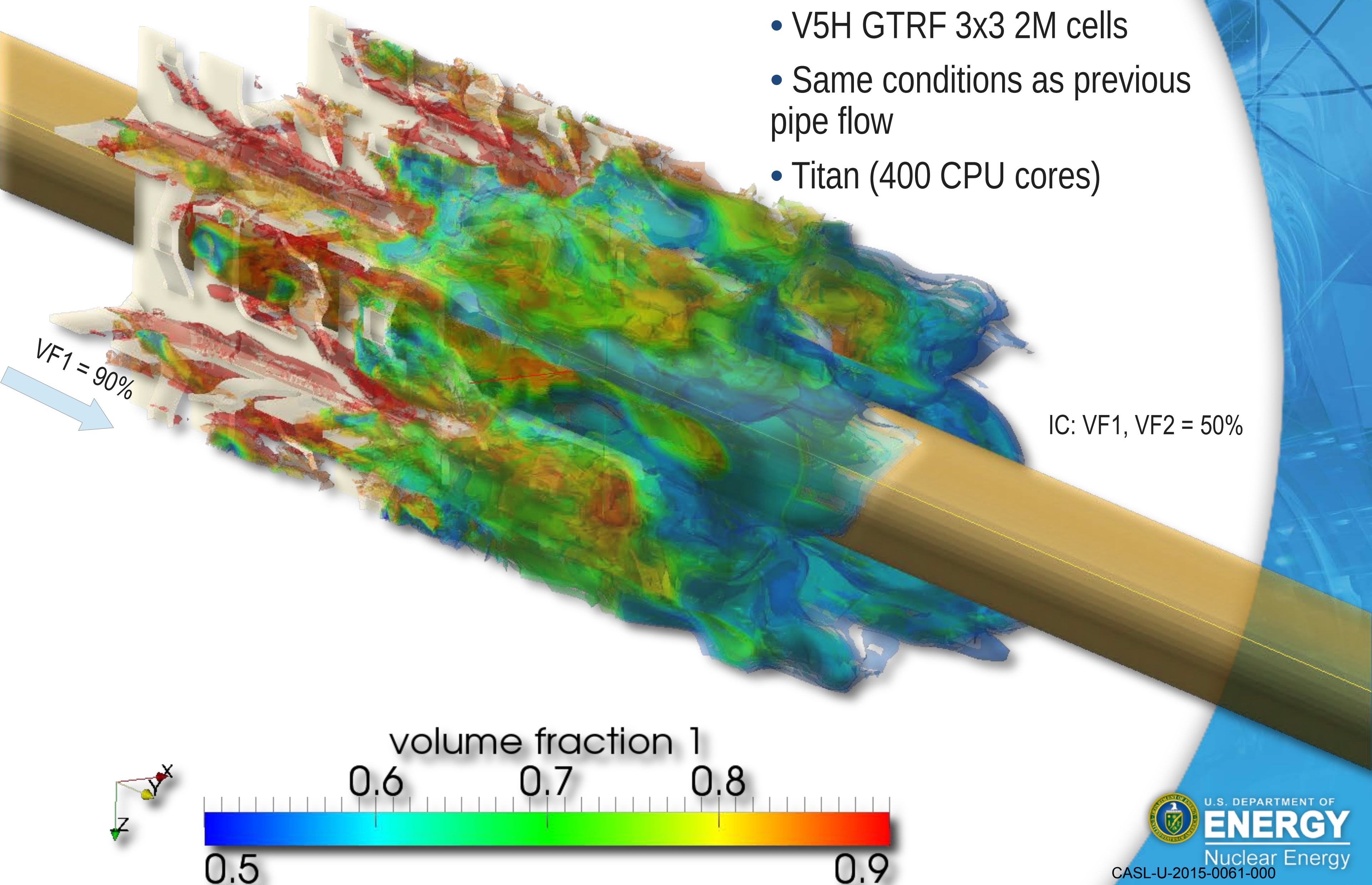
Parameter	**Experimental Range**
Orientation Angle [°]	0, 30, 45, 60, 90, 180
Mass Flux [kg/m^{2}s]	250, 300, 350, 400
Subcooling [°C]	10, 20
Heat Flux [MW/m^2]	0.05, 0.10
Pressure [kPa]	101, 202, 505

- Compared data to mechanistic force model by Klausner et al. (1993) and recent update by Yun et al. (2011) (used in STAR-CD).
- Average error and SD are 35.7±24.2% for Klausner's and 16.6±11.6% for Yun's

- Large errors in bubble departure diameter result in enormous errors in boiling heat transfer ($\propto D^3$)
- Currently modifying Yun's model to improve accuracy. Adopted in VERA-CFD

Multi-Field Flow – Proof of Concept

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



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CASL Results to Date

CASL
Consortium for Advanced Simulation of LWRs

- Developed and released Virtual Environment for Reactor Applications (VERA) to CASL core partners through ORNL's Radiation Safety Information Computational Center
- Established baseline industry capability and advanced R&D capability in VERA for neutronics, thermal hydraulics, and corrosion chemistry
- Applied selected aspects of VERA to operational PWR core scenarios with conditions relevant to corrosion buildup ("crud"), pellet-clad interaction, and grid-to-rod fretting
- Integrated within VERA a state-of-the-art sensitivity and optimization capability to support uncertainty analysis of reactor operational and safety scenarios
- Demonstrated that newly established multidimensional simulation capabilities exceed industry capabilities in physics modeling

Scientific output

- 261 publications
- 30+ invited talks
- 247 milestone deliverables in CASL database

Questions?

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

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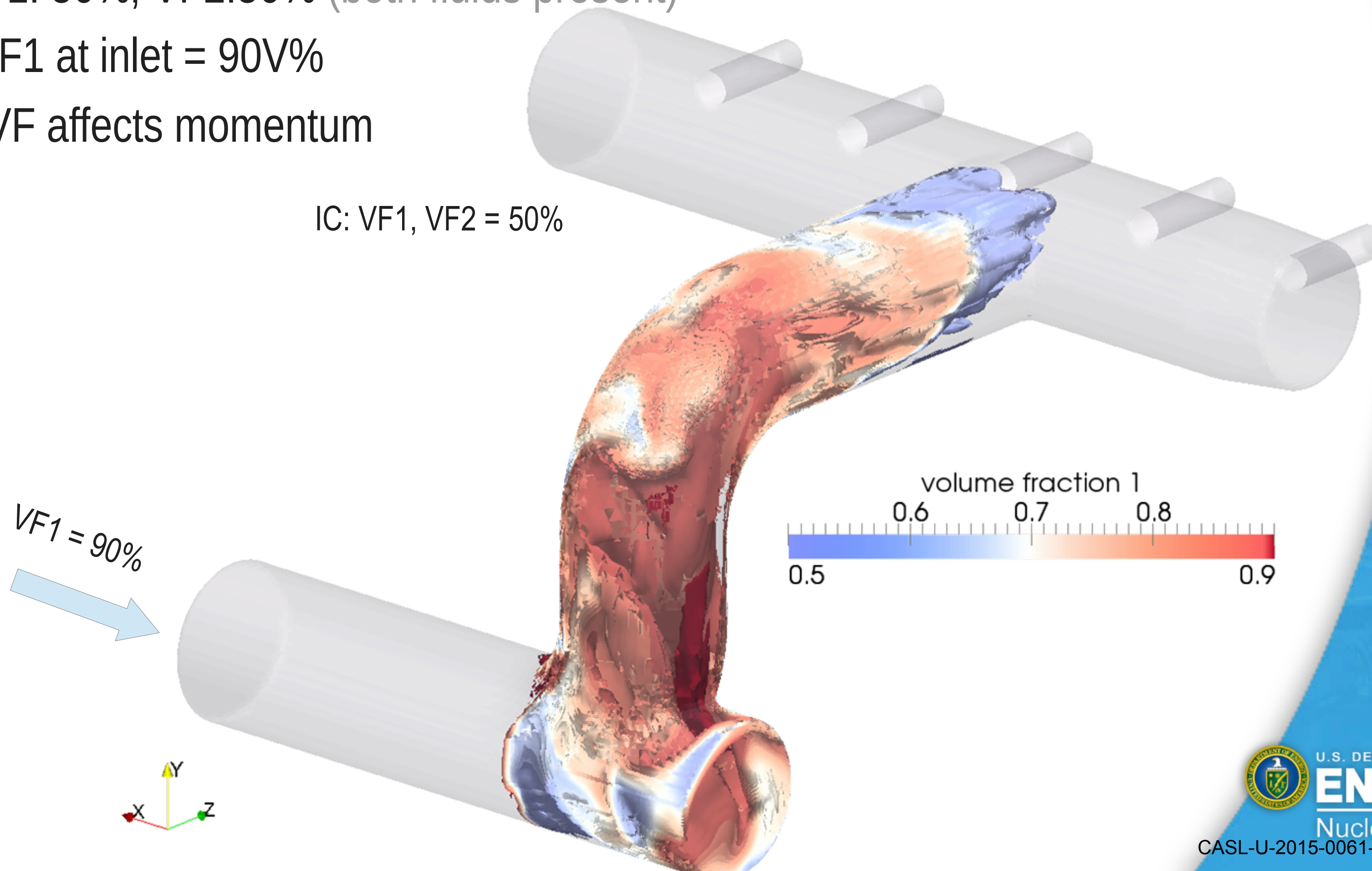
Supplemental Material

Multi-Field Flow – Proof of Concept

- Hybrid mesh generated by Spider
- 2 fields, same densities
- Coupled through single pressure via projection algorithm
- IC: VF1: 50%, VF2:50% (both fluids present)
- BC: VF1 at inlet = 90V%
- Now VF affects momentum



“Option 1” gov. eqs. for *k* = 1,...,*N* fields

$$\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k \overline{\mathbf{v}}_k) = 0$$

$$\alpha_k \overline{\rho}_k \left(\frac{\partial \overline{\mathbf{v}}_k}{\partial t} + \overline{\mathbf{v}}_k \cdot \nabla \overline{\mathbf{v}}_k \right) = -\alpha_k \nabla \overline{p} + \nabla \cdot (\alpha_k \overline{\boldsymbol{\tau}}_k)$$

$$\alpha_k \overline{\rho}_k C_{pk} \left(\frac{\partial \overline{T}_k}{\partial t} + \overline{\mathbf{v}}_k \cdot \nabla \overline{T}_k \right) = -\nabla \cdot \overline{\mathbf{q}}_k + \overline{q}_k'''$$

$$\nabla \cdot \textstyle\sum_k (\alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k) = 0$$

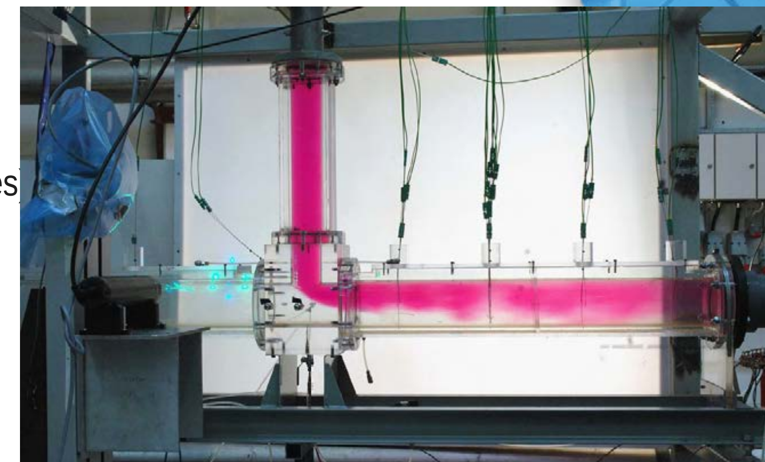
- Overbars – ensemble average
- Solve Poisson eq. for single pressure

$$\nabla^2 \left(\overline{p}^{n+1} - \overline{p}^n \right) = \nabla \cdot \sum_k \left(\alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k \right)^* / \Delta t$$

- Project velocities to div-free subspace

$$\overline{\mathbf{v}}_k^{n+1} = \overline{\mathbf{v}}_k^* - \frac{\Delta t}{\alpha_k^{n+1} \rho_k^{n+1}} \left(\alpha_k^{n+1} \nabla p^{n+1} - \alpha_k^n \nabla p^n \right)$$

Verification, Validation, and Uncertainty Quantification



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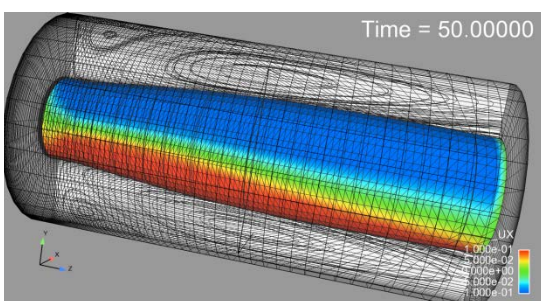
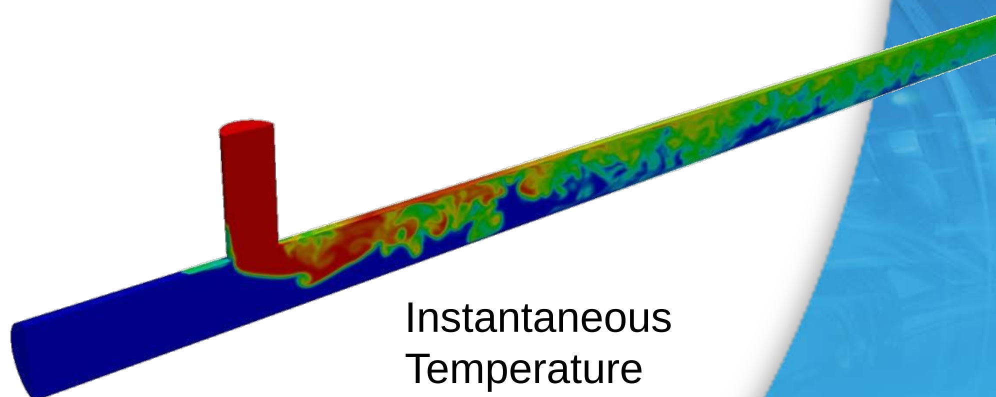




Instantaneous Temperature

In a nutshell...

- Initial multi-phase flow capability in place
- Fully-implicit time marching in place, exercised for single-phase

Milestone accomplishments

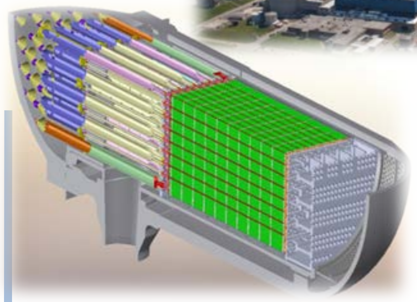
- Multi-field flow:
  - *N* volume fractions, momentum, and energy equations integrated
  - Coupling (at this time) via volume fractions and single pressure
  - No inter-field mass, momentum, or energy transfer (next months)
  - Extended user input-deck
  - <u>Demonstration:</u> proof-of-concept calculations
- Fully-implicit time marching:
  - Projection-method as preconditioner to implicit scheme with Picard iterations
  - Provides stability, removes any time step size limitation, 2nd order in time
  - Crucial for stiff phase-coupling terms
  - Next: Newton method (to reduce number of Picard iterations) + multi-field
  - <u>Demonstration:</u> proof-of-concept calculations

Advanced Modeling Applications (AMA)

Driving development of VR to support real-world applications

Objectives and Strategies

- Establish CASL's M&S needs for achieving plant power uprates, life extension, and higher burnup fuels
- Ensure that CASL research and development (R&D) meets the needs and requirements of the stakeholders
- Engagement with regulatory authorities to enable future application of the results
- Leverage industry contribution to include en users in the development and evaluation process



Requirements Drivers

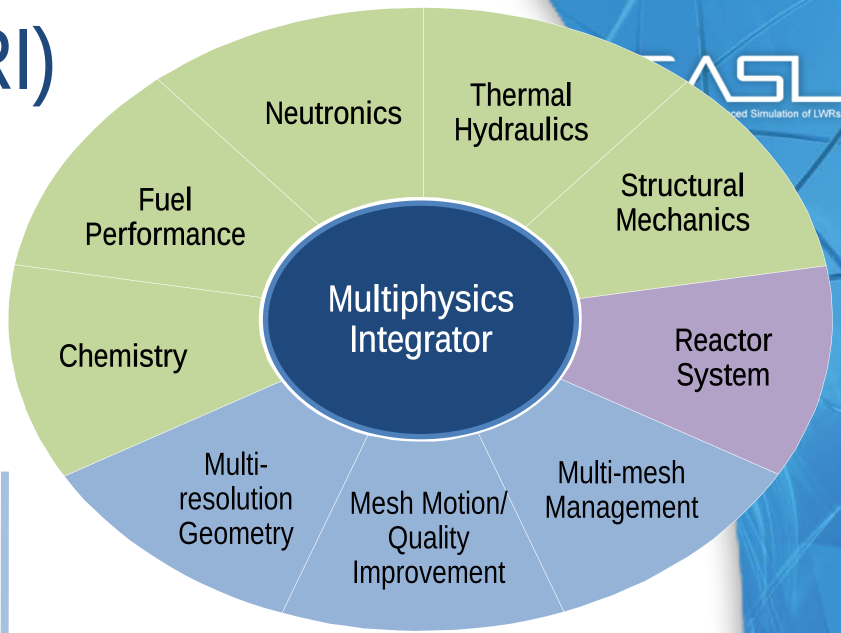
- Connect end uses with CASL R&D by:
  - Providing a conduit for end-user input
  - Defining requirements for and performing capability assessments of the Virtual Reactor
  - Integrating with other DOE and NRC programs that support improvements in light water reactors
- Simulating operational and safety challenge problems and physical nuclear reactors

Outcomes and Impact

- AMA will demonstrate the applicability of VERA's capabilities to current industry challenges through successful application to the CASL challenge problems
- VERA will be benchmarked with operational data from commercial reactors
- AMA will support early deployment for industry partners through CASL test stands.

Virtual Reactor Integration (VRI)

Bridging the gap between research and engineering.



Objectives and Strategies

- VRI will deliver a suite of robust, verified, and usable tools within a common multi-physics environment for the design and analysis of nuclear reactor cores, with quantified uncertainties.
- Agile software development processes and partner strengths in large-scale code development are key to meeting VRI challenges.

Requirements Drivers

- VRI is the conduit between targeted research and engineering analysis
  - guided by current and future simulation and workflow requirements developed with AMA
  - in collaboration with VUQ on improved tools and methodologies for quantification of uncertainties,
  - research, development, and Integration of advanced capabilities with the MPO, THM, and RTM focus areas.

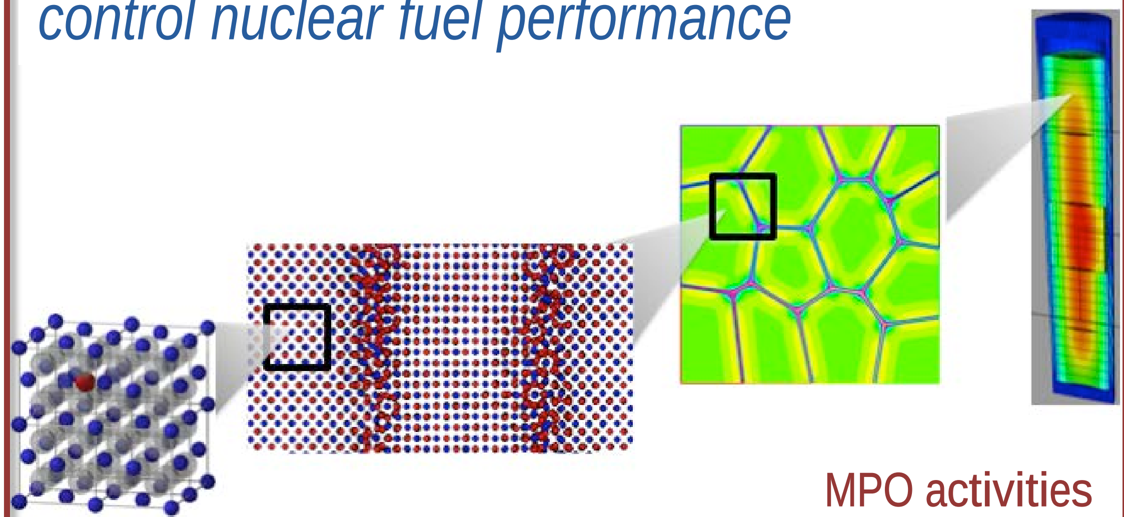
Outcomes and Impact

- VRI will deliver the environment described above, portions of which will be openly-available.
- VRI success can be measured by
  - measurable use of VERA by industry partners in understanding and mitigating key issues
  - downloads of the open portion(s) of VERA
- VRI success will improve industry analysis, bringing coupled, high-fidelity simulation into engineering workflows.

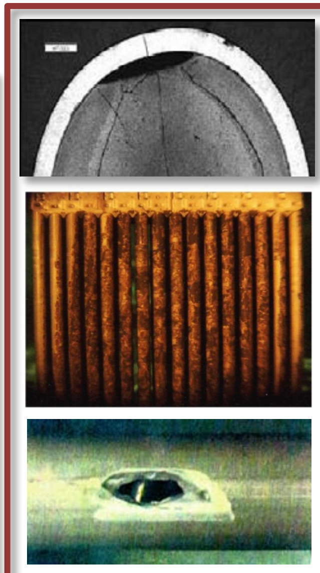
Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

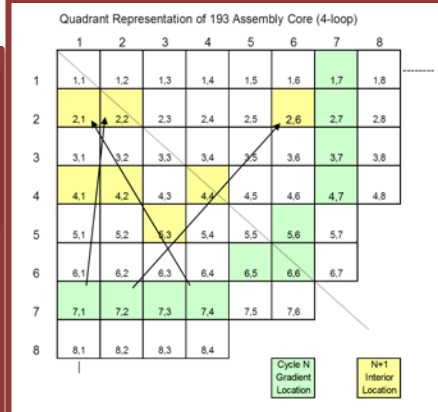
Challenging, multiscale processes control nuclear fuel performance



MPO activities



CASL Challenge Problems

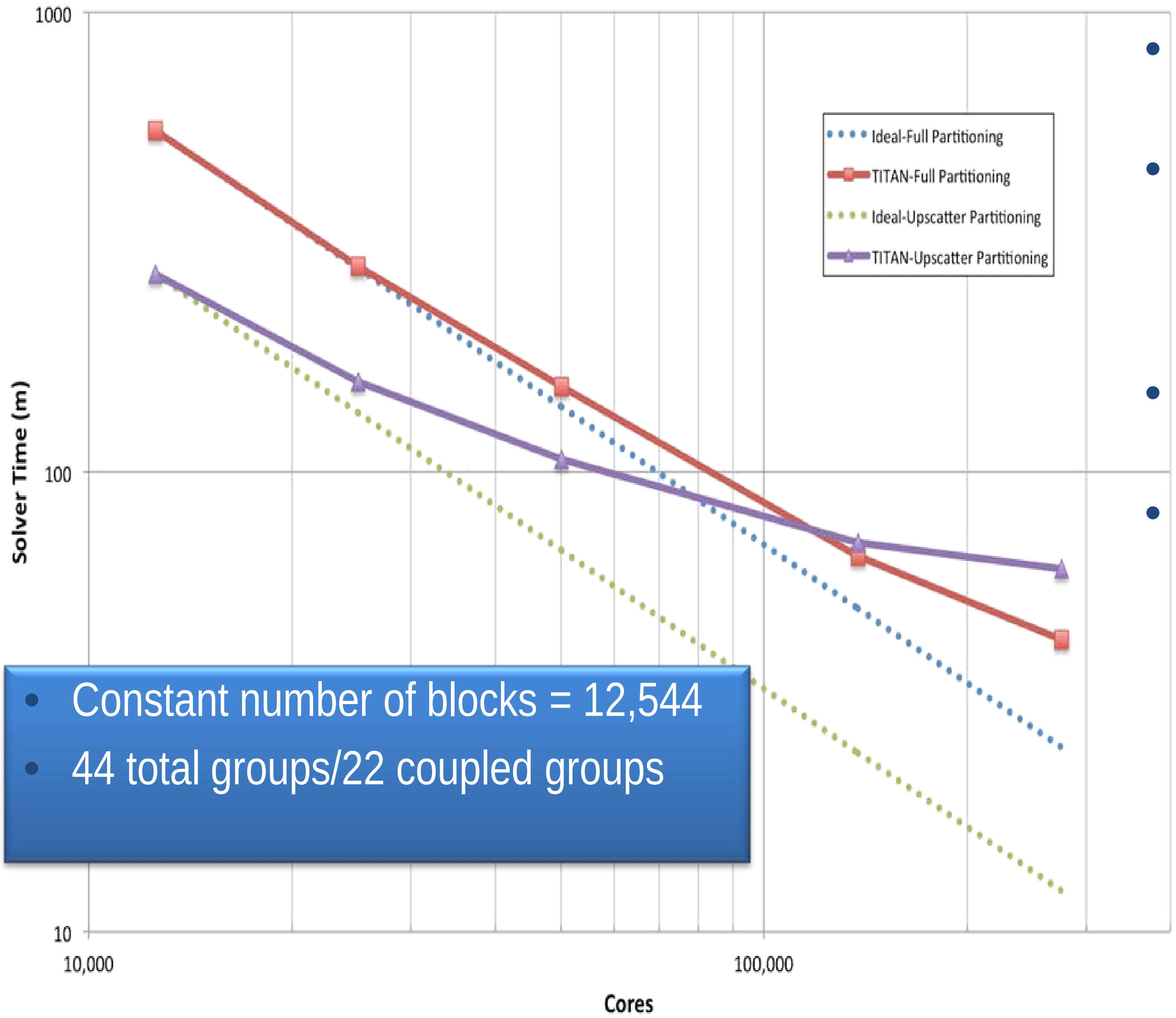


VERA CS (Core Simulator)

- Deliver engineering-scale fuel performance models and physics-based constitutive and behavioral models to CASL fuel and structural materials related challenge problems
- Improved physics and chemistry insight delivered via constitutive relations and behavioral models

- VERA CS (Core Simulator) will be used to highlight assemblies of interest, and provide conditions of specific fuel rods.

Performance at scaling on ORNL Titan (Cray XK6)

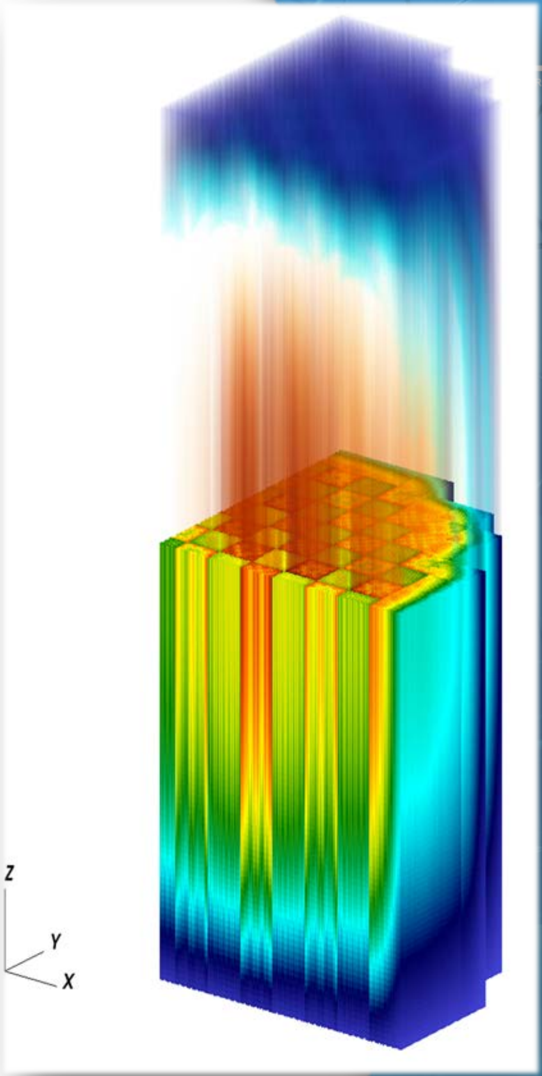


- Constant number of blocks = 12,544
- 44 total groups/22 coupled groups

- full partitioning scales well to 275K cores
- improved interconnect + reduce-scatter have dramatically reduced global reduction cost
- upscatter partitioning more efficient at lower set counts
- roll-over occurs between 4 and 11 sets (5 and 2 groups per set) where serial work in GS solver dominates

Is it hopeless?

- according to industry partners, a fully-consistent 3D calculation in 1 week would be acceptable
  - factor of 7 (20 EF/s)
- valuable insight possible without reproducing full 2D fidelity
  - factor of 150-200 (100 PF/s)
- utilize GPUs
  - if current projections hold, we can potentially get a factor of 3x-4x improvement by executing sweep kernels on the GPU
- further solver research (multigrid-in-energy) shows promise for reducing iteration counts as well



a 30-40 PF/s machine could allow fully-consistent, 3-D neutronics simulations

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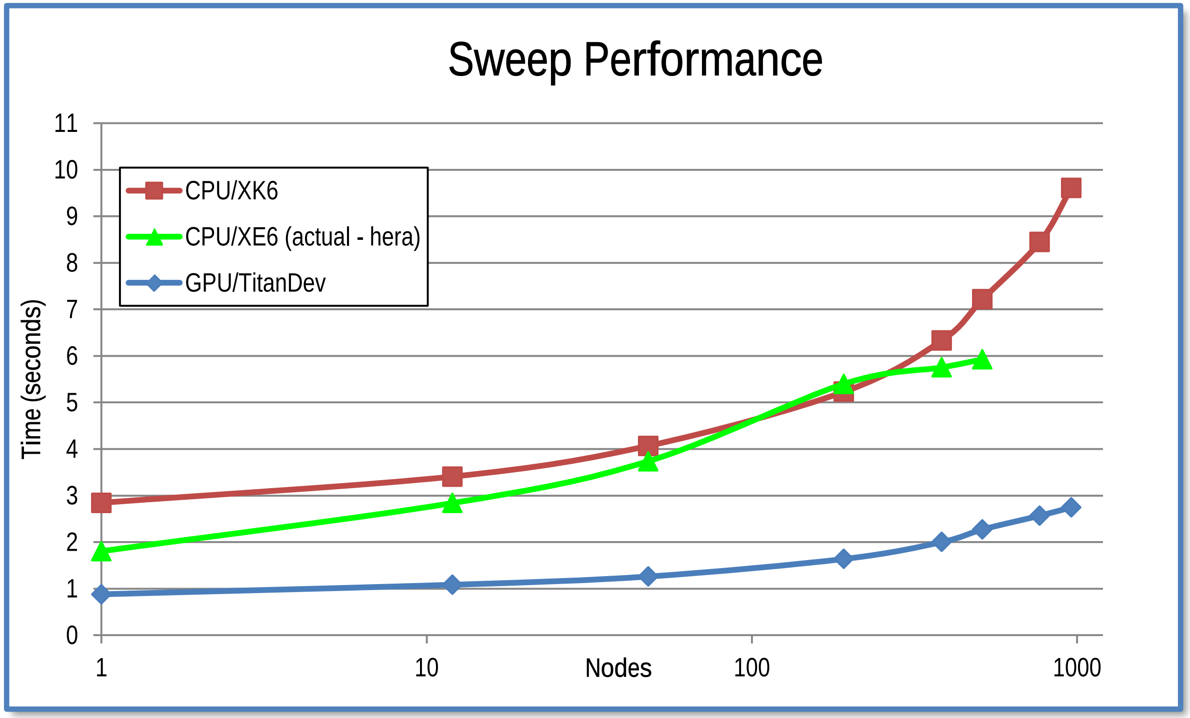
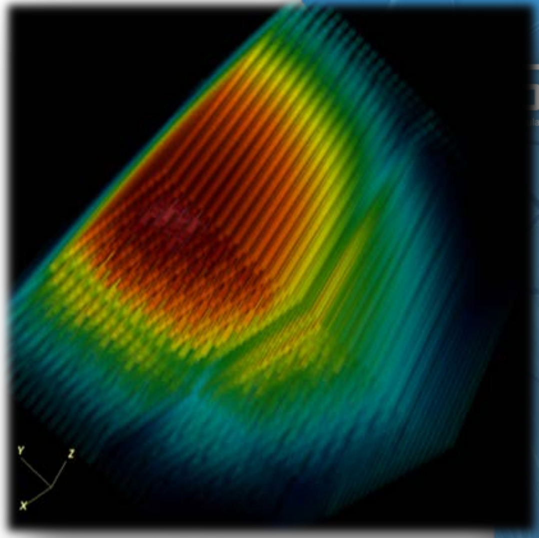
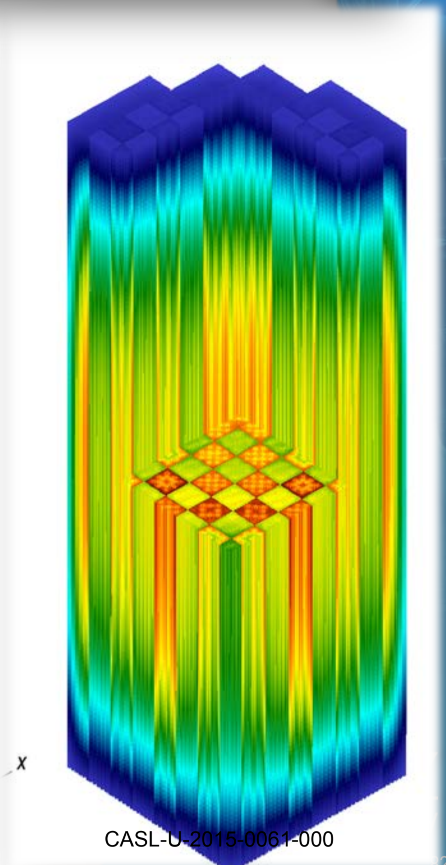
GPU Sweep Kernel



Performance Improvement factors		GPU
		XK6 Fermi
CPU	*XK6 / Interlagos*	3.5
	XE6 / dual Interlagos	3.3

- Krylov multigroup solvers allow space-angle sweeps to be performed over all groups concurrently
- ideal for exploiting thread-based concurrency on GPUs
- space-angle sweep for all groups on GPU





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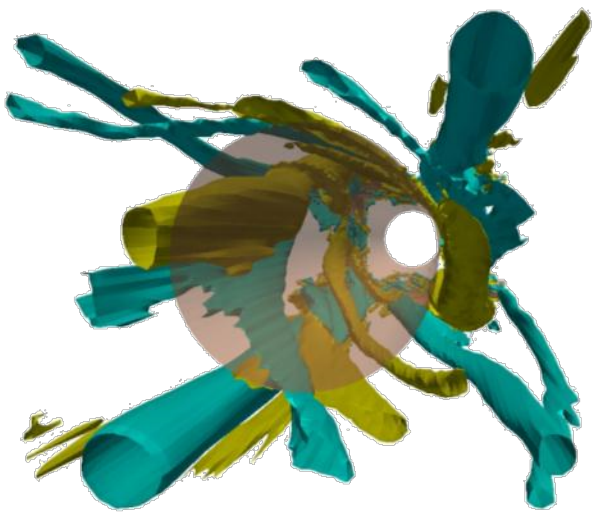
Turbulent Flow in Grid-to-Rod-Fretting

Scoping simulations – towards optimal resolution

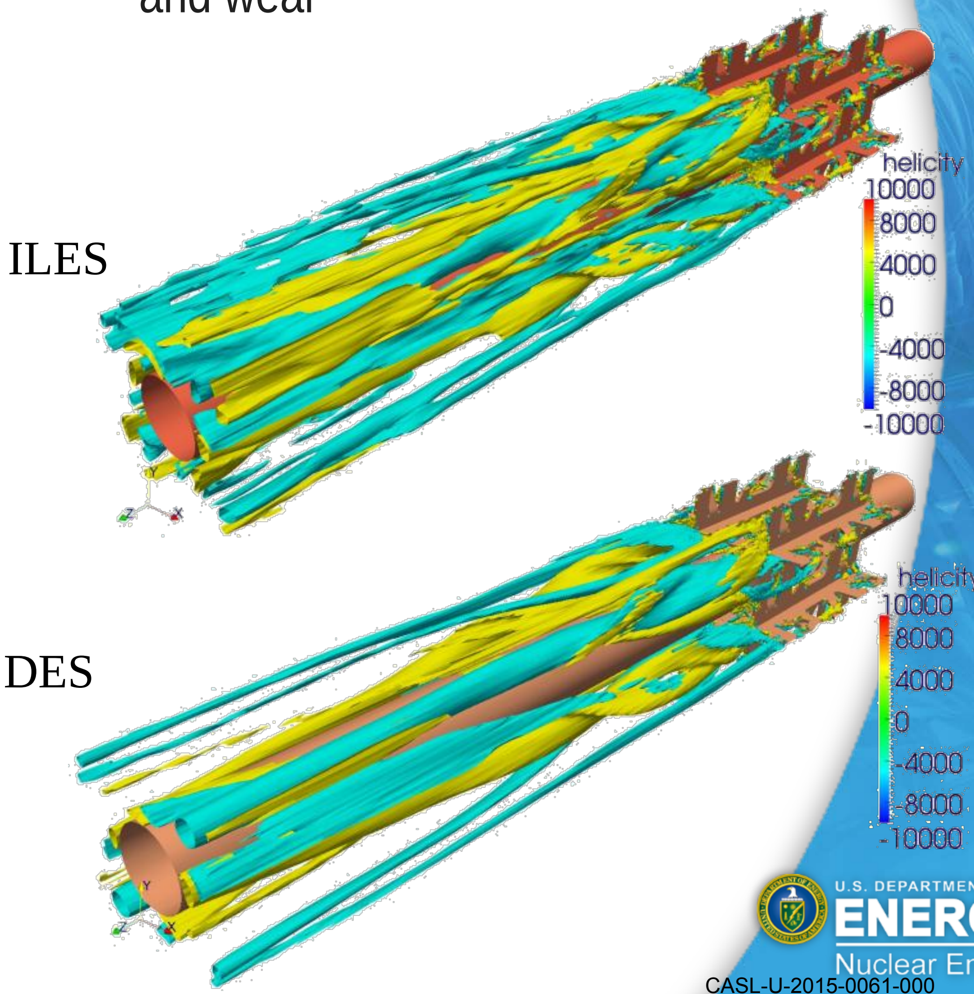
<u>Helicity isosurfaces</u>

- All models capture some level of detail in the longitudinal vortical structures and swirl
- How much is "enough"
- Towards self-adapting Models

- Ultimate goal is accurate turbulent excitation forces to predict rod vibration and wear



End-view of fuel rod showing swirl in coherent structures



CASL-U-2015-0061-000

Verification, Validation, and Uncertainty Quantification

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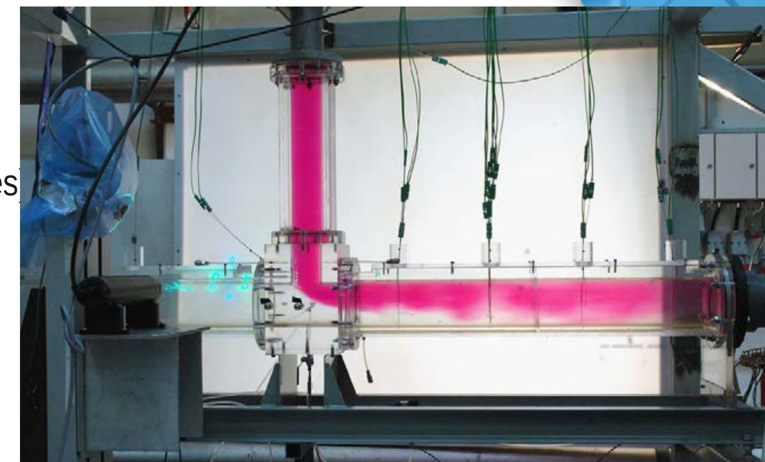

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  - Fully-coupled, Newton-Krylov Stabilized FEM
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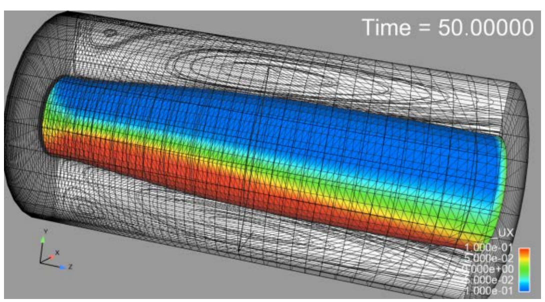
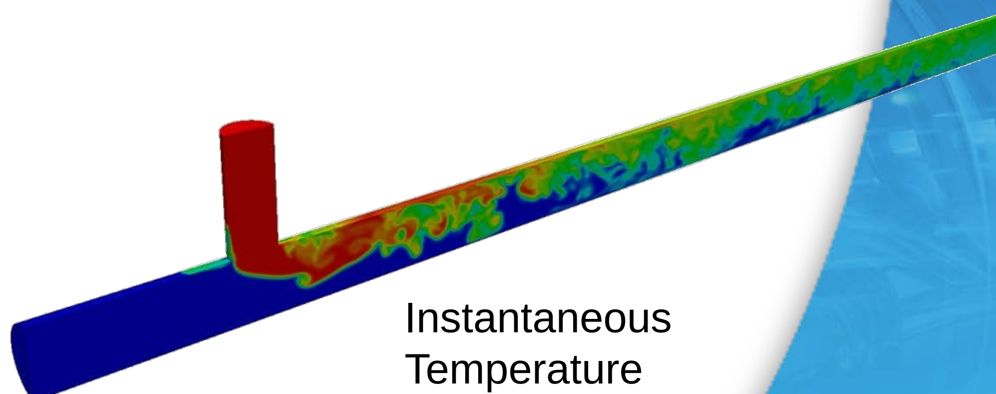
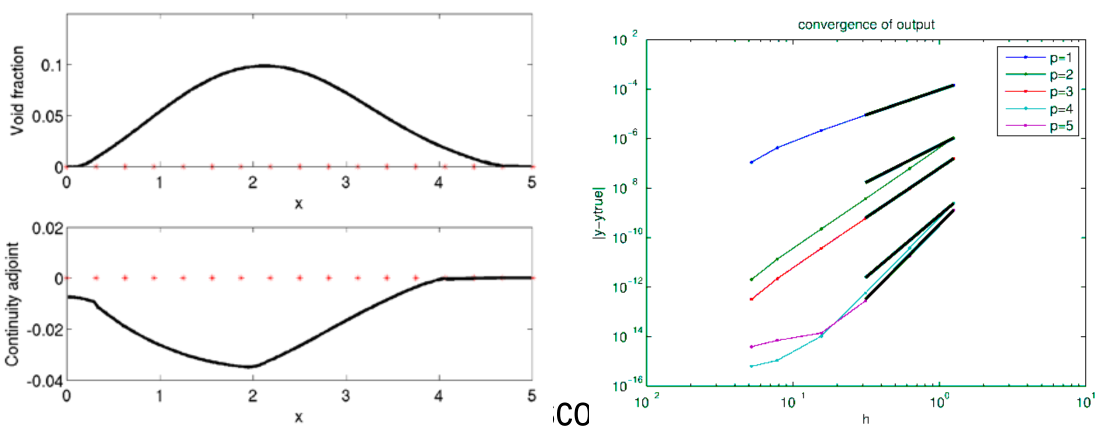




Instantaneous Temperature

Verification, Validation, and Uncertainty Quantification (Cont.)

- Adjoint-based UQ for THM (Fidkowski, U. Michigan): Multiphase thermal-hydraulics models contain a large number of not-so-well known parameters and numerical error. This effort is developing and applying methods for efficiently quantifying these errors and uncertainties through adjoint methods.
- Sample convergence and primal/adjoint solutions of 1D code

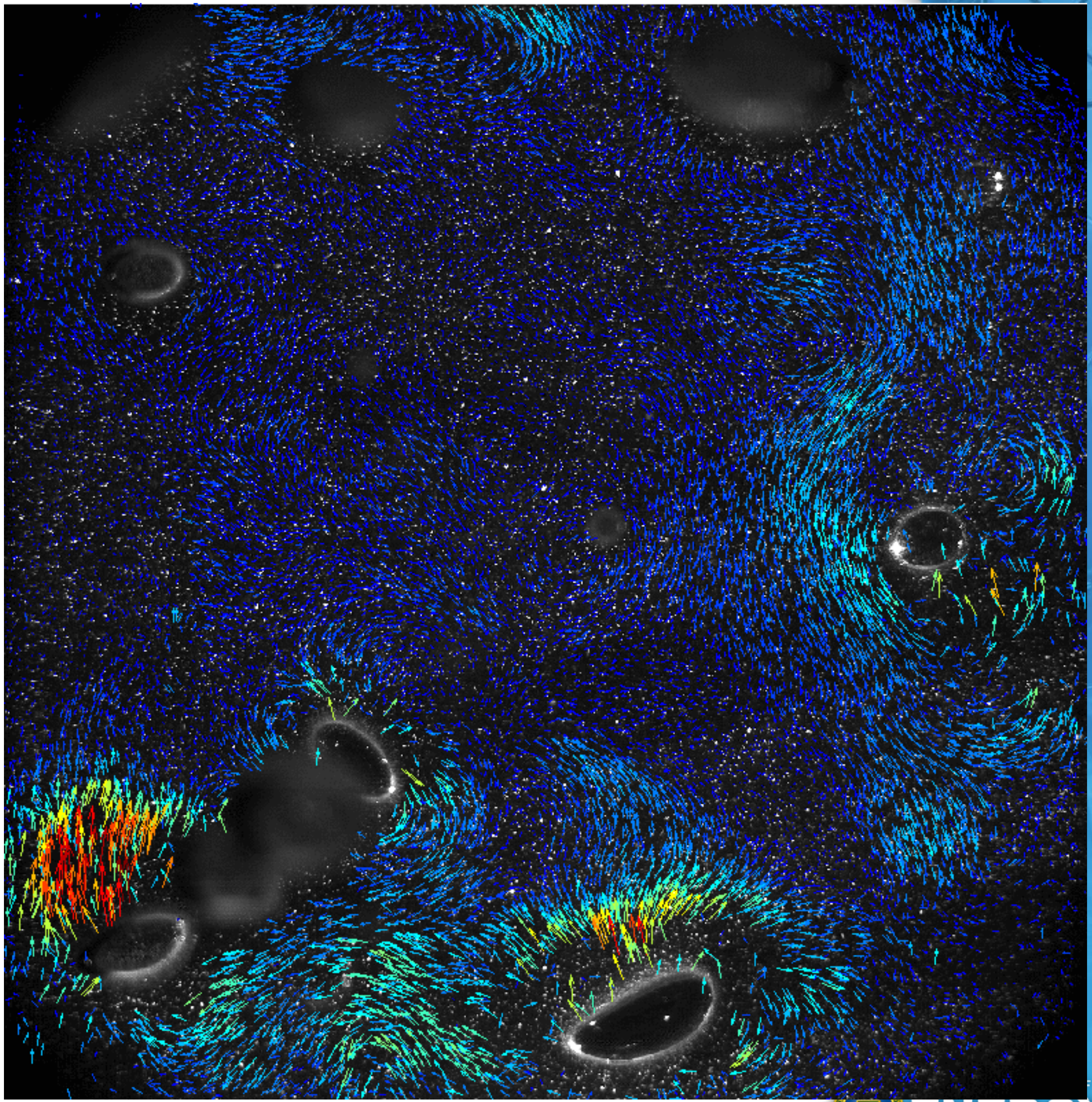


  - co comparisons to PATHS ongoing)
  - Discrete adjoint for 1D code implemented and verified
  - Adjoint-based output error estimation implemented/verified
  - 1D mesh adaptation working, driven by output error estimates

Validating ITM Methods

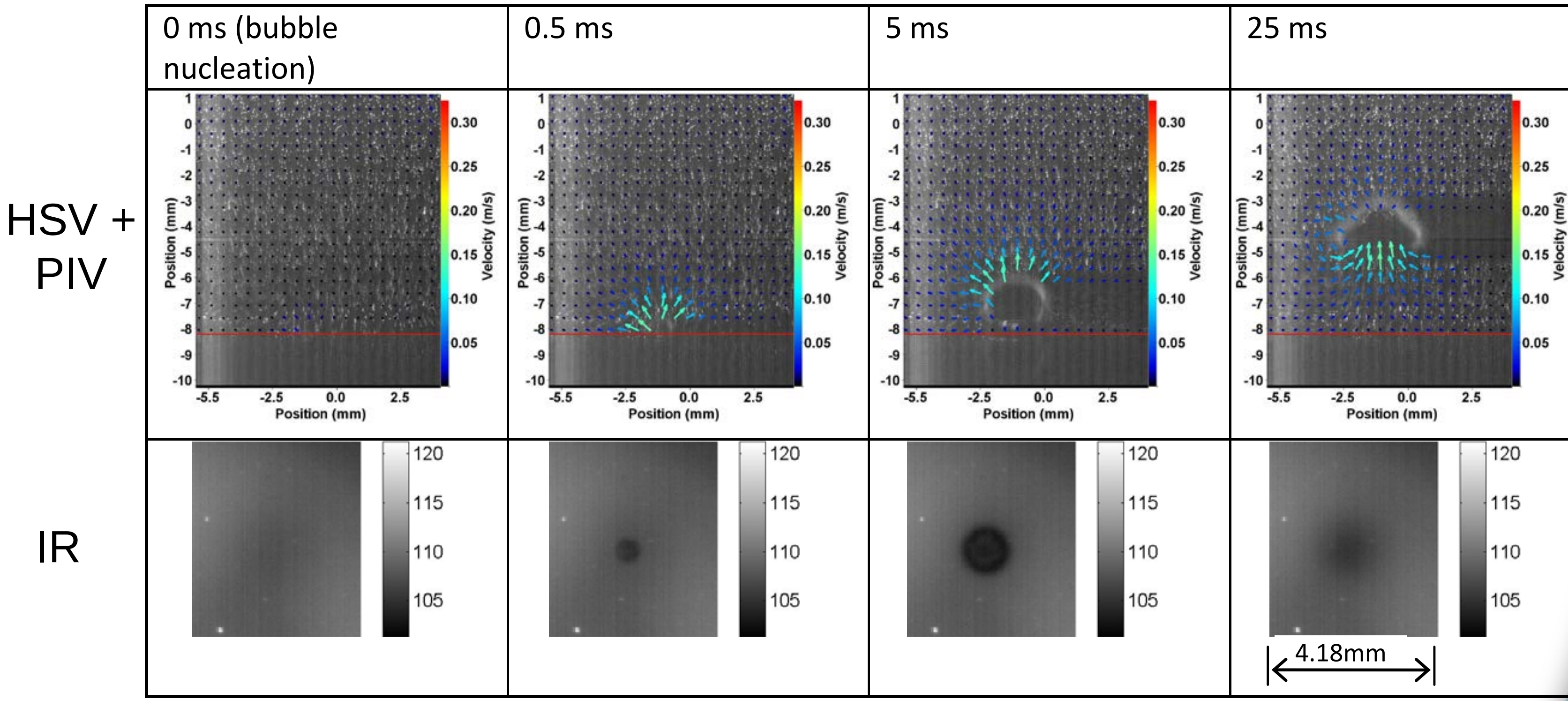
Two-phase Flow PTV (Hassan, TAMU)

- The use of fluorescent particles and optical filters allowed for an efficient discrimination tool between the two phases.
- The liquid phase is analyzed.
- Note that no vectors exist within the bubble domain.



Pool Boiling (data)

Used synchronized high-speed video (HSV), infrared (IR) thermography and PIV to generate experimental database for validation of ITM Boiling

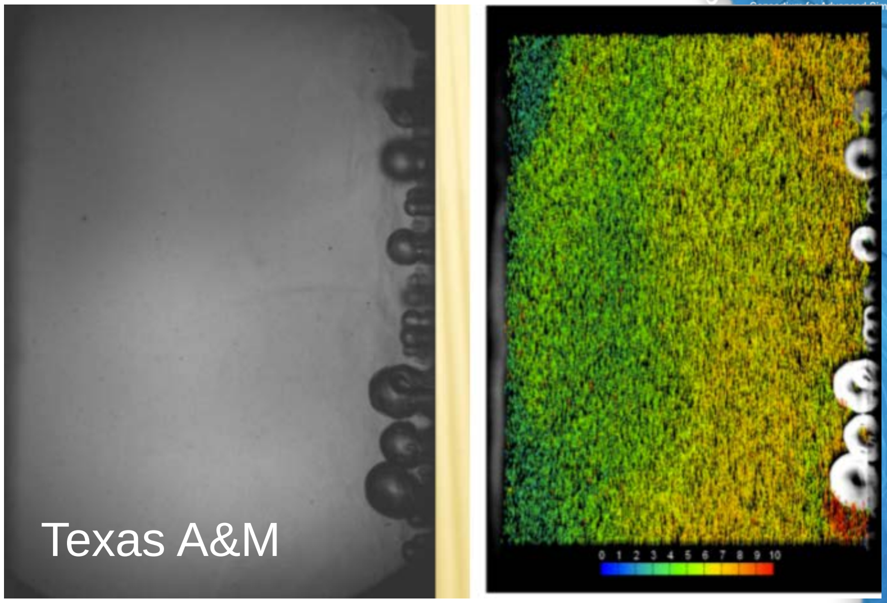


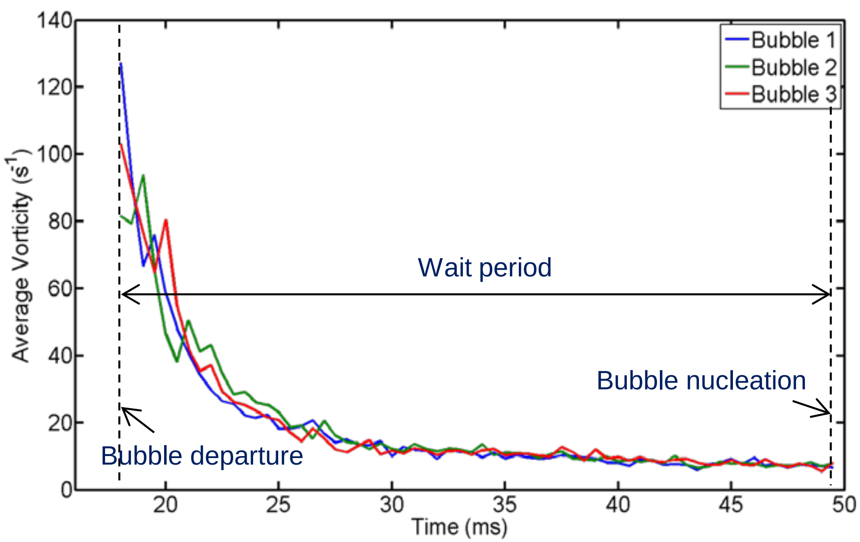
- **HSV gives bubble shape, size and departure frequency**
- **IR gives temperature distribution, wait and growth period**
- **PIV gives velocity distribution**

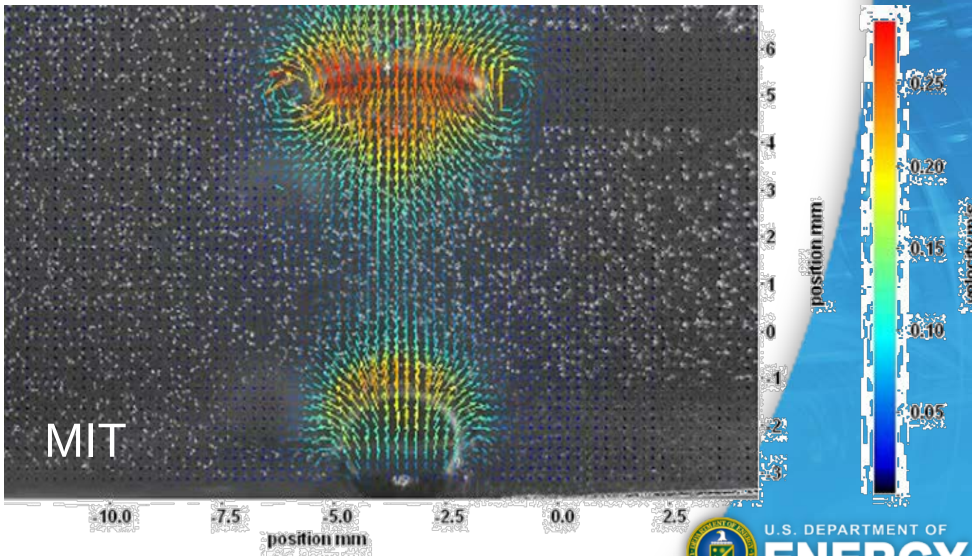
“Doubling up” on boiling experiments

MIT + Texas A&M

Quantitative analysis of PIV videos generates considerable insight into physical phenomena

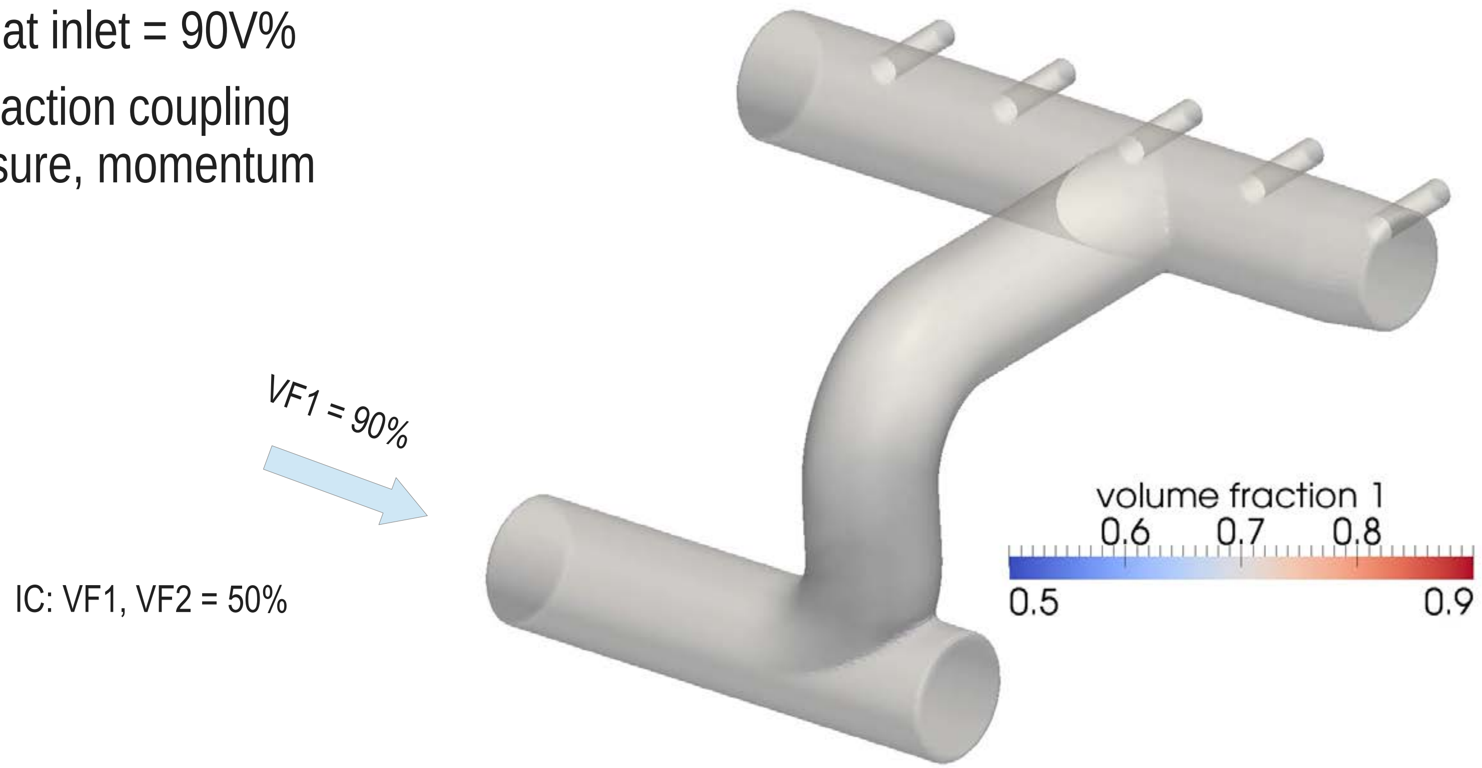






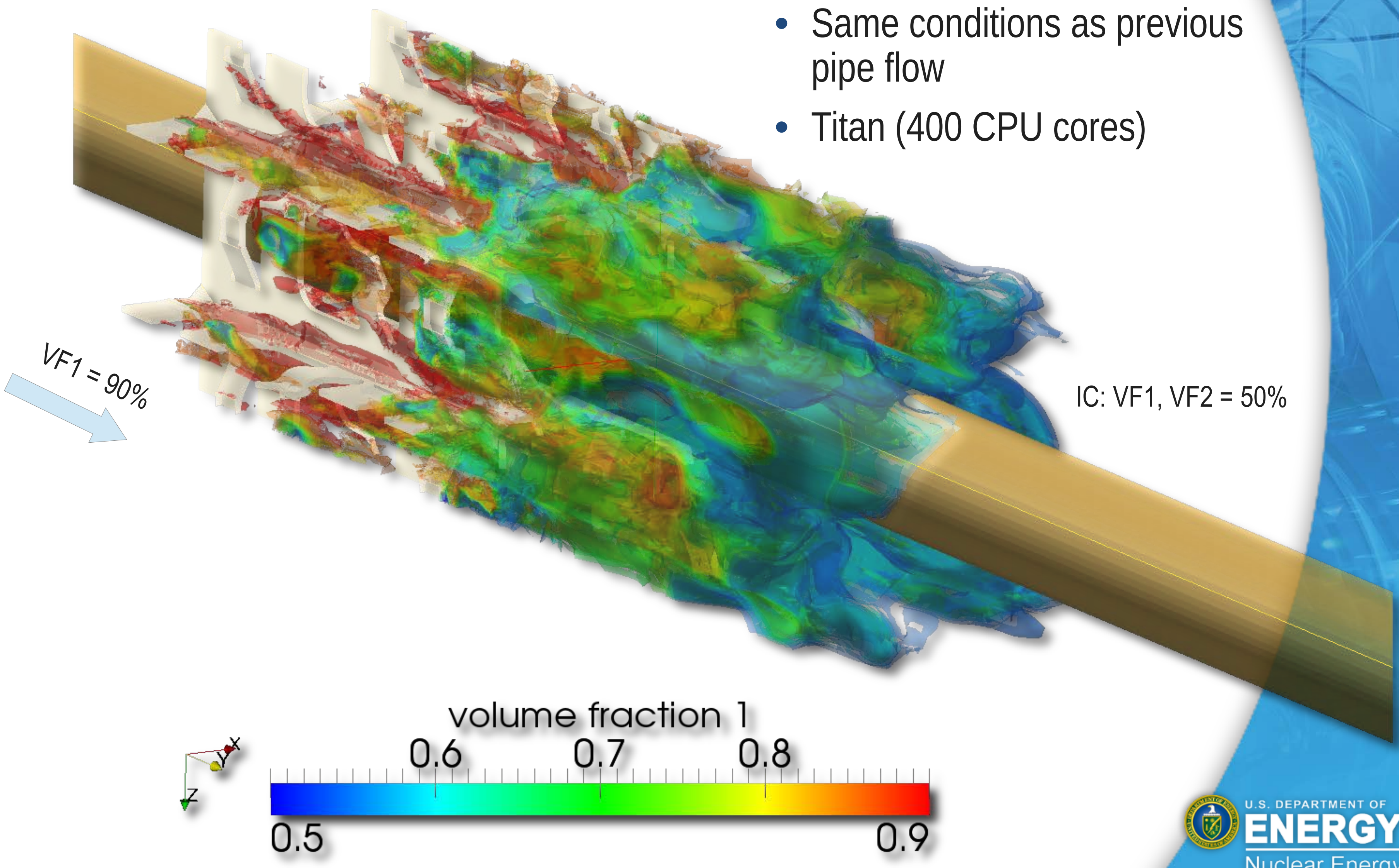
MultiPhase Flow – Modified 2nd-Order Projection Algorithm

- Hybrid mesh generated by Hexpress/Hybrid
- 2 fields, same densities
- Coupled through single pressure via projection algorithm
- IC: VF1: 50%, VF2:50% (both fluids present)
- BC: VF1 at inlet = 90V%
- Volume-fraction coupling with pressure, momentum



MultiPhase Flow – Complex Geometry, Reactor Flow Conditions

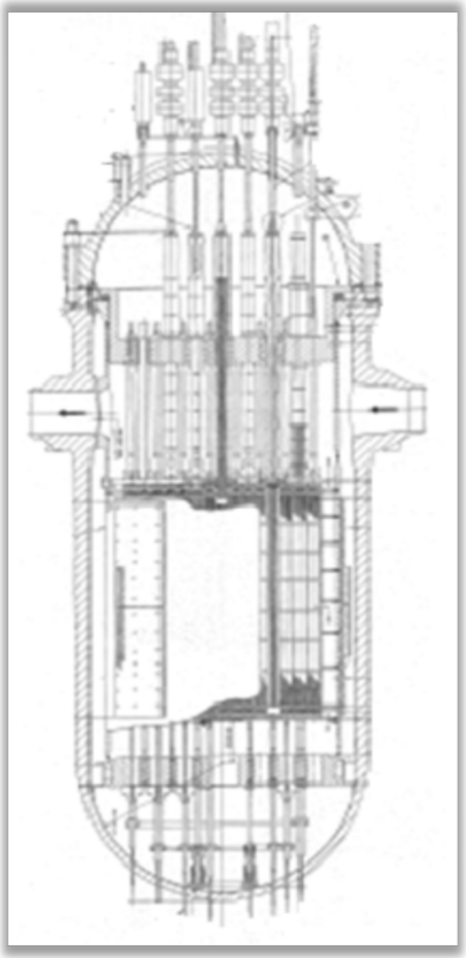
- V5H GTRF 3x3 2M cells
- Same conditions as previous pipe flow
- Titan (400 CPU cores)



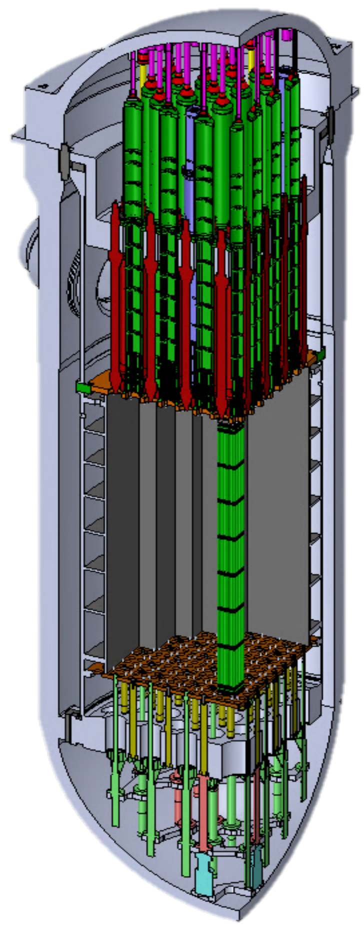
4-Loop Westinghouse PWR Multi-Physics Model Development

Consortium for Advanced Simulation of LWRs

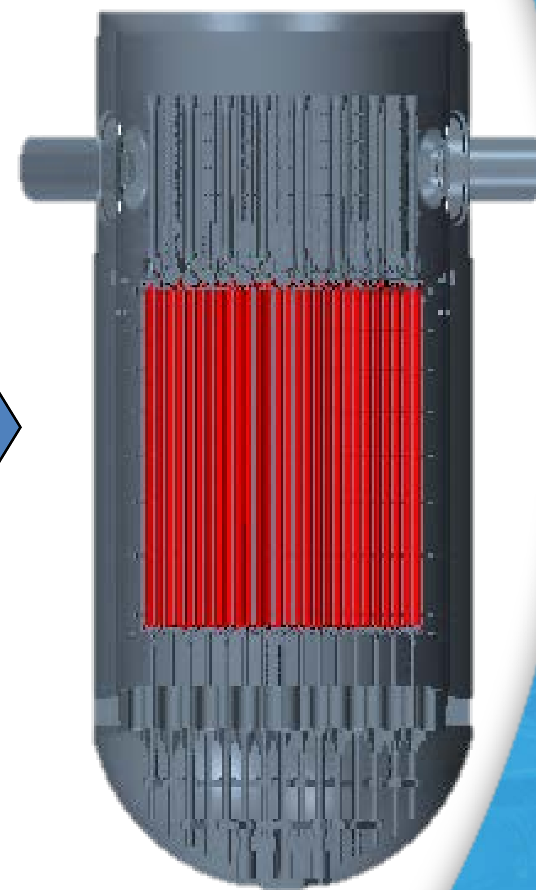
- RPV ID 173”, 193/4 Fuel Assemblies,13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; 1.2 billion cells



Drawings



CAD Model



CFD Model

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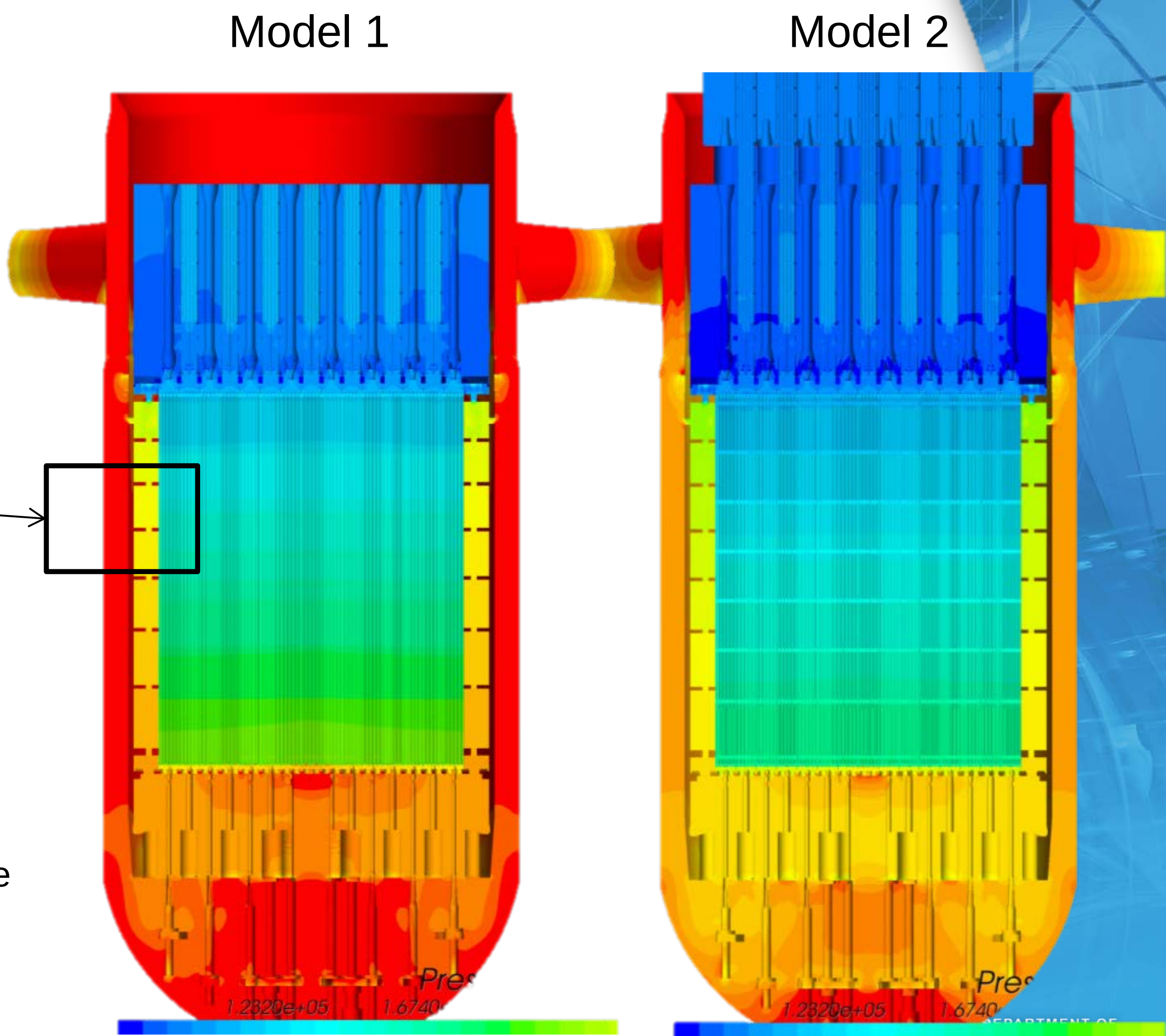
A "Typical" Multi-Scale Problem

Full-core performance is affected by localized phenomena

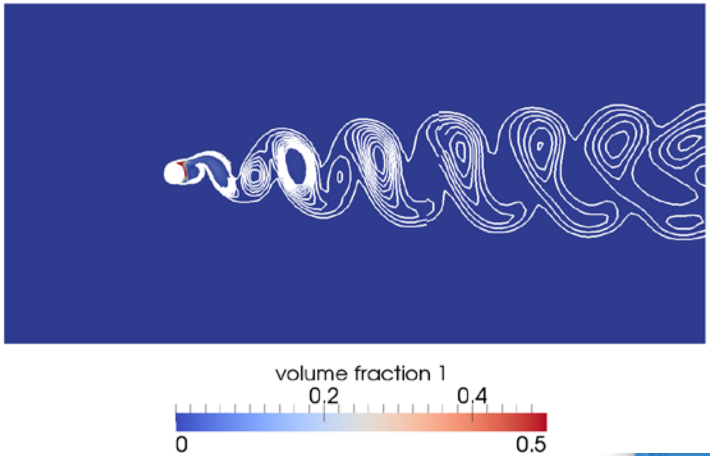
- Local T&H conditions such as pressure, velocity, cross flow magnitude can be used to address challenge problems:
  - o **GTRF**
  - o **FAD**
  - o **Debris flow and blockage**
- The design TH questions under normal operating and accident conditions such as:
  - o **Lower plenum flow anomaly**
  - o **Core inlet flow mal-distribution**
  - o **Pressure drop**
  - o **Turbulence mixing coefficients input to channel code**
  - o **Lift force**
  - o **Cross flow between fuel assemblies**
  - o **Bypass flow**
- The local low information can be used as boundary conditions for micro scale models.

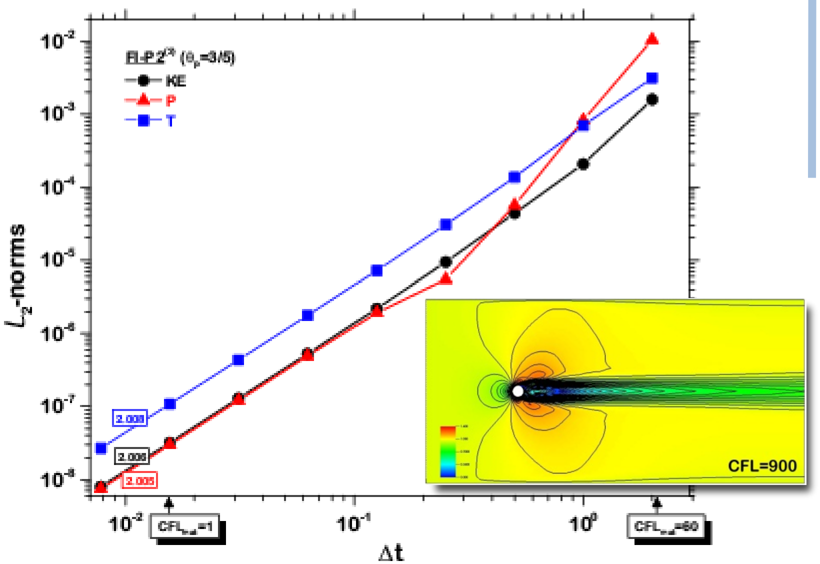


Development of Advanced Multiphase Thermal Hydraulics Capability

Multi-Field Flow, Fully Implicit Time-Marching

- Initial multi-field flow capability implemented in Hydra-TH
- Extended semi-implicit projection algorithm to *N* flow fields
- Coupling (at this time) via volume fractions and single pressure
- Derived and implemented a fully-implicit projection-based Picard time-marching technique





Key personnel: Bakosi, Christon, Pritchett-Sheats (LANL), Nourgaliev (INL)

Milestone Accomplishments

- The efficiency and accuracy of projection methods for incompressible flows are extended to multi-phase flow
- Fully-implicit time-marching provides stability, removes any time step size restrictions, and second-order accurate in time

Future Work

- Newton-based implicit time-marching to reduce the number of iterations required for Picard
- State-of-the-art algorithms for multi-phase thermal-hydraulics with various options for inter-phase mass, momentum, and energy transfer