CASL Energy Innovation Hub: Delivering Multi-scale Multiphysics Solutions for Commercial Nuclear Industry Challenges

Jess C. Gehin, CASL Director

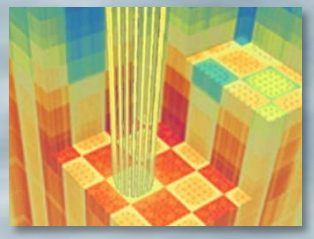
Brian Kendrick, CASL FMC Focus Area

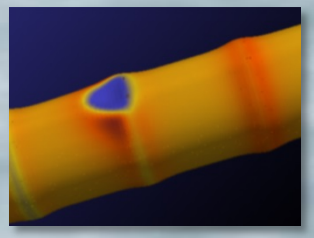
Kevin Clarno, CASL PHI Focus Area

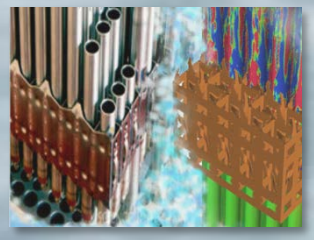
Jeffrey Secker, CASL CRUD CPI

ANS Webinar

October 21, 2015







The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

U.S. DEPARTMENT OF ENERGY

What is the Consortium for the Advanced Simulation of Light Water Reactors?

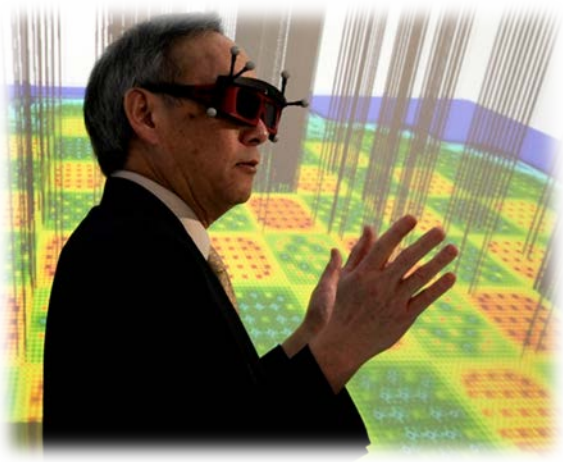
CASL is the first U.S. DOE Energy Innovation Hub connecting fundamental research and technology development through an integrated partnership of government, academia, and industry.

Our primary objective is to provide leading-edge modeling and simulation (M&S) capability to improve light water reactor performance.

With a vision for safer and more productive commercial nuclear power production via comprehensive science-based predictive M&S technology.

What is a DOE Energy Innovation Hub?

- Established by Former DOE Energy Secretary Steven Chu
- Modeled after the scientific management characteristics of Manhattan Project and AT&T Bell Labs:
  - Addressing critical problems
  - Combines basic and applied research with engineering
  - Integrated team to take discovery to application
- Four Hubs are in operation



"Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges"
– *Steven Chu*

JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

JCESR JOINT CENTER FOR ENERGY STORAGE RESEARCH

CASL A DOE Energy Innovation Hub

CMI Critical Materials Institute AN ENERGY INNOVATION HUB

For more info: http://http://energy.gov/science-innovation/innovation/hubs

CASL is a National Laboratory, Industry, University Partnership

CASL Founding Partners

CASL Contributing Partners

THE UNIVERSITY OF TEXAS AT AUSTIN

THE UNIVERSITY of TENNESSEE KNOXVILLE

Pacific Northwest NATIONAL LABORATORY

ANATECH

ASCOMP MULTIPHASE FLOW SCIENCE AND TECHNOLOGY

CD-adapco

Core Physics, Inc.

THE UNIVERSITY of WISCONSIN MADISON

PENNSTATE 1855

AREVA

Imperial College London

The City College of New York

TEXAS A&M UNIVERSITY

GNF Global Nuclear Fuel A Joint Venture of GE, Toshiba, & Hitachi

SOUTHERN STATES ENERGY BOARD

UF UNIVERSITY of FLORIDA

THE UNIVERSITY OF TENNESSEE CHATTANOOGA

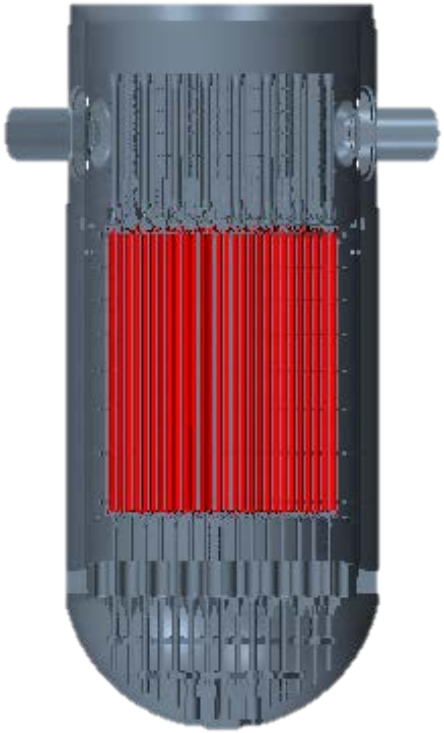
Rensselaer

UNIVERSITY OF NOTRE DAME

CASL The Consortium for Advanced Simulation of LWRs A DOE Energy Innovation Hub

CASL Scope: Develop and apply a "Virtual Reactor" to assess reactor operation and safety

- Deliver improved predictive simulation of Light Water Reactors
  - Focus on fuel, vessel, internals
  - First five year focus on PWRs, broadened to BWR and Light Water Small Modular Reactors
- Execute work in six technical focus areas to:
  - Equip the Virtual Reactor with necessary physical models and multiphysics integrators
  - Build the Virtual Reactor with a comprehensive, usable, and extensible software system
  - Validate and assess the Virtual Reactor models with quantified uncertainties



Focus on Addressing Challenge Problems to Drive CASL Development

Our Challenge Problems are Focused on Key Industry Reactor Performance Areas

Pellet-Clad Interaction

Predict Core Wide PCI Margin and Missing Pellet Surface PCI

Neutronics, Thermal-hydraulics, Fuel/Cladding Performance

CRUD

Predict CRUD Thickness Boron Uptake and Impact on Core Power Distribution (CIPS) and Cladding Corrosion (CILC)

Neutronics, Thermal-hydraulics/Fluid Flow, Chemistry

Core Operation Environment

Conditions for fuel rod depletion over operating cycle

Neutronics, Thermal-Hydraulics, Fuel Performance

Cladding Integrity Reactivity Insertion Accident

Predict Pellet-Clad Mechanical Interaction

Reactor kinetics, Transient fuel/cladding Performance

Cladding Integrity Loss of Coolant Accident

Predict Peak Clad Temperature and Oxidation Margin given Thermal-Hydraulic Conditions

Fuel/cladding performance

Departure from Nucleate Boiling

Predict DNB Margin for Steam Line Break and RIA and Predict Mixing & DNB

Neutronics, Thermal-hydraulics/Fluid Flow

Grid-to-Rod Fretting

Predict Fluid-Structure Excitation Forces, Grid Gap, and Cladding Wear

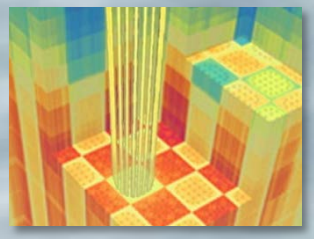
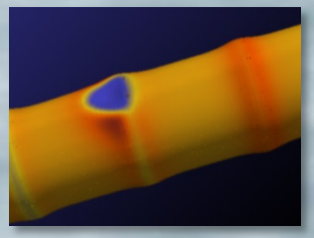
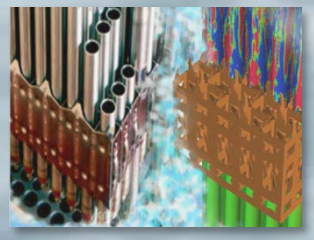
Fluid flow, Fuel/Clad Performance, Materials Performance

CASL Researchers Presenting Today

- **Brian Kendrick - Fuels, Materials and Chemistry Focus Area**
  - Multi-scale aspects of modeling CRUD including chemistry physics of CRUD deposition on to fuel rod surfaces
- **Kevin Clarno – Physics Integration Focus Area**
  - Multi-physics aspects of CRUD Challenge problem including integration of neutronics, thermal-hydraulics and CRUD chemistry
- **Jeff Secker – CRUD Challenge Problem Integrator**
  - Significance of the CRUD Challenge problem for industry and recent CASL simulation results

Overview of the CASL Crud Challenge Problem

Jeff Secker
Westinghouse Electric Company
October 21, 2015

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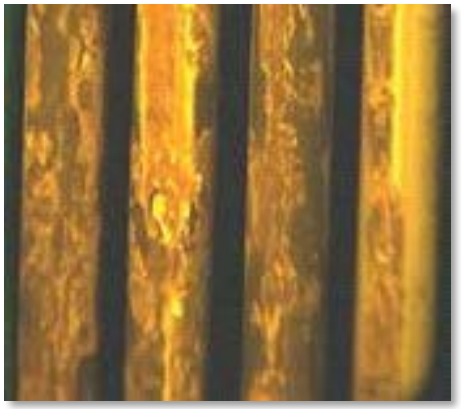
What is crud?

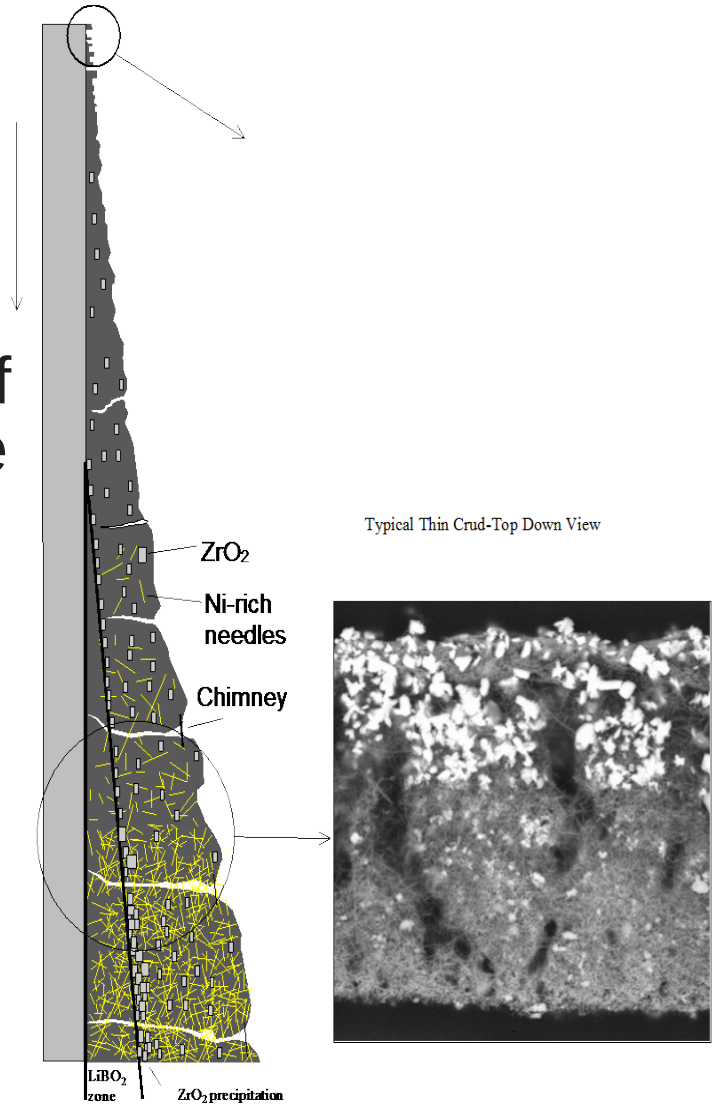
- Corrosion product materials from reactor coolant system surfaces that deposit on the fuel cladding are referred to as crud deposits
  - System materials are highly corrosion resistant – stainless steel and nickel based alloys
  - However, some corrosion does occur, and the resulting iron and nickel ions and oxides circulate in the reactor coolant system
  - The circulating corrosion products can then deposit on the reactor core
  - Crud deposition is strongly enhanced if the core is undergoing sub-cooled boiling
    - Steam bubbles on fuel cladding surface that then condense once they move in to the bulk coolant
    - Bulk coolant remains below saturation temperature, but fuel cladding surface temperature exceeds saturation in local hot spots



CRUD deposits

What is Crud Induced Power Shift (CIPS)?

- CIPS is an unexpected shift in axial power distribution toward the core inlet
- CIPS is caused by crud deposition in the upper spans of the fuel cladding surfaces of the reactor core in the presence of sub-cooled nucleate boiling
  - Sub-cooled boiling draws liquid containing iron and nickel corrosion products to the cladding surface, which is then deposited on the cladding since the steam does not contain iron or nickel

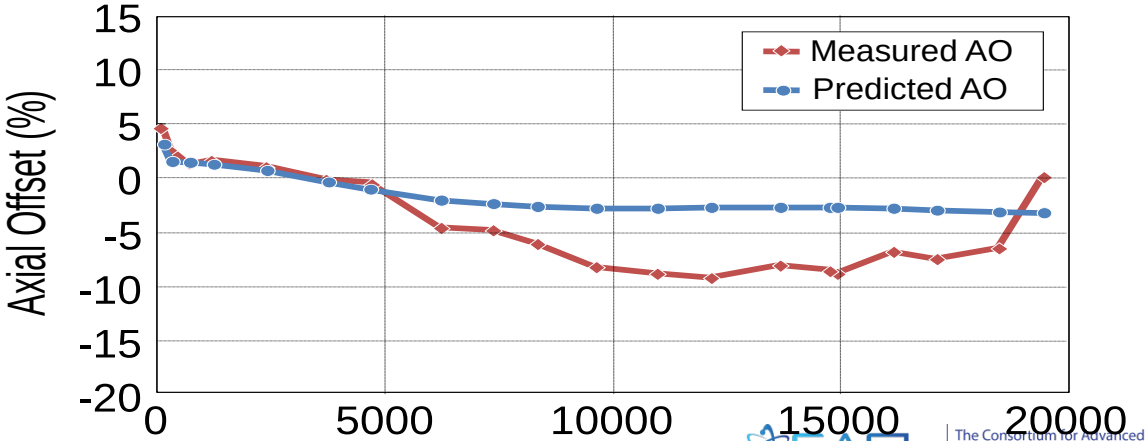


Typical thick AOA crud in cross section

What is Crud Induced Power Shift (CIPS)?

- The sub-cooled boiling process in the porous crud deposits lead to concentration of boric acid (used for PWR reactivity control) and lithium hydroxide (to maintain a neutral pH in the presence of boric acid) in the crud layer
  - Liquid containing B and Li is drawn into the crud by the sub-cooled boiling process, but the steam exits the crud without appreciable B or Li
  - If B and Li concentrate sufficiently within the crud deposit, a lithium boron compound (believed to be $Li_2B_4O_7$) will precipitate in the crud
- When boron is deposited in the upper spans of the core in the crud deposits, the flux distribution shifts toward the lower portions of the core that do not contain the neutron absorbing boron

$$\text{Axial Offset} = \frac{P^{top} - p^{bot}}{P^{top} + p^{bot}}$$



Effects of crud and boron deposition

- Unexpected shift in flux distribution leading to unpredictable core power distribution
- Core reactivity is altered
  - Can be transient effect as reactor power level is changed since $Li_2B_4O_7$ has retrograde solubility – more soluble at low temperatures when power is reduced, so it dissolves out of the crud
- Can cause loss of shutdown margin
  - Deposited boron present at 100% power, dissolves at 0% power
- Thick crud deposits have also led to fuel cladding failures (Crud Induced Localized Corrosion – CILC) as heat transfer is impeded

In extreme cases, CIPS required a PWR to operate at reduced power for many months

Multi-Physics Needs for CIPS modeling

- A robust neutronics code is needed to accurately predict the core power (heat flux) distribution
- The neutronics model also needs to model the effect on the neutron flux and core reactivity as crud and boron are deposited
- A thermal-hydraulics model is needed to model the local thermal conditions in the core including the sub-cooled boiling distribution
- A crud deposition model is needed to grow the deposits during plant operation
- A crud chemistry model is needed to predict the concentration of B and Li in the crud and the precipitation of $Li_2B_4O_7$

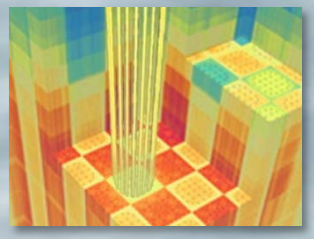
CRUD Modeling: MAMBA (FMC Advanced Model for Boron Analysis) development and applications

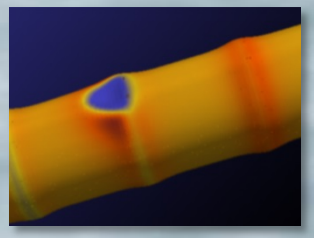
ANS Webinar

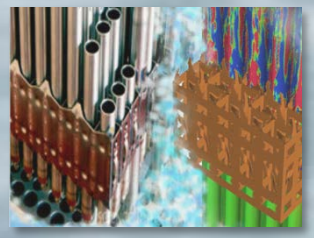
October 21, 2015

Brian Kendrick

Los Alamos National Laboratory







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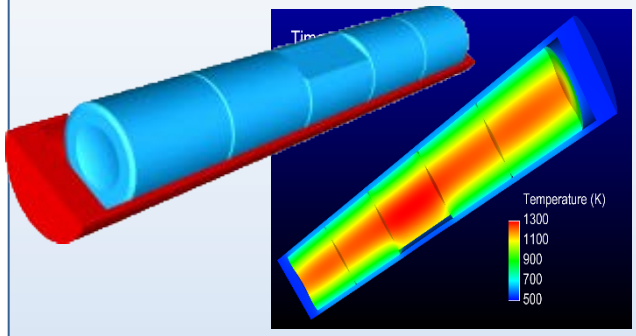
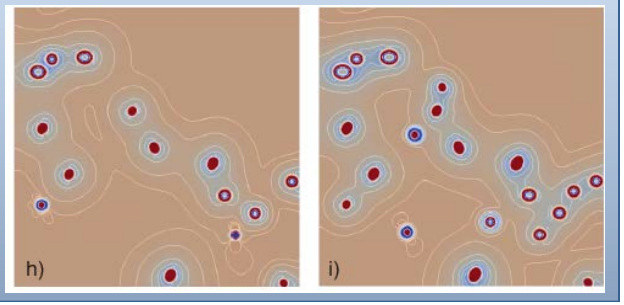
FMC (Fuels, Materials, & Chemistry) focus area: Delivers Engineering Scale Fuel Performance Models and Materials Physics-based Constitutive Models for CASL Challenge Problems

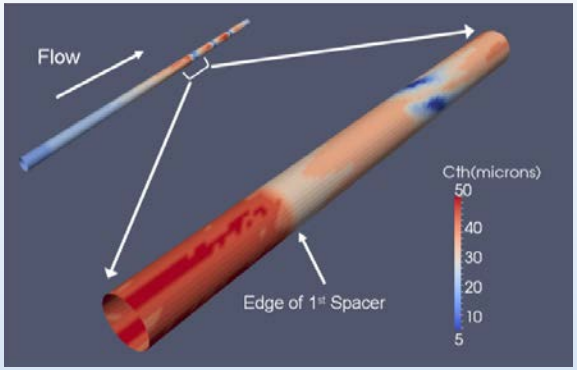
PCI
(Pellet Clad Interaction)



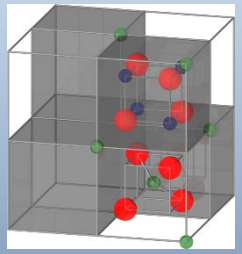
Peregrine
(Fuel Performance)

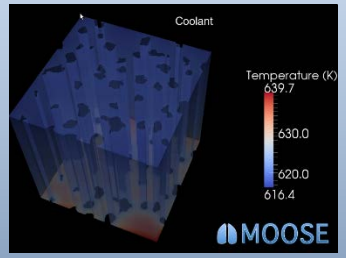


CRUD
(Chalk River Unidentified Deposit)

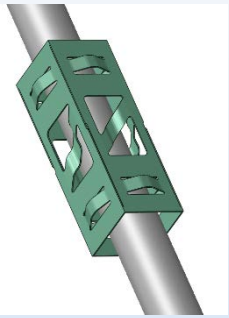


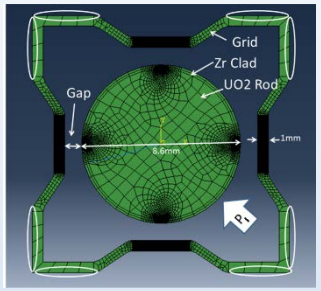
MAMBA
(FMC Advanced Model for Boron Analysis)



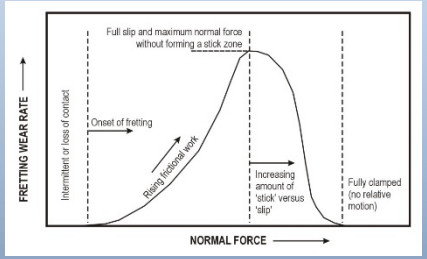


GTRF
(Grid To Rod Fretting)





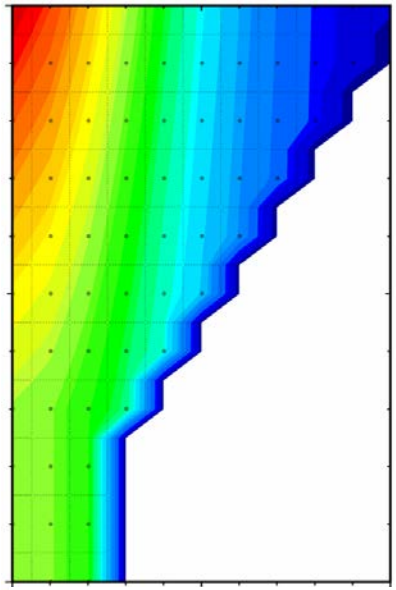
Structural Mechanics & WEAR MODELS



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

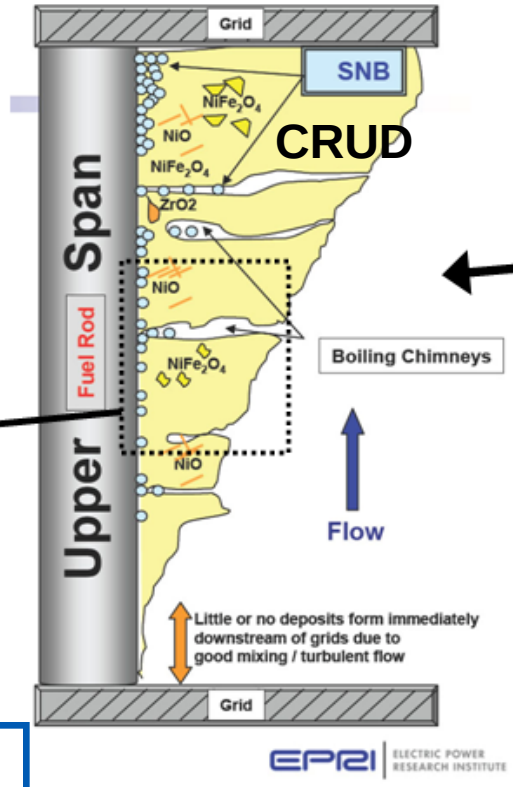
MAMBA's 3D Computational Grid Covers the Entire Surface of the Fuel Rods

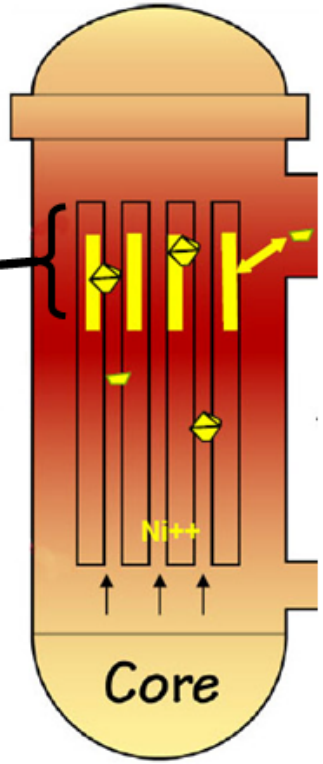
2D profile view



1 – 400 cm

50 – 150 microns





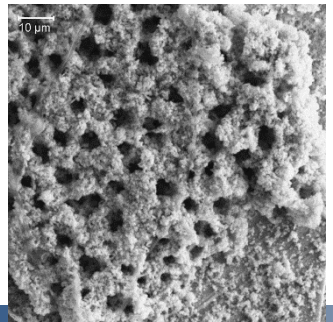
CRUD
(Chalk River Unidentified Deposit)

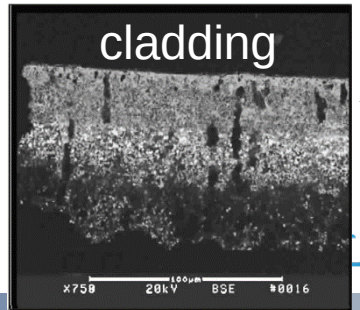
Industrial relevant issues:

1) Crud Induced Power Shift (**CIPS**)
2) Crud Induced Localized Corrosion (**CILC**)

CRUD

top view

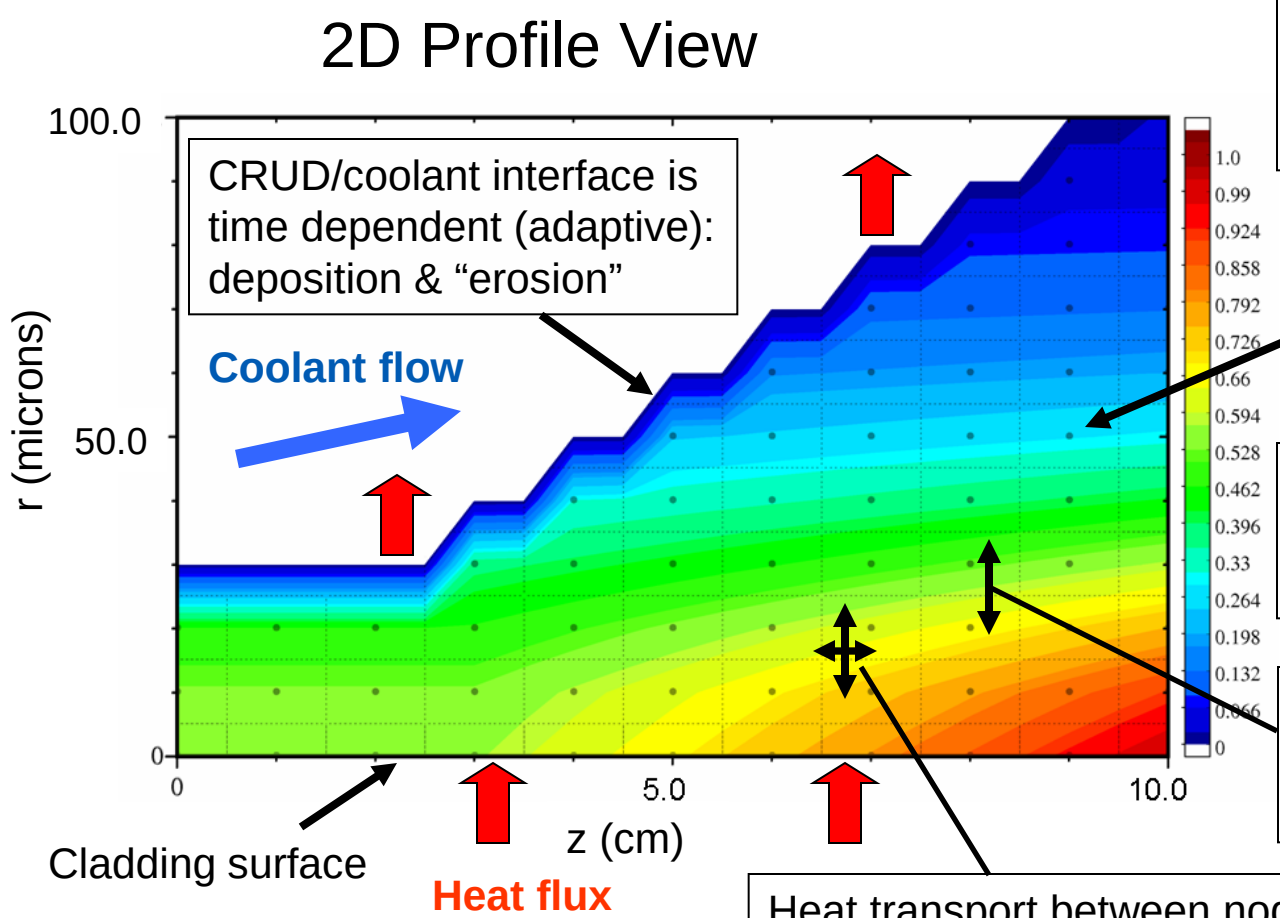




side view

80 microns

MAMBA's Computational Grid: Modeling CRUD is a Coupled Multi-Scale Multi-Physics Problem



CRUD/coolant interface is time dependent (adaptive): deposition & "erosion"

Colored contours: normalized boron concentration

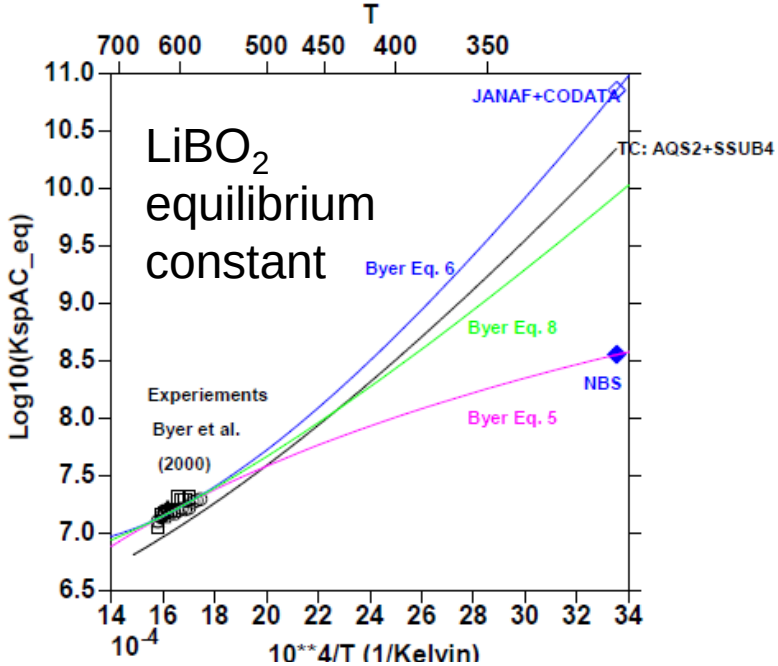
Compute node and volume element

Thermodynamics and chemical kinetics computed at each node and time step

Boiling induced convective & diffusive transport between nodes and coolant

Heat transport between nodes:
3D non-linear, iterative, numerical solution
at each time step, with local "sinks" due to boiling

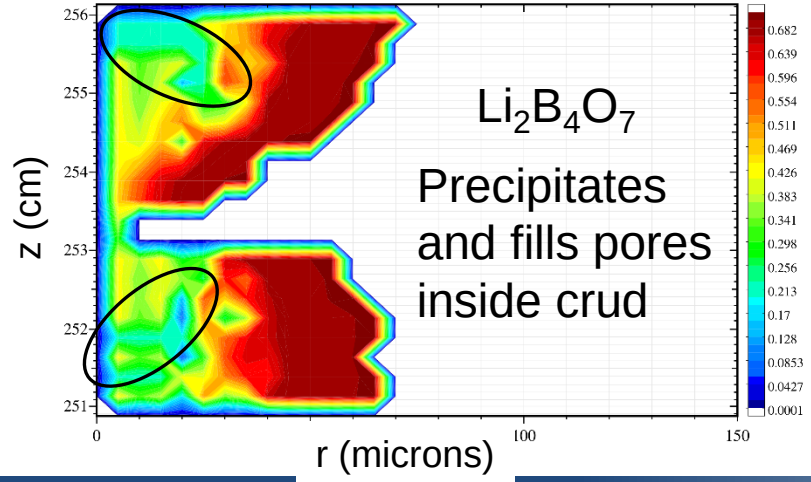
Fundamental DFT-Based Free Energies and Thermodynamic Correlations Have Been Incorporated into MAMBA

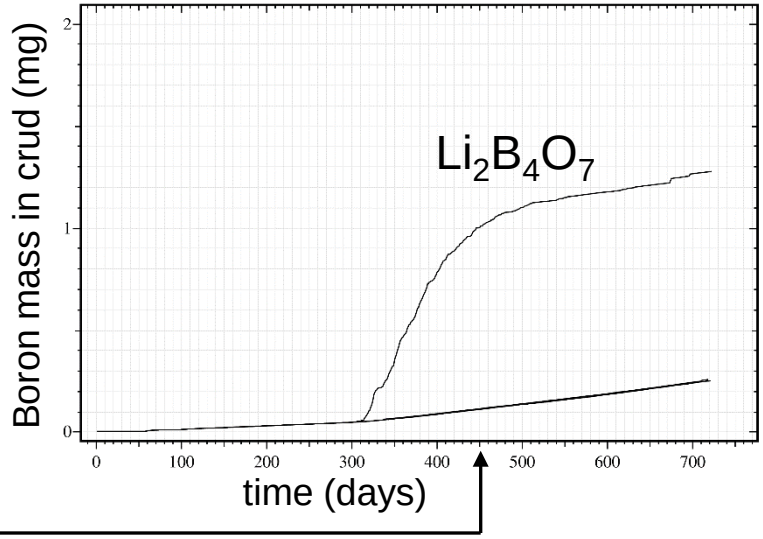


Solubility correlations also developed for $Li_2B_4O_7$ and Ni_2FeBO_5 (bonaccordite)

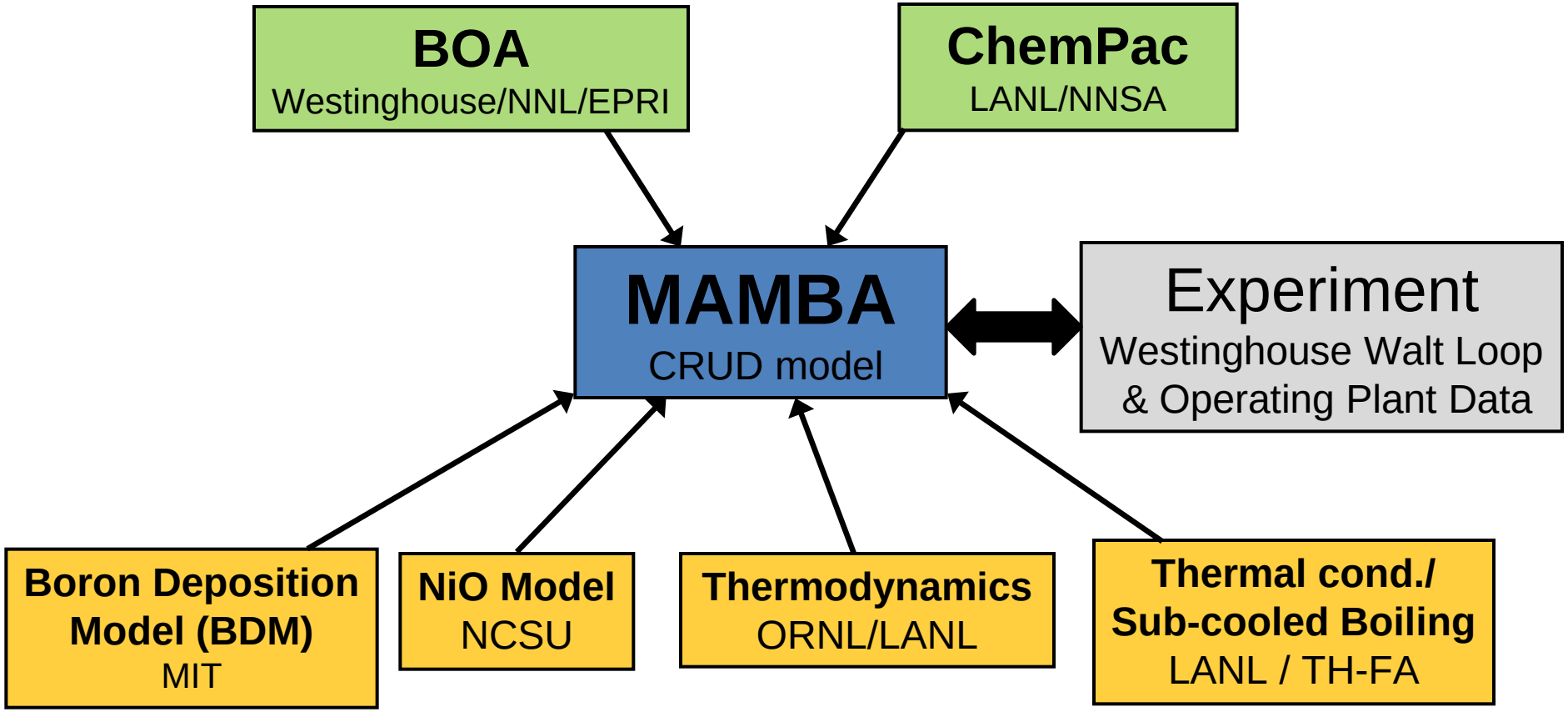
Thermodynamic correlations + MAMBA transport / boiling models determine precipitation threshold and boron uptake

Crud porosity at 450 days



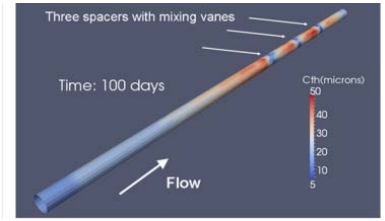


Material Modeling Framework for the CRUD Challenge Problem

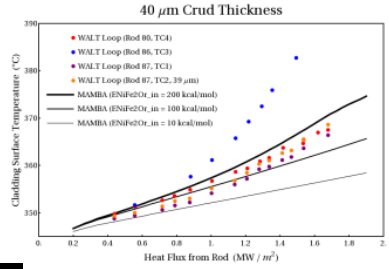


MAMBA Development, Applications, and Validation

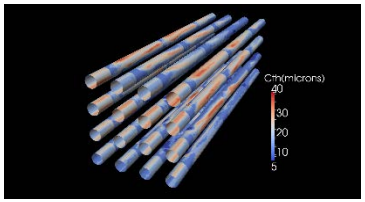
- Coupled MAMBA / STAR-CCM$^+$ / DeCART initial demonstration simulation for a 3D single pin cell geometry (Annals of Nuclear Energy **85**, 1152 (2015)).



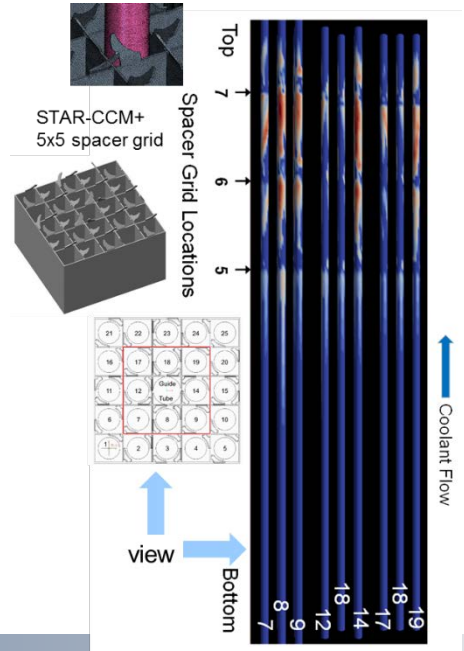
- Initial Validation and Benchmark Study of 3D MAMBA v2.0 against the Walt Loop Experiment and BOA v3.0 Lead to improved boiling models in industry's BOA v3.1 code (CASL internal report).



- Coupled MAMBA/STAR-CCM$^+$/DeCART simulations for 4x4 subassembly (CASL internal report).

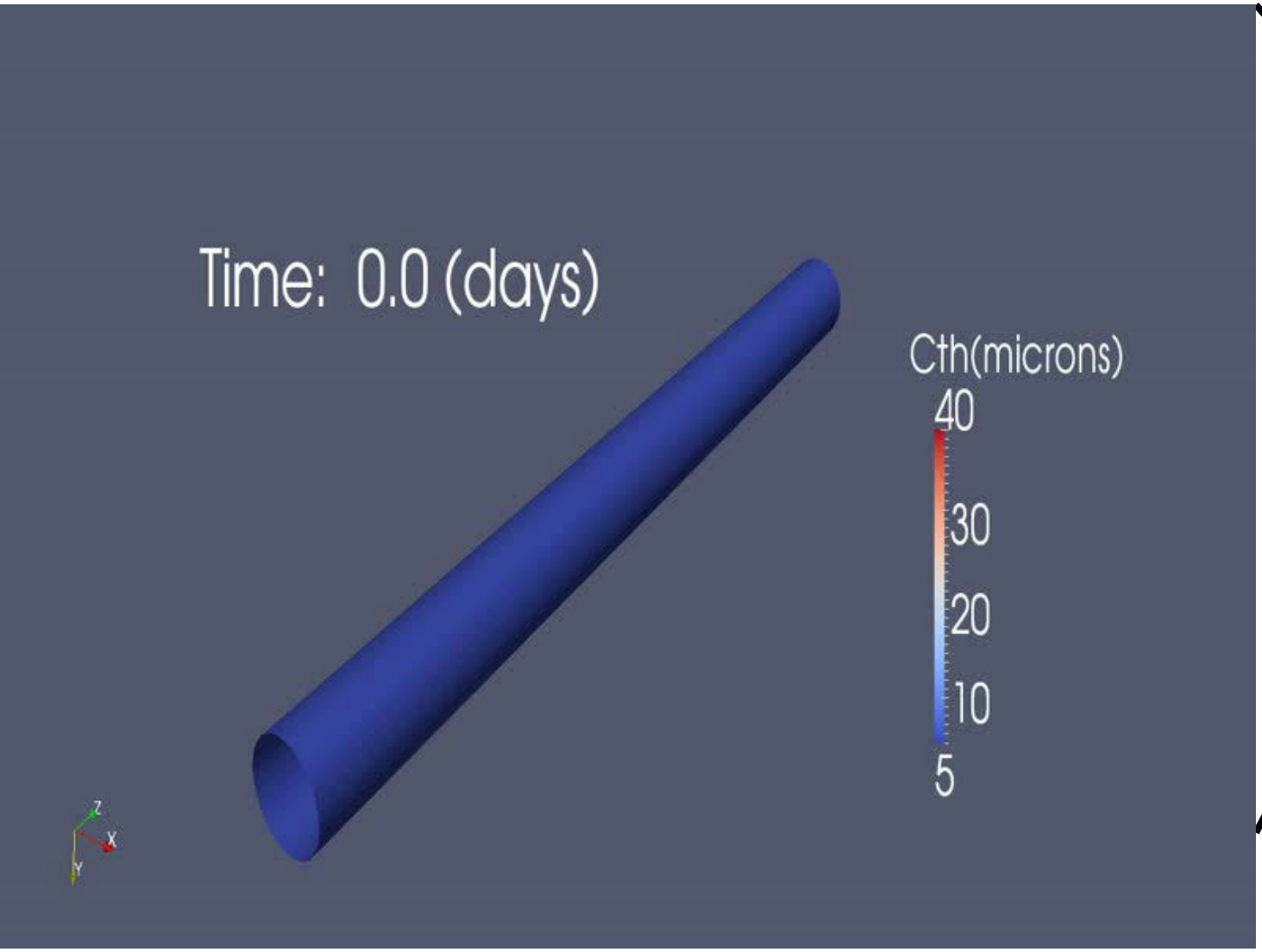


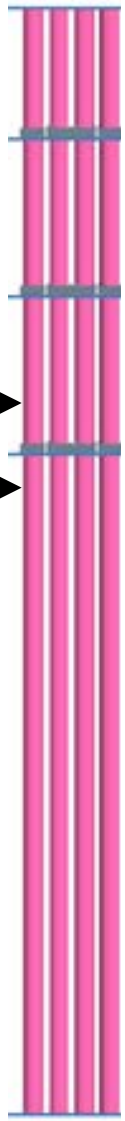
- Coupled MAMBA/STAR-CCM$^+$/ANC simulations for 5x5 subassembly for Seabrook Unit 1 cycle 5 (Nuclear Engineering & Design, in press).



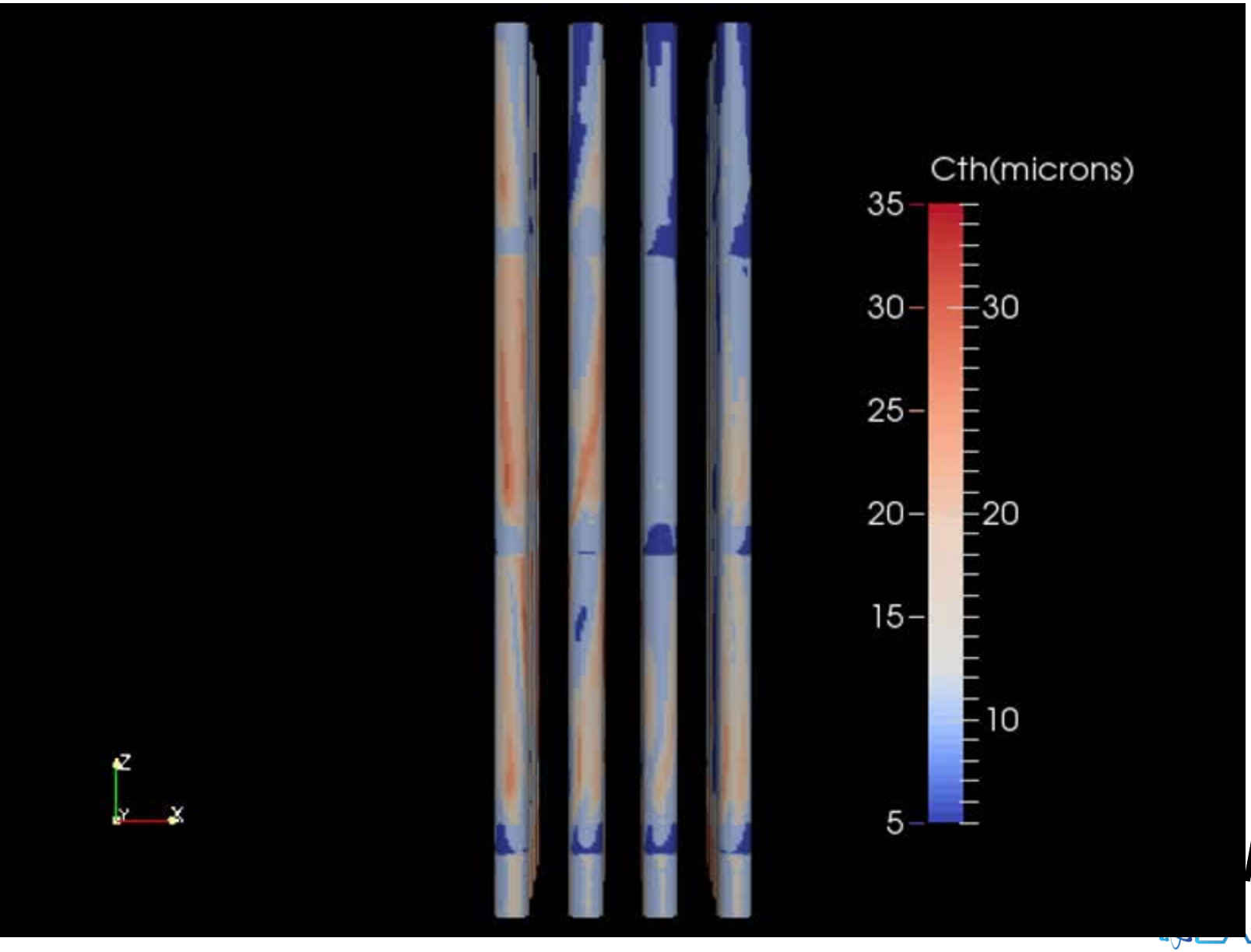
- Coupled MAMBA/MPACT/CTF quarter core simulation Watts Bar Unit 1 cycle 7 (see following presentations).

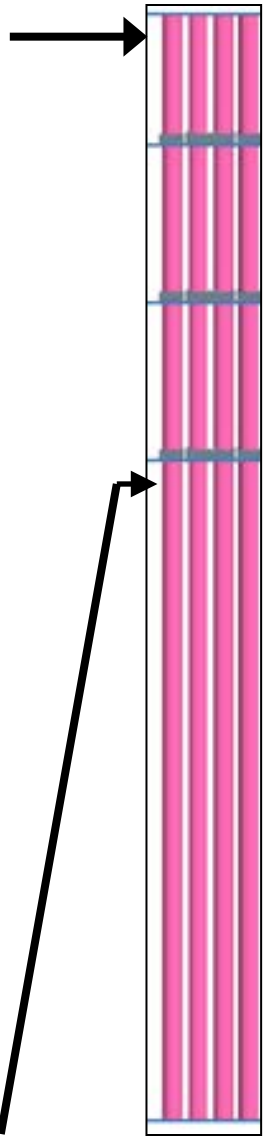
Movie: CRUD Simulation Near Grid Spacer



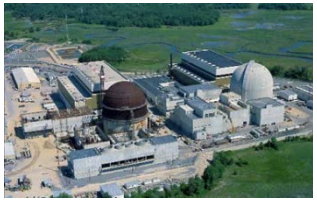


Movie: CRUD Simulation Results for 4x4



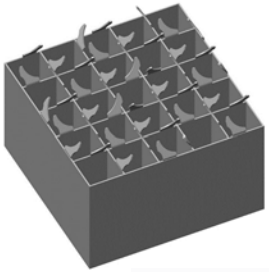


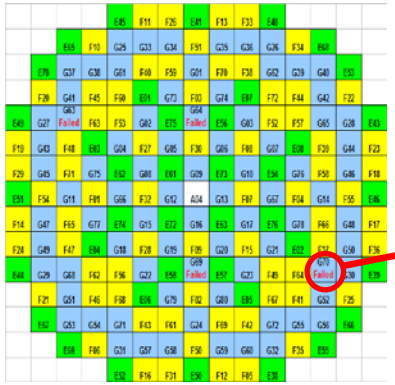
Seabrook Unit 1 PWR - Cycle 5 : Selected 5x5 subassembly

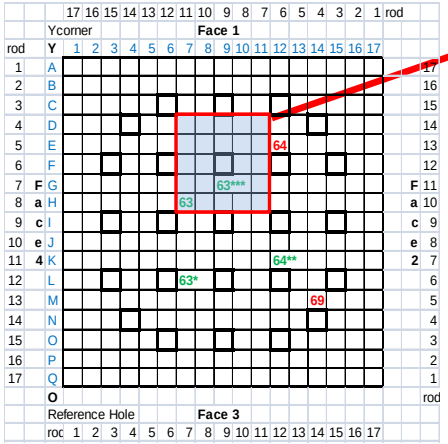


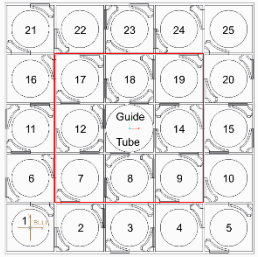
- 5-rod by 5-rod array for which qualitative and quantitative plant data is available was selected for analysis
- First high-fidelity, two-way coupled CFD/CRUD simulation of an industrial relevant plant cycle
- Input power provided by industry simulations
- Showed that <u>both</u> axial and azimuthal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

STAR-CCM+
5x5 spacer grid

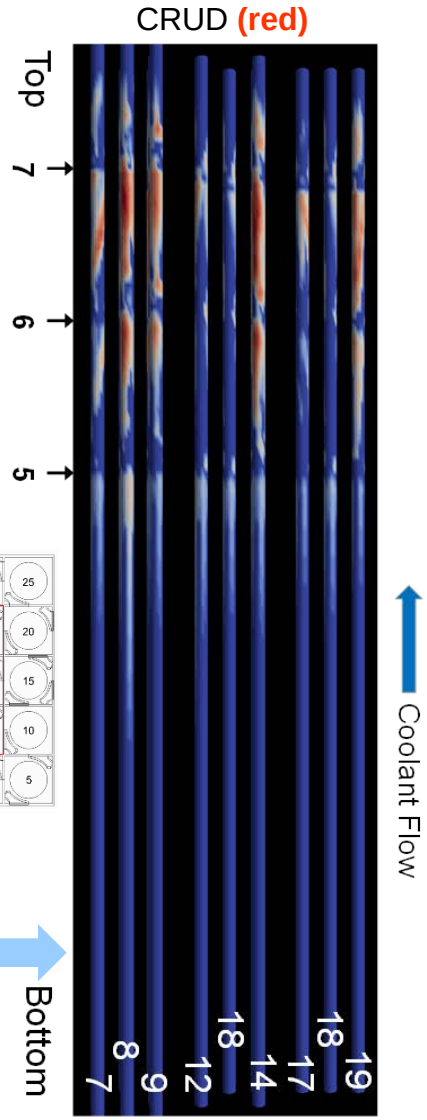




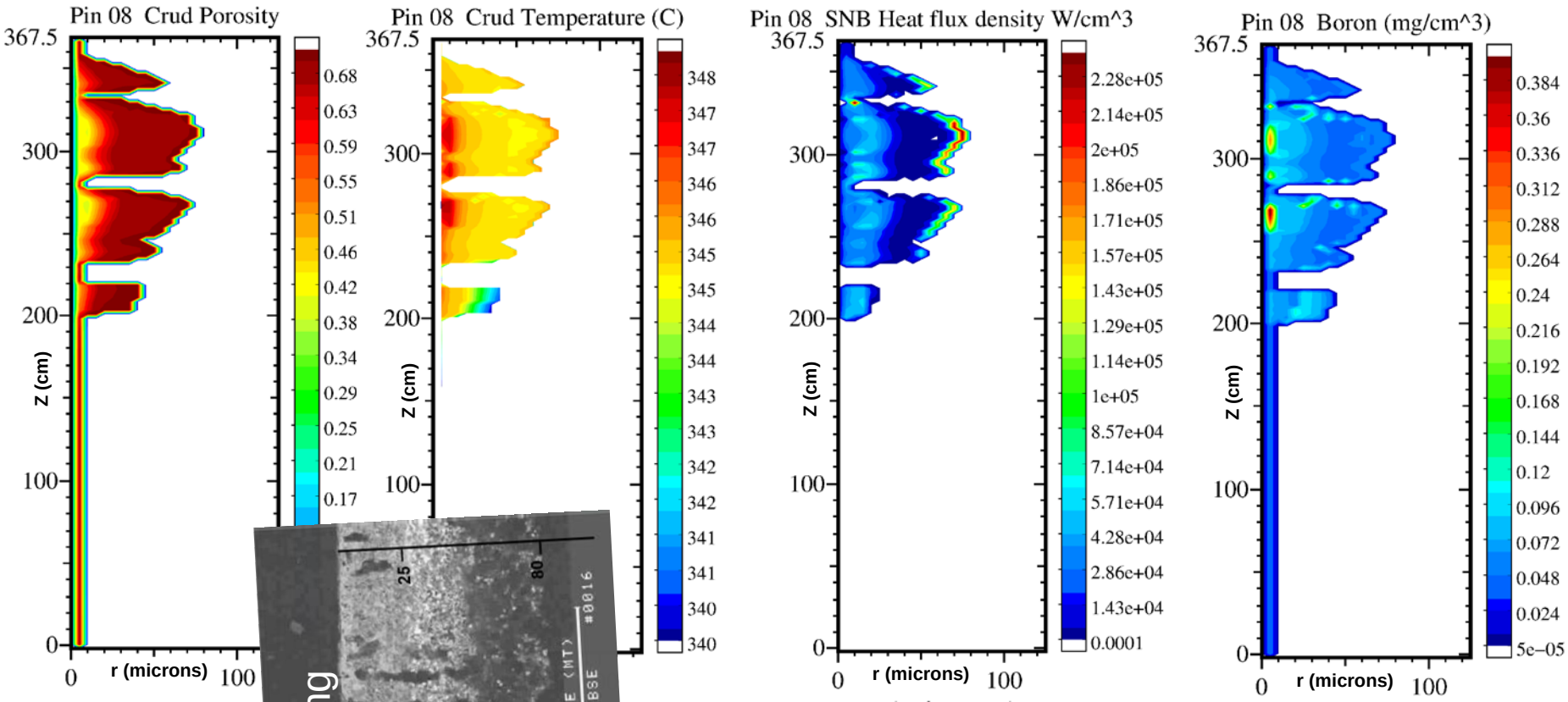


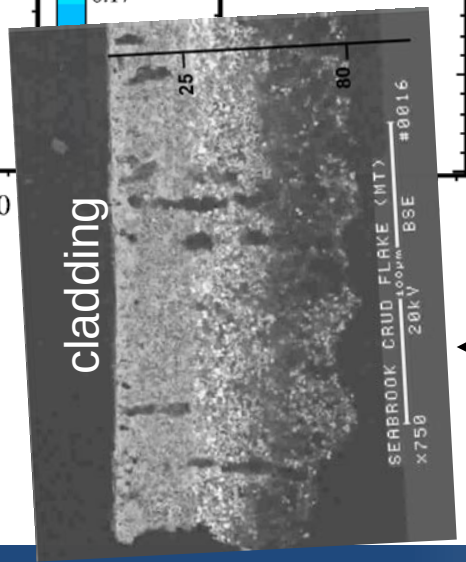


view



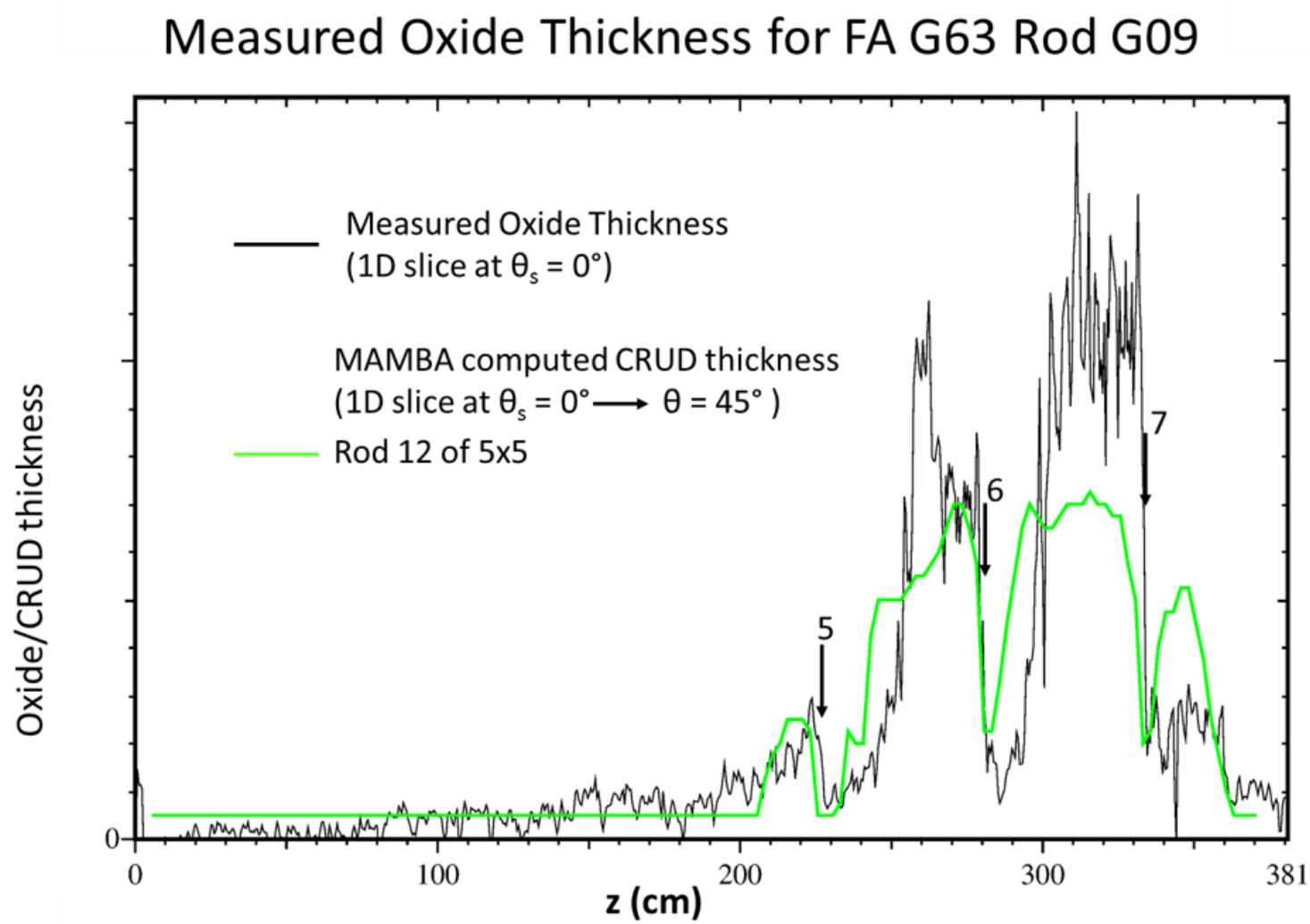
Profile View of CRUD Layer for Pin 8 at 502 days





Actual Seabrook CRUD flake (80 microns thick)

Comparisons with Seabrook Cycle 5 Oxide Data



Summary

- Reviewed CRUD modeling framework (MAMBA development)
  - crud growth + erosion
  - heat transfer + chimney boiling
  - soluble transport: convection (boiling induced Darcy flow) + diffusion
  - thermodynamic models + boric acid chemistry
  - microstructure models (porosity)
  - external coupling to fluid and neutronics codes

- Simulation results for a coupled MAMBA/STAR-CCM+/DeCART single pin simulation

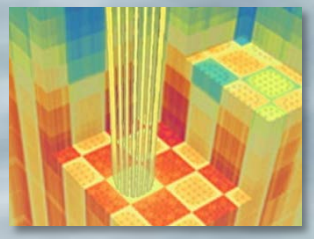
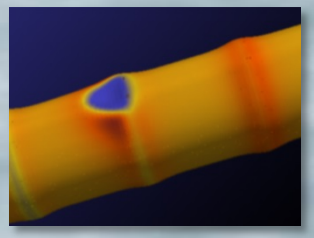
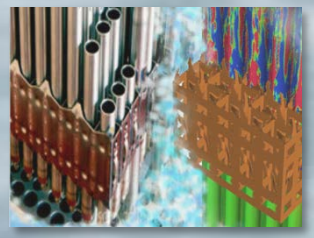
- Simulation results for a coupled MAMBA/STAR-CCM+/DeCART 4x4 subassembly

- Results from the first coupled MAMBA/STAR-CCM+ simulation of an <u>operating PWR</u> (Seabrook Unit 1 Cycle 5): predicted CRUD surface distributions are consistent with measured oxide data

- MAMBA subgrid module developed and used in quarter core Watts Bar Unit 1 cycle 7 simulations (see next presentations)

CASL Physics Integration and Multi-Scale Challenges: A CRUD Example

Kevin T. Clarno
Oak Ridge National Laboratory
October 21, 2015

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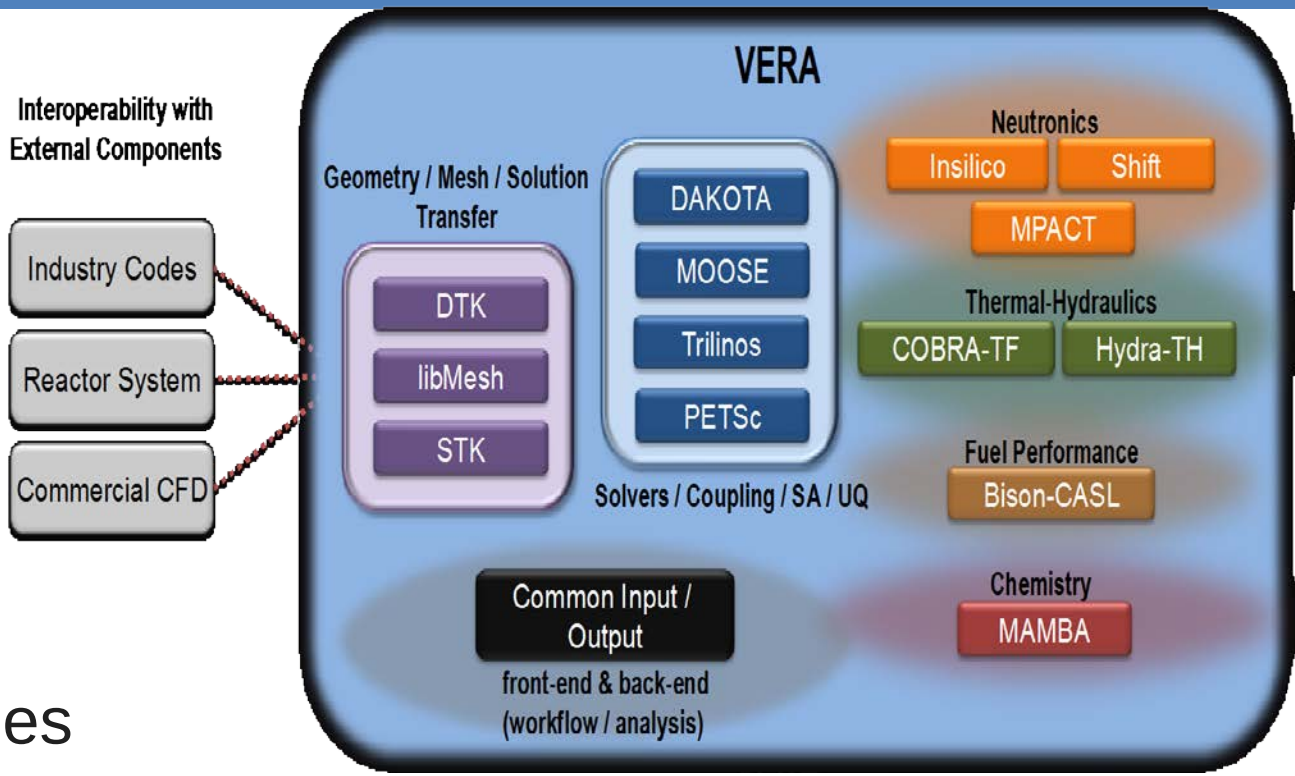
Outline

- VERA: Virtual Environment for Reactor Analysis
  - Prediction of normal operation with modest computers
- Multi-scale challenges
  - Demonstrated with CRUD and discussed for other applications
- Validation with 12 cycles of Watts Bar Unit 1
  - Discussion of results and limitations
- Extensions for CRUD analysis
  - Improvements to Watts Bar Unit 1 models using MAMBA

VERA



- Collection of codes
  - Covering all physics
  - Covering a breadth of scales
  - Some are coupled; some enable coupling
  - All leverage common infrastructure to simplify use and development

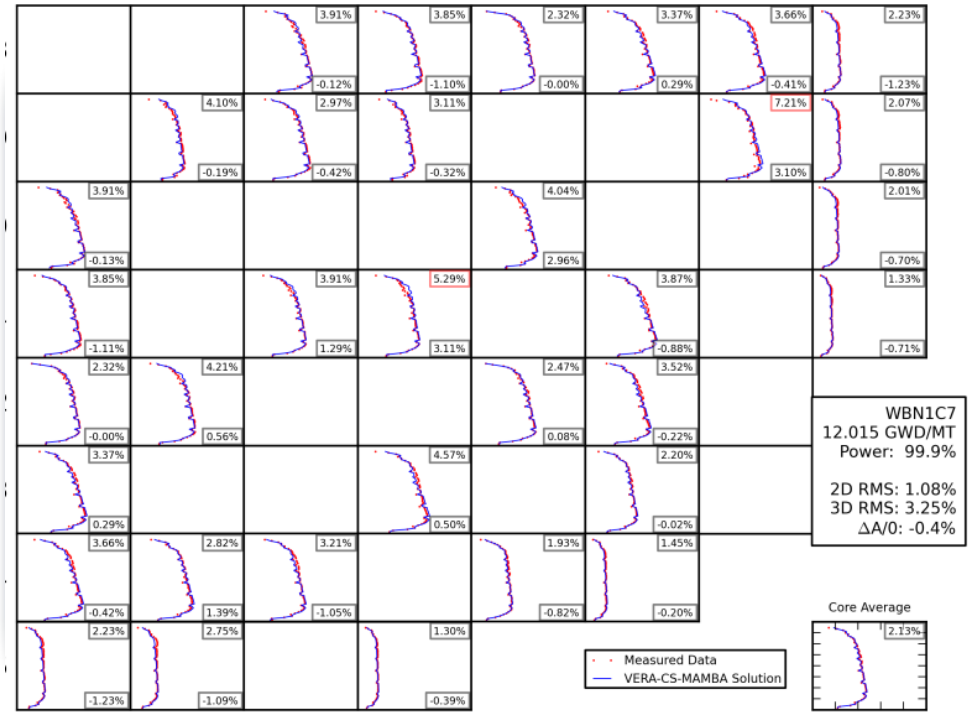
VERA: a reactor analysis code suite

Multi-Scale Physics Integration Challenges

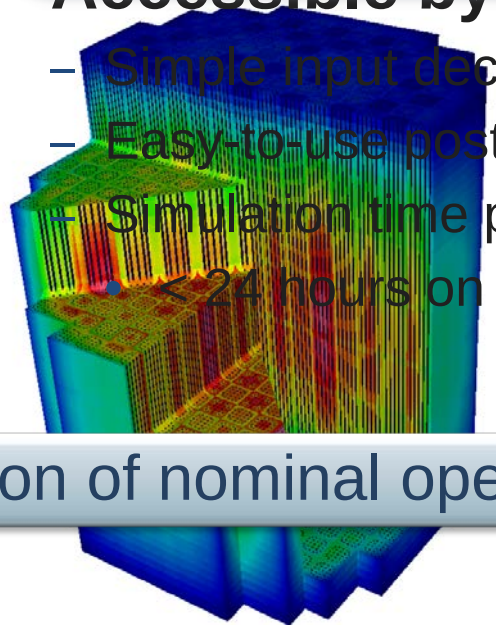
- **CFD:**
  - CFD-informed spacer grid models for CTF
  - CTF boundary and source-terms for CILC analysis
- **Monte Carlo transport:**
  - Continuous-energy Monte Carlo to understand deterministic errors
  - Monte Carlo with MPACT source for ex-core detectors
- **Fuel performance:**
  - Core Simulator source and BCs for 3D fuel analysis
  - Simplified Bison models to improve VERA temperature estimates

Bridging scales within VERA

Full Core Simulation



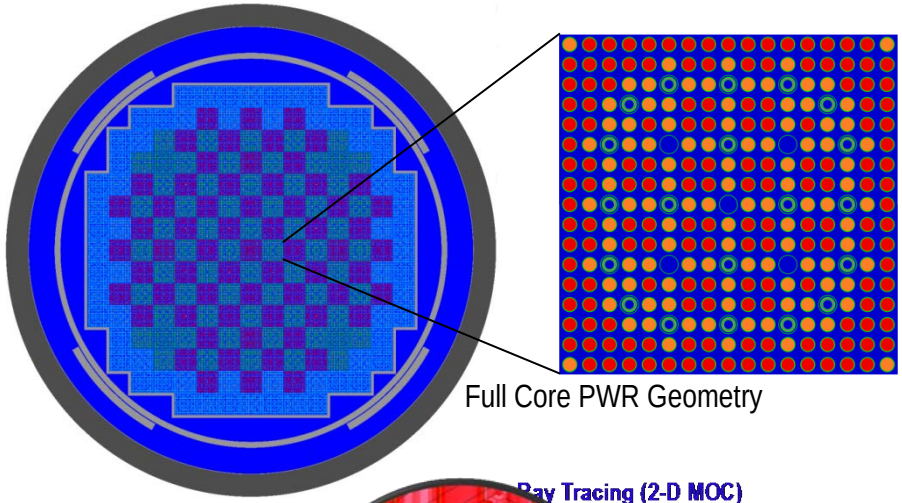
- **Nominal operation**
  - Quasi-static neutronics
  - Steady-state coolant flow
  - Simplified pin heat transfer
- **Multi-cycle analyses**
  - Rotation and shuffling of fuel
  - Comparisons with operational data
    - Zero-power physics tests
    - Boron letdown curves
    - In-core flux detectors
- **Accessible by industry**
  - Simple input deck
  - Easy-to-use post processing tool
  - Simulation time per cycle:
    - < 24 hours on < 4000 cores

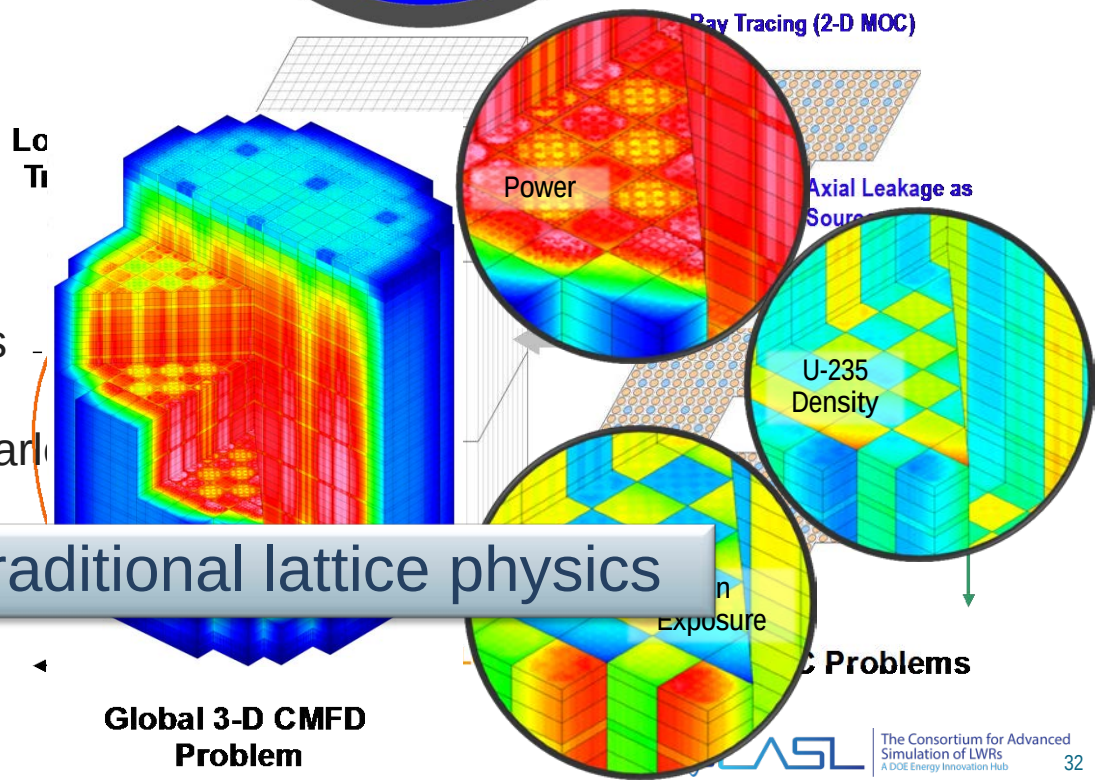


High-resolution simulation of nominal operation

MPACT: pin-resolved neutronics

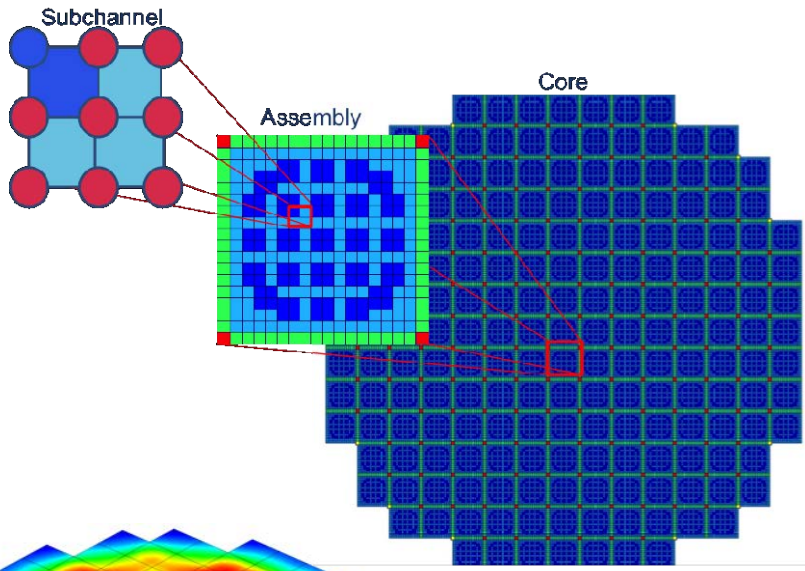
- **Integrated neutronics**
  - Cross section processing
  - Full-core radiation transport
  - Isotopic depletion & decay
- **3D pin-resolved transport**
  - 2D radial MOC
  - 1D axial SPn
  - 47 energy groups
  - Scales to O(10^4) cores
- **Validation in progress**
  - Critical experiment benchmarks
  - Comparisons to plant data
  - Comparisons with CE Monte Carl



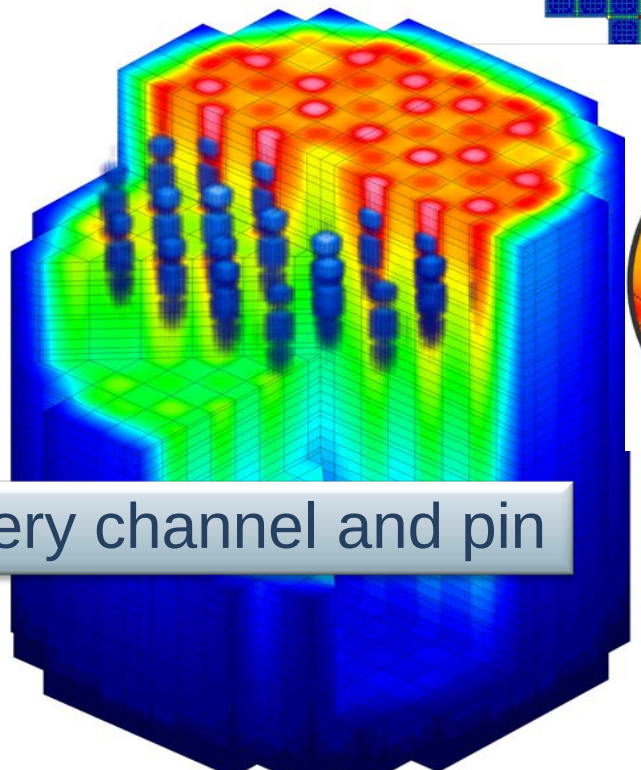


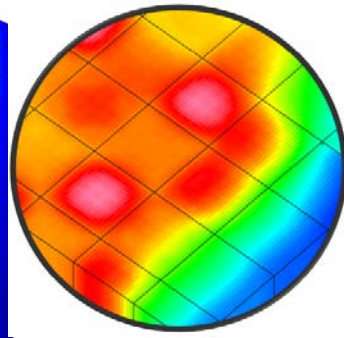
Eliminating traditional lattice physics

CTF: channel-resolved heat transfer



- **Conjugate heat transfer**
  - Radial heat transfer within each pin
  - Thermal-hydraulics throughout core
    - Two-fluid, three-field model
  - Static or transient mode
- **Resolving flow in every channel**
  - Axially resolved to less than one inch
  - Models each quadrant in every cell
    - 30 million clad surfaces in the core
  - Scales to $O(10^2)$ cores
- **Validation in progress**
  - Single and two phase benchmarks
  - Comparisons with CFD



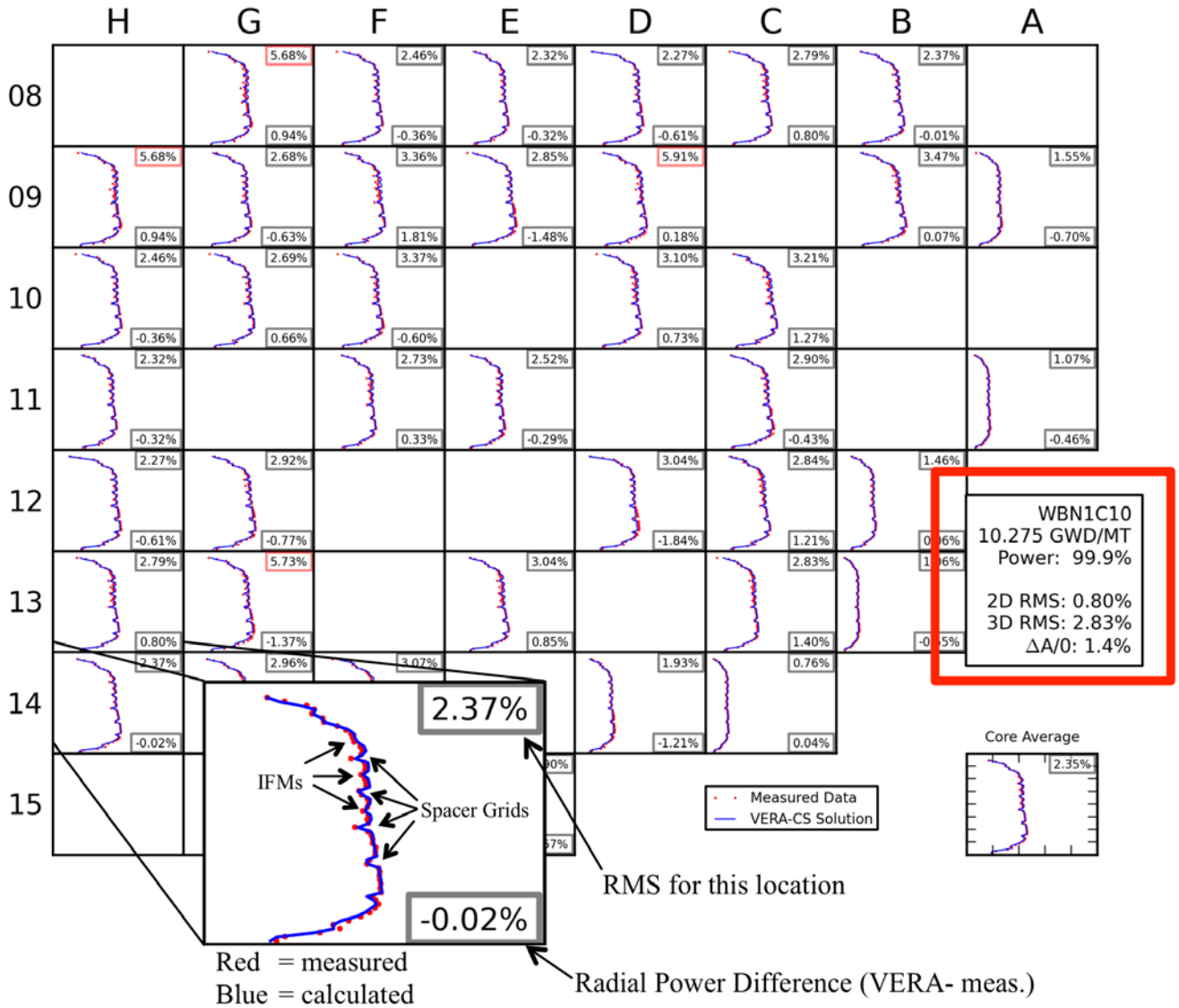


TH modeling of every channel and pin

Watts Bar Nuclear Unit 1 Simulations

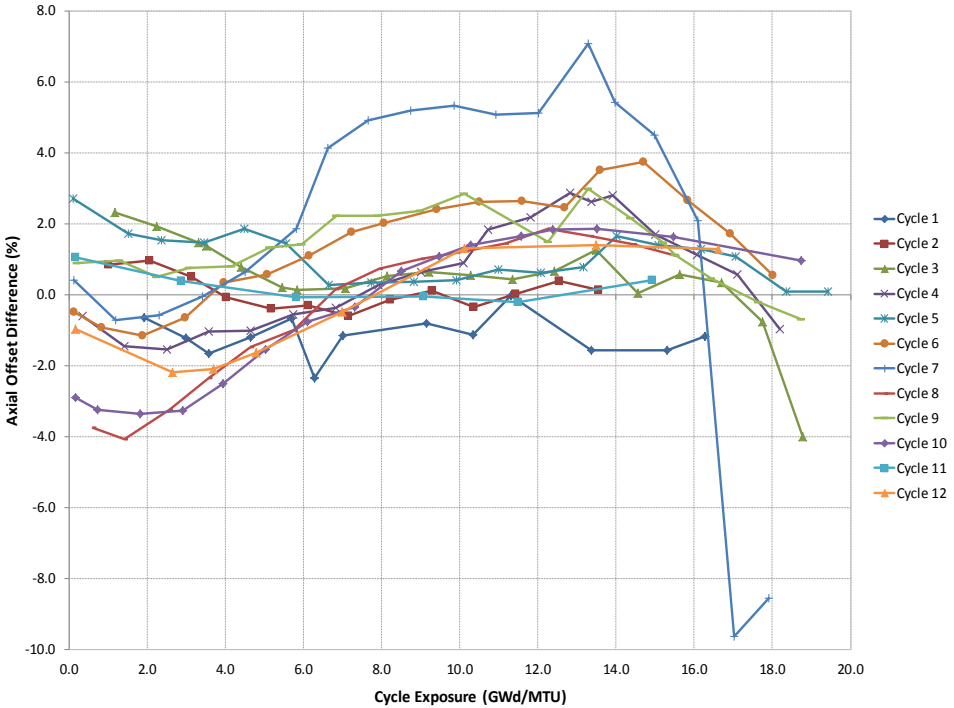
- Operated by Tennessee Valley Authority in Spring City, TN
- Traditional four-loop Westinghouse PWR
- Began operation in 1996
- Currently in 13th fuel cycle
- 3459 MW_{th} thermal power
- Unit 2 will startup soon!

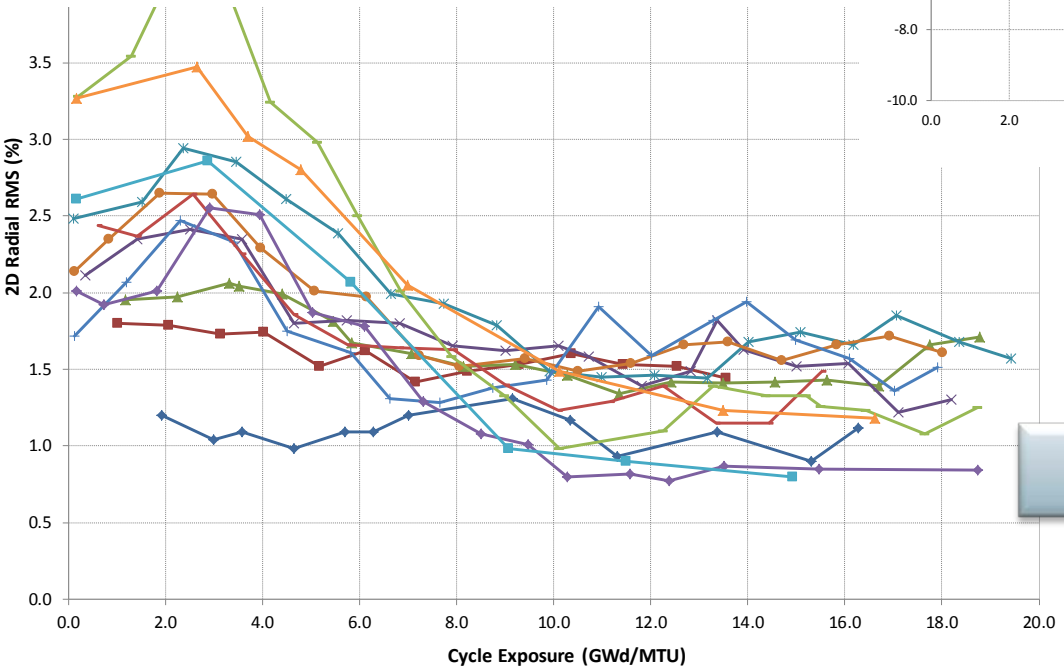
Validation using Watts Bar 1, Cycles 1-12



Validation using Watts Bar 1, Cycles 1-12

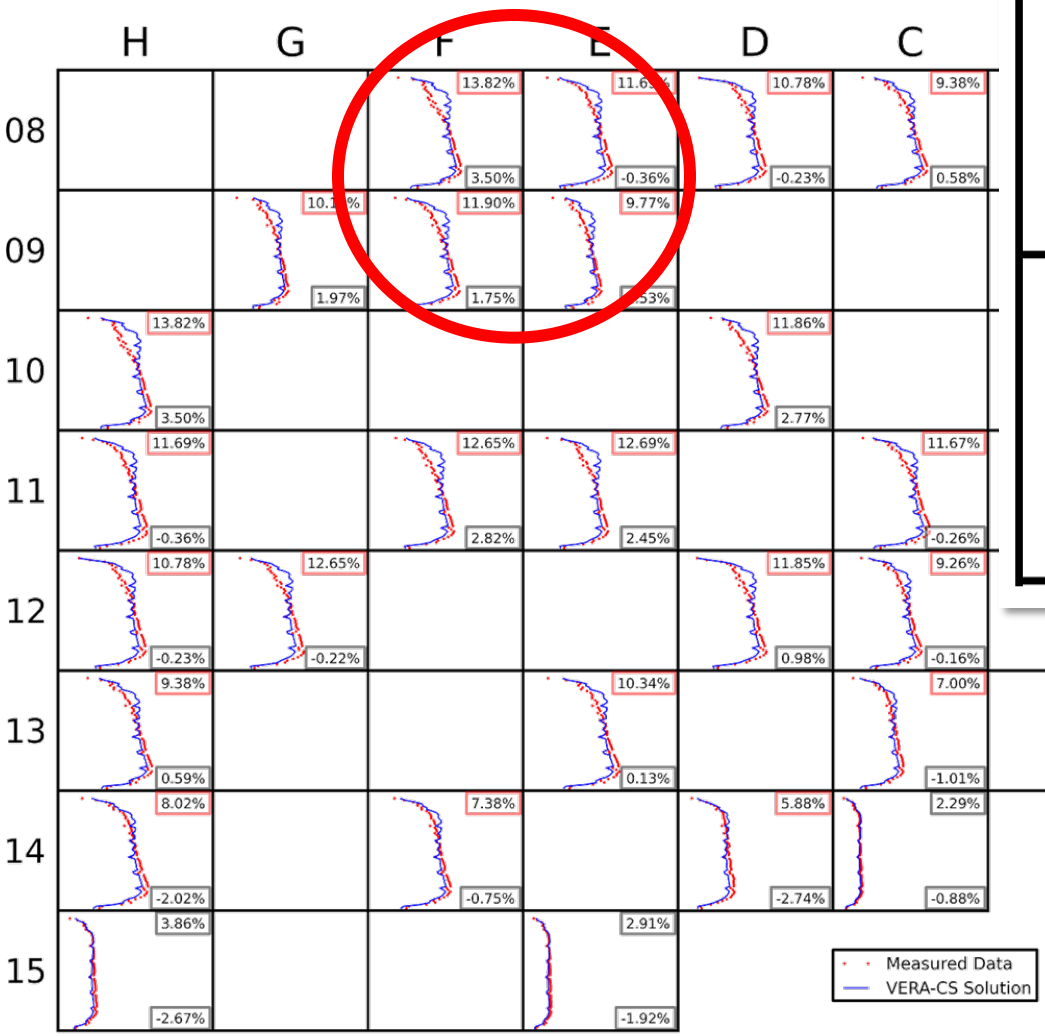
Cycle	Count	ΔAO	1D RMS	2D RMS	3D RMS	2D Max	Det Max
1	13	-1.17	2.55	1.10	3.29	3.37	7.25
2	13	0.08	1.11	1.60	2.70	3.99	7.29
3	19	0.45	1.87	1.67	2.92	5.95	8.34
4	19	0.52	2.14	1.77	3.23	4.82	8.37
5	19	1.04	2.33	2.05	3.64	8.02	9.61
6	18	1.38	2.60	1.92	3.77	6.15	9.60
7	18	1.79	5.17	1.74	6.73	5.94	15.70
8	15	-0.35	3.03	1.77	4.00	7.67	10.27
9	19	1.32	2.41	2.35	3.94	10.03	11.88
10	16	-0.43	2.79	1.56	3.64	7.55	9.62
11	6	0.25	1.52	1.88	2.77	7.36	7.85
12	8	-0.43	2.23	2.47	3.72	11.54	12.32
Total	**183**	**0.50**	**2.75**	**1.95**	**4.08**	**11.54**	**15.70**
St. Dev.		**0.85**	**0.98**	**0.32**	**1.05**		

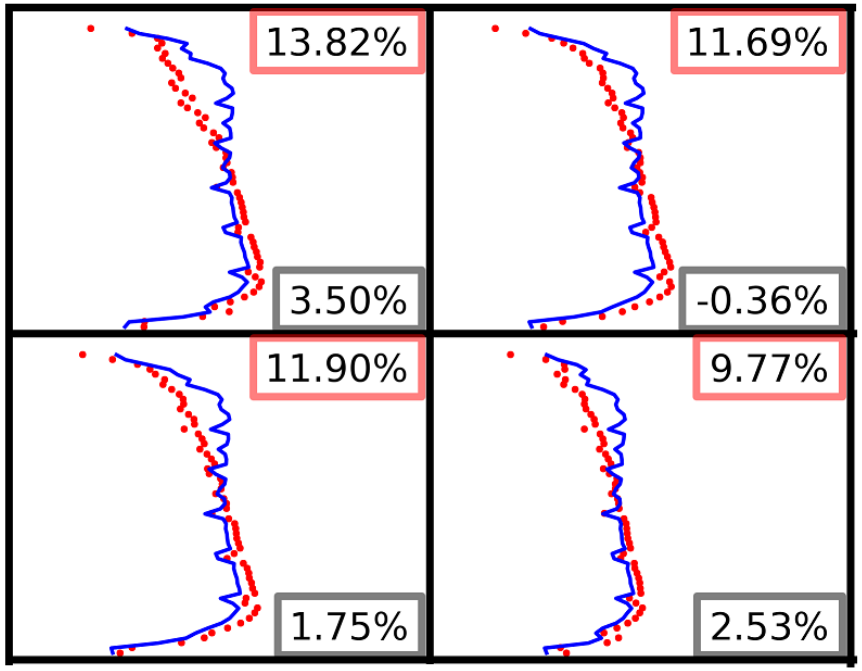




CIPS in Cycle 7

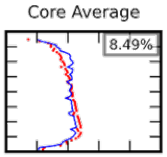
WBN1 Cycle 7 Results without CRUD models





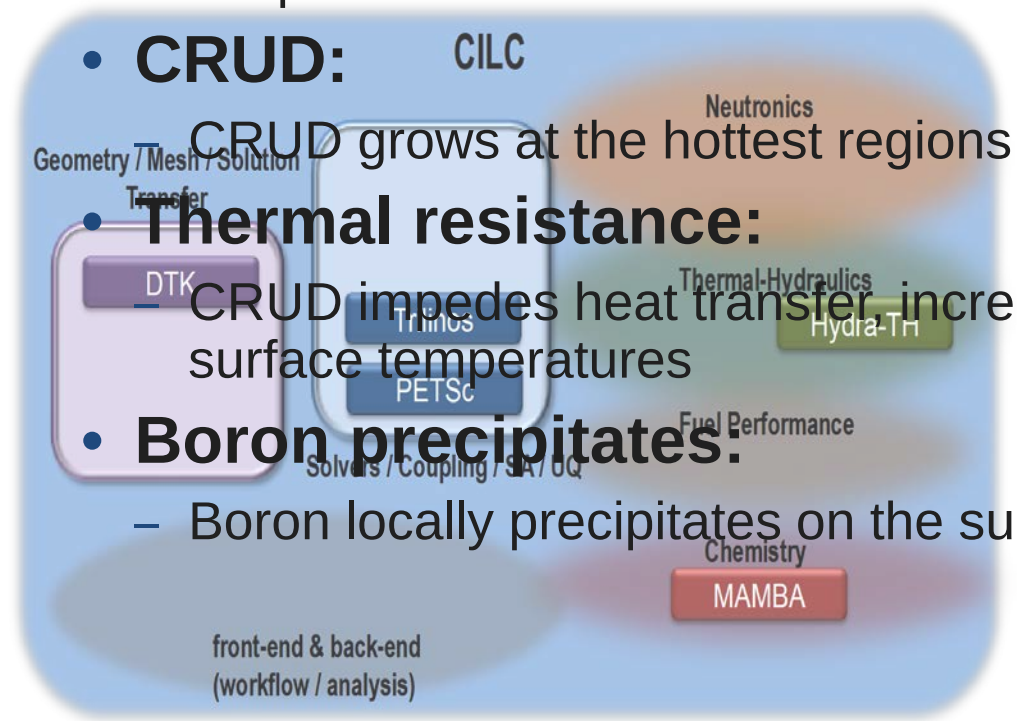
WBN1C7
13.283 GWD/MT
Power: 99.9%

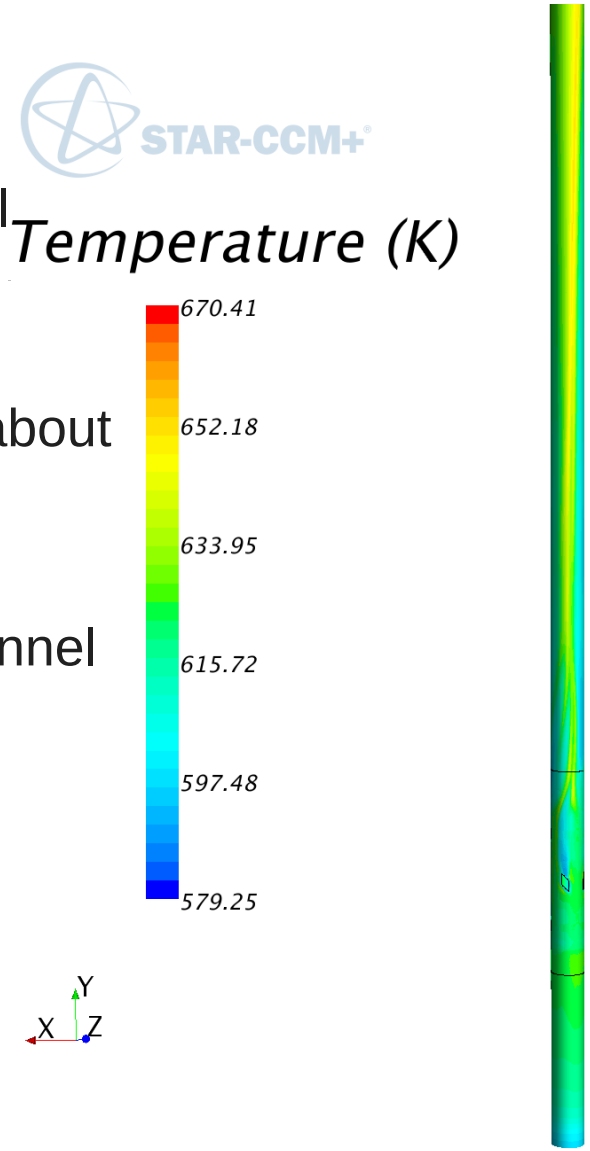
2D RMS: 1.82%
3D RMS: 9.58%
ΔA/0: 7.1%

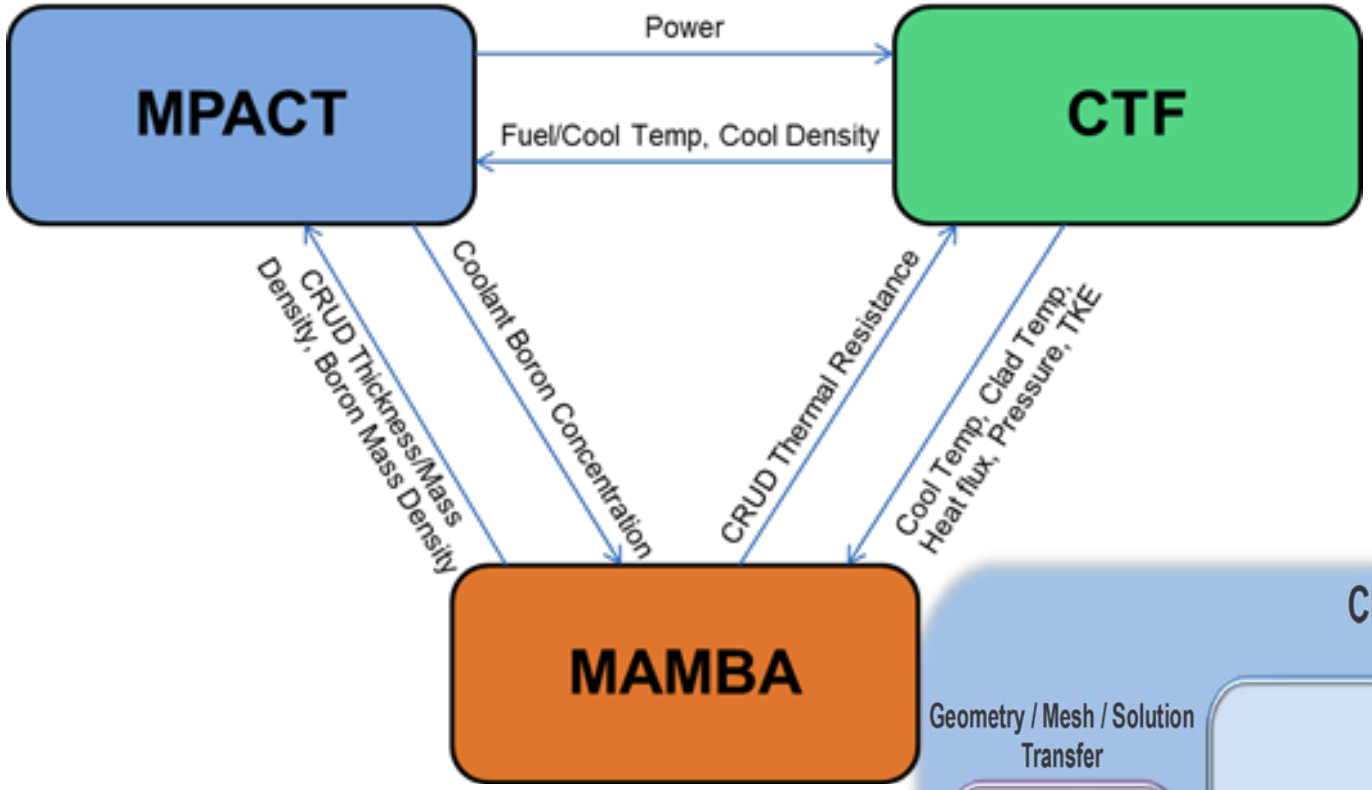


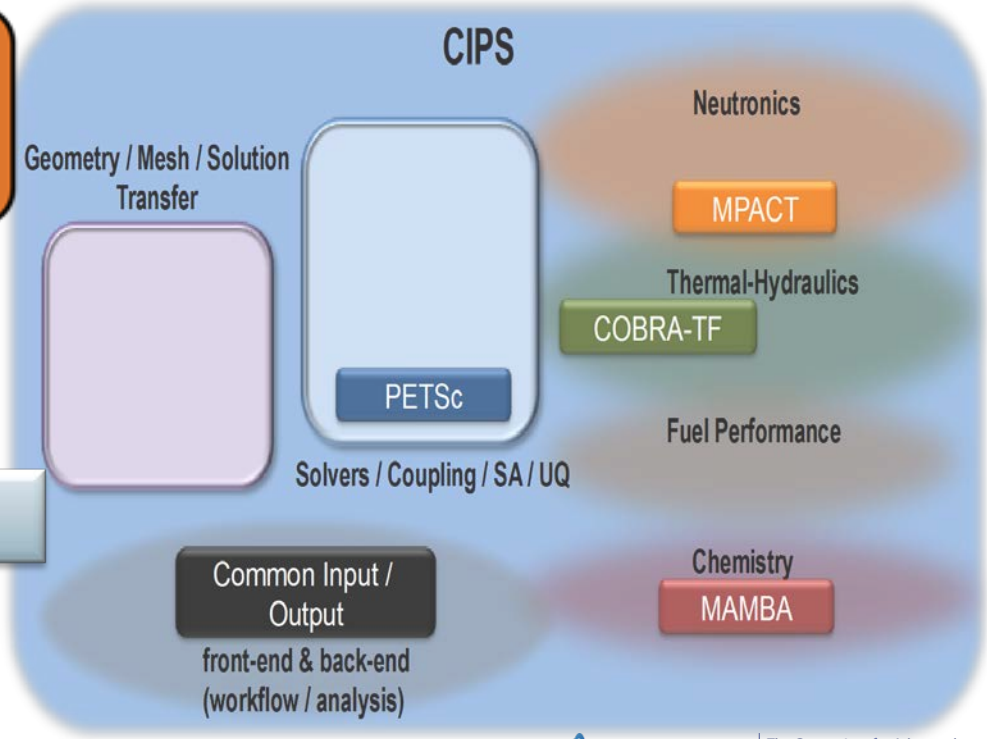
CRUD is a very localized deposit

- **Flow:**
  - Grids and mixing vanes induce within-channel variations
- **Temperature:**
  - Clad surface temperature varies azimuthally about the pin
- **CRUD:**
  - CRUD grows at the hottest regions of the channel
- **Thermal resistance:**
  - CRUD impedes heat transfer, increasing clad surface temperatures
- **Boron precipitates:**
  - Boron locally precipitates on the surface









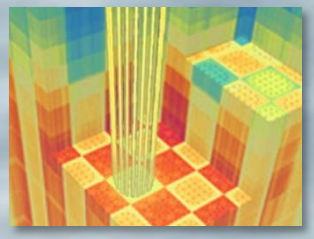
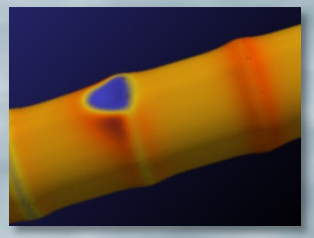
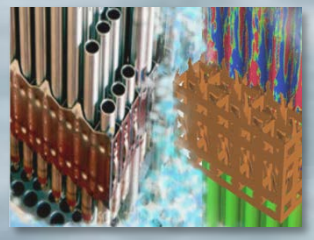
Application of VERA for CIPS

Physics Integration Conclusions

- **Virtual Environment for Reactor Analysis (VERA)**
  - Suite of tools for high resolution analysis of reactors and fuel
  - Coupled in several ways to enable the prediction of reactor performance
- **CRUD-Induced Power Shift (CIPS)**
  - Directly depends on local quantities (sub-cooled boiling) that are globally-dependent (power distribution)
  - Azimuthal variation of CRUD growth on the rod cannot be predicted by CTF and requires leveraging CFD
  - Requires multi-cycle full core simulations to predict growth on each rod
- **Application of VERA for Cycles 1-12 of Watts Bar Unit 1**
  - Demonstrated accuracy of VERA through many cycles of commercial operation
  - Highlighted the limitations of neglecting CRUD growth and CIPS
  - Incorporating MAMBA dramatically improved VERA for cycle 7 and beyond
- **Physics Integration efforts to account for multi-scale problems**
  - Multi-scale physics integration challenges remain while addressing many other Challenge Problems

CASL Crud Challenge Problem – Multi-physics Applications

Jeff Secker
Westinghouse Electric Company
October 21, 2015

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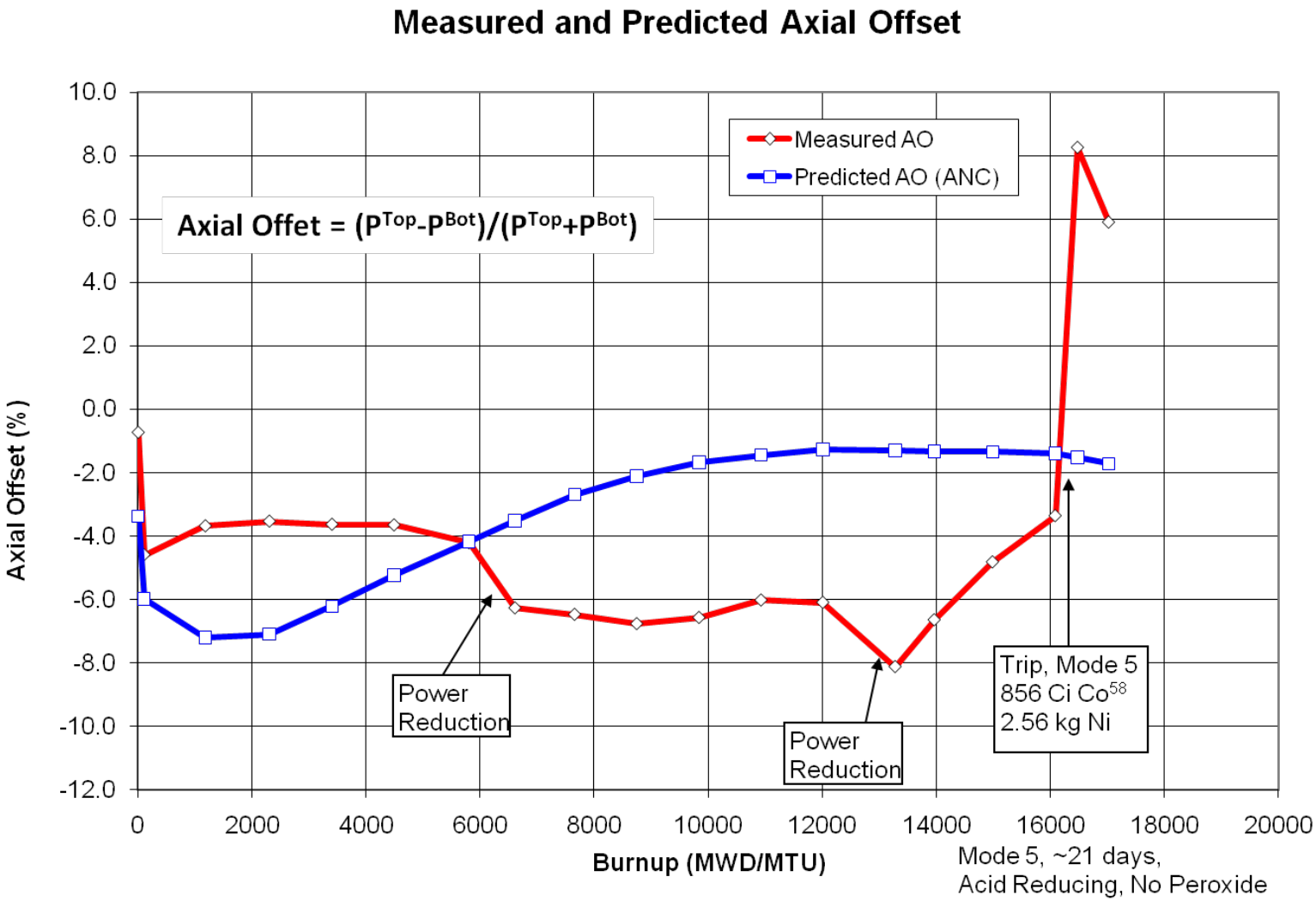
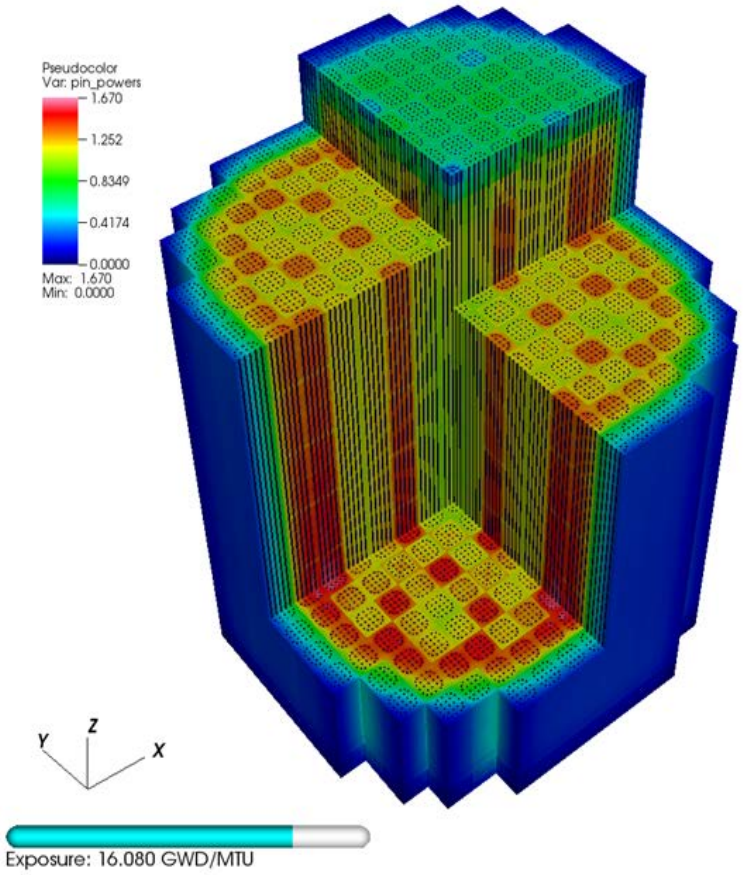
Watts Bar Unit 1 Cycle 7 CIPS



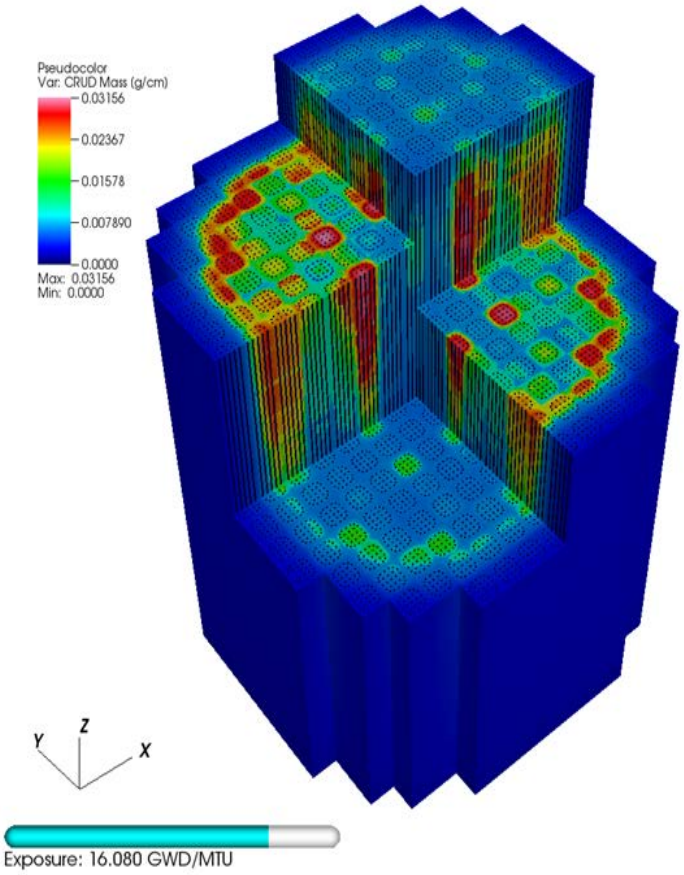
Cycle 7 Experienced CIPS

Watts Bar 1 Cycle 7 Predicted Crud Distribution

Power Distribution

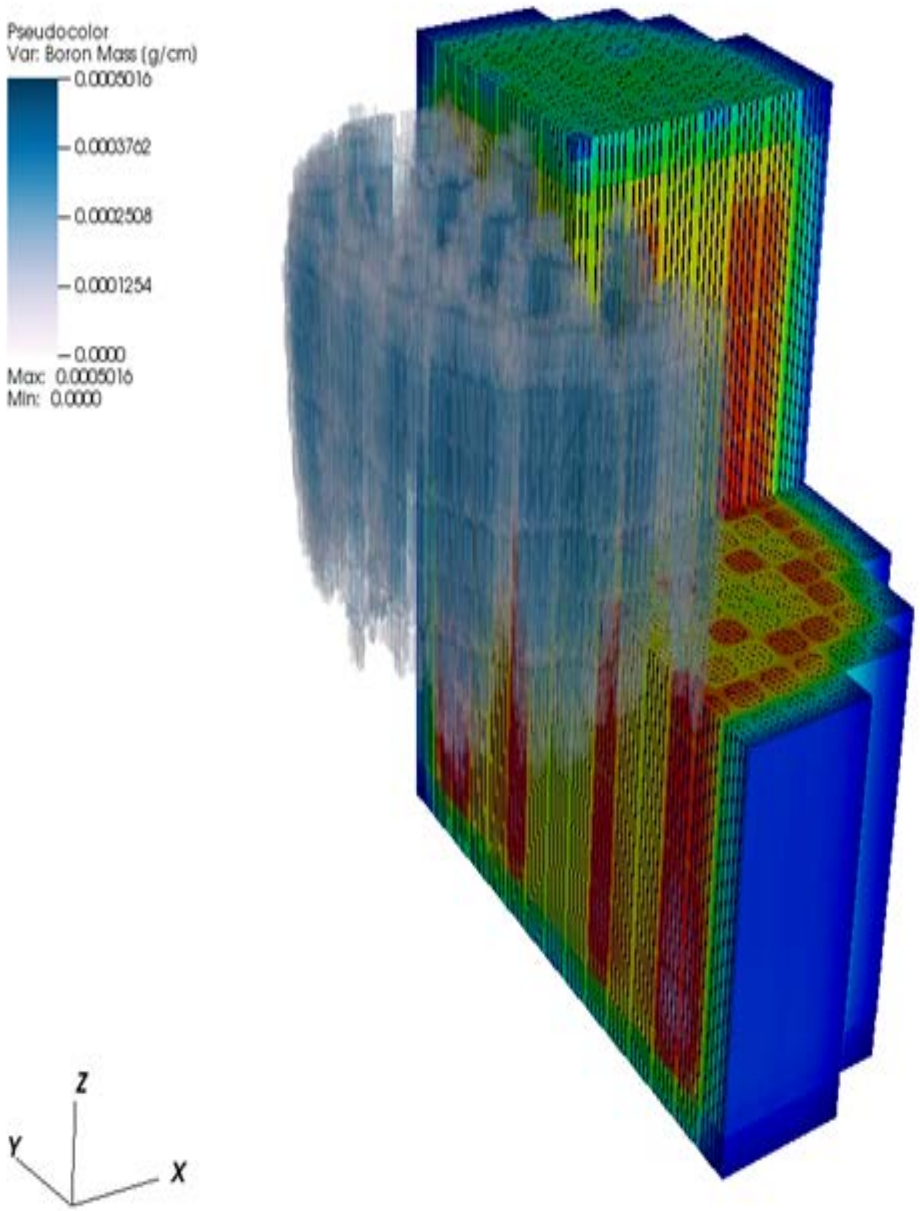


Crud Distribution

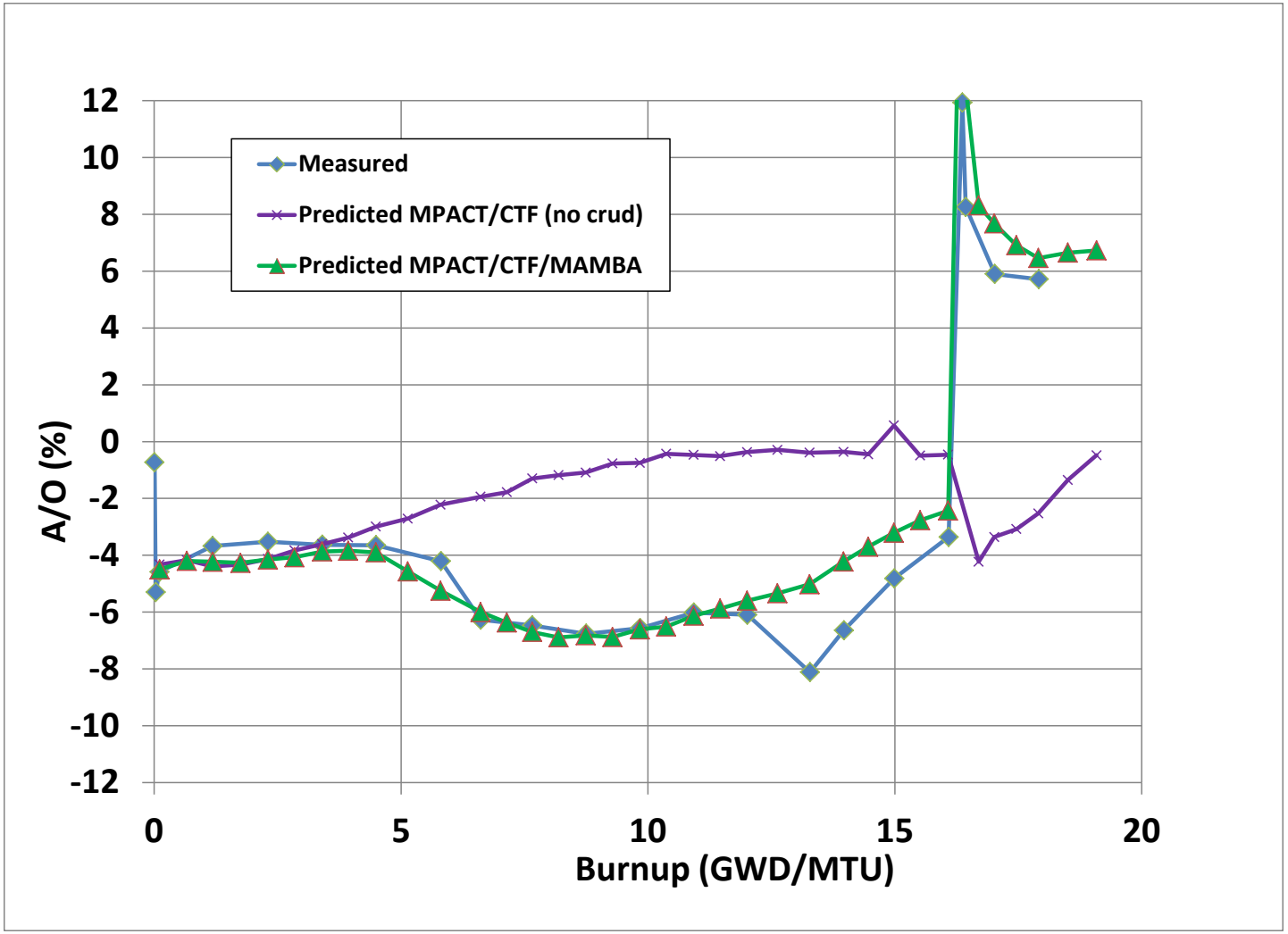


Watts Bar 1 Cycle 7 Predicted Boron Distribution

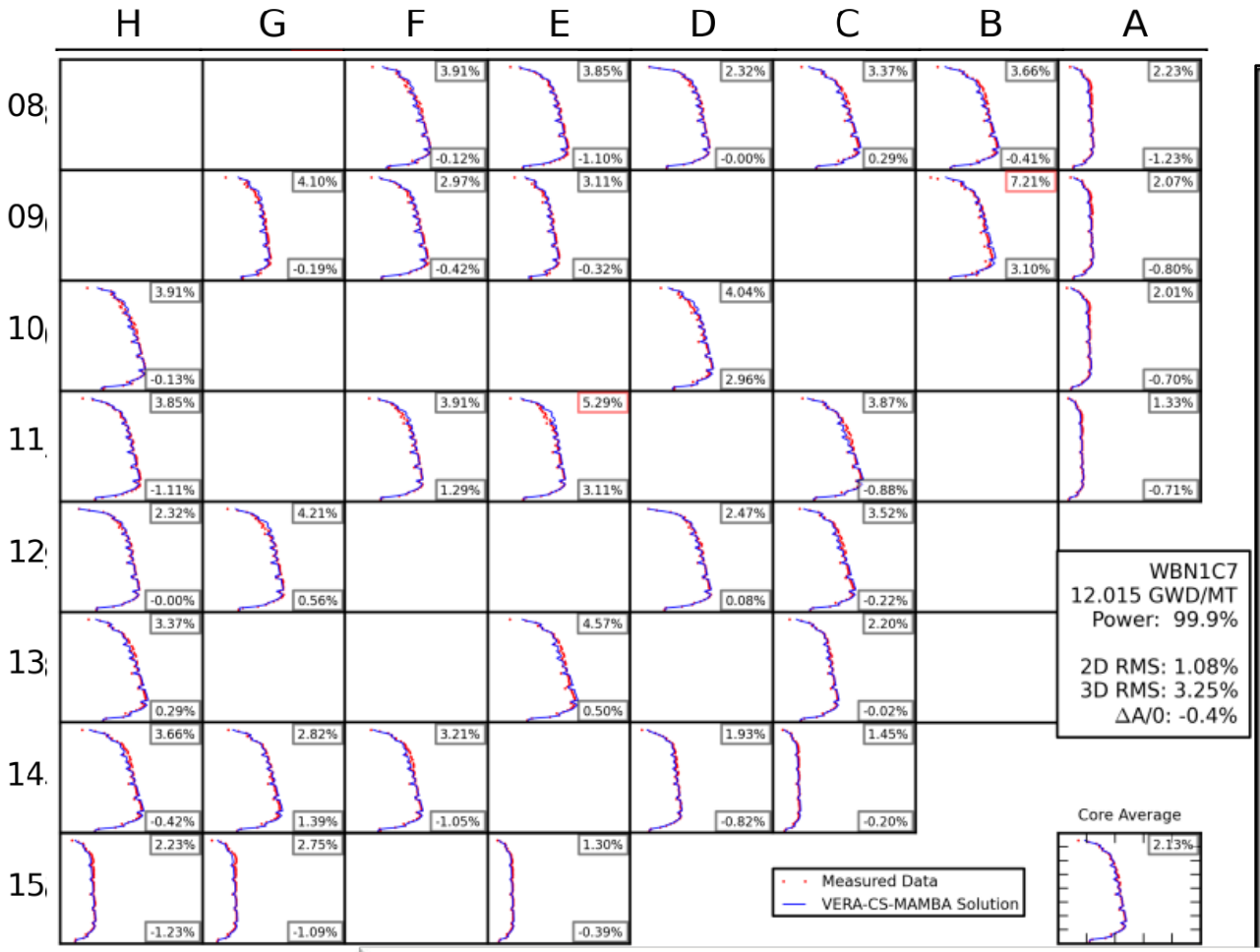
Boron Distribution at 16.08 GWD/MTU

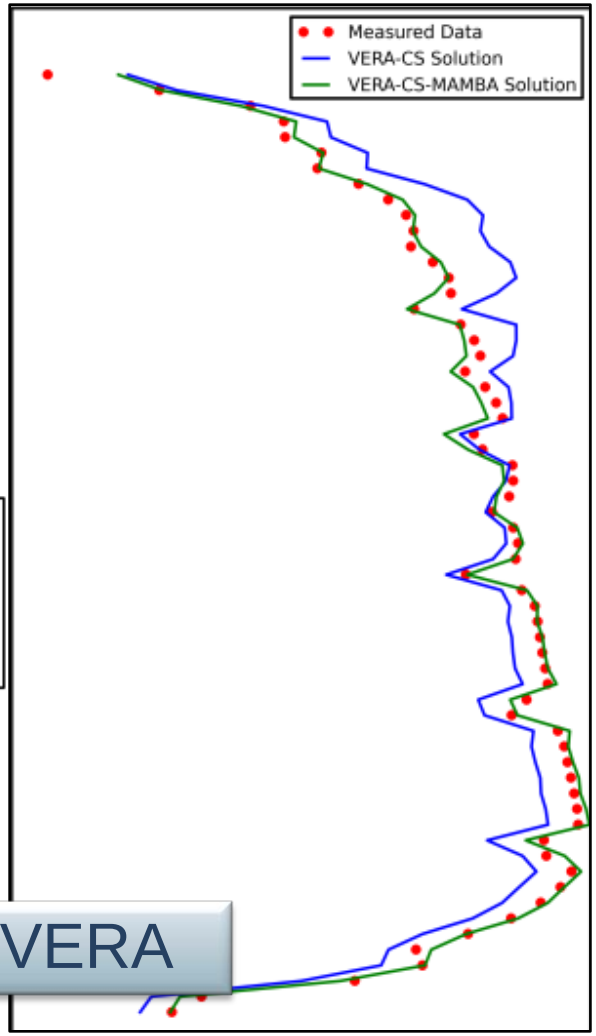


Watts Bar 1 Cycle 7 Measured and Predicted Axial Offset Behavior



Cycle 7 Predictions Improved Dramatically





CIPS in Cycle 7 simulated by VERA

CASL CIPS Modeling Conclusions

- CASL has developed multi-physics tools to model crud deposition on PWR cores and the resulting effects on core behavior
- Pin resolved 3D transport neutronics (MPACT) has been coupled with sub-channel thermal-hydraulics (CTF) and crud/chemistry models (MAMBA) to create a multi-physics crud modeling and simulation tool
- The CASL CIPS modeling tools accurately model the CIPS behavior experienced at Watts Bar Unit 1 Cycle 7
- Addition improvements to the models are planned and underway

CASL CIPS Challenge Problem

CASL

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