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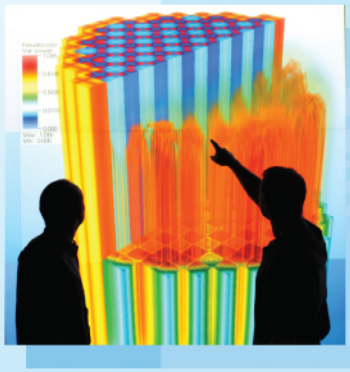
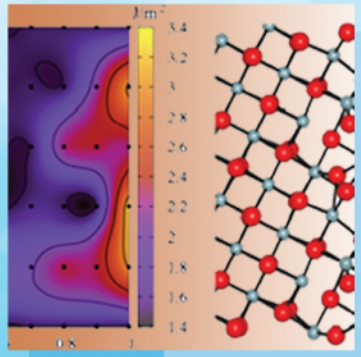
Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

L3:AMA.NRC.P5.01

CASL NRC Commissioner Technical Seminar

Jess Gehin
Oak Ridge National Laboratory

December 22, 2012

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2012-0076-000-a

CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

NRC Commissioner Technical Seminar
November 30, 2012

Doug Kothe (ORNL) CASL Director
Doug Burns (INL) CASL Deputy Director
Paul Turinsky (NCSU) CASL Chief Scientist
Jess Gehin (ORNL) CASL AMA FA Lead
Jeff Binder (ORNL) Associate Laboratory Director
Trevor Cook (DOE-NE) Director, Advanced Modeling and Simulation Office

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Presentation Outline

- **CASL Overview [Doug Kothe]**
  - Mission
  - Scope/Goals
  - Challenge Problems
  - Organization/Councils
- **Science and Virtual Reactor [Paul Turinsky]**
  - Virtual Environment for Reactor Applications
  - CRUD modeling
  - Grid-to-Rod Fretting
  - Pellet Clad Interaction
- **Reactor Simulation and NRC Engagement [Jess Gehin]**
- **Summary**

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

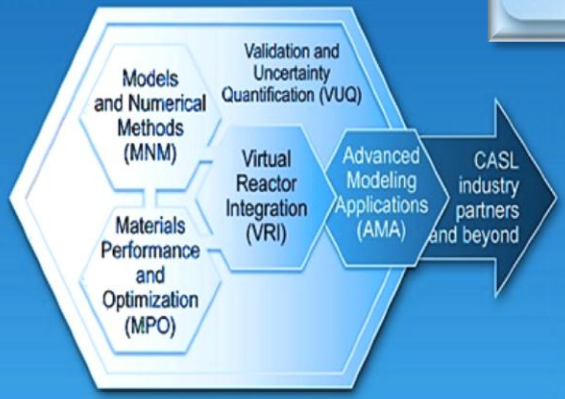
- Key nuclear energy vendor, utility, R&D institute
- Leading DOE labs in science, nuclear energy, national security
- Preeminent university nuclear engineering programs
- World leaders in high-performance computing (HPC) and computational science

Tackling tough industry challenges that matter

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

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



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

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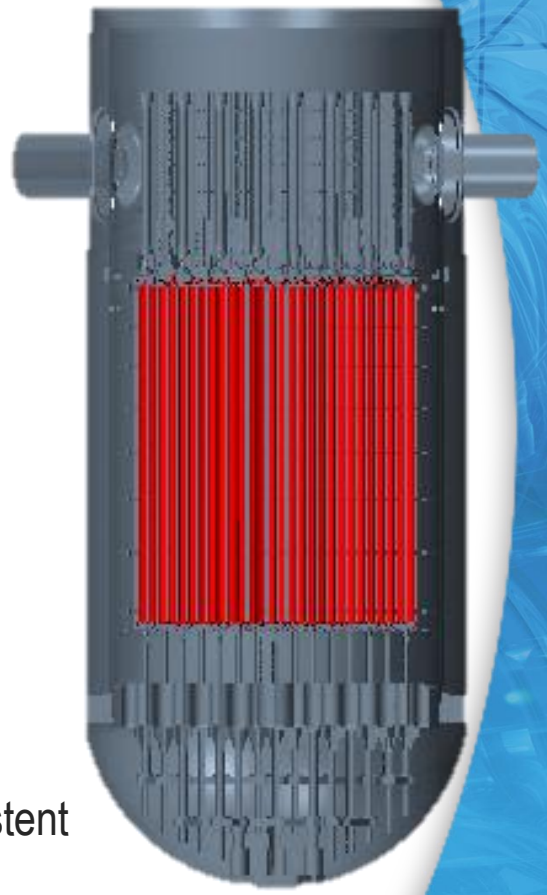
Nuclear Energy

CASL Scope: Develop and apply a "Virtual Reactor" to assess fuel design, operation, and safety criteria

- Deliver improved predictive simulation of **PWR core, internals, and vessel**
  - Couple Virtual Reactor to evolving out-of-vessel simulation capability
  - Maintain applicability to other NPP types
- 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 self-consistent quantified uncertainties

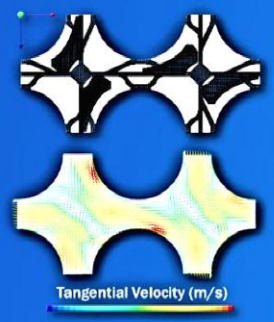


Focus on Addressing Challenge Problems to Drive Development and Demonstration

CASL Challenge Problems

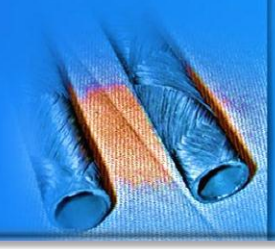
Key safety-relevant reactor phenomena that limit performance

Departure from Nucleate Boiling

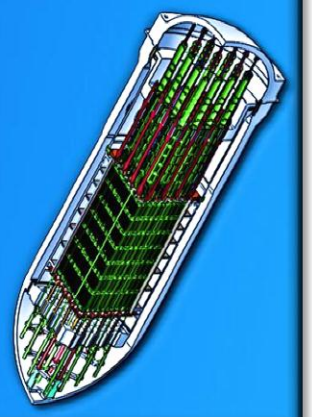


Cladding Integrity

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



Reactor Vessel and Internals Integrity

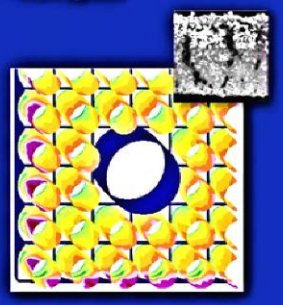


CASL is committed to delivering simulation capabilities for

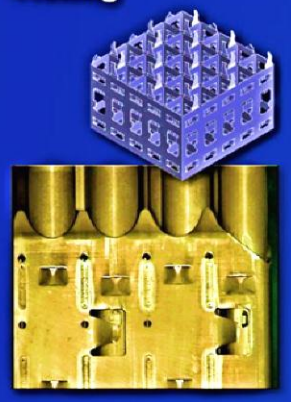
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

Crud

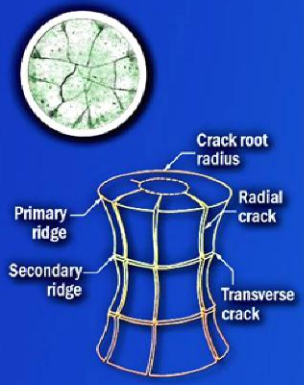
- Deposition
- Axial offset anomaly
- Hot spots



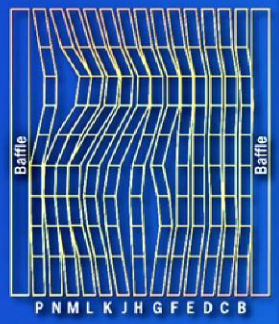
Grid-to-Rod Fretting



Pellet-Clad Interaction



Fuel Assembly Distortion



CASL Consortium for Advanced Simulation of LWRs
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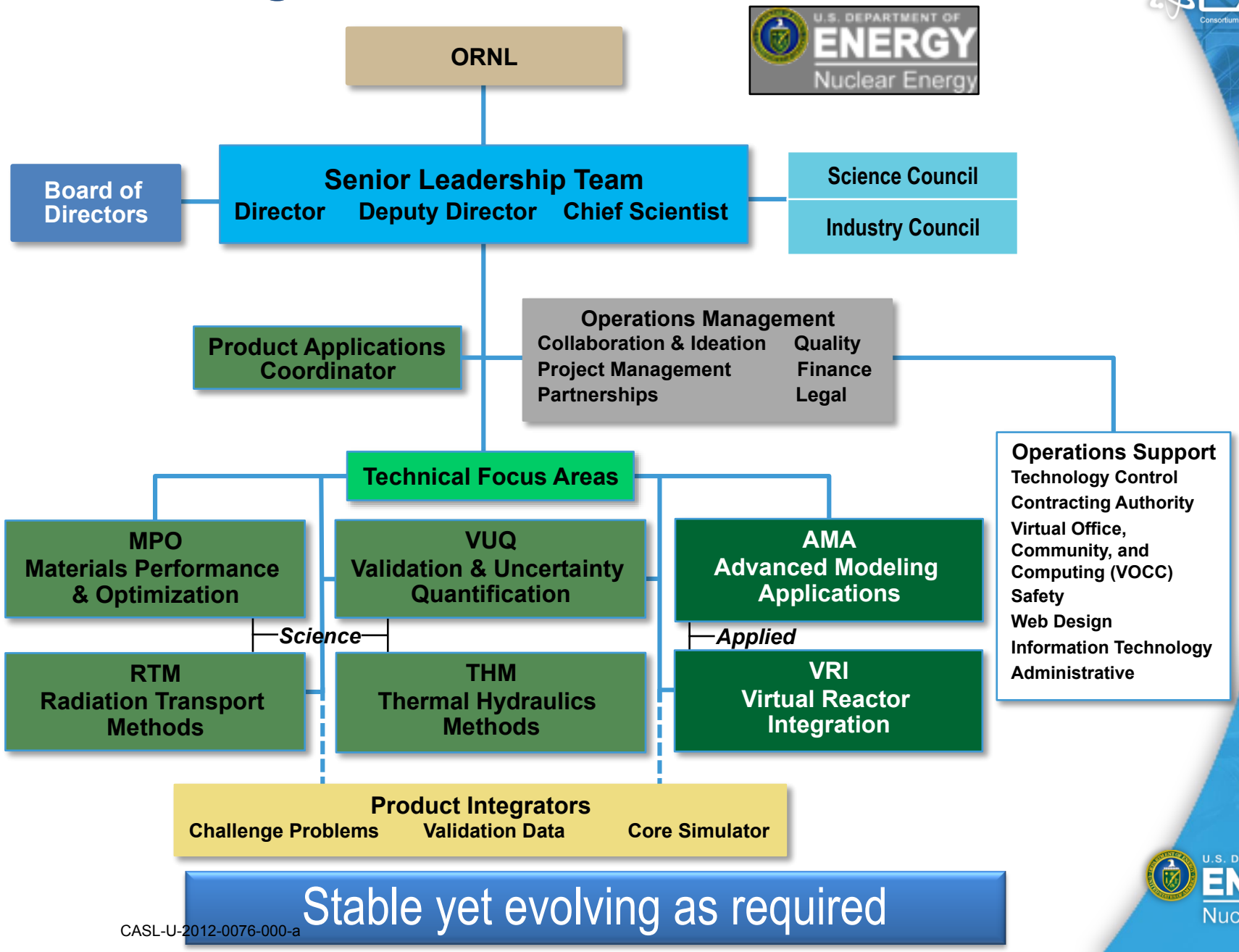
CASL: Challenge Problem (CP) Objectives

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

Significant Progress on CRUD, GTRF, PCI CPs

Increasing effort on DNB, Cladding Integrity CPs

CASL Organization



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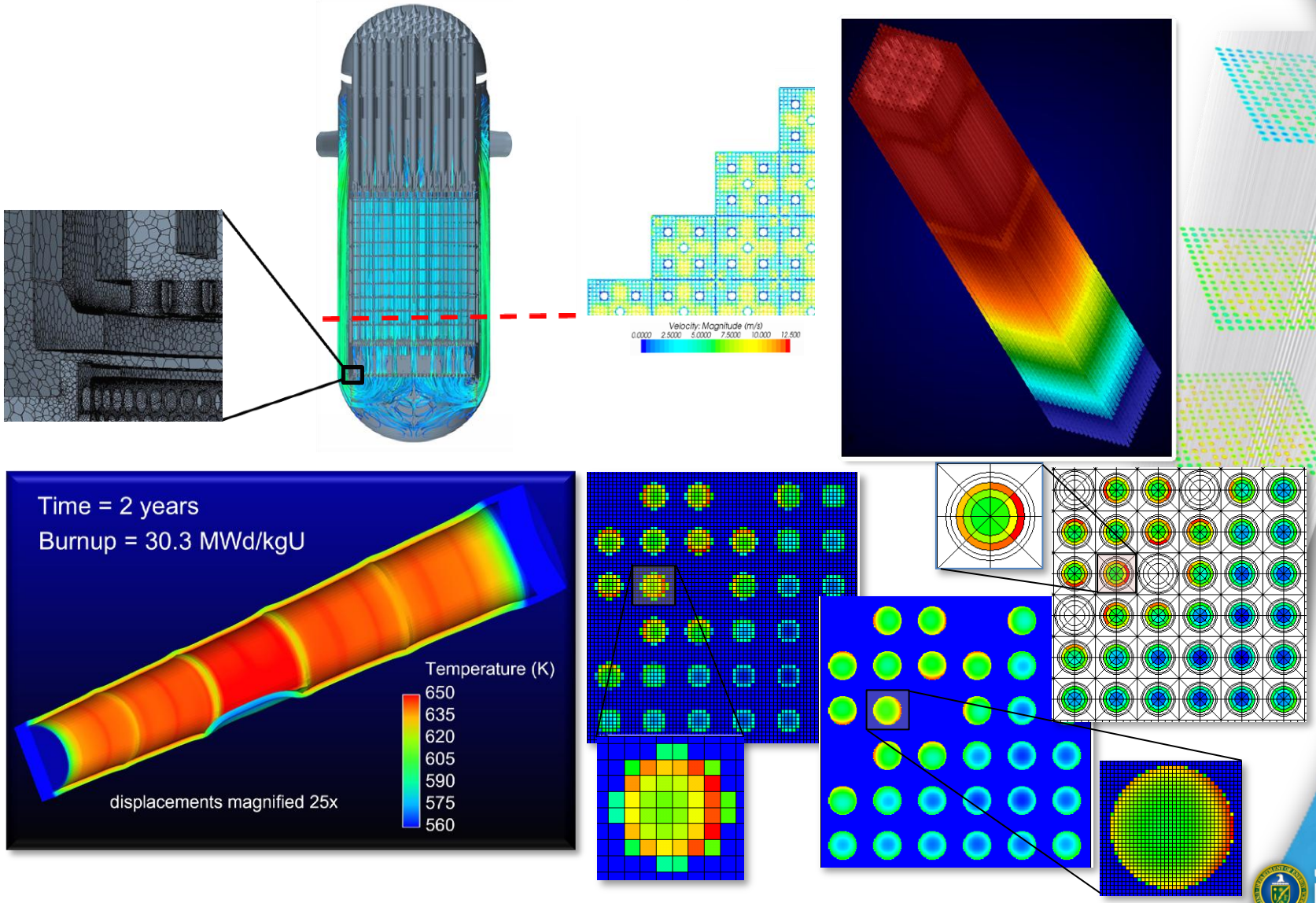
CASL Tackles the Multi-Scale Challenge of Predictively Simulating a Reactor Core



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

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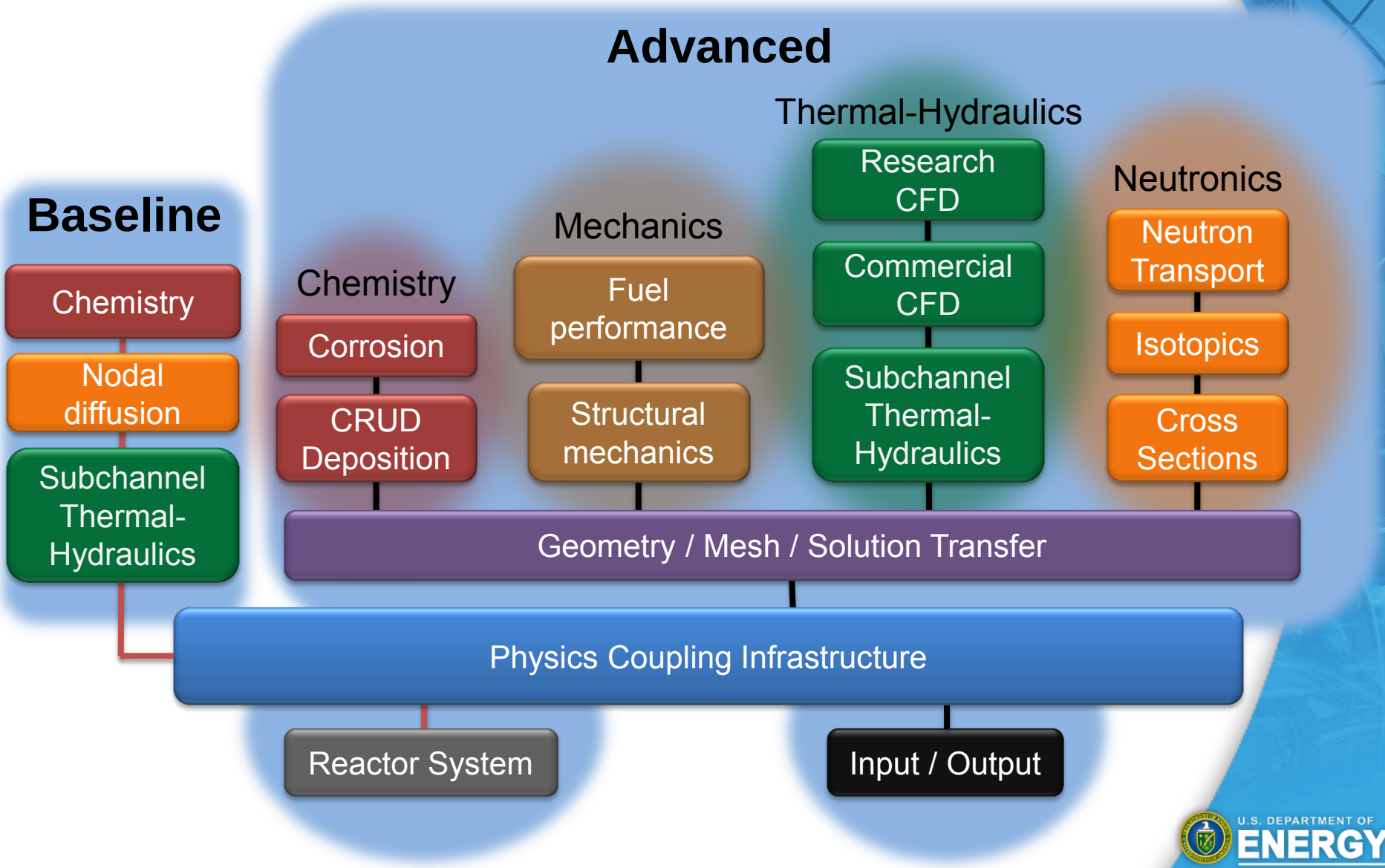
Virtual Environment for Reactor Applications (VERA)

Virtual Environment for Reactor Applications (VERA)

CASL's virtual reactor for in-vessel LWR phenomena



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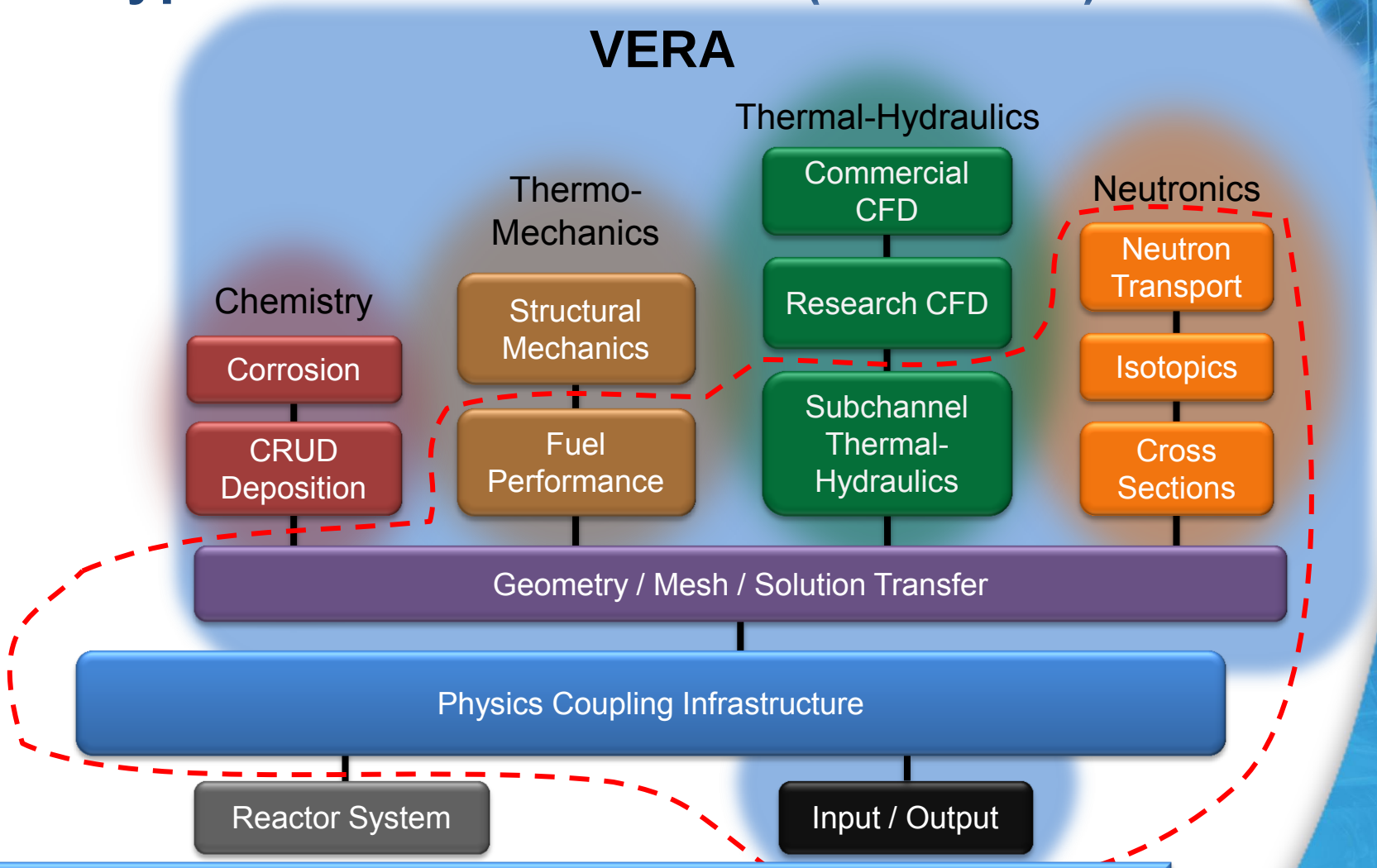
Some of our VERA components comprise a new type of "Core Simulator" (VERA-CS)



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.

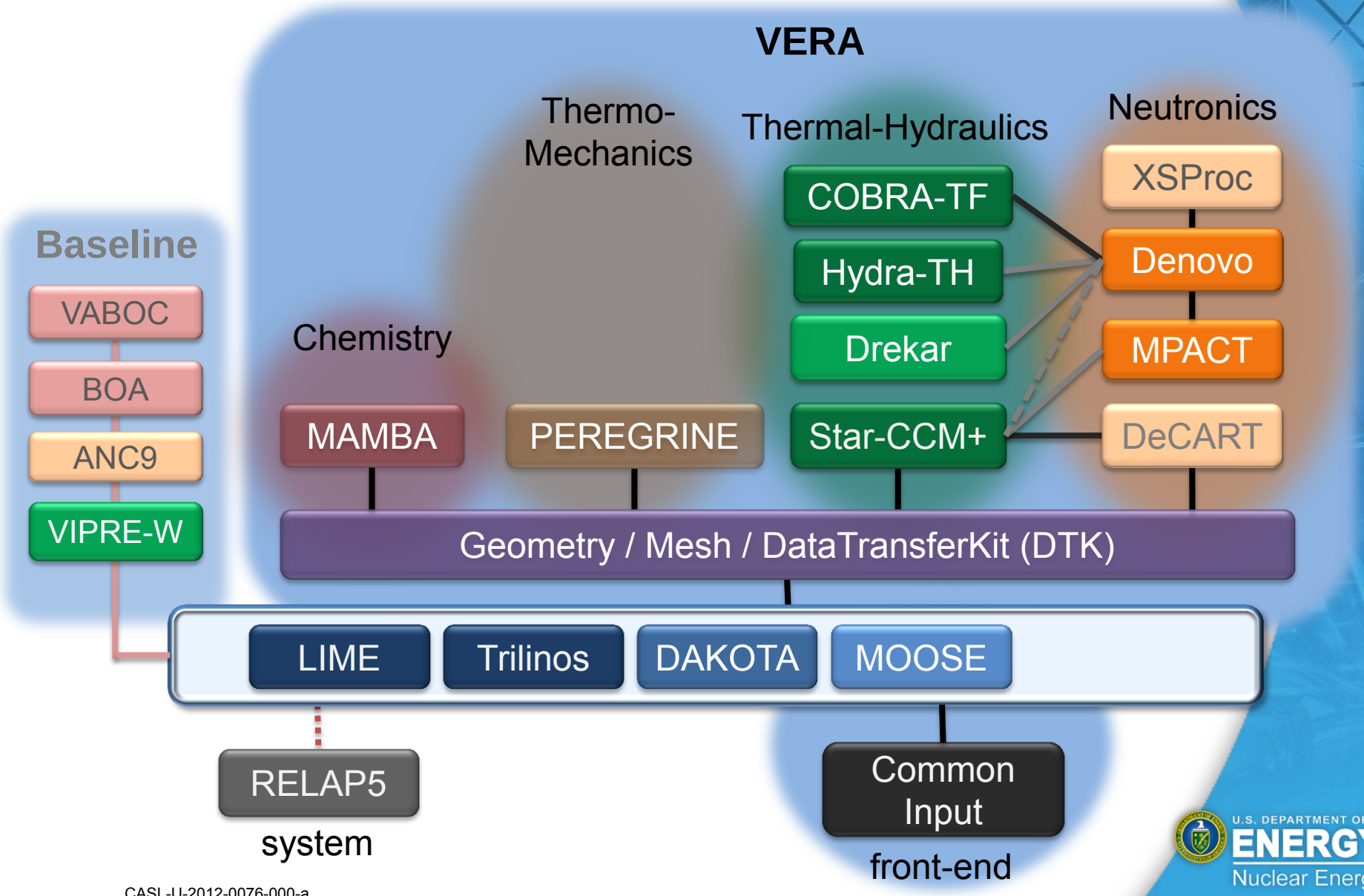
VERA-CS vs. Industry Core Simulators

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

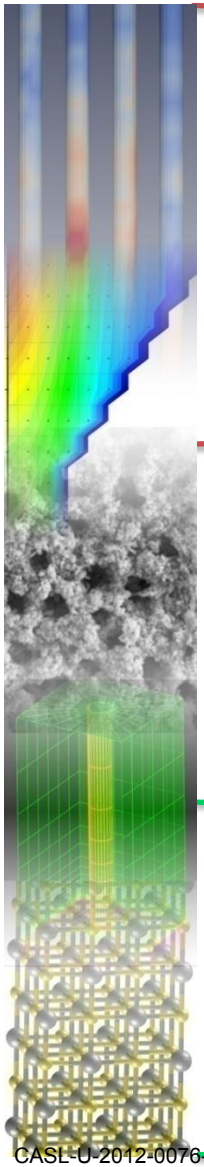
- What's "good enough"? Quantified margins and uncertainties will guide us

Next Development Snapshot: VERA 3.0 (03/2013)



CRUD Challenge Problem Progress

The CASL Approach to Multiscale Materials Modeling: CRUD as an Illustrative Example



- Top-Down Approach
- Ultimate Goal: 3D Engineering Framework (MAMBA)
  - Predict :
    - CRUD thickness
    - Peak cad temperature
    - Boron loading
  - Couple to fuel performance codes
- High-Fidelity Info from the Mesoscale (MAMBA-BDM)
  - Finer level of granularity
  - Couples CRUD to cladding corrosion
  - Same parameters at MAMBA
  - Higher computational cost
- CRUD Formation Atomistics & Thermodynamics
  - Develop fundamental data
  - Pass info up to MAMBA-BDM, such as:
    - NiO cluster formation
    - Species-dependent boron compound precipitation
    - Thermodynamic phase stability

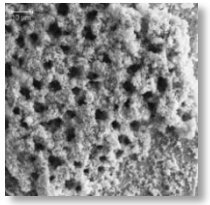
Coolant Chemistry and CRUD Growth

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

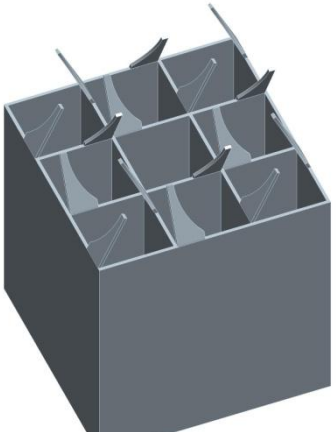
Reduced crud and boron due to turbulence behind mixing vanes

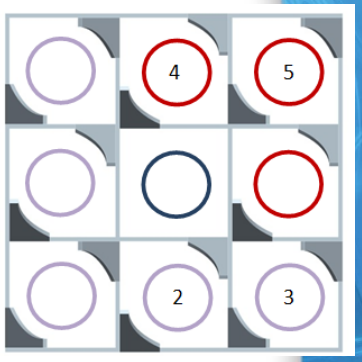


80 cm section of fuel rod

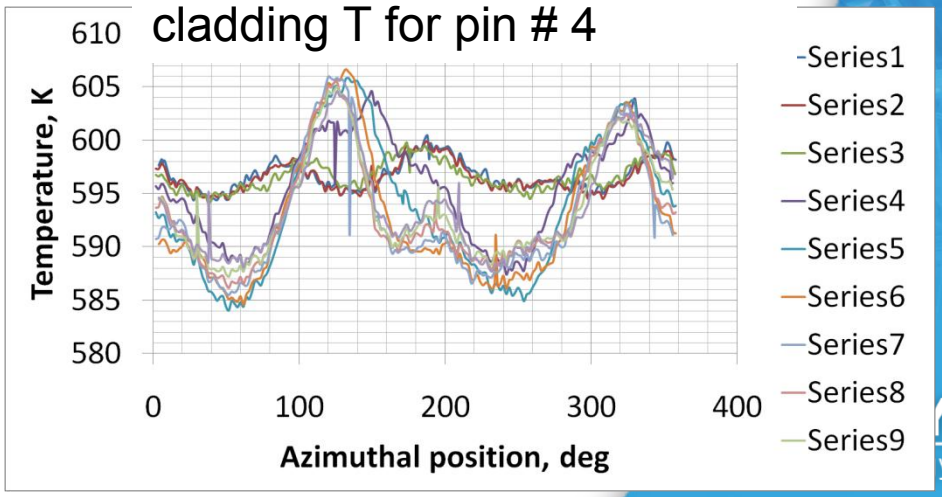
Large azimuthal variation in fluid/cladding temperature computed

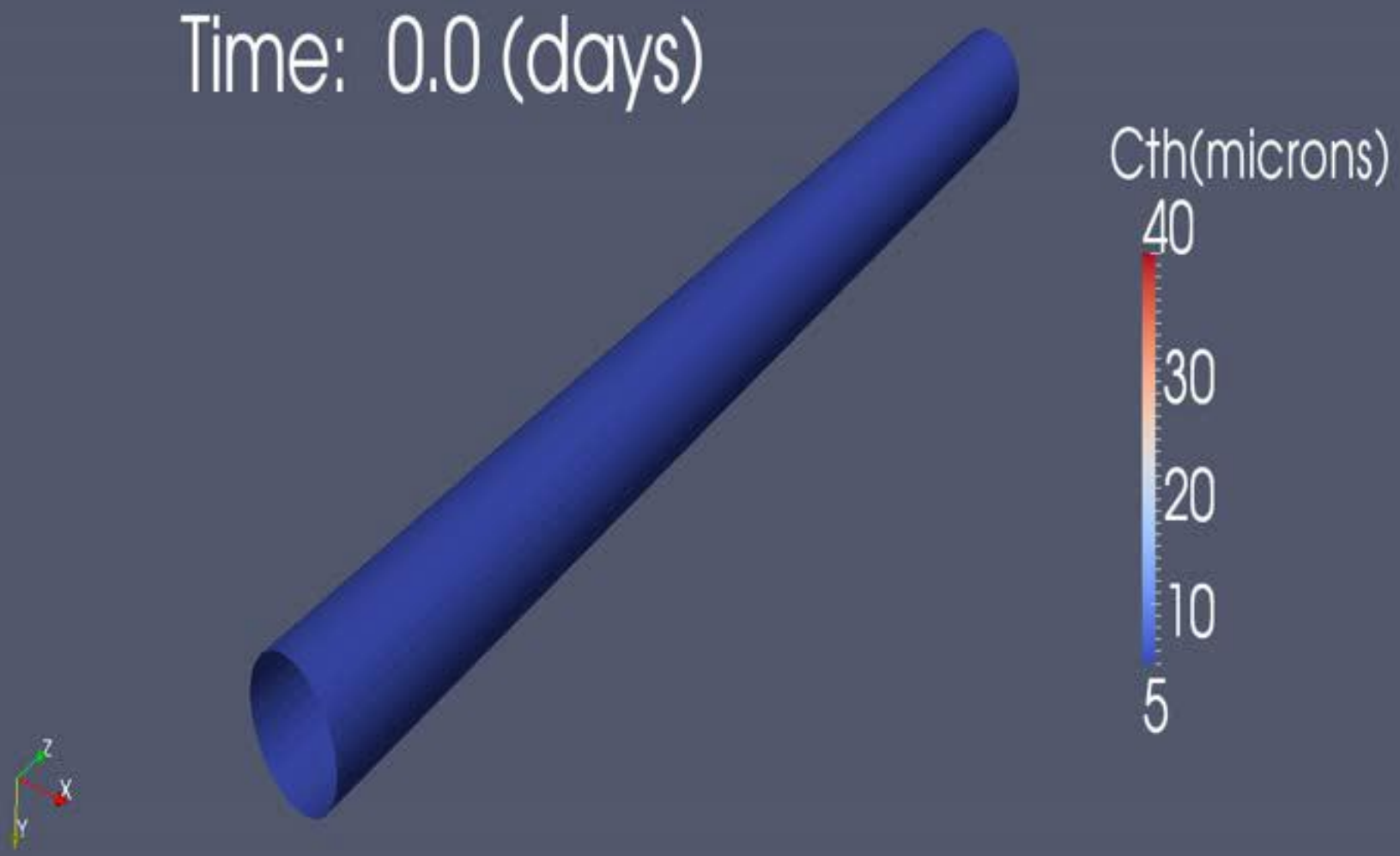
Spacer with mixing vanes





CFD computed cladding T for pin # 4



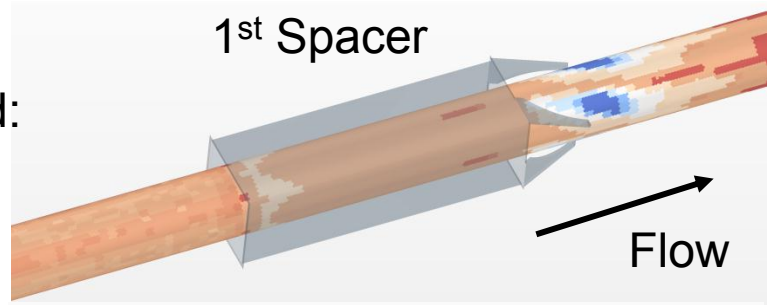

Time: 0.0 (days)
Cth(microns)
40
30
20
10
5
Z
X
Y

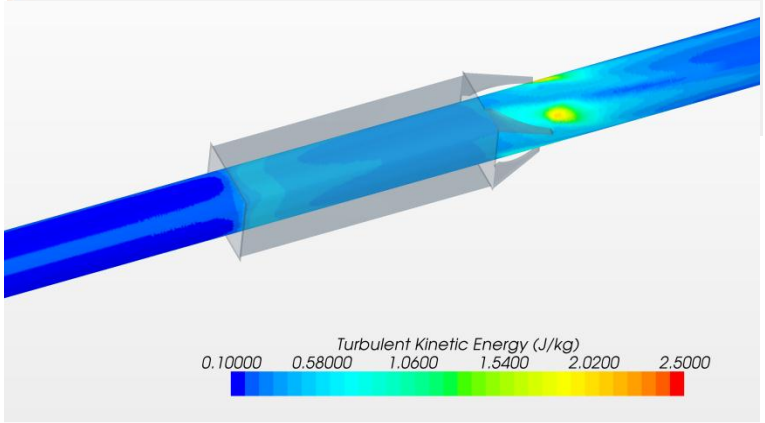
Positive Feedback between CRUD growth and CFD

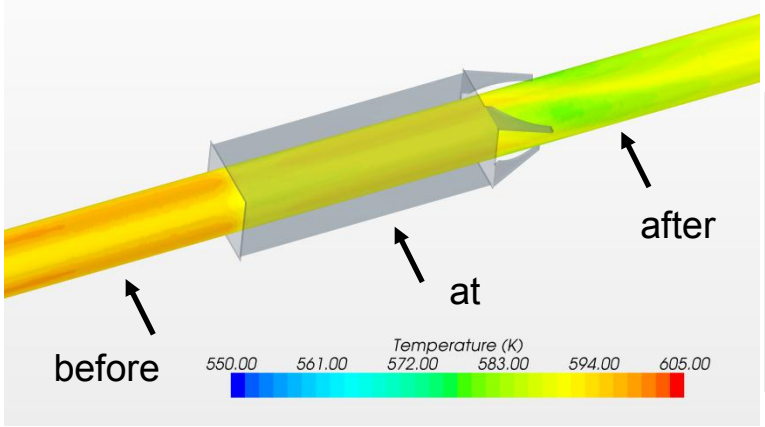
Chemistry computed: Crud Thermal Resistance

CFD computed: Turbulent Kinetic Energy

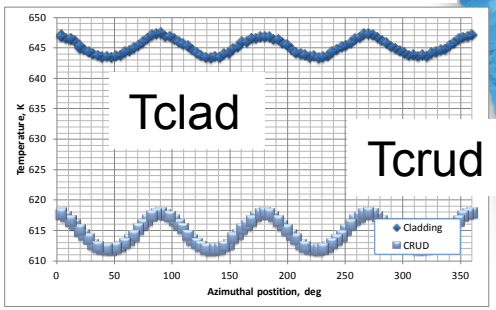
Fuel computed: Cladding Temperature



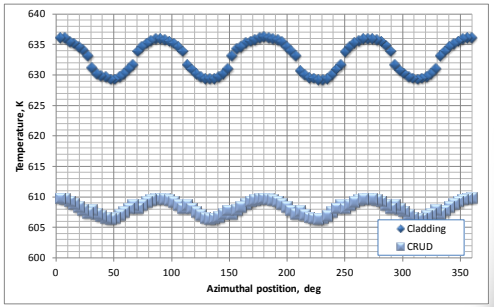




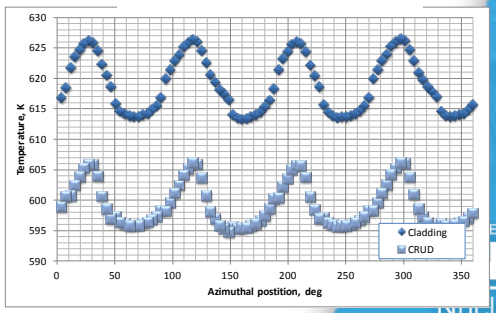
Before Spacer



At Spacer

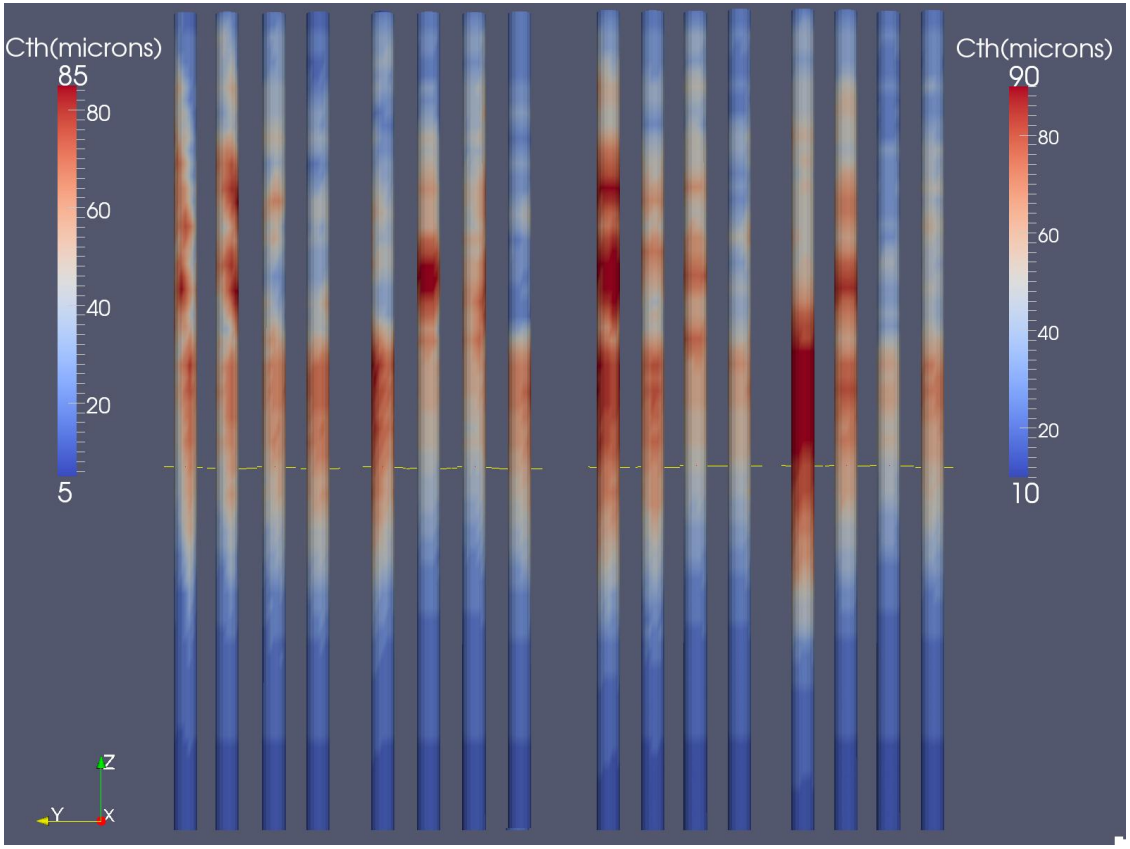


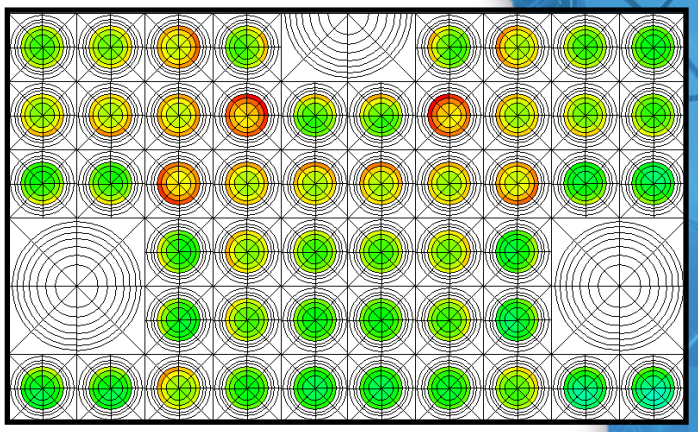
After Spacer

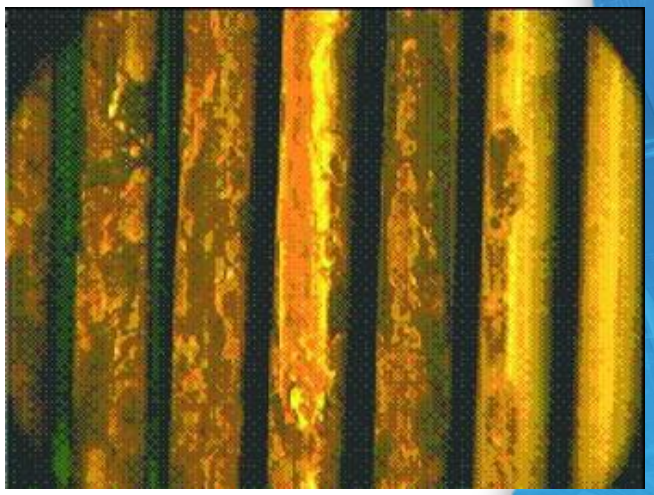


Extension to 4x4 Subassembly:

Qualitative Comparison to CRUD Formations







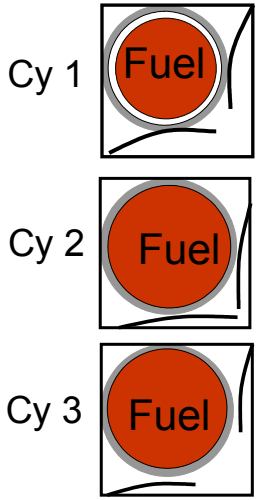
Quantitative benchmarking to industry code benchmarks and experimental data currently underway

Grid-to-Rod Fretting Challenge Problem Progress and T/H-CFD Development

Grid To Rod Fretting (GTRF)

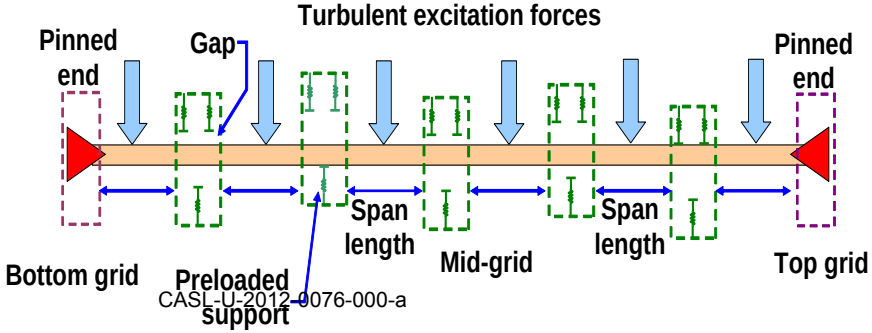
Definition of Problem

- 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 and 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 and wear any location in core



What is Success

- Develop CASL capability to predict turbulent excitation force, grid to rod gap, rod vibration and rod wear for any rod in core
- Benchmark tools and apply to experimental data and plant data

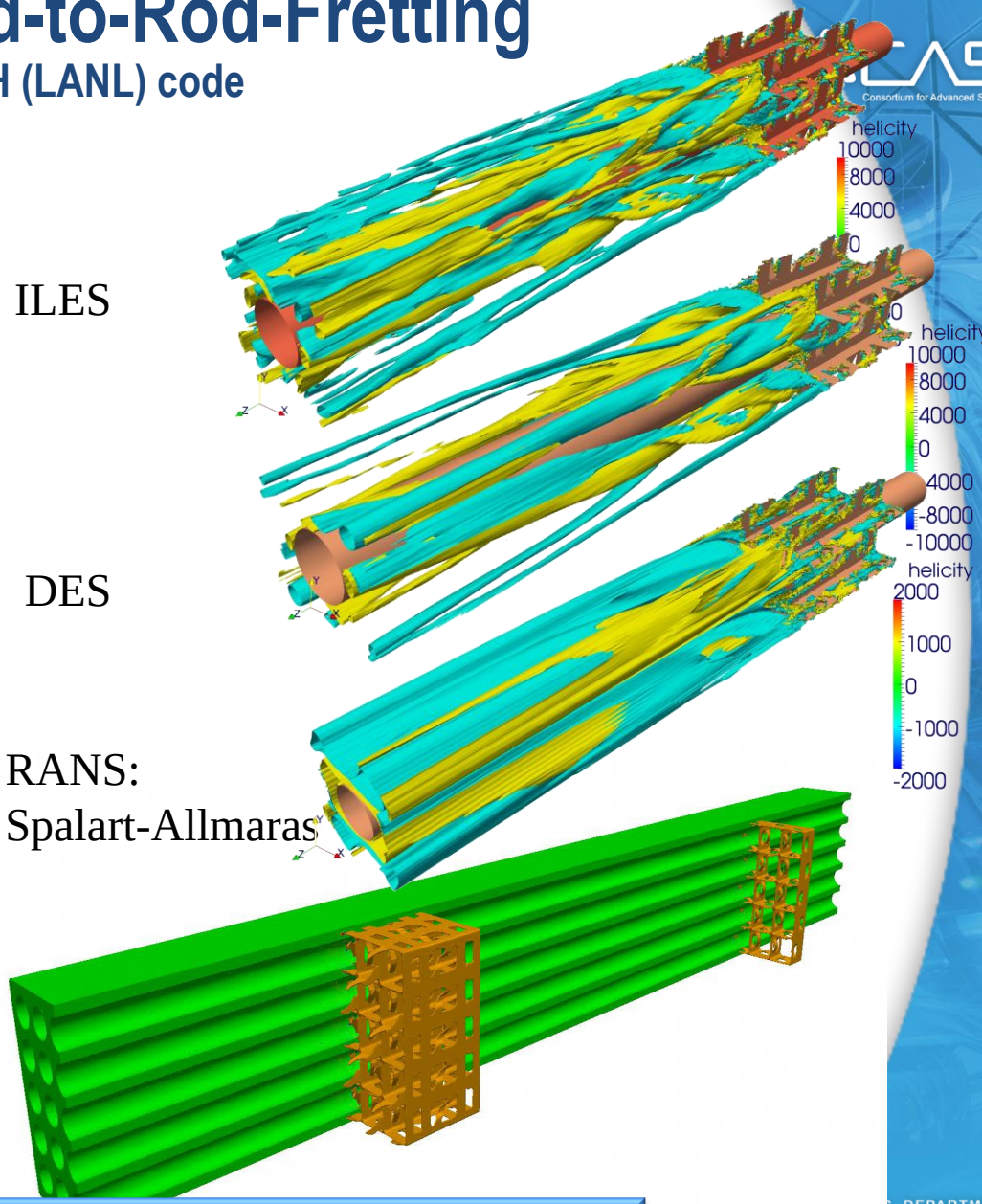
Turbulent Flow in Grid-to-Rod-Fretting

Scoping simulations with the Hydra-TH (LANL) code

Helicity isosurfaces $(v \cdot w)$

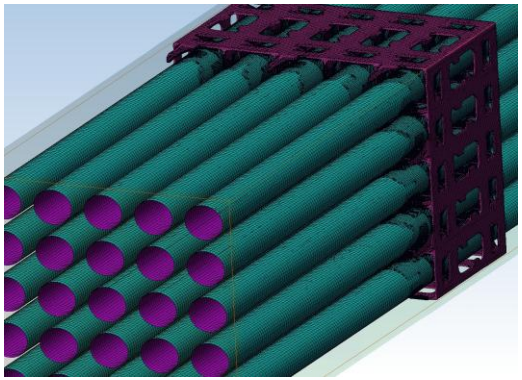
- All models capture some level of detail in the longitudinal vortical structures and swirl
- With Spalart-Allmaras, eddies appear more damped, rotation around rod is smeared

End-view of fuel rod showing swirl in coherent structures

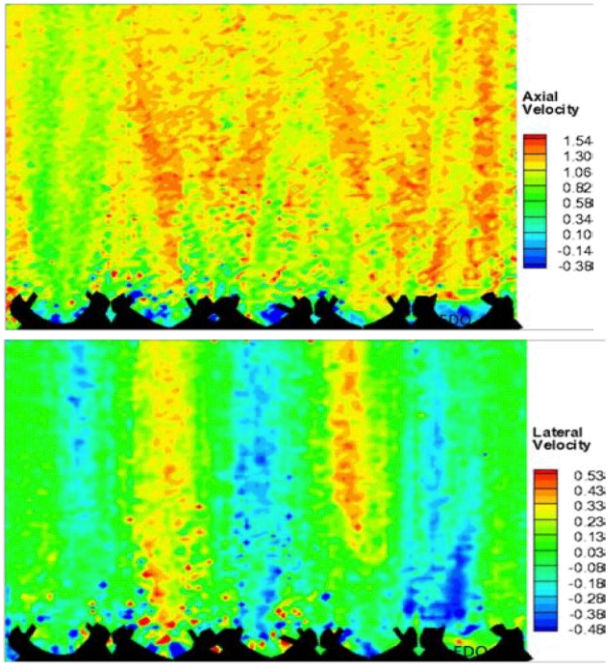


CFD RANS Models May Not Be Sufficient for Capturing Fluid Flow Effects Important for GTRF

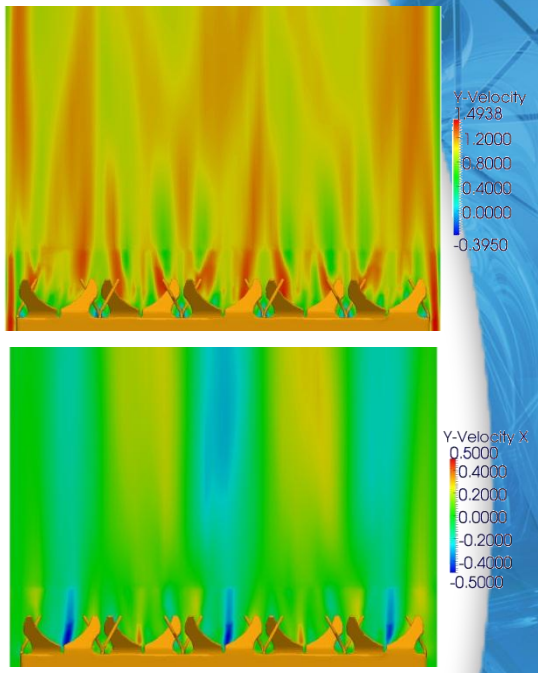
5x5 V5H grid study shows good agreement with experimental data



- Predicted mean peak velocities within 5% of experiments

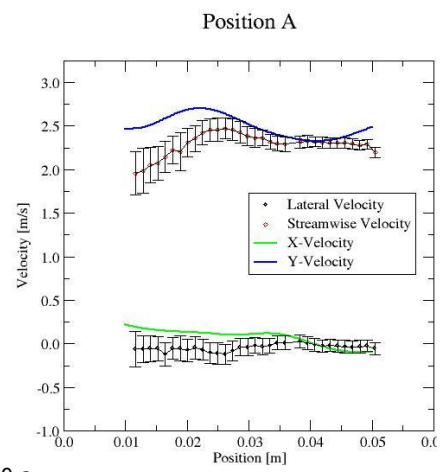


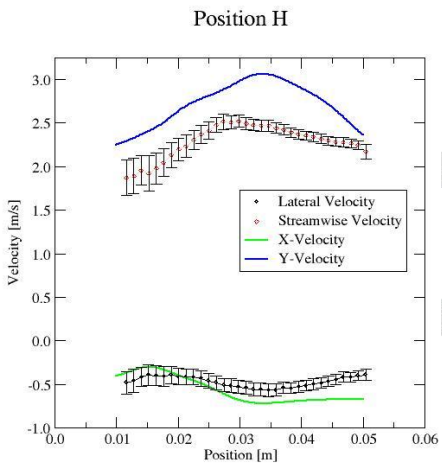
Texas A&M experiments

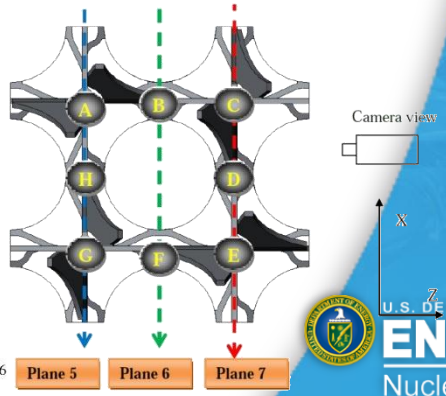


Hydra-TH calculations

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







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Thermal Hydraulics 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)

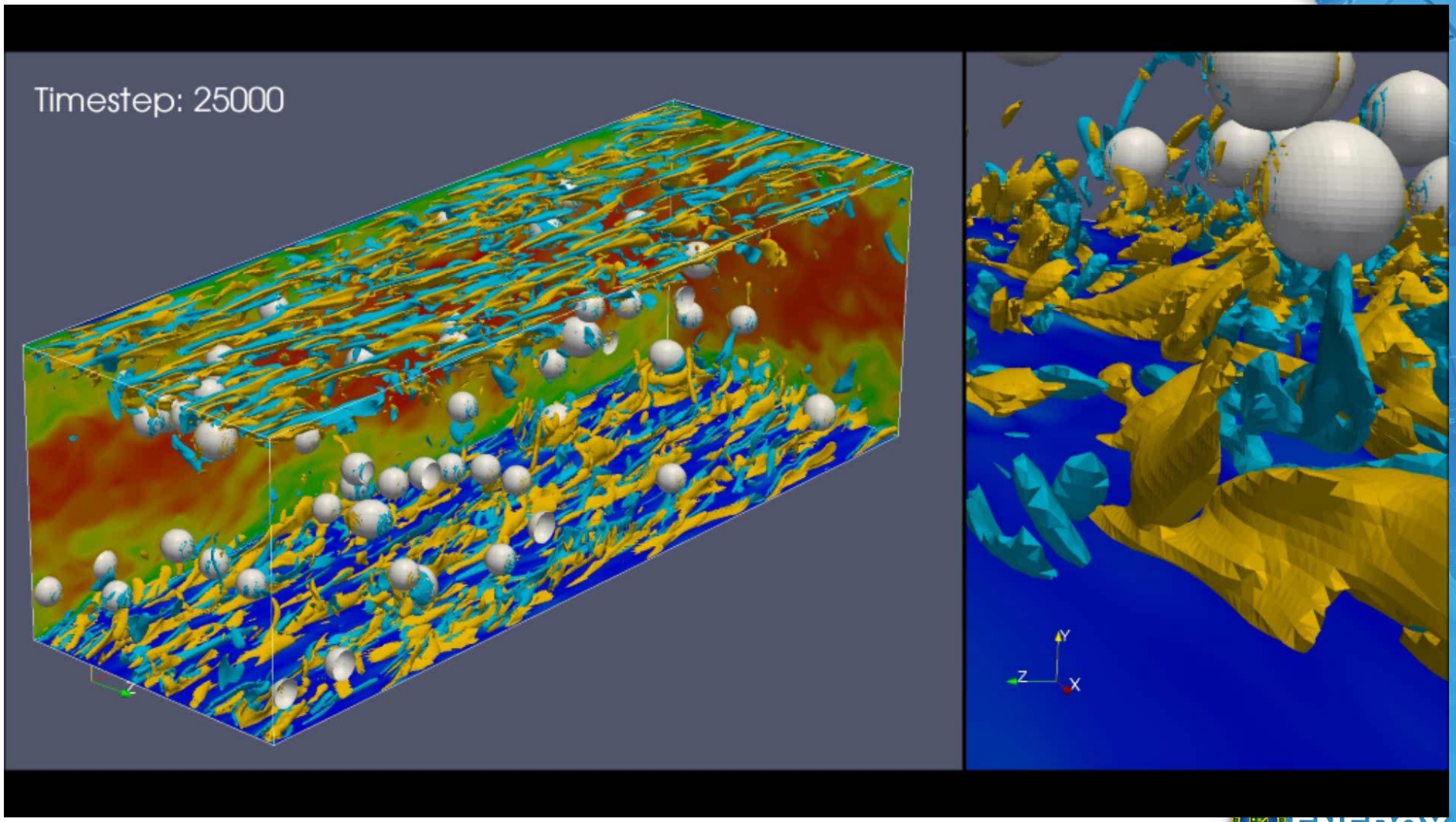
- Generate microscale simulation results data for CFD closure models and validation

Experiments

- Provide validation data for CFD/ITM and fundamental understanding

Multiphase: Track every bubble?

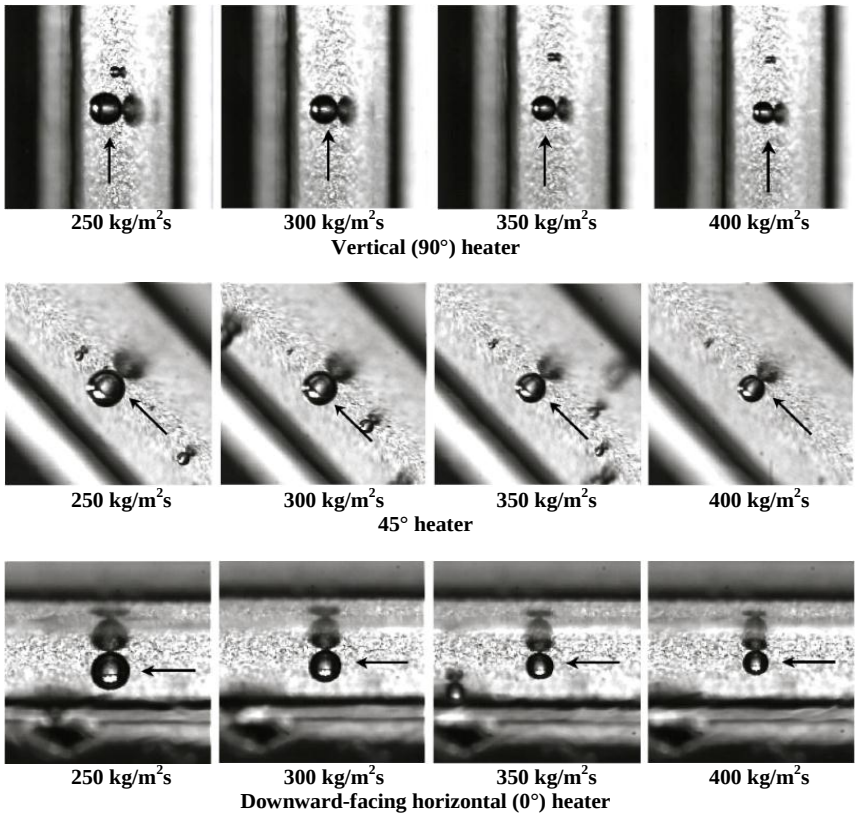
Example: 60 bubble simulation for upscaling



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



Parameter	Experimental Range
Orientation Angle [°]	0, 30, 45, 60, 90, 180
Mass Flux [kg/m²s]	250, 300, 350, 400
Subcooling [°C]	10, 20
Heat Flux [MW/m²]	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

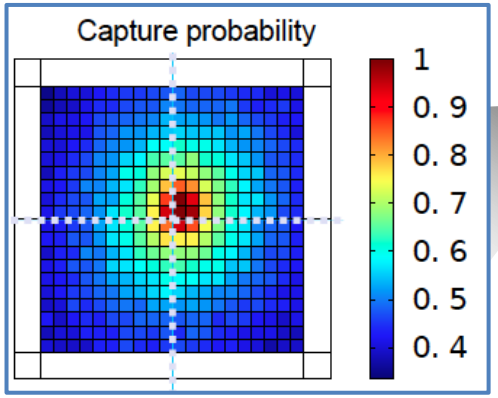
Fuel Performance: Pellet Clad Interaction Challenge Problem Progress

Cladding Deformation

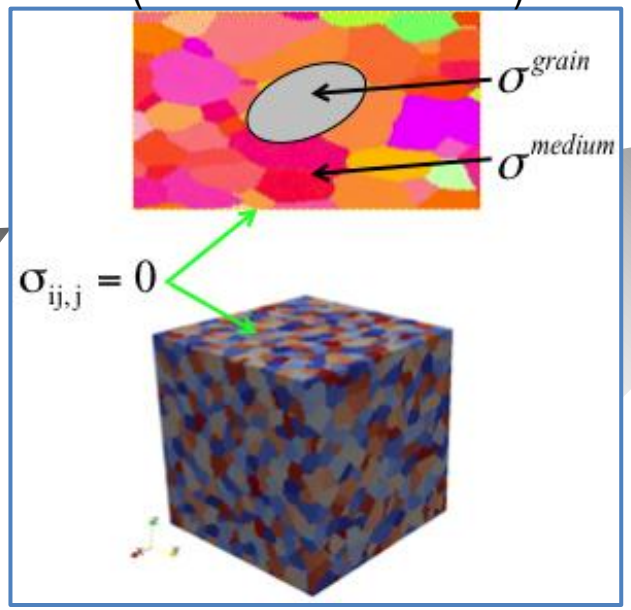
Viscoplastic Self Consistent (VPSC) creep and growth model implemented in Peregrine for clad deformation

Improved models for clad deformation required for PCI and safety assessments.

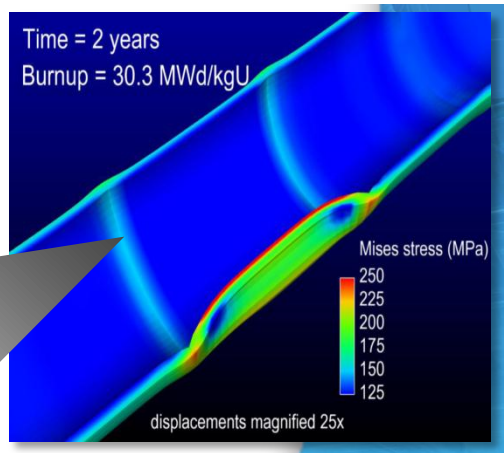
Atomistic simulation for defect behavior, including mobility and interaction with dislocations



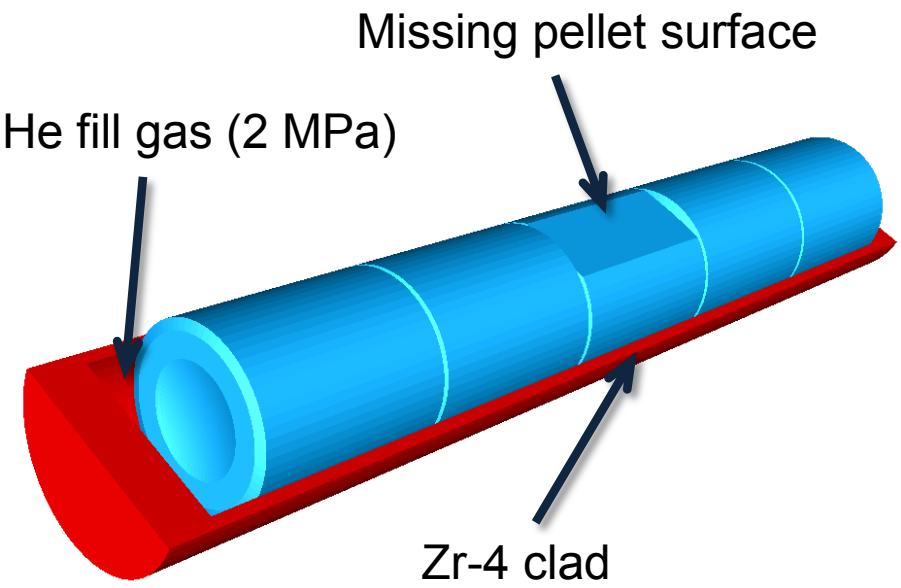
Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)



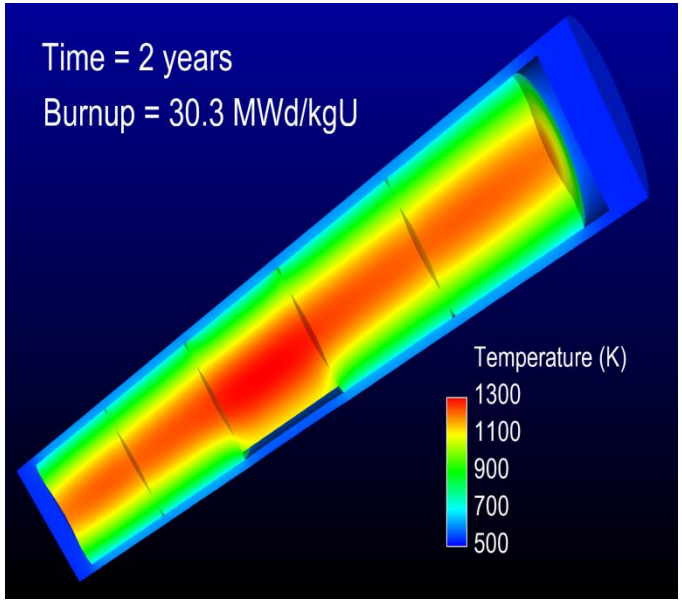
Peregrine engineering scale fuel performance



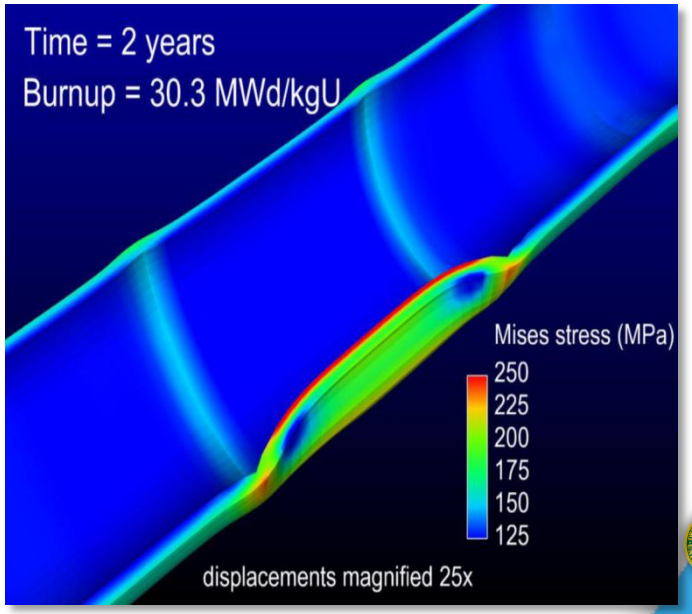
3D Fuel Performance Model: Peregrine



- Defective (MPS) pellet placed midway between four intact pellets
- Simulation from fresh fuel state with a typical power history, followed by a late-life power ramp



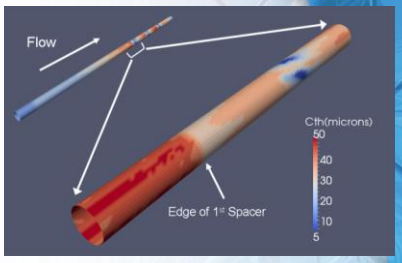
Fuel Temperature

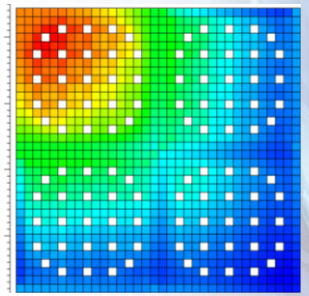


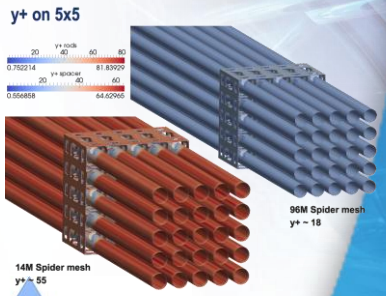
Von Mises Effective Stress

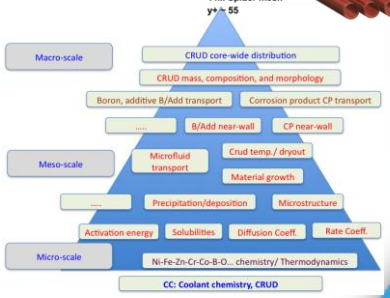
Enabling R&D Objectives

- 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





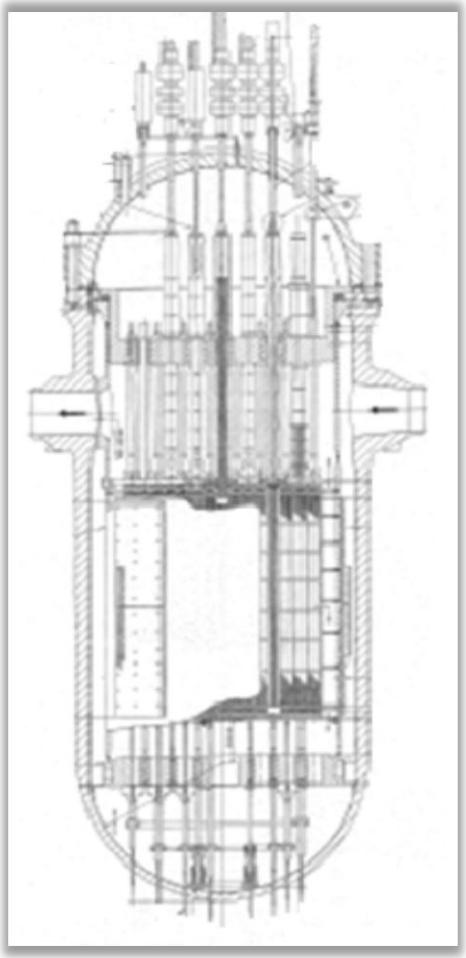




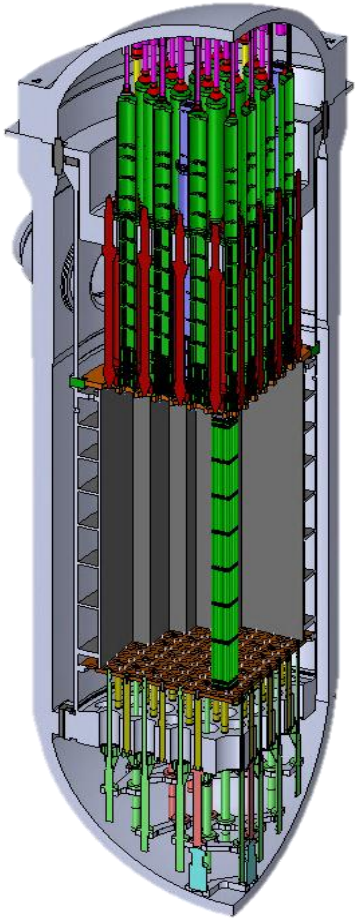
Advanced Modeling Applications

4-Loop Westinghouse PWR Multi-Physics Model Development

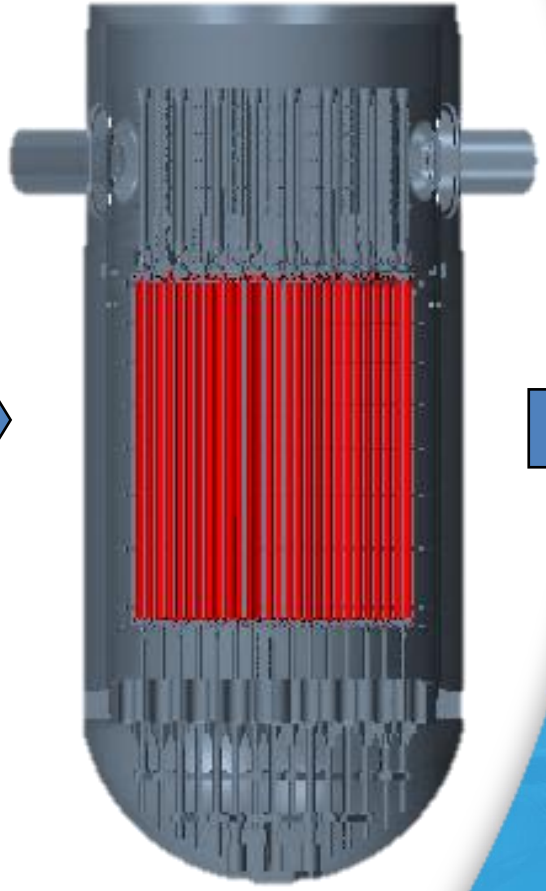
- RPV ID 173”, 193/4 Fuel Assemblies,13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; 1.2 billion cells



Drawings



CAD Model

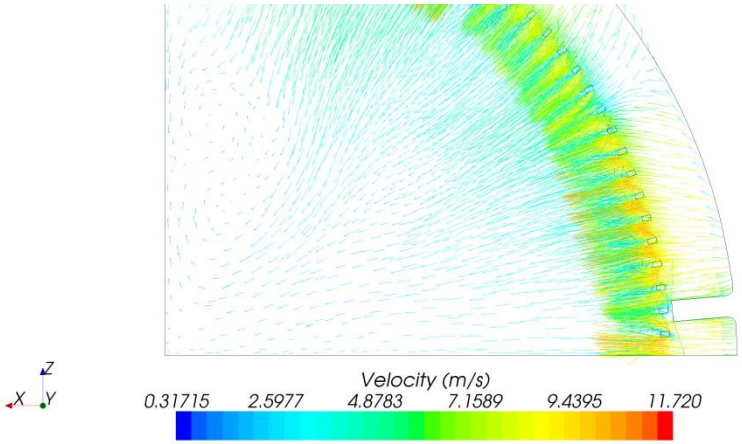


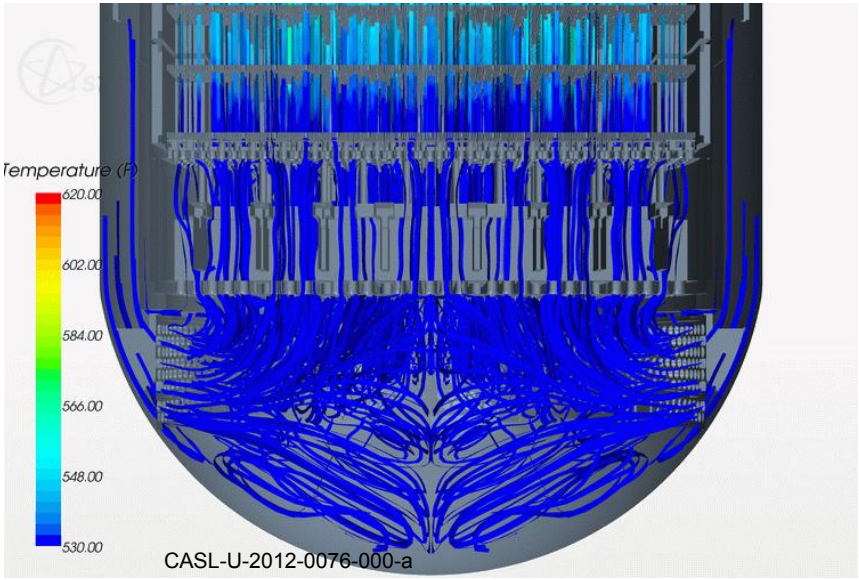
Star-CCM+ CFD Model

CASL-U-2012-0076-000-a

CFD Flow Distribution Results

Flow Distribution Through Flow Skirt





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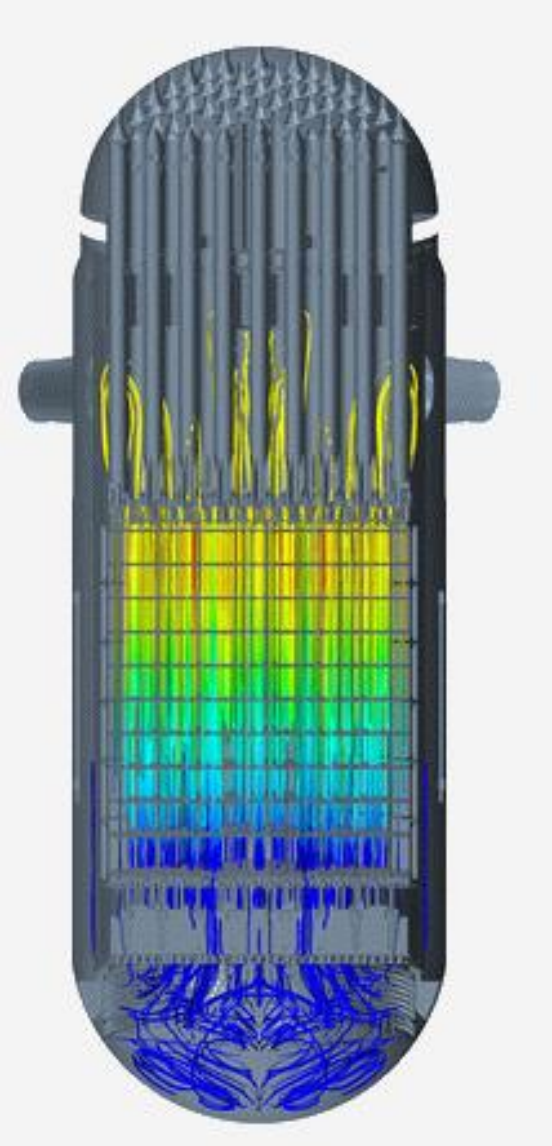
Flow Distribution Through Vessel



Core Physics Modeling

- A set of progression problems developed to guide progress from pin cell modeling to full core with depletion and T/H feedback
- Reference solutions used for problems that do not correspond to reactor conditions/geometries
- Problems #5, #8, #9 correspond to problems with measured plant data
- Models are being developed with existing tools to compare with measured data
- Neutronics methods based on pin-by-pin radiation transport

Benchmark Progression Problems

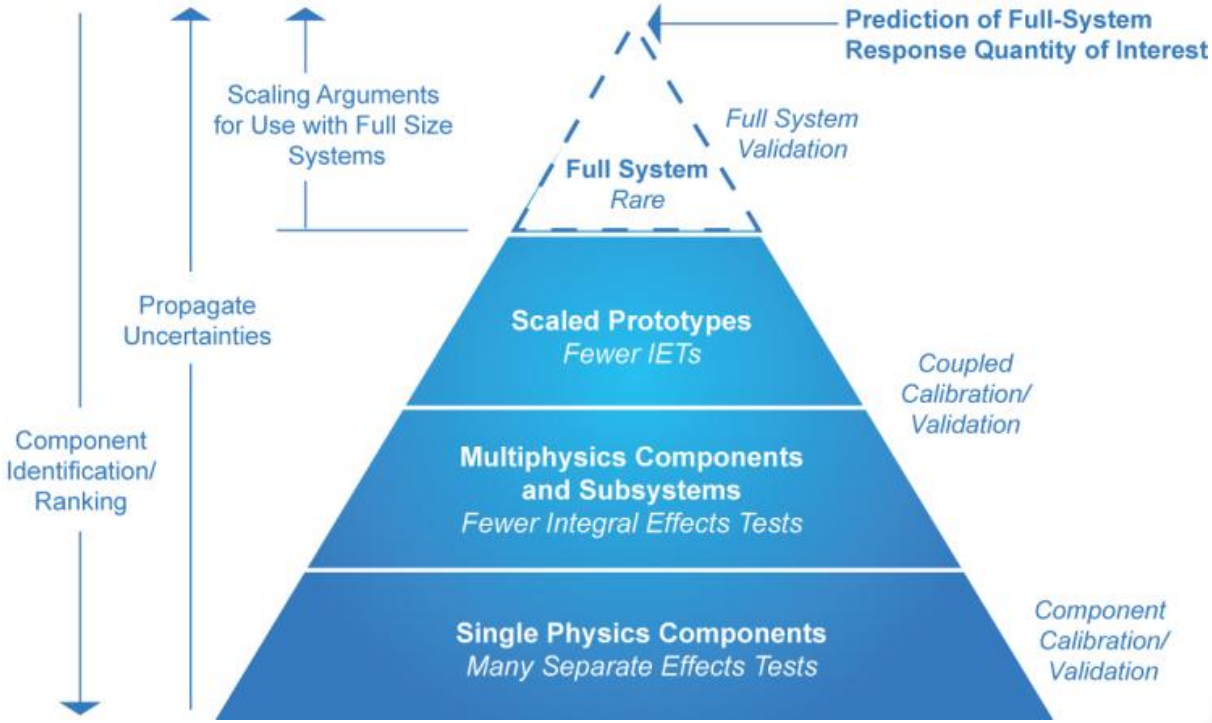
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- **#5 Physical Reactor Zero Power Physics Tests (ZPPT)**
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical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

Key Validation / Prediction Principle

*Efficiency and effectiveness of validation and prediction assessments are often improved by exploiting the **hierarchical composition** of computational and mathematical models.*

Key Point:
Validation data needed at each of these levels in the hierarchy.

Key Challenge:
Identifying and obtaining the data!



"Generic" Validation Hierarchy
(from our CASL Proposal, 2010)

CASL Consortium for Advanced Simulation of LWRs
U.S. DEPARTMENT OF ENERGY Nuclear Energy

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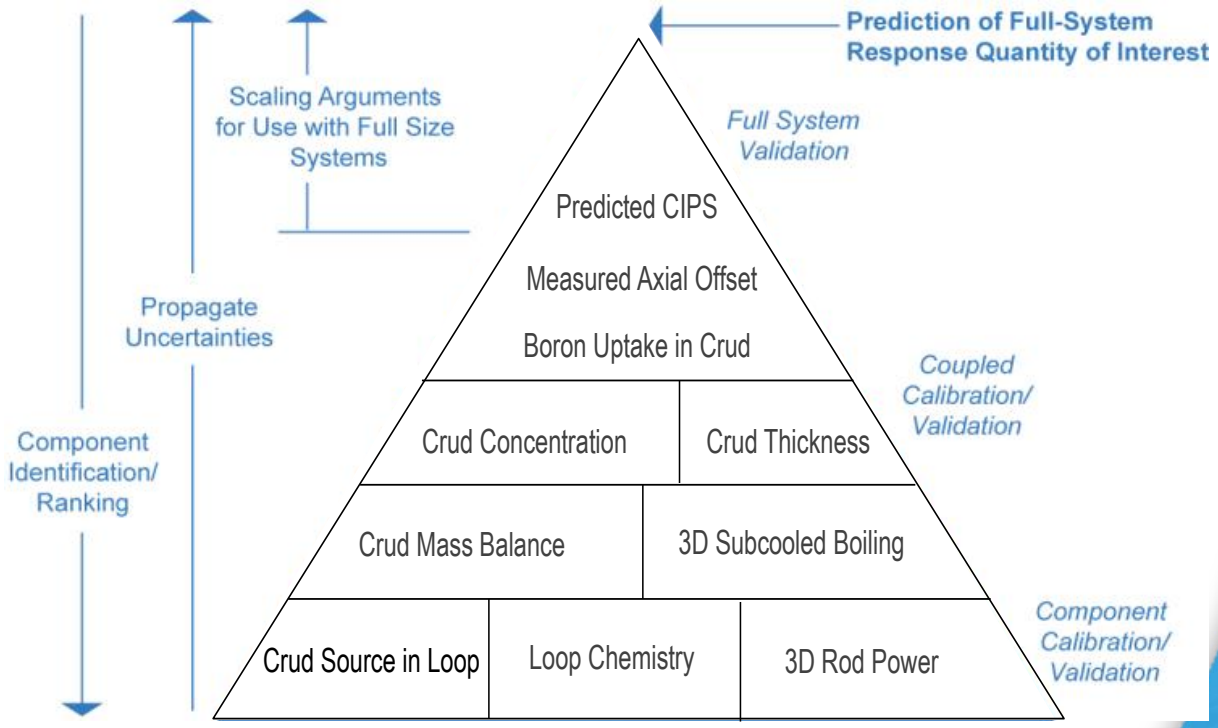


Validation Hierarchy for CRUD Challenge Problem

Validation Data Review

For CRUD-related and GTRF Challenge Problems

Relevance, Scaling, Uncertainty: Grade 0-4

		Relevance	Scaling	Uncertainty
PMO	International Fuel Performance Experiments IPFE Recommendation: Low-to-medium priority	CRUD: 2 GTRF:2 PCI: 3	CRUD: 1 GTRF:1 PCI: 3	CRUD: 0 GTRF:0 PCI: 2
PMO	Data collected from operational plants Recommendation: High priority	CRUD: 4 GTRF: TBI	CRUD: 4 GTRF: TBI	CRUD: 0-2 GTRF:0-1
In-pile IET	Studsvik Cladding Integrity Project SCIP Recommendation: High priority	CRUD: 2 GTRF:3 PCI: 4	CRUD: 2 GTRF:2 PCI: 4	CRUD: 0 GTRF:0 PCI: 2
In-Pile IET	Halden Reactor Project Axial Offset Anomaly AOA Tests Recommendation: High priority	CRUD: 3 PCI: 2	CRUD: 2 PCI: 1	CRUD: 2 PCI: 1
Out-of-pile IET	Westinghouse Advanced Loop Tester WALT Recommendation: High priority	CRUD: 4 DNB: 3	CRUD: 2 DNB: 3	CRUD: TDB DNB: TBD
Out-of-pile IET	New Experimental Studies of Thermal-Hydraulics of Rod Bundles NESTOR Recommendation: High priority	CRUD: 3 DNB: 3	CRUD: 2 DNB: 2	CRUD: TDB DNB: TBD
SET	Rod Bundle Heat Transfer RBHT : PSBT /BFBT (for PWR focus in Phase 1) Recommendation: High priority PSBT	CRUD: 3/1 GTRF:3/1 DNB: 4/1	CRUD: 3/2 GTRF:3/2 DNB: 3/2	CRUD: 3/3 GTRF:3/3 DNB: 3/3
SET	Subcooled flow boiling SFB: covering a range of SETs on participating phenomena (over 20 data sets) Recommendation: New, well-controlled, VUQ-grade SETs on SFB	CRD/GTRF/DNB: range [2-4]	1 (low pressure) 3 (high P tests)	In range [1-2]
SET	Vibration Investigation of Small-scale Test Assemblies VISTA Fuel Assembly Compatibility Test System FACTS	GTRF: 4	GTRF: 4	GTRF: TBD

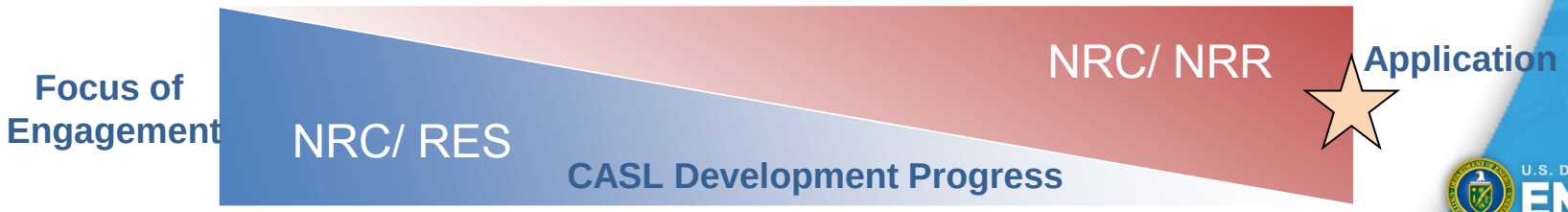
Major gap: data for validation of multi-physics simulation capability

Recommend: Provide guidance for experiments in FCRD, LWR-S, NEUP programs

SET: Separate-Effect Test; IET: Integral-Effect Test
PMO: Plant Measurements and Observations, incl. PIE

CASL/NRC Engagement Overview

- **Objective: Inform, discuss, and exchange information with NRC Staff on CASL activities and approaches**
  - Familiarize NRC with CASL R&D and use of advanced M&S for nuclear reactors
  - Seek feedback and exchange on scope of work, developments, and approaches
  - Work within constraints to avoid conflict of interest issues
- **Approach: Engage with RES and NRR**
  - RES: Interface in development of new M&S capabilities
    - Provide for exchange on V&V plans and results – a key issue of interest to NRC
    - Exchange of information, data, benchmark results, etc. for joint benefit
    - Expected to the be focus of the first five years but can continue with CASL extension and application to BWRs
  - NRR: Interface in the approval of new M&S capabilities
    - Keep NRR informed via RES [feedback not solicited or expected] No submittals to NRC from CASL
    - Vendors (e.g. Westinghouse) will engage with NRR to license CASL technology codes at the appropriate time
    - Utilities (e.g. TVA) will submit license amendment requests based upon NRC-approved vendor codes



Summary

- CASL continues to follow its originally proposed 2010 technical plan, as defined by our Challenge Problems and high-level L1/L2 milestone roadmap. We are paying careful attention to our industry partners, Industry Council members, and other Federal Programs to ensure relevance, timeliness, and consistency.
- CASL has initiated, committed to, and maintained an aggressive technical plan
  - Approaches and solutions to our Challenge Problems
  - Development, application, V&V/UQ, and deployment of VERA and its Core Simulator component
  - Proactively responding to feedback from Board of Directors, Science & Industry Councils, and DOE NE sponsor
- The CASL Program Plan lays out technical roadmaps having clear, measurable mileposts and outcome-based performance metrics tied to its strategic goals
- CASL is committed to delivery of its technology to the nuclear community
  - Release and support of VERA, Test Stands, Pilot Studies, Collaborative Applications, External User Collaboration

Outstanding technical challenges focus our efforts in the near term

Thermal Hydraulics: Multiphase turbulence modeling and closure relationships selection, generation and validation; DNS/ITM bubble nucleation, coalescence and condensation

Virtual Reactor Integration: "Tight" multiphysics coupling development; different physics time scales; software complexity & usability, structural mechanics

Validation and Uncertainty Quantification: Multiphysics & multiscale uncertainty quantification (particularly epistemic errors) and data assimilation

Materials Performance and Optimization: Predictive (minimum free tuning parameters) CRUD predictive capability; microscale informed macroscale

Advanced Modeling Applications: Meshing complex geometries; CPs' solution paths that are realizable within computational resource capabilities

Questions?

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