U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

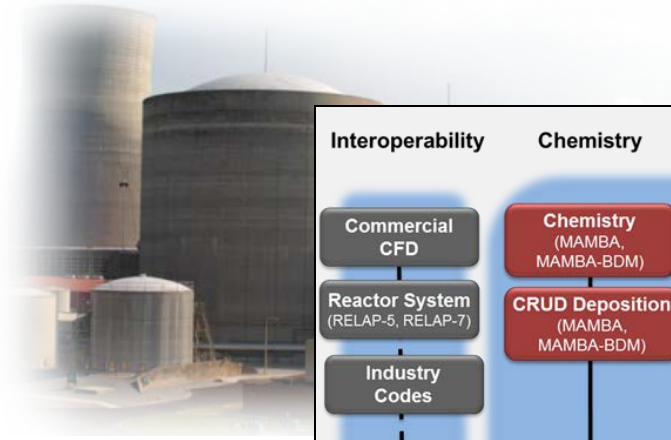
2015 Update
The Power of Use Inspired Advanced Modeling and Simulation Research

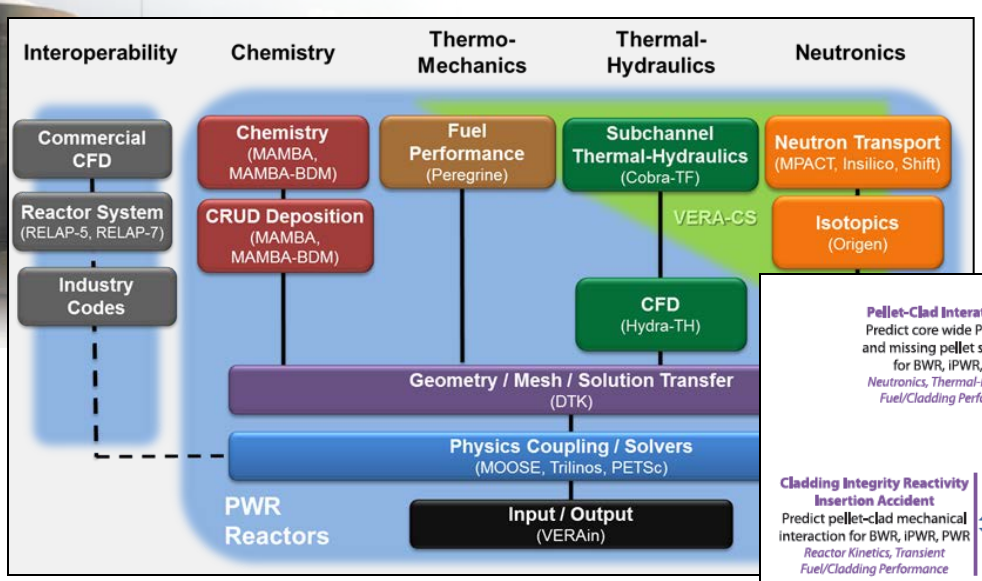
Alex Larzelere
Federal Director, Modeling and Simulation Energy Innovation Hub
Office of Nuclear Energy
U.S. Department of Energy

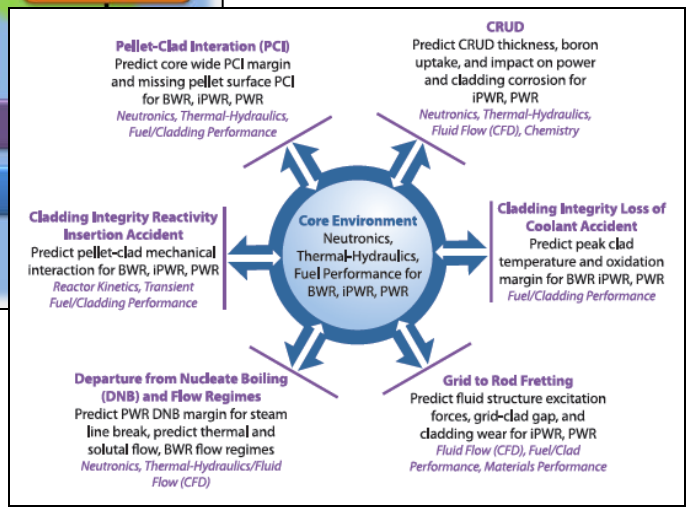
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

In 2015, CASL Completed its First Five Year Phase

They Built a Virtual Version of the TVA Watts Bar #1 Reactor



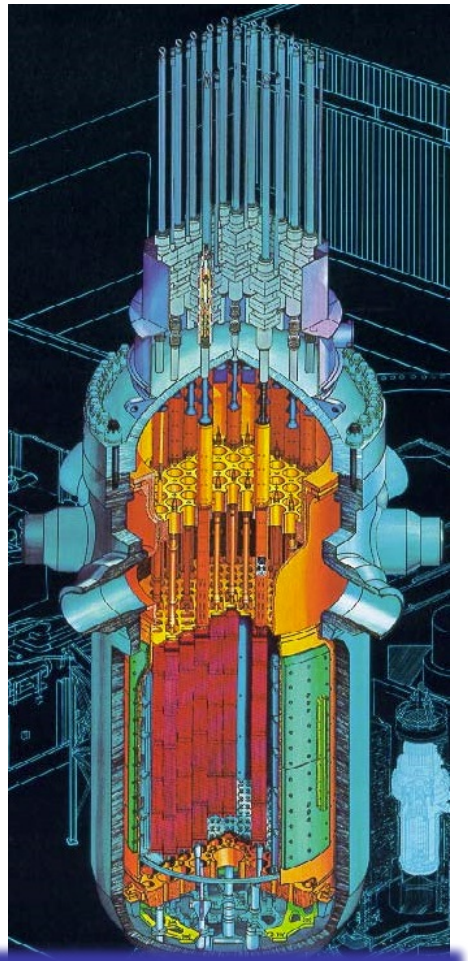




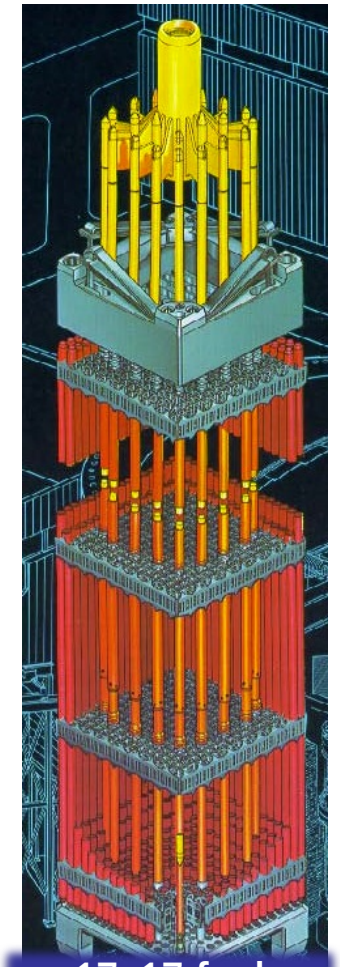
To Be Used to Address Industry Defined Performance and Safety Challenge Problems

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

TVA's Watts Bar #1 Westinghouse 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

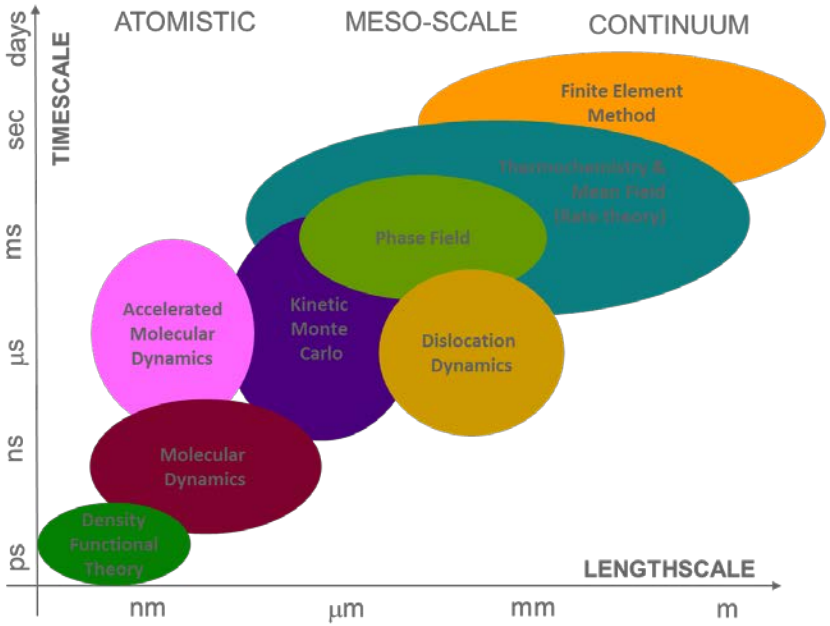
Fuel Temperatures
- 4140° F (max centerline)
- 657° F (max clad surface)

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

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

ModSim Challenges of Creating the "Virtual"

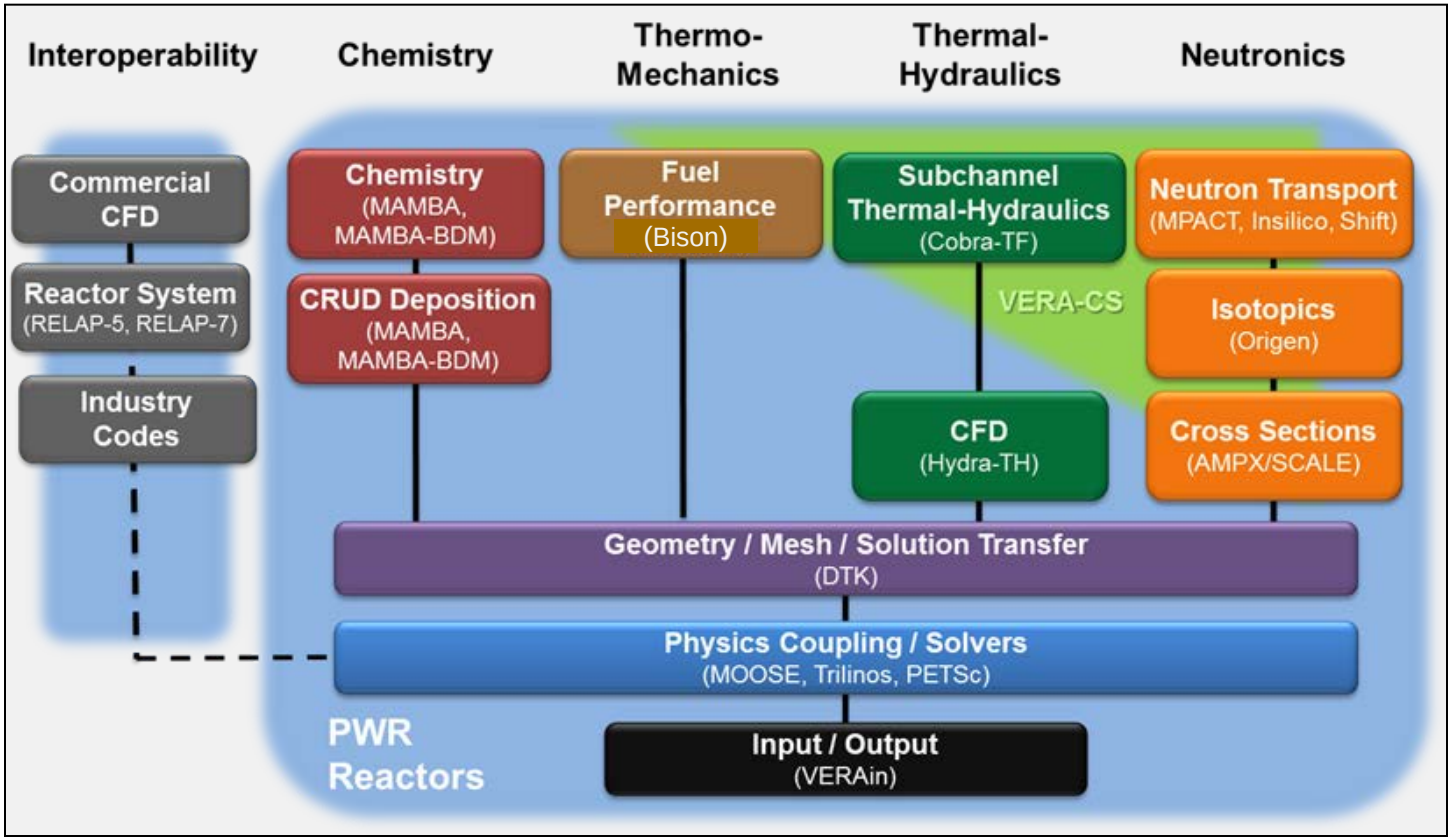
- 3-Dimensions (4D with time)
- Coupled Multi-physics, multi-scale
- High resolution
- High fidelity (as much 1st principle physics as possible)
- Sufficient simulation time
- Sufficient simulation space
- Enabled by high performance parallel processing computing
- Rigorous verification, validation & uncertainty quantification



M. Stan, Materials Today, 12 (2009) 20.

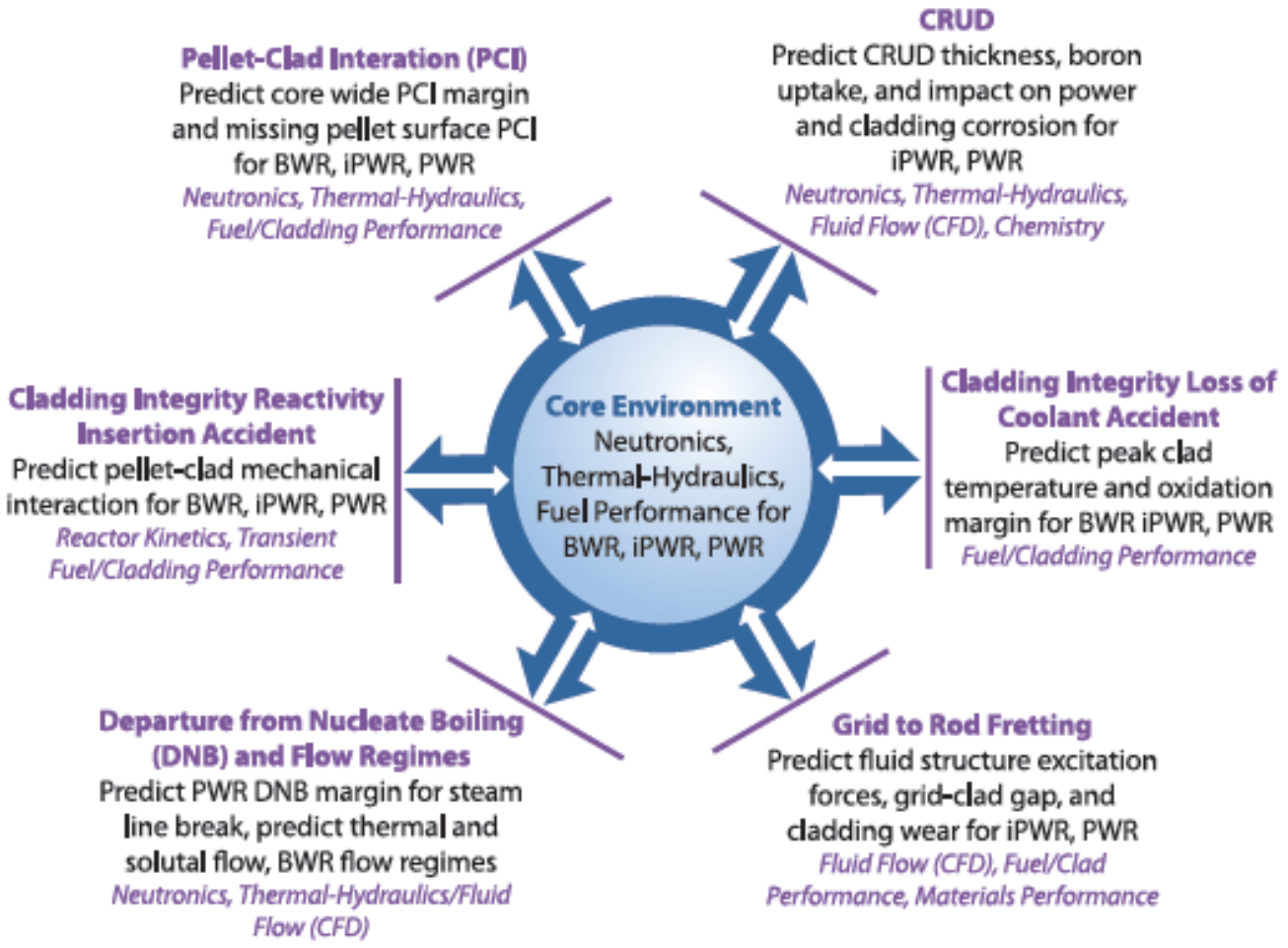
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL Virtual Reactor



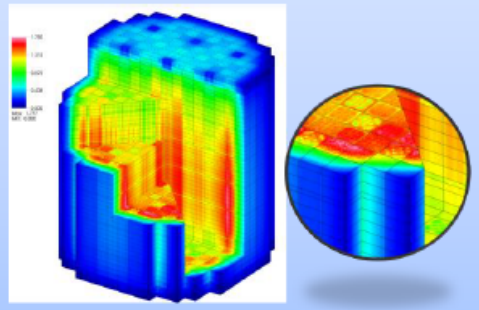
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Used to Create Insights Into Industry Defined Challenge Problems

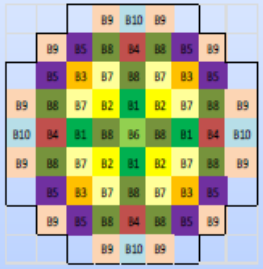


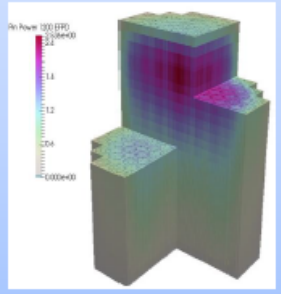
Key Accomplishments in FY15

VERA Simulation of Watts Bar Nuclear Unit 1 Operational History

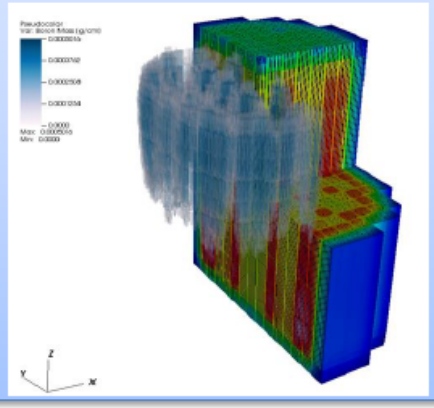


iPWR SMR Modeling Demonstration

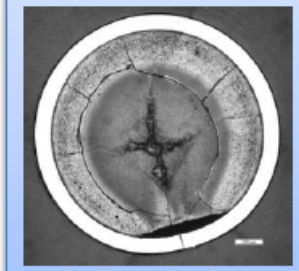


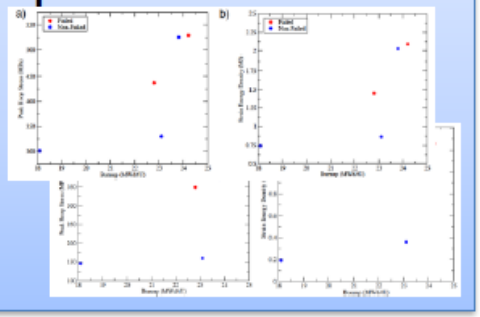


Simulation of Crud Induced Power Shift Challenge Problem (WBN1C7)

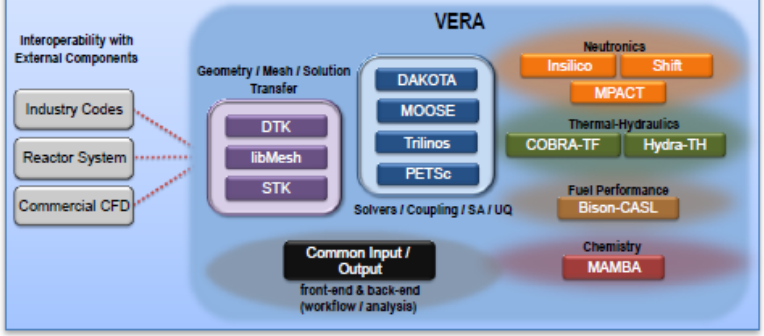


3D Modeling of Pellet-Clad Interaction and Comparison with Braidwood Experience



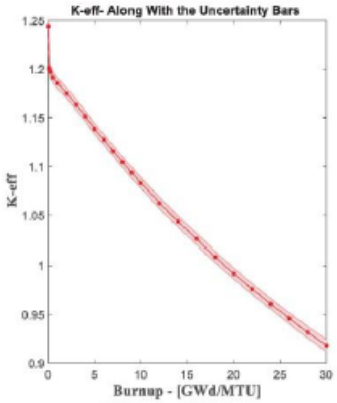


Second Major Externally-available Release of VERA

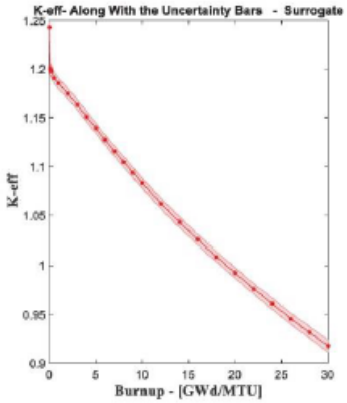


Joint Uncertainties– Depletion Dependent

Keff

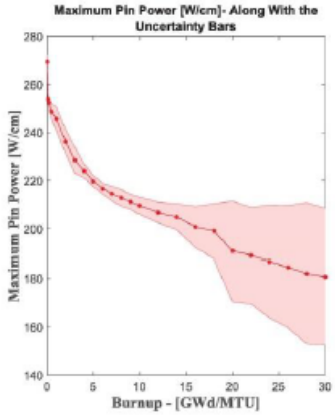


Monte Carlo

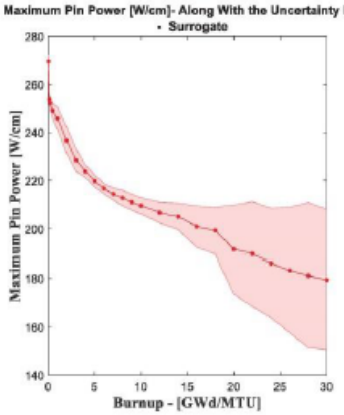


Surrogate

Maximum Pin Power

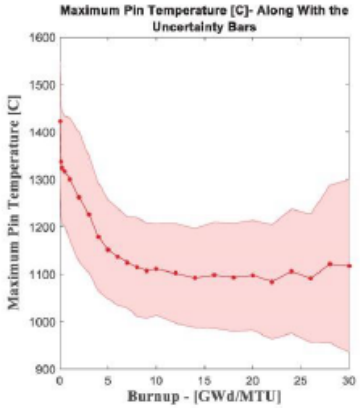


Monte Carlo

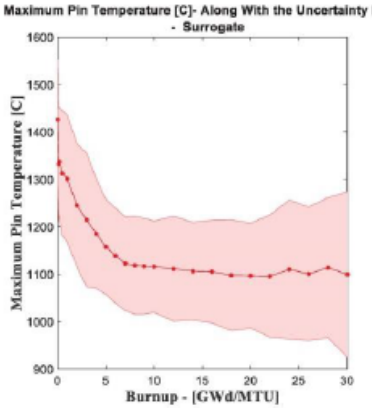


Surrogate

Maximum Pin Temperature



Monte Carlo



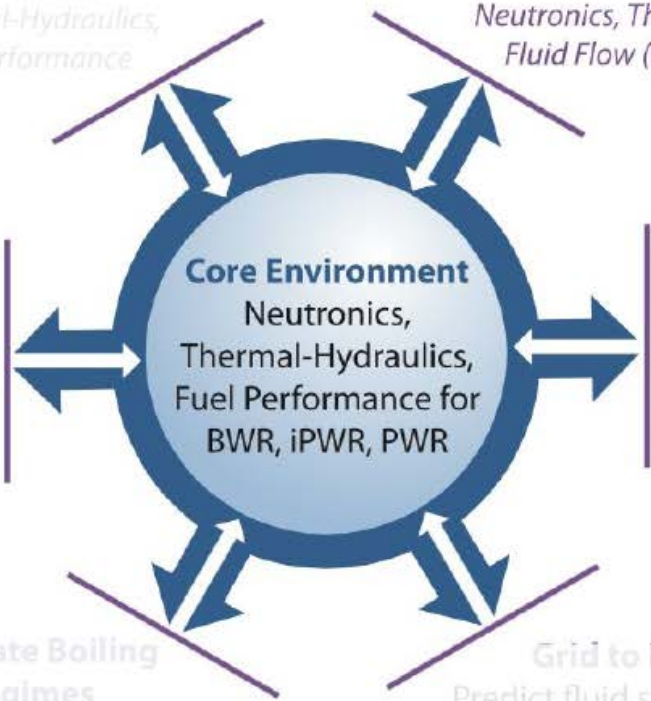
Surrogate

Difference of MC & Surrogate within MC Associated Uncertainty

Progress on CRUD Challenge Problem

CRUD
Predict CRUD thickness, boron uptake, and impact on power and cladding corrosion for iPWR, PWR
Neutronics, Thermal-Hydraulics, Fluid Flow (CFD), Chemistry

Pellet-Clad Interation (PCI)
Predict core wide PCI margin and missing pellet surface PCI for BWR, iPWR, PWR
Neutronics, Thermal-Hydraulics, Fuel/Cladding Performance



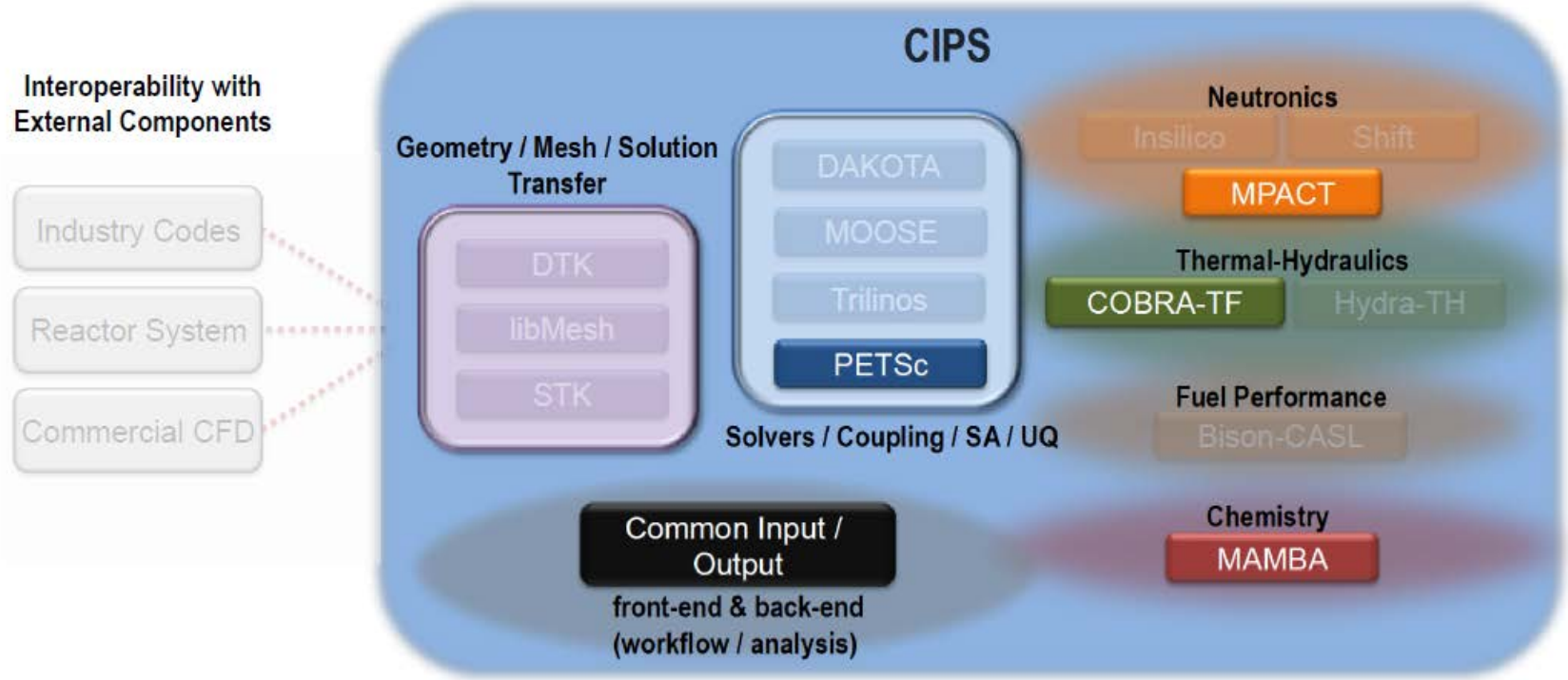
Cladding Integrity Reactivity Insertion Accident
Predict pellet-clad mechanical interaction for BWR, iPWR, PWR
Reactor Kinetics, Transient Fuel/Cladding Performance

Cladding Integrity Loss of Coolant Accident
Predict peak clad temperature and oxidation margin for BWR iPWR, PWR
Fuel/Cladding Performance

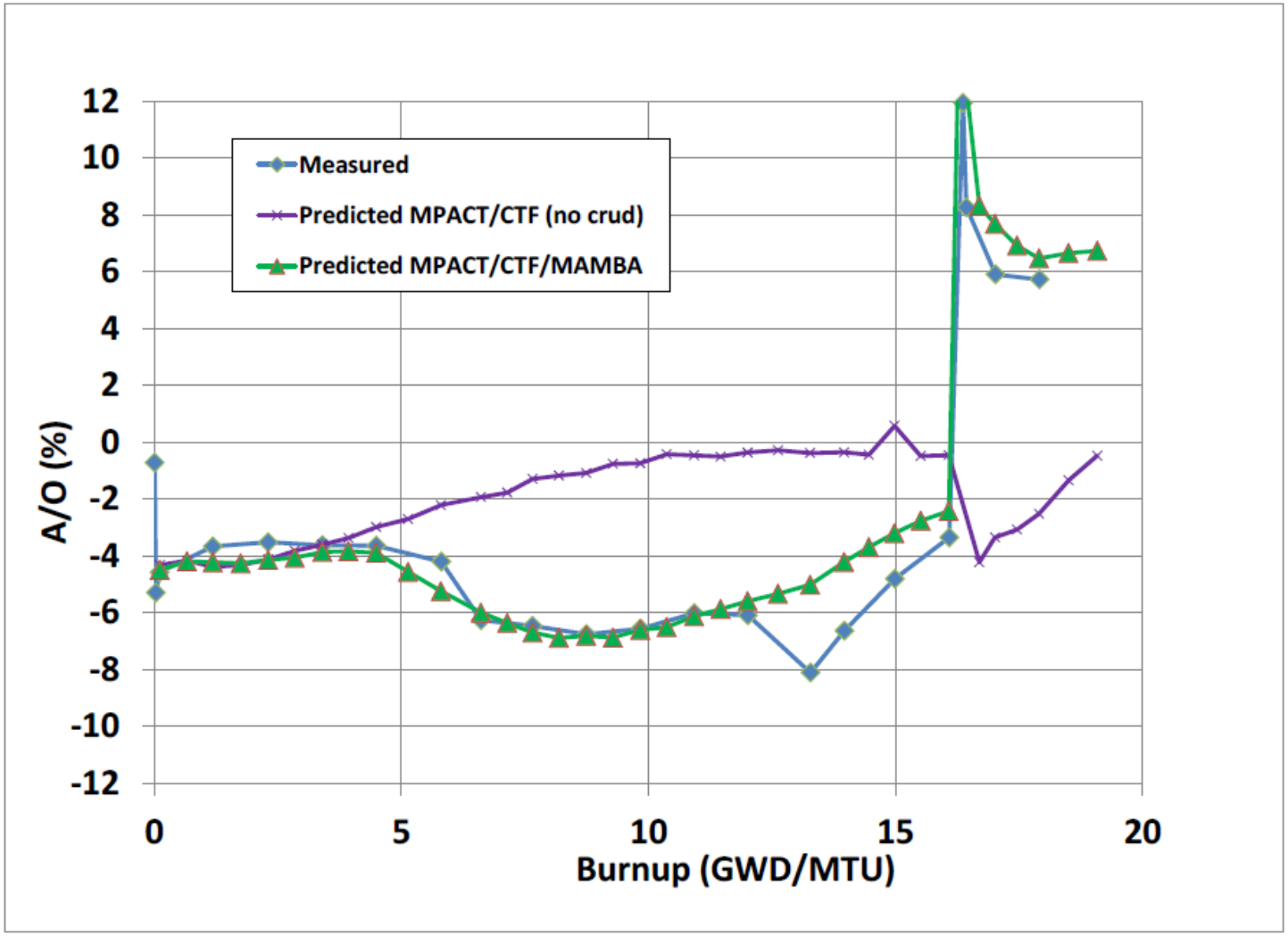
Departure from Nucleate Boiling (DNB) and Flow Regimes
Predict PWR DNB margin for steam line break, predict thermal and solutal flow, BWR flow regimes
Neutronics, Thermal-Hydraulics/Fluid Flow (CFD)

Grid to Rod Fretting
Predict fluid structure excitation forces, grid-clad gap, and cladding wear for iPWR, PWR
Fluid Flow (CFD), Fuel/Clad Performance, Materials Performance

VERA for CRUD Induced Power Shift Component Coupling



Updated Watts Bar 1 Cycle 7 Measured and Predicted Axial Offset Behavior

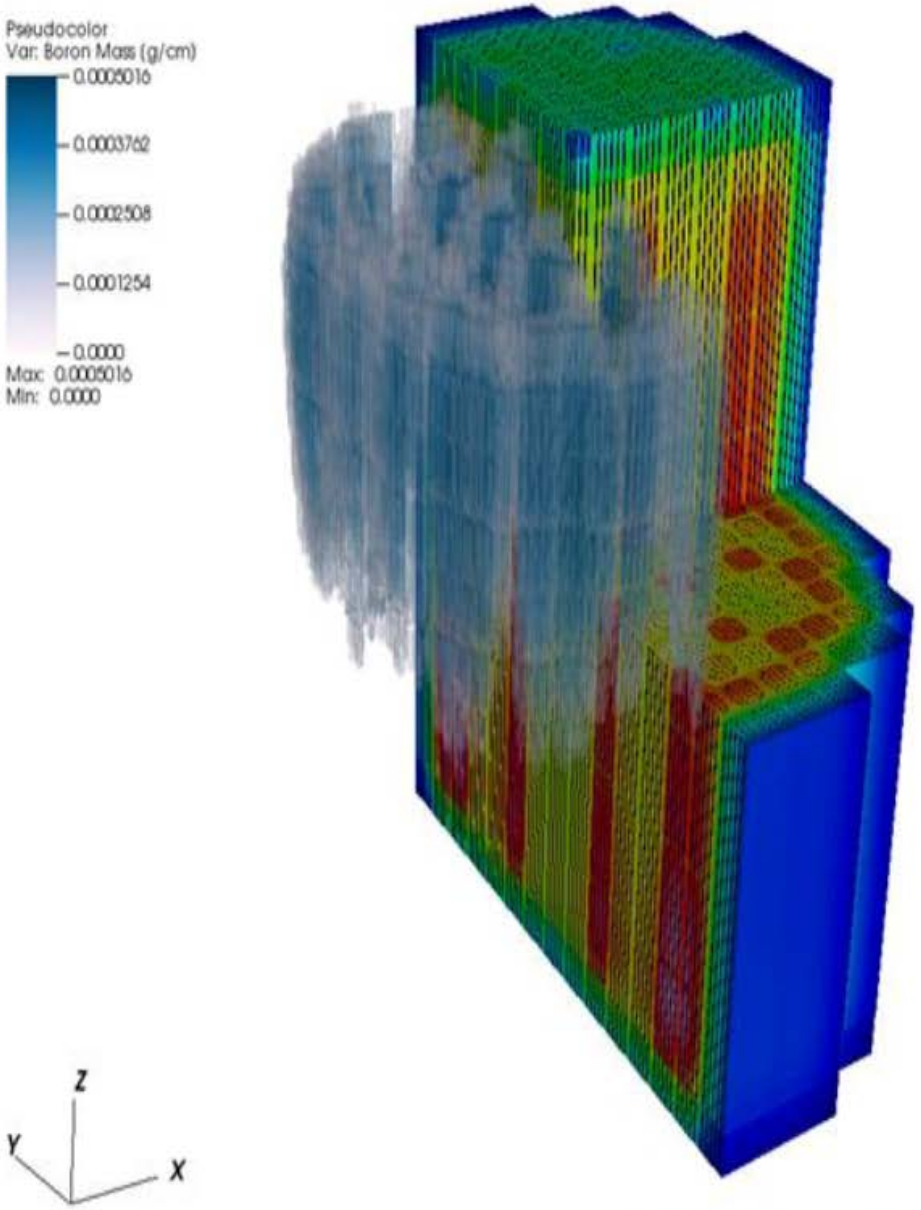


Concentration Threshold For Boron Precipitation Decreased 5X

Fraction of Crud Available For Boron Deposition Increased 3X

Watts Bar 1 Cycle 7 Predicted Boron Distribution

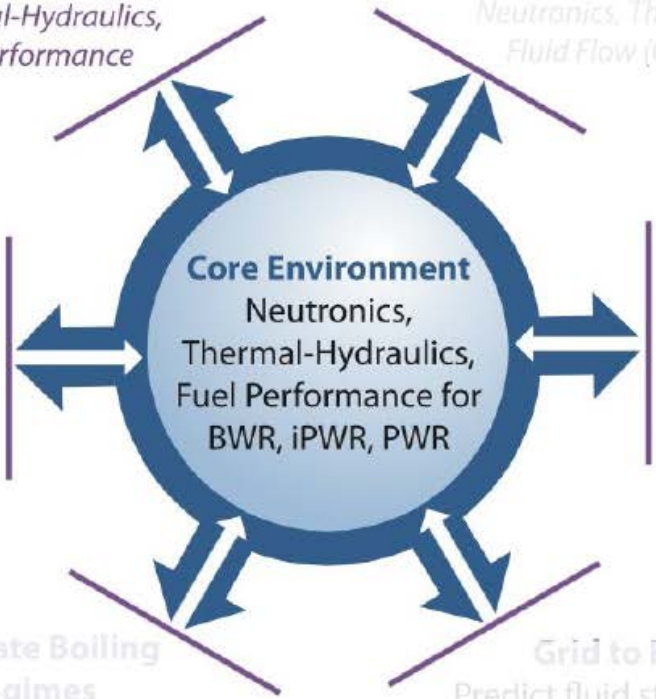
Boron Distribution at 16.08 GWD/MTU



Progress on PCI Challenge Problem

Pellet-Clad Interation (PCI)
Predict core wide PCI margin and missing pellet surface PCI for BWR, iPWR, PWR
Neutronics, Thermal-Hydraulics, Fuel/Cladding Performance

CRUD
Predict CRUD thickness, boron uptake, and impact on power and cladding corrosion for iPWR, PWR
Neutronics, Thermal-Hydraulics, Fluid Flow (CFD), Chemistry



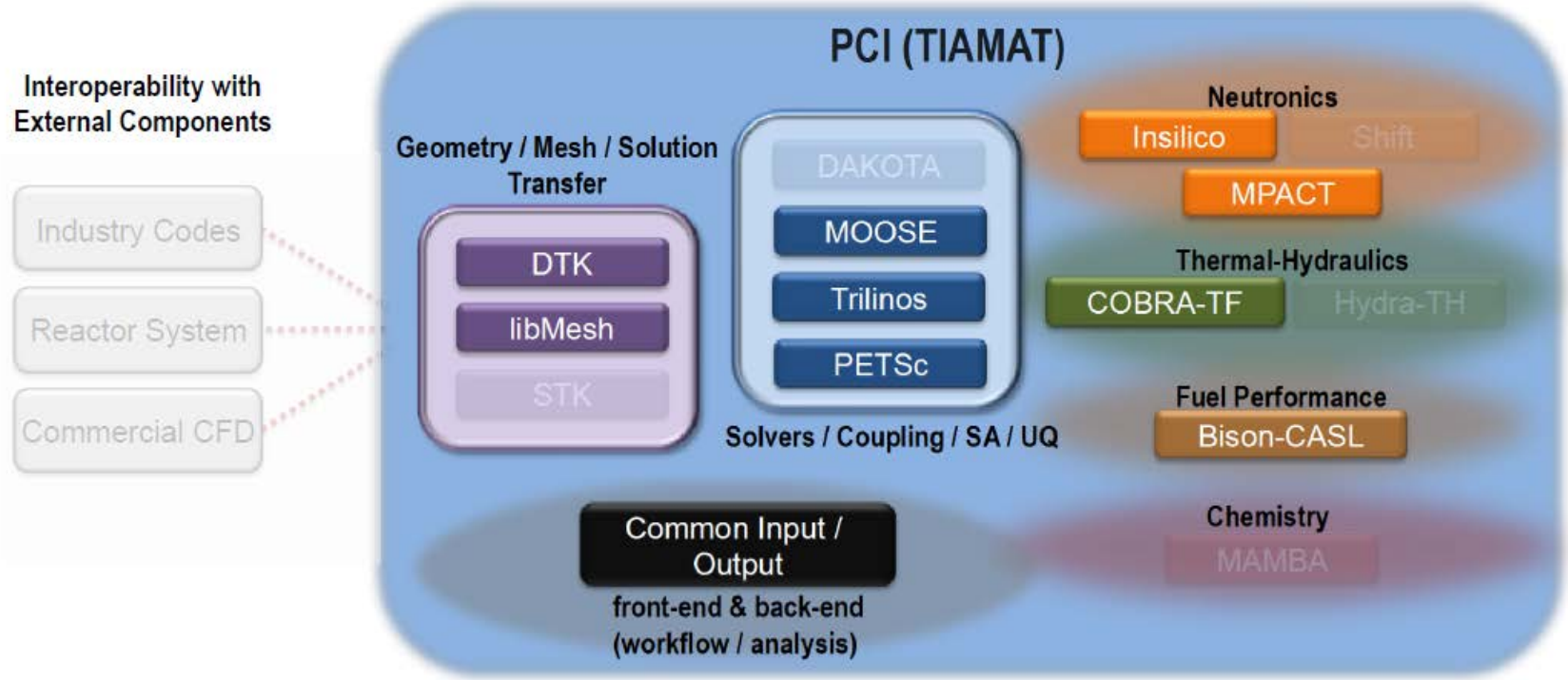
Cladding Integrity Reactivity Insertion Accident
Predict pellet-clad mechanical interaction for BWR, iPWR, PWR
Reactor Kinetics, Transient Fuel/Cladding Performance

Cladding Integrity Loss of Coolant Accident
Predict peak clad temperature and oxidation margin for BWR iPWR, PWR
Fuel/Cladding Performance

Departure from Nucleate Boiling (DNB) and Flow Regimes
Predict PWR DNB margin for steam line break, predict thermal and solutal flow, BWR flow regimes
Neutronics, Thermal-Hydraulics/Fluid Flow (CFD)

Grid to Rod Fretting
Predict fluid structure excitation forces, grid-clad gap, and cladding wear for iPWR, PWR
Fluid Flow (CFD), Fuel/Clad Performance, Materials Performance

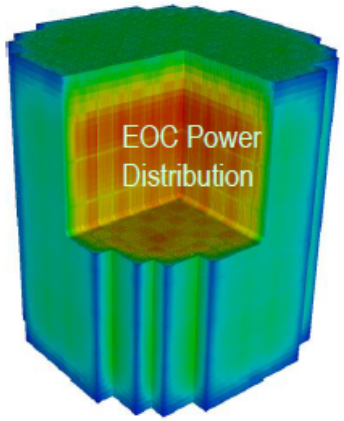
VERA for Pellet Clad Interaction Component Coupling



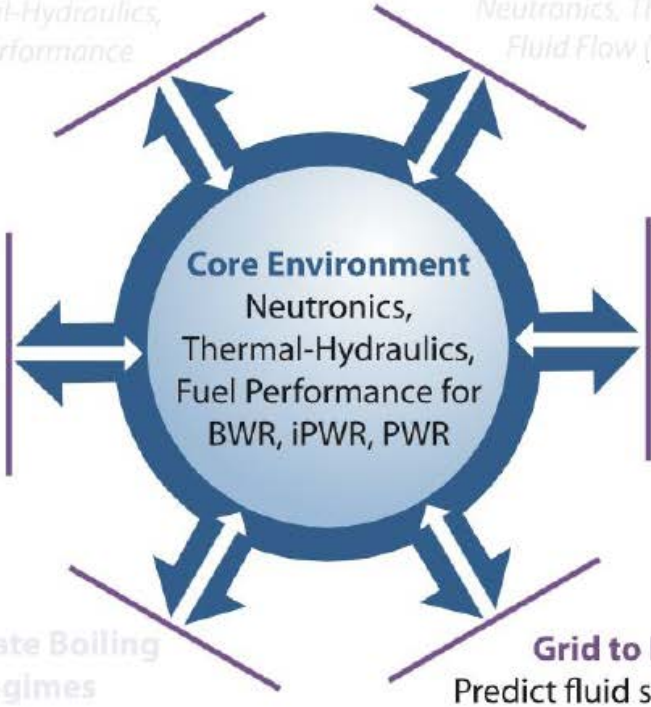
Part 1 Accomplishments

- Development for 2-D and 3-D modeling for both full-length and local effects geometry
- Lower-length scale material modeling of cladding
  - Visco-plastic self consistent model (VPSC) for thermal and irradiation creep and growth
  - Dislocation density crystal plasticity model for Zr-cladding fracture
  - Corrosion and hydriding behavior of Zr-alloys
- Integration into VERA-CS (Tiamat) for multi-rod/multi-assembly simulations
- EPRI Test Stand focus on PCI modeling
  - Initial focus on fuel performance modeling with CASL-BISON

Cladding deformations and stress contour around MPS defect (displacements x20)

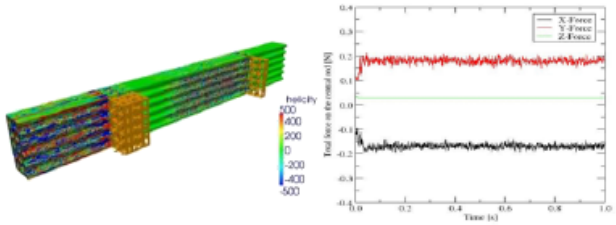


Progress on GTRF Challenge Problem

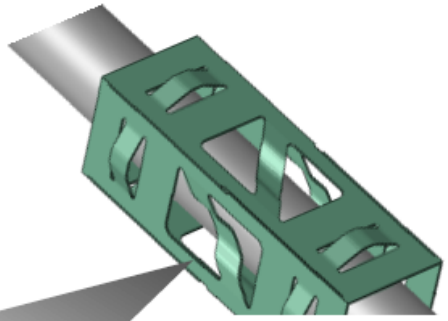


Grid to Rod Fretting
Predict fluid structure excitation forces, grid-clad gap, and cladding wear for iPWR, PWR
Fluid Flow (CFD), Fuel/Clad Performance, Materials Performance

GTRF Challenge Problem



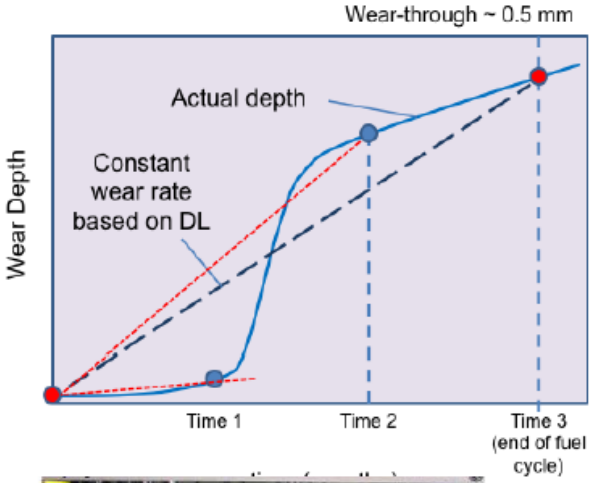
CFD Pressure Load History (Hydra-TH & limited fluid-structure interaction sims)

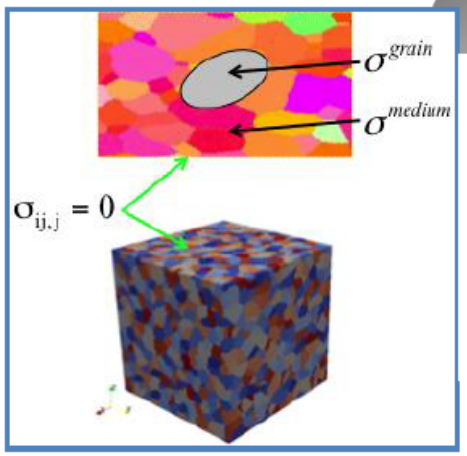


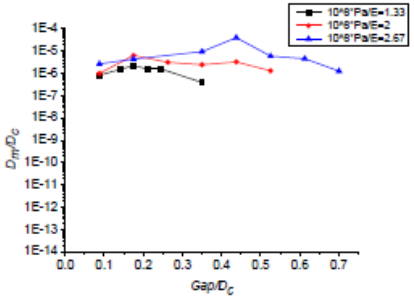
Structural mechanics thru interoperability with ISVs

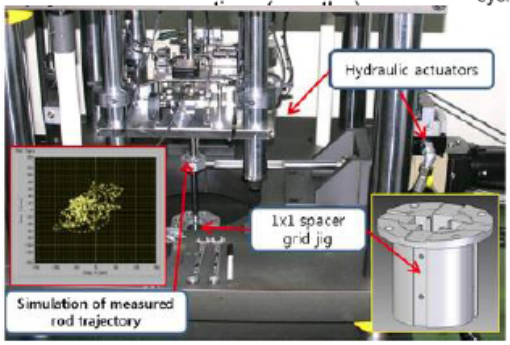
TEAM: Dave Parks, Ken Kamrin, Michael Demkowicz, Sam Sham, Peter Blau. Jun Qu, Roger Lu, Michael Thouless, Wei Lu,

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







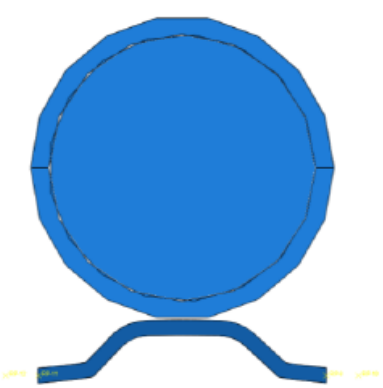


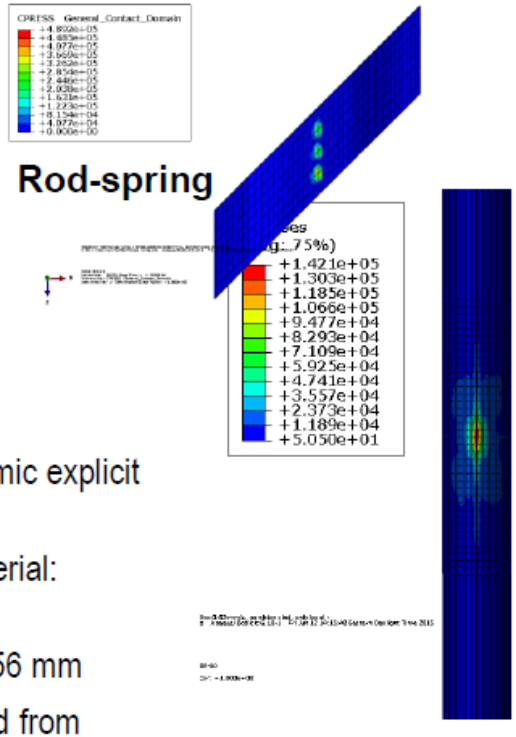
ORNL controlled fretting wear measurements

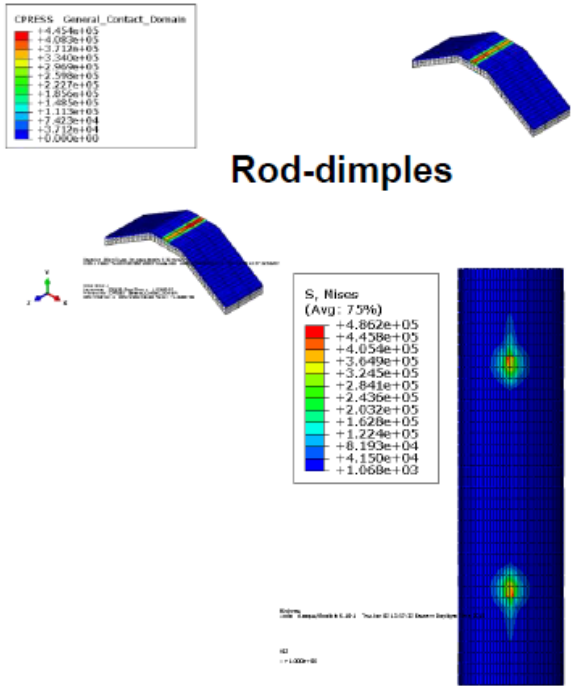
Grid-rod gap evolution, mechanical property evolution & parametric studies of gap size/rod stiffness on wear shapes

Fretting mechanics: recent progress

Finite element modeling used to evaluate and refine design for new fretting tester under procurement







- 3-D FEA model using dynamic explicit code
- Rod and spring/dimple material: Zircaloy-4
- Rod modeled with length 356 mm
- Spring/two dimples modeled from scanned profile
- Contact defined between clad and spring/ dimples surfaces
- Initial velocity of clad upon impacting spring/dimples estimated as 0.25~0.62mm/s

Impact	FEA simulated reaction force (N)
Rod against spring	0.08 ~ 0.16
Rod against dimple	0.17 ~ 0.40

Used to define the specs of contact forces in bench tests.

Summary - Overall Challenge Problem Progress

	Development	Innovation	Validation
Operational			
CRUD-induced power shift (CIPS) – PWR/iPWR			
CRUD-induced localized corrosion (CILC) – PWR/iPWR			
Grid-to-rod fretting failure (GTRF) – PWR/iPWR			
Pellet-clad interaction (PCI) – PWR/iPWR			
Pellet-clad interaction (PCI) - BWR			
Safety			
Departure from nucleate boiling (DNB) – PWR/iPWR			
Cladding integrity during (LOCA) – PWR/iPWR			
Cladding integrity during (RIA) – PWR/iPWR			
Predict Thermal & Solutal Flows – iPWR/BWR			
Cladding integrity during (LOCA) – BWR			
Cladding integrity during (RIA) – BWR			

Significant Progress

Planning & Scoping

Good Progress

Not Started

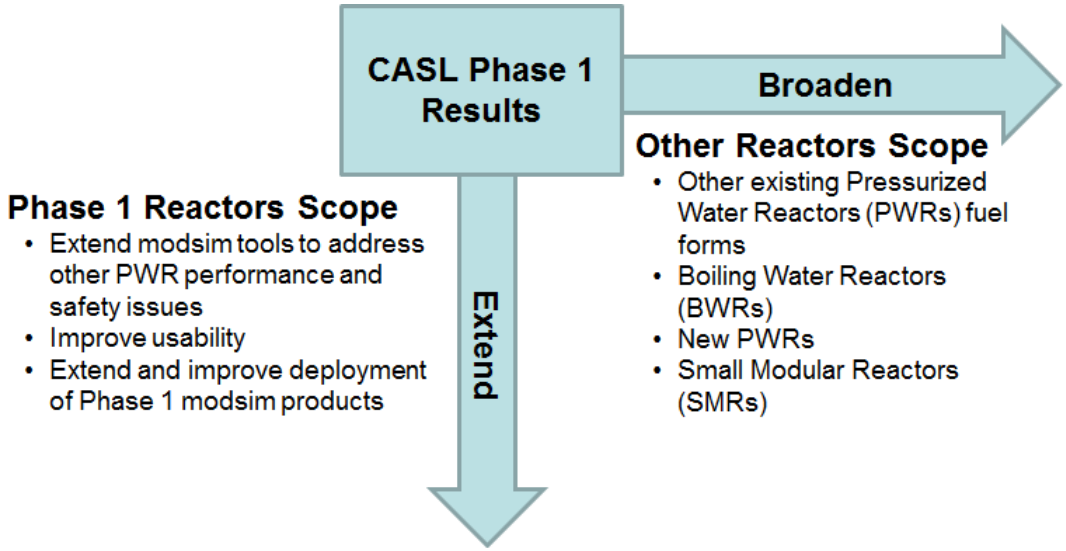
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Phase 2 Application Process

Demonstrated CASL Met Criteria to Qualify for Phase 2

- **Technical Performance** – Meeting Milestones
- **Annual Reviews** – Successful Completion
- **Impact on Science and Engineering** – Publications, Presentations, Students
- **Technology Deployment** – Demonstrated Success

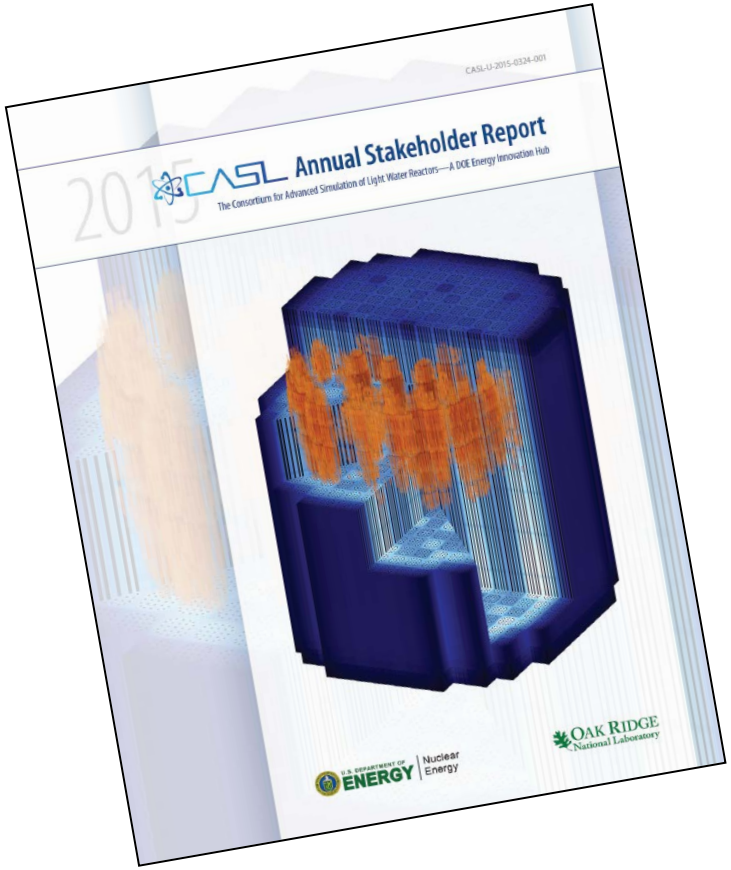
Generated Plans for Phase 2



- **Most Importantly** – Phase 2 is not a repeat of Phase 1!

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

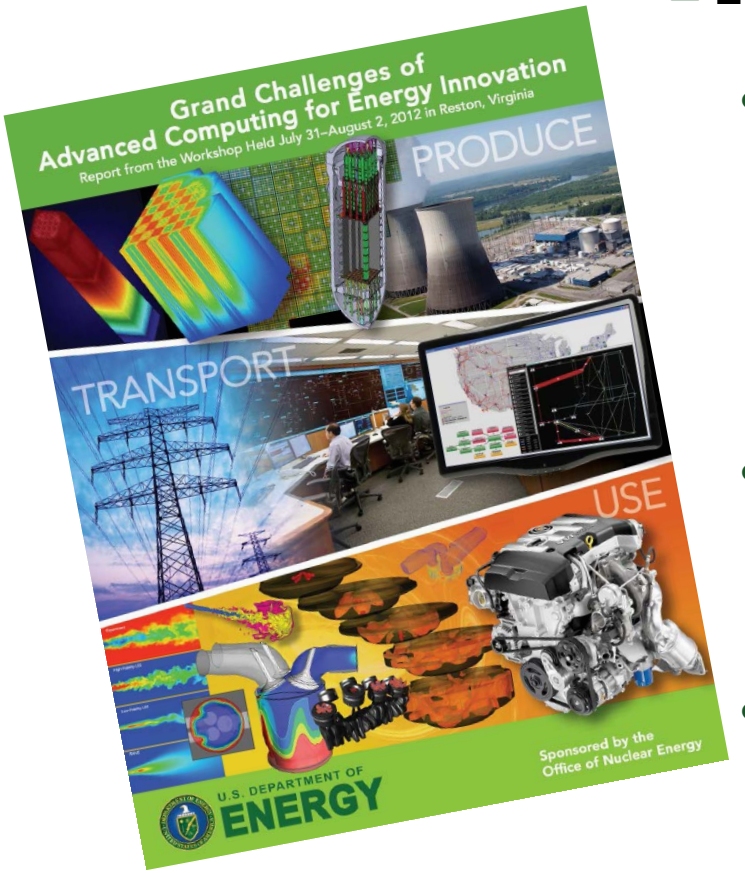
Phase 2 Light Federal Touch Oversight to be Provided by an Annual Stakeholder Report



- **End Nuclear Energy Modeling and Simulation Users**
  - Simulated all 13 fuel cycles of the Watt Bar #1 Reactor with depletion, fuel shuffling and discharge
  - Extended VERA tools to SMRs & BWRs
  - Accurately simulated (pin by pin) simulation of the cycle 7 CRUD induced power shift
- **Science and Engineering**
  - Extensive publications
  - Recognition of CASL with individual research awards and journal special editions
- **Workforce Training and Education**
  - Created VERA-EDU
  - Initiated VERA training, documentation and course curriculum
  - CASL Undergraduate Research Scholars Program
- **Sustaining Taxpayer Investments**
  - Initiated the creation of the VERA-Working Group based on the RELAP5 model to collect funds for code maintenance and ongoing user support.
  - NCSU Business School study of CASL

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL is Overcoming the Barriers for Successful Advanced Computing Deployment



2012 Workshop Identified Barriers

- **Technical** – Simulation Tools that are Useful and Usable
  - CASL Responses Includes
    - Focused on industry defined challenge problems
    - Standard input based on industry workflows and standards
    - Improved computational efficiency to allow running simulations on industry class systems
- **Structural** – IP and Legal Agreements
  - CASL Responses Includes
    - Established export control protocols
    - Released Intellectual Property Management Plan
- **Motivation** – Demonstration of the value CASL tools
  - CASL Responses Includes
    - Deployment of VERA Test Stands
    - Return on investment studies
    - Ongoing engagement through the Industry Council