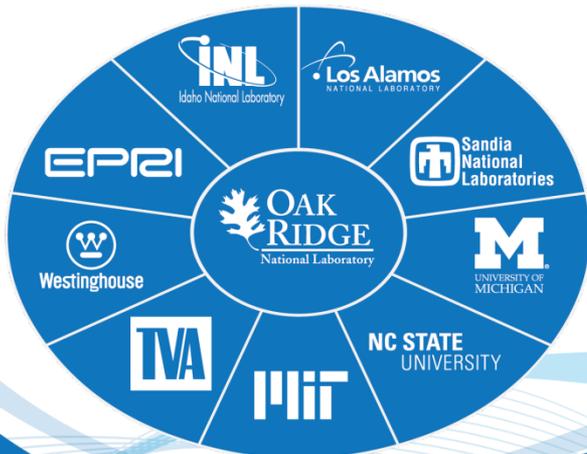


# CASL: The Consortium for Advanced Simulation of Light Water Reactors

## A DOE Energy Innovation Hub

Douglas B. Kothe  
Oak Ridge National Laboratory  
Director, CASL



# CASL

## A DOE Energy Innovation Hub in the Office of Nuclear Energy



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

- A Different Approach

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

### Mission

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

### Vision

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

### Goals

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

# CASL Key Elements

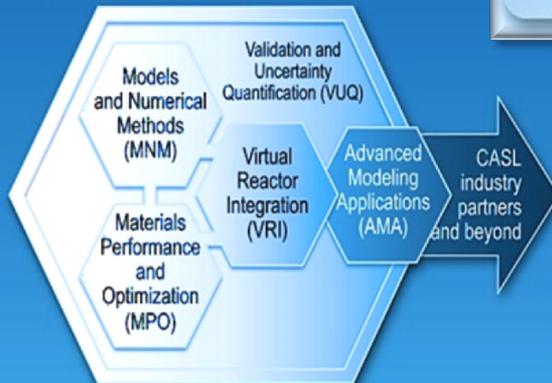
Outstanding team, industry challenges, compelling plan

## U.S. team with a remarkable set of assets

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

## Executing a compelling and urgent plan

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



## Tackling tough industry challenges that matter

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

## DOE Energy Innovation Hubs

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

# CASL Key Elements

Creative collaboration, fostering innovation, predictive simulation solutions

## Teaming at the speed of human insight

- CASL resources extended and enhanced under virtual one roof
- Virtual Office, Community, and Computing Project: Highly collaborative work space
- Immersive telepresence, desktop collaboration, data sharing, HPC connectivity
- New paradigm driven by CASL culture

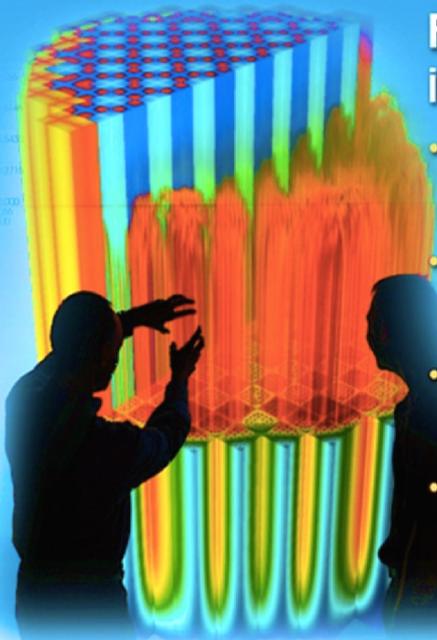


## Delivering industry solutions through predictive simulation

- Improved reactor performance and output
- Technology step change: CASL Virtual Reactor (VERA)
- Imparting innovation and agility to nuclear reactor analysis, design, and safety
- Informing the design and licensing of new reactors
- Public-private partnerships

## Fostering innovation where it is most needed

- Essential understanding reactor fuel and structural materials
- Novel numerical algorithms ready for current and future HPC systems
- Quantified uncertainties to inform operational and safety margins
- Multiphysics HPC-based tools embedded in reactor design and analysis workflows



# The CASL Team

## Core partners

- Oak Ridge National Laboratory
- Electric Power Research Institute
- Idaho National Laboratory
- Los Alamos National Laboratory
- Massachusetts Institute of Technology
- North Carolina State University
- Sandia National Laboratories
- Tennessee Valley Authority
- University of Michigan
- Westinghouse Electric Company



## Contributing Partners

- ASCOMP GmbH
- CD-adapco
- City College of New York
- Florida State University
- Imperial College London
- Rensselaer Polytechnic Institute
- Texas A&M University
- Pennsylvania State University
- University of Florida
- University of Tennessee – Knoxville
- University of Wisconsin
- Notre Dame University
- Anatech Corporation
- Core Physics Inc.
- Pacific Northwest National Laboratory
- G S Nuclear Consulting, LLC
- University of Texas at Austin
- University of Texas at Dallas

# CASL is addressing industry needs

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

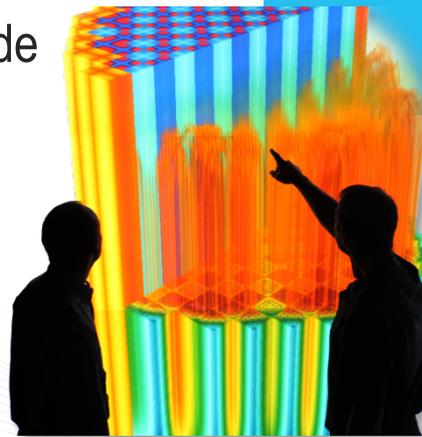
## CASL advisory groups

### Industry Council

- Reviews plans, specifications, and products
- Advises on gaps and critical needs
- Advises on incremental technology deployment

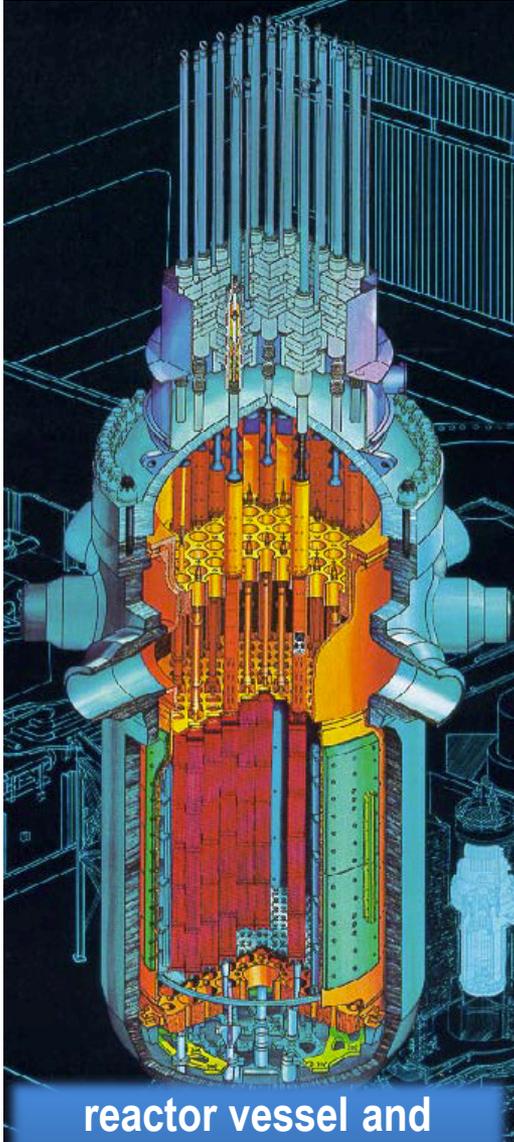
### Science Council

- Provides independent assessments of alignment between scientific work, as planned and executed, and overall goals

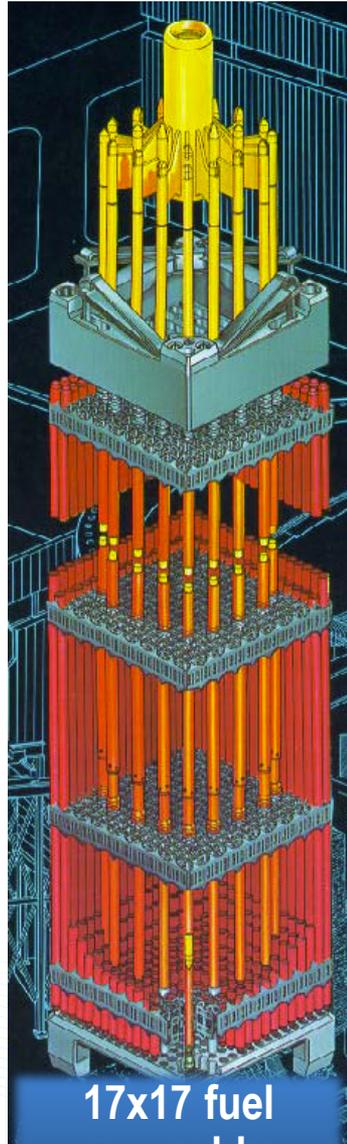


# Anatomy of a Nuclear Reactor

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



reactor vessel and  
internals



17x17 fuel  
assembly

### Core

- 11.1' diameter x 12' high
- 193 fuel assemblies
- 107.7 tons of  $\text{UO}_2$  (~3-5%  $\text{U}_{235}$ )

### Fuel Assemblies

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

### Fuel Pins

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

### Fuel Pellets

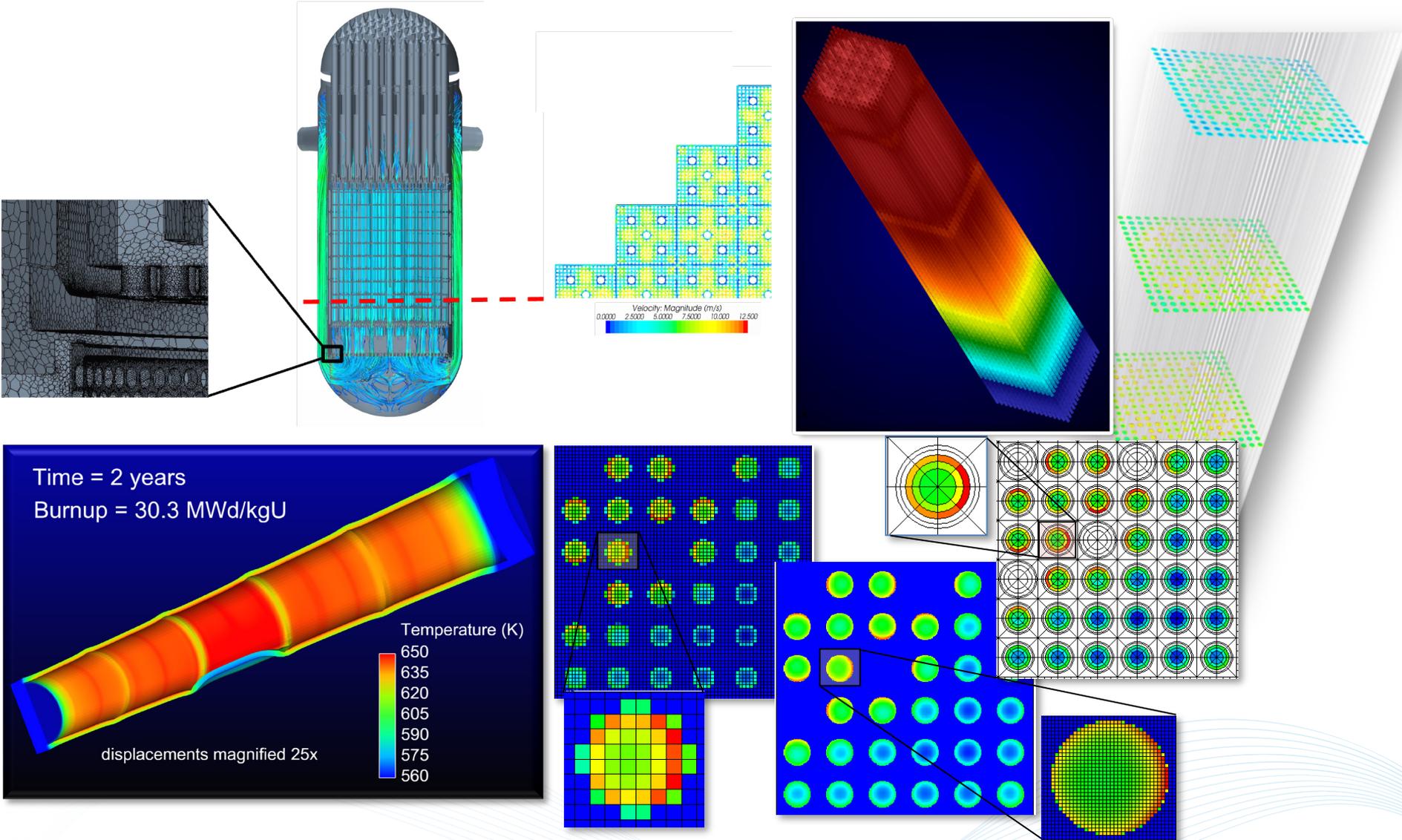
- 9.29 mm diameter x ~10.0 mm high

### Fuel Temperatures

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

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

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



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



# Navigate Transforming Landscape via CASL

Source: Heather Feldman (EPRI)

## Flexible Nuclear Plant Operation

- Gray control rods
- Flow induced vibration
- Flow accelerated corrosion

## License Extension

- Higher burn up fuel
- Enhanced core design

## Accident Tolerant Fuel

- Concept refinement
- Test Planning
- Margins

## Power Up-rate

- Fuel modifications
- Safety margin assessment

## CASL Test Stand - Potentials

- Peregrine validation
- Inform mods to Falcon
- Technical Challenges



# Hopes and Expectations for CASL

Source: Dan Stout, Rose Montgomery (TVA)

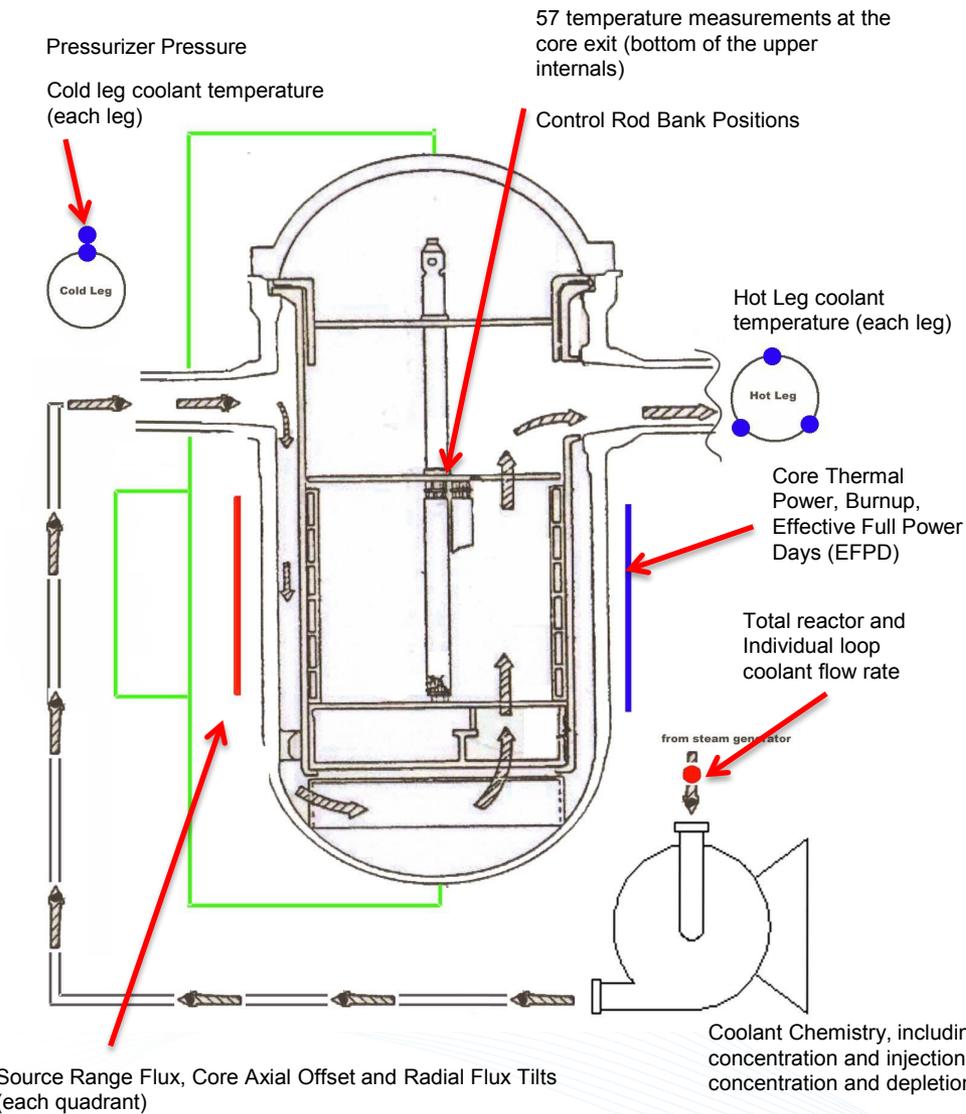
- Advance the state of the art in understanding nuclear concepts and performance
- Produce a rigorous, fully-coupled, first principles simulation code package usable by the full range of domestic fuel vendors and power utilities
  - Ensure key performance models are fully described for industry implementation
  - Provide a flexible path to industry implementation
- Strategically address power-limiting operating scenarios
  - Design Basis Accidents (DBAs), Power Ramp rates
  - Departure from Nucleate Boiling (DNB)
  - Potential for better understanding of beyond design basis events

Phase 1: Insights from CASL enable a utility to realize more aggressive core loading saving on fuel costs with applicability to multiple utilities/reactors;

Phase 2: Insights from CASL result in multiple vendors making code modifications to existing licensed codes that enable utilities to seek license amendments that could add ?? GW(e) of nuclear energy on the grid

Long Term: CASL tools are broadly used to enhance nuclear energy safety and capacity

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

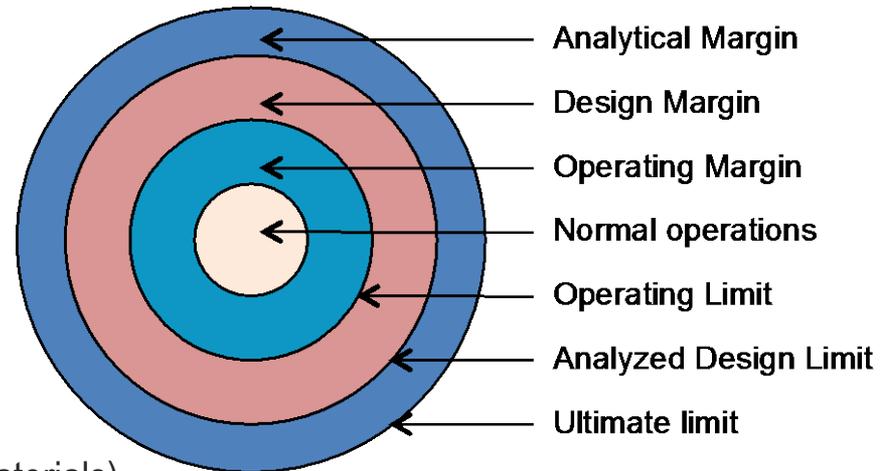


- TVA provided detailed information on Watts Bar Unit 1 Cycles 1 through 10
  - Core cycle design
  - Core performance observations
  - Measured operating data from various instrumented locations (see graphic) on a 5-day average basis for the complete cycle
  - Cycle 1 startup testing information
  -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

# Margin Management

Source: Sumit Ray (Westinghouse)

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

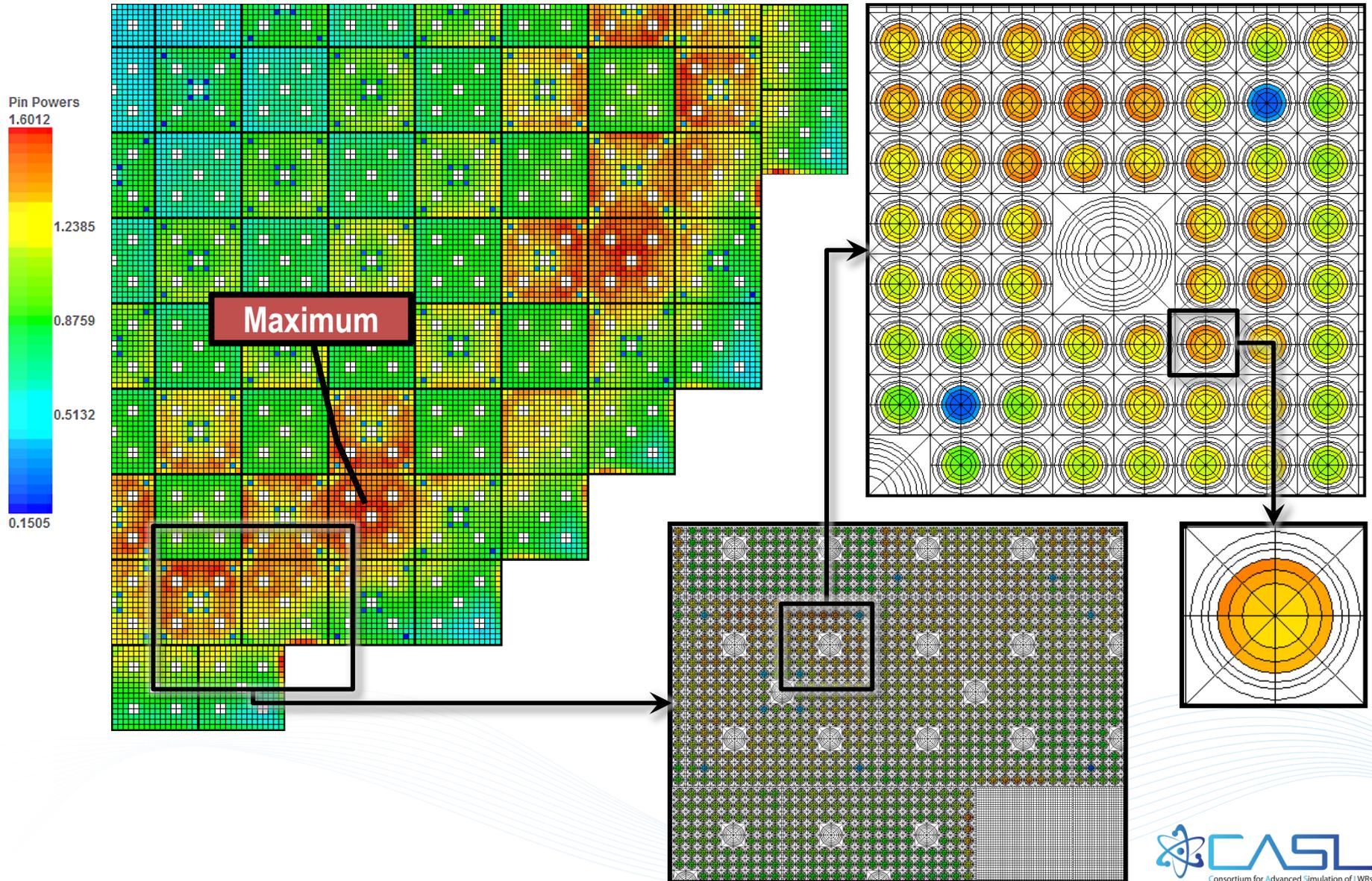


Margin trade-offs and evaluation of risks require involvement of many stakeholders within the Utility (Fuels and Plant Operations) and suppliers (BOP, NSSS, T/G, etc.)

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

# Pin-Resolution of Neutron Behavior is Required

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



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

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

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

# Creating a Virtual Reactor

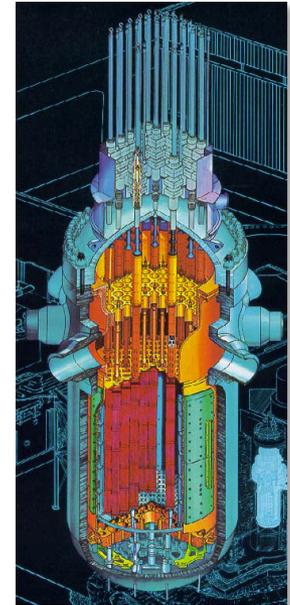
## Enable assessment of fuel design, operation, and safety criteria

Deliver improved predictive simulation of PWR core, internals, and vessel

- Couple Virtual Reactor (VR) to evolving out-of-vessel simulation capability
- Maintain applicability to other nuclear power plant (NPP) types

Execute work in 6 technical focus areas

- Equip VR with necessary physical models and multiphysics integrators
- Build VR with a comprehensive, usable, and extensible software system
- Validate and assess the VR models with self-consistent quantified uncertainties



### MPO

Materials performance and optimization

### RTM

Radiation transport methods

### THM

Thermal hydraulics methods

### VUQ

Validation and uncertainty quantification

### PHI

Physics integration

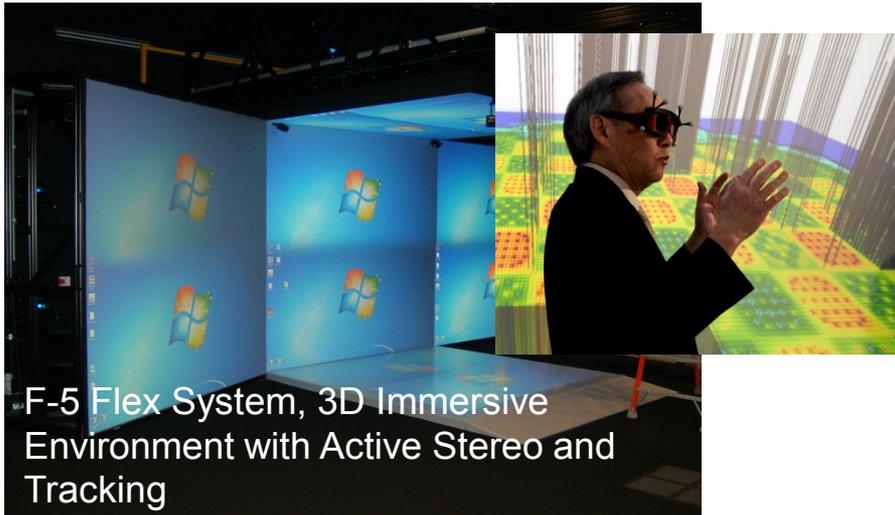
### AMA

Advanced modeling applications

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

# Challenge: One-Roof Execution

## CASL's virtual one roof (April Lewis, CASL CIO)



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



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



VOCC Immersion Room



3D Mobile Immersive Environment With Active Stereo and Tracking



Virtual Meetings

**Virtual Office, Community, and Computing**



See more about VOCC at [voccnnet.org](http://voccnnet.org)

# CASL Challenge Problems

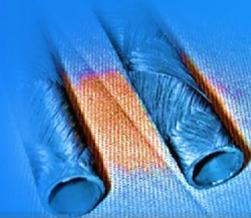
Key safety-relevant reactor phenomena that limit performance

## Departure from Nucleate Boiling



## Cladding Integrity

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



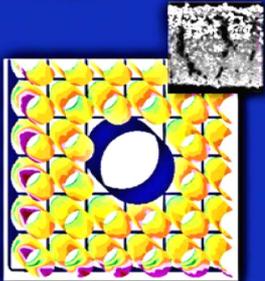
## Safety Related Challenge Problems

CASL is committed to delivering simulation capabilities for

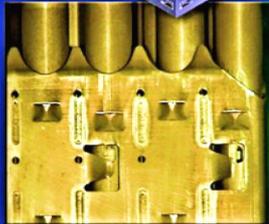
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

## Crud

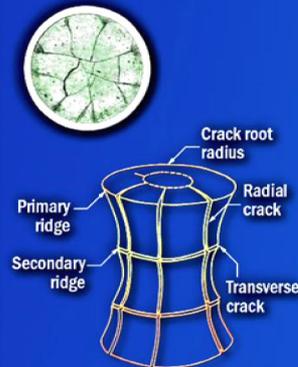
- Deposition
- Axial offset anomaly
- Hot spots



## Grid-to-Rod Fretting



## Pellet-Clad Interaction



## Operational Challenge Problems

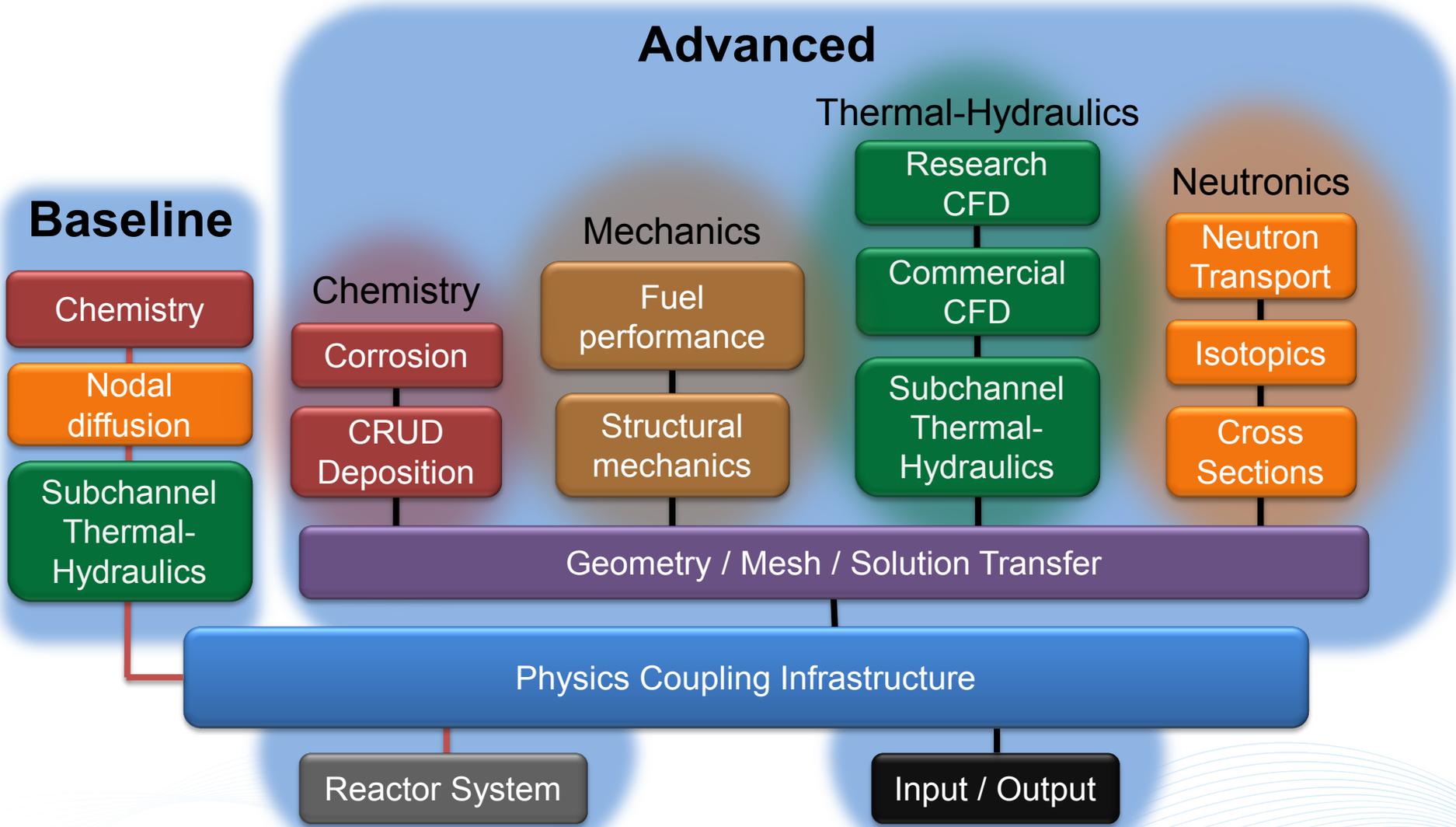
# Challenge Problems

## Product Integrators are in place and driving metrics, products, and plans

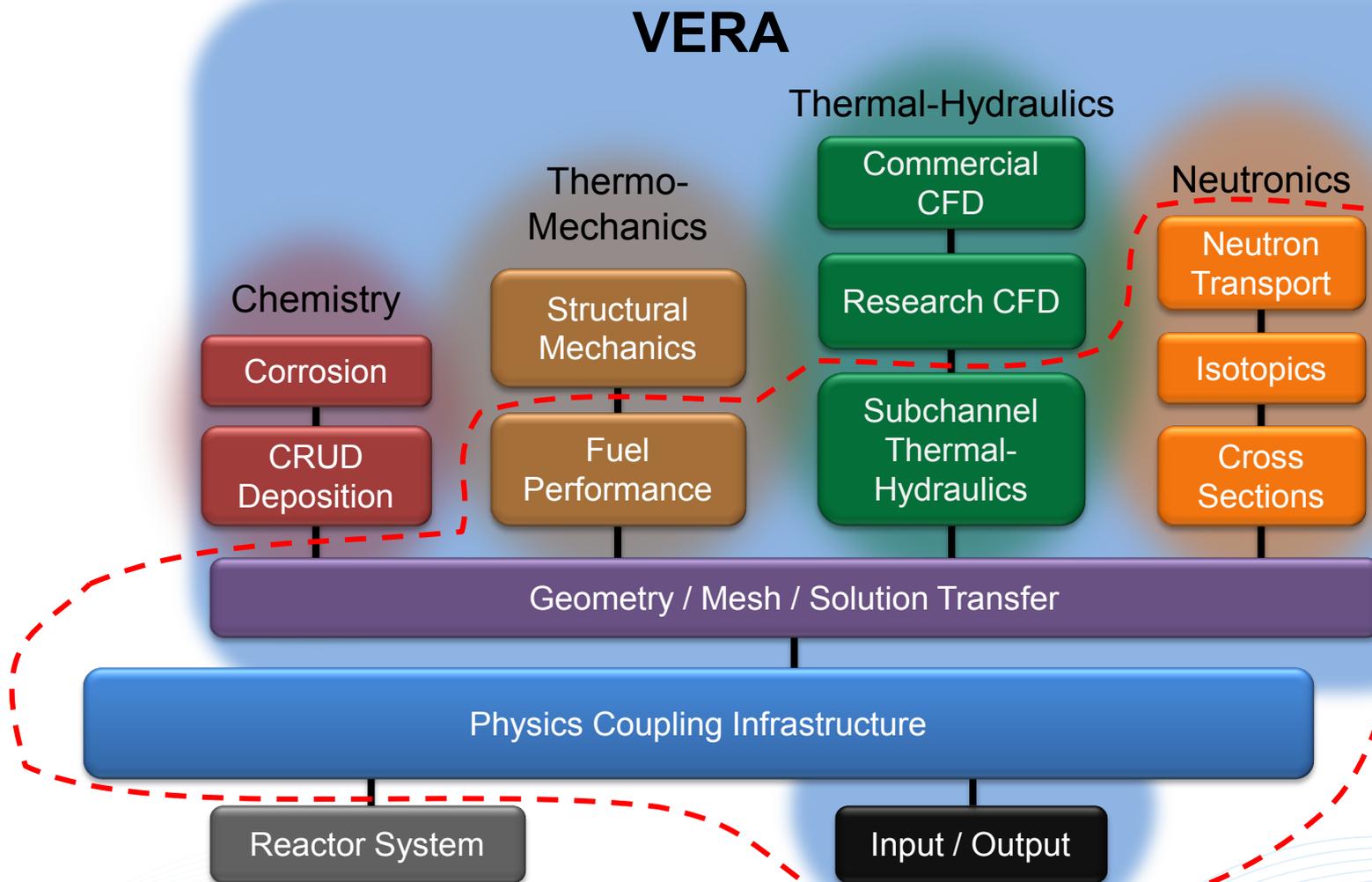
CP	Description and Impact	Simulations Gaps and Drivers
<b>Crud-induced power shift; crud-induced localized corrosion</b>	High uncertainties in crud source, thickness, boiling surface area, and margin to fuel leakage affect fuel management and thermal margin in many plants, limiting power uprates	More accurate, higher resolution models for boiling surface area, crud deposition, boron uptake and cladding oxidation rate for each rod in core, with boron feedback in neutronics
<b>Grid-to-rod fretting</b>	Rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation affect wear, especially for fuel near the core shroud	Reliable predictions of grid to rod gap, turbulent flow excitation, and resulting rod vibration and wear at any location in core
<b>Pellet-clad interaction</b>	Cladding creep-down onto pellets, followed by pellet expansion, creates local cladding stresses at pellet imperfections, resulting in clad failure sometimes assisted by SCC	Sufficient 3D geometric detail of fuel rod material property changes; pellet growth, cracking and fission product release; cladding stresses, creep, fracture and SCC attach; fuel-cladding binding; and coupling to neutronics and T-H
<b>Fuel assembly distortion</b>	Forces from radiation-induced growth and fluid flow may cause distortion and alter power distributions, challenge fuel handling, retard control rod insertion, and restrict plant operation	Fully 3D structural models of fuel assemblies accounting for material property changes, growth and creep; coupled with neutronics and TH
<b>Reactor vessel and internals integrity over reactor lifetime</b>	Damage from radiation results in increased temperature for onset of brittle failure and higher failure probability due to thermal shock stresses with safety injection for RV, and damage from radiation, thermal & mechanical fatigue render upper internal package more susceptible to distortion under blow-down or seismic loads.	3D prediction of temperature, force, stress, fluence and resulting material property changes of reactor internal structures and vessel; and solid mechanics prediction of vessel fracture and internals distortion
<b>Departure from nucleate boiling</b>	Local clad surface dryout, affected by detailed flow patterns and mixing, cause dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures	3D subchannel and CFD tools to model detailed flow patterns downstream of mixing grids for single and two-phase flow, coupled to detailed pin-resolved radiation transport and fuel performance models for application to DNB transients (e.g., RIA, Loss of Flow)
<b>Cladding integrity during a reactivity insertion accident and loss of coolant accident</b>	Physical changes during transient (e.g., swelling and burst, oxidation mechanics), leading to clad failure followed by fuel dispersal	Enhanced fuel rod models, with improved predictive capability for normal operations to obtain fuel initial conditions at initiation of accident simulation, and transient fuel rod behavior

# Virtual Environment for Reactor Applications (VERA)

CASL's virtual reactor for in-vessel LWR phenomena



# Some of our VERA components comprise a new type of “Core Simulator” (VERA-CS)

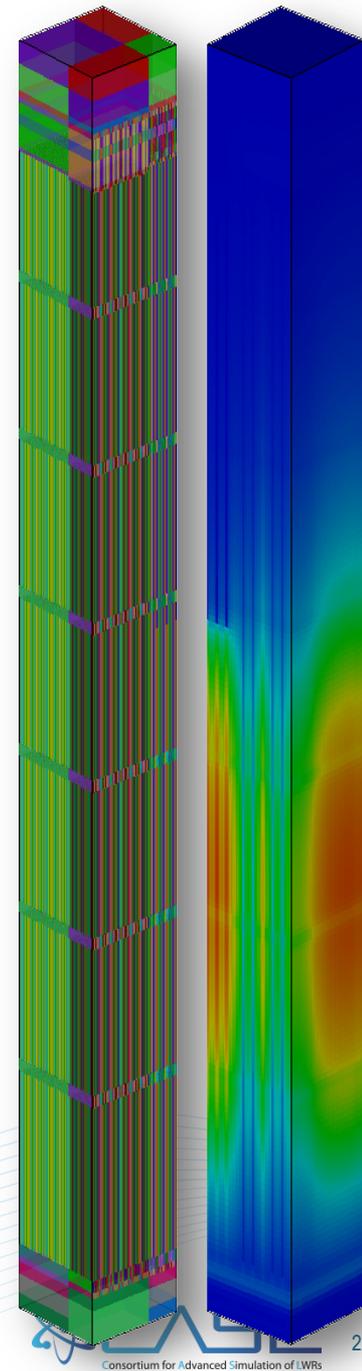


The Core Simulator facet of VERA (VERA-CS) is a code system for modeling steady-state LWR conditions and depletion, providing reactor conditions and distributions *needed to solve our Challenge Problems*. VERA-CS includes components for neutron transport, cross sections, thermal-hydraulics, fuel temperature,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

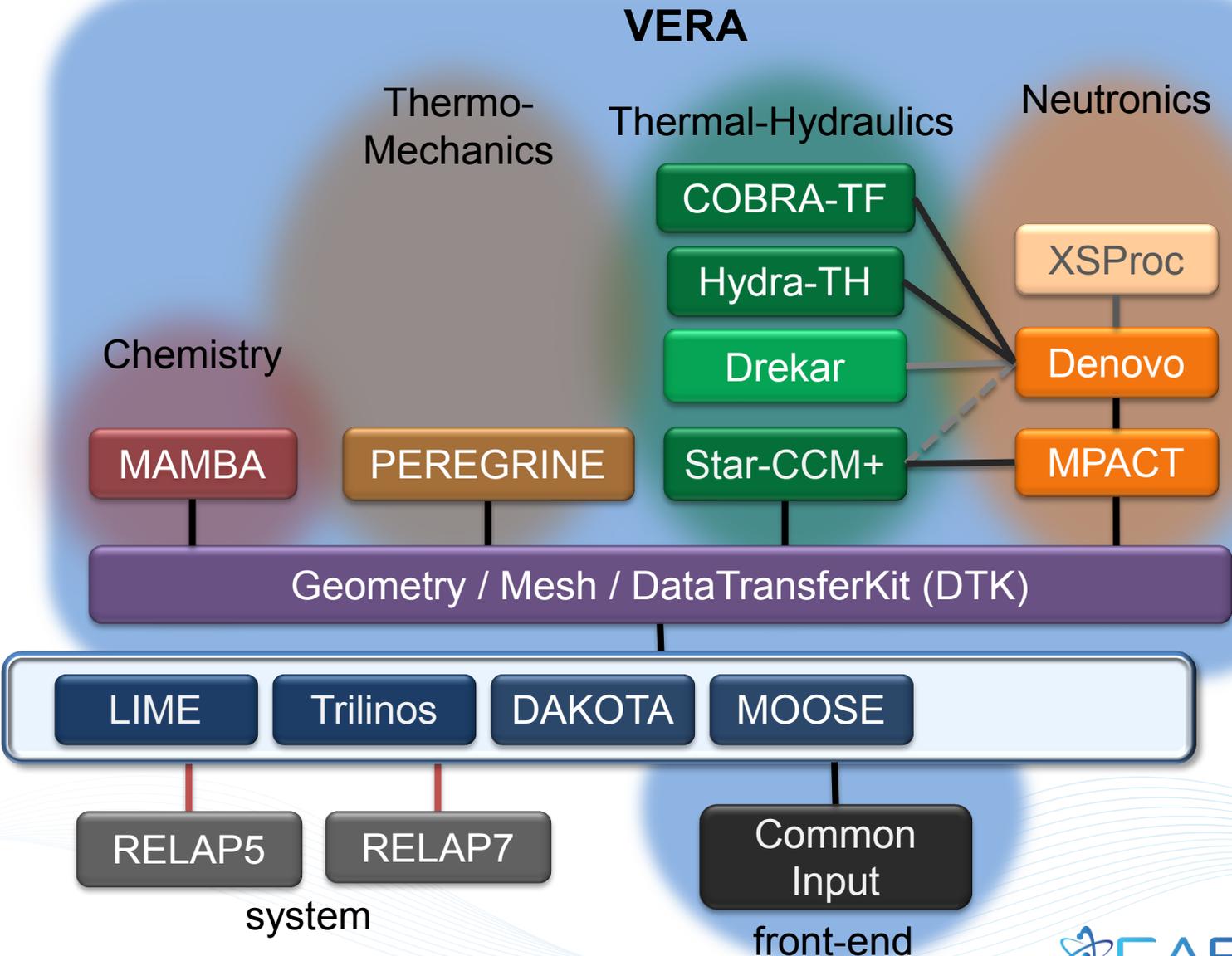
# VERA-CS vs. Industry Core Simulators

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

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

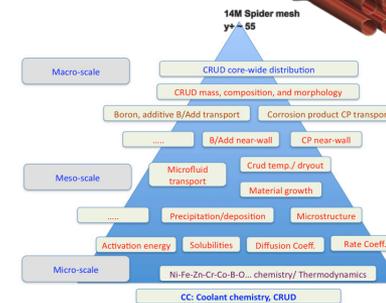
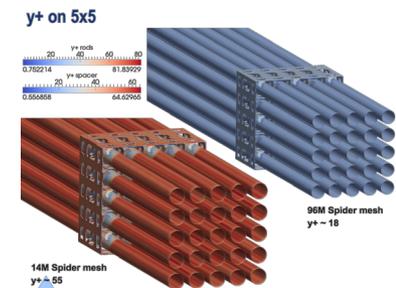
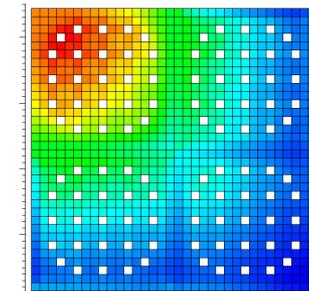
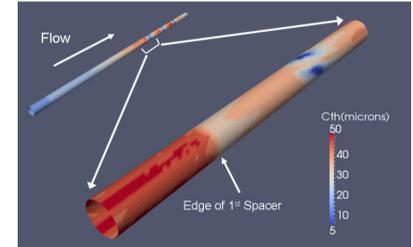


# VERA 5.0 snapshot (03/2015)



# 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



By 2015

# What enhanced capabilities over current practices will CASL provide?

## **Predictive capabilities**

- Utilization of more science based models
- Utilization of micro and mesa scale models to increase understanding and provide closure relationships

## **Phase-space resolution**

- Space, time, energy and angle
- Pin-resolved detail

## **VUQ practices**

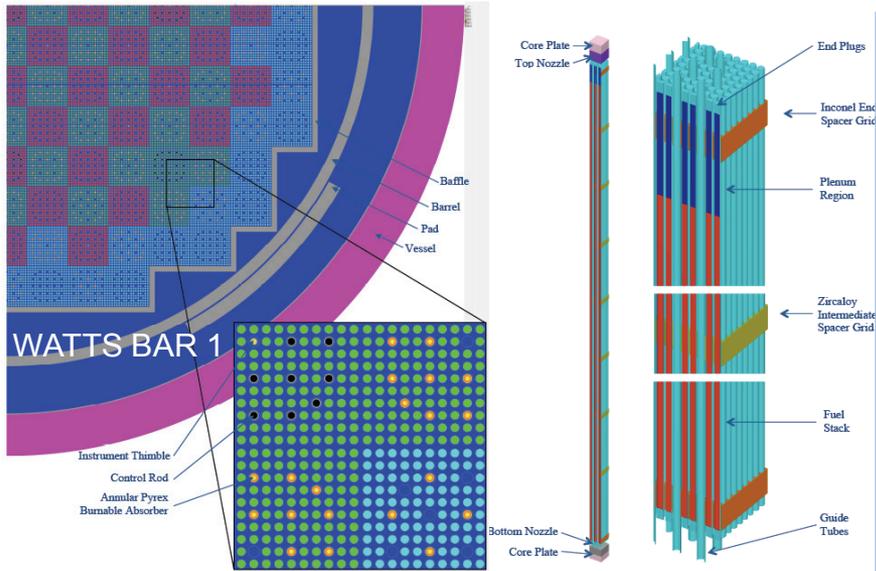
- Verification & validation
- Data assimilation
- Uncertainty quantification

## **Computational resource utilization**

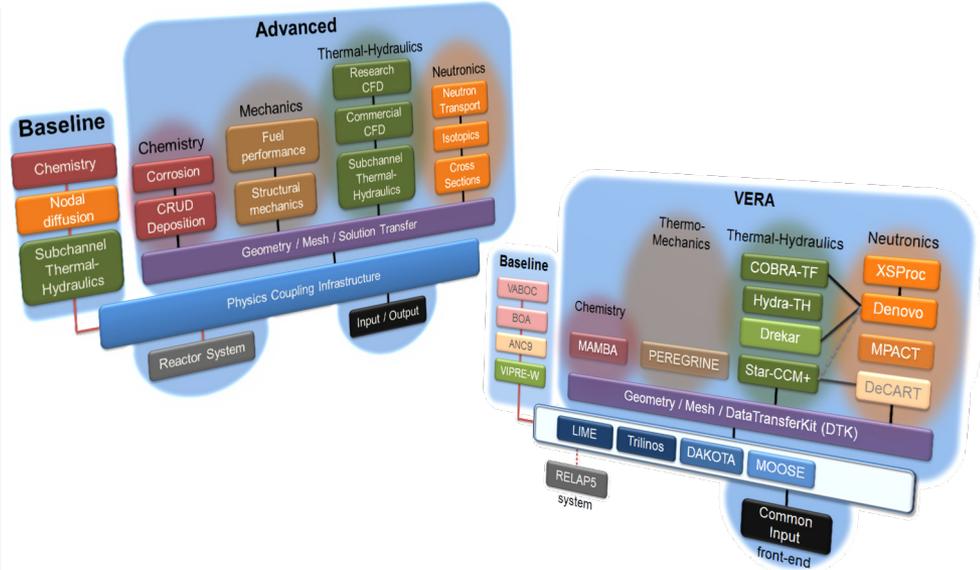
- Hardware: multiprocessor, multicore & GPUs
- Software: object oriented, I/O standards, third-party software (modern solvers)

# Highlights, Accomplishments, Capabilities

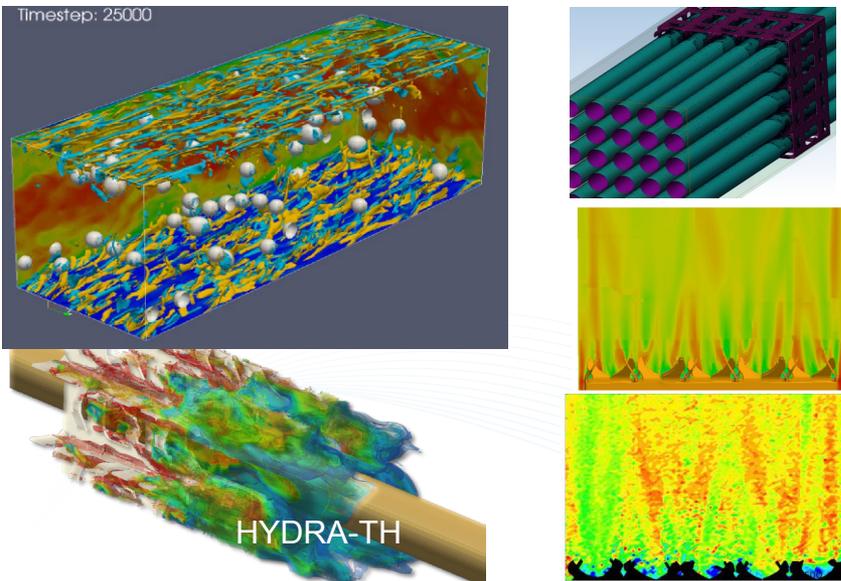
## Advanced Modeling Applications



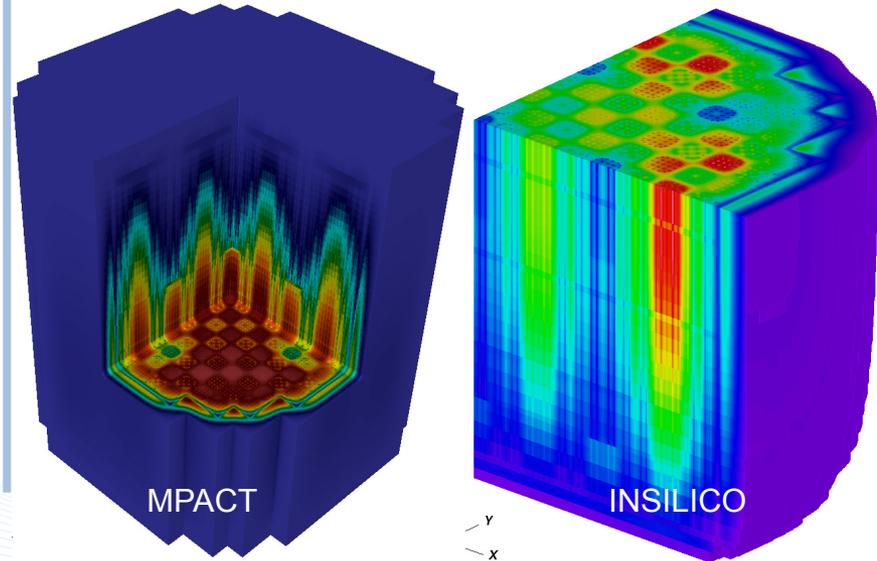
## Physics Integration



## Thermal Hydraulic Methods

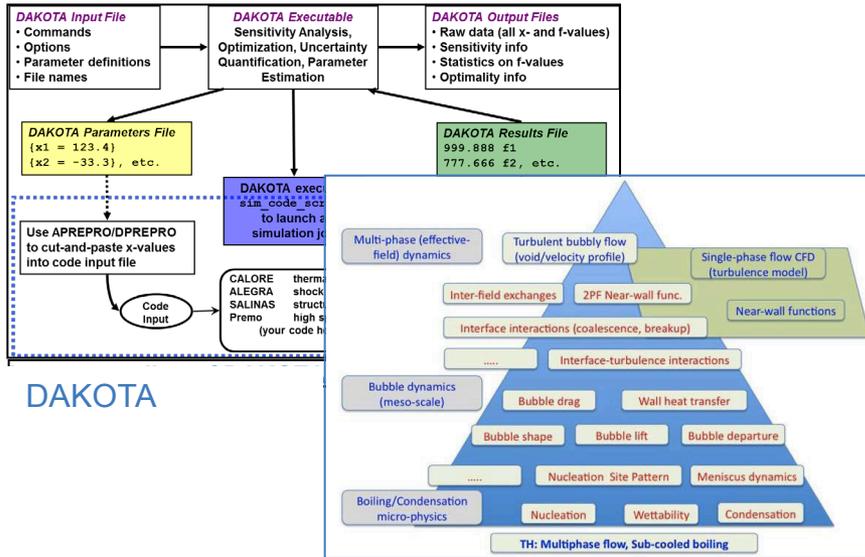


## Radiation Transport Methods



# Highlights, Accomplishments, Capabilities

## Validation & Uncertainty Quantification

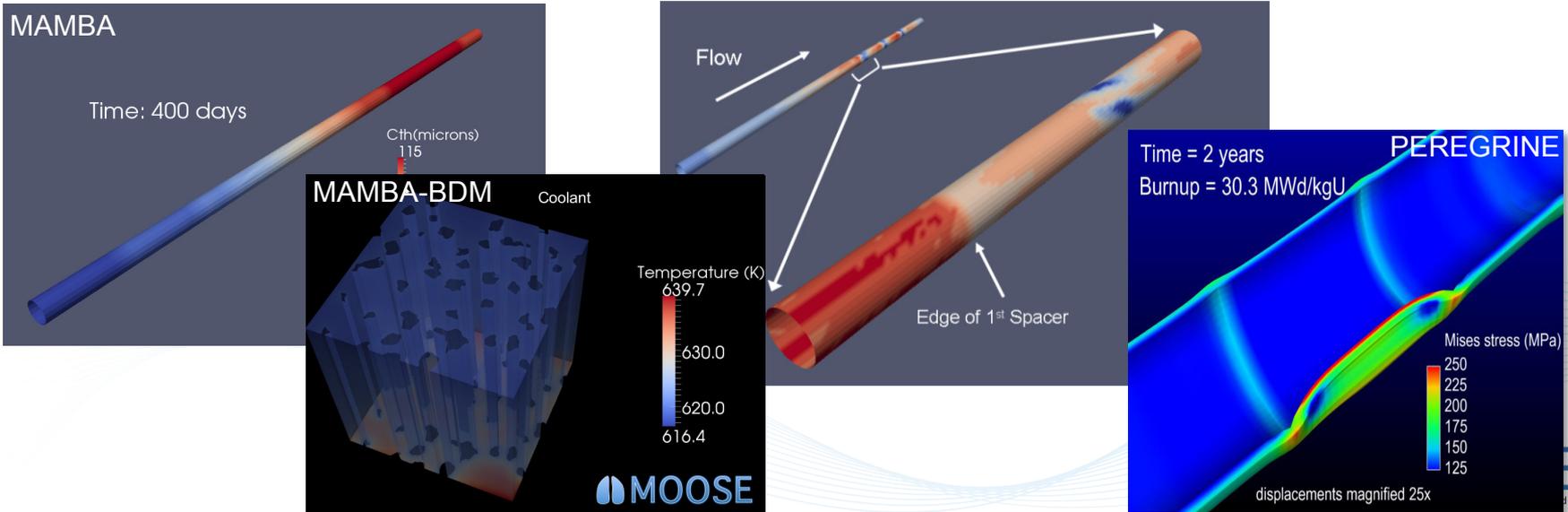


DAKOTA

## VOCC

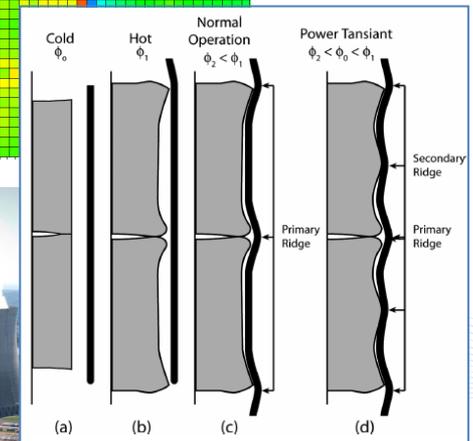
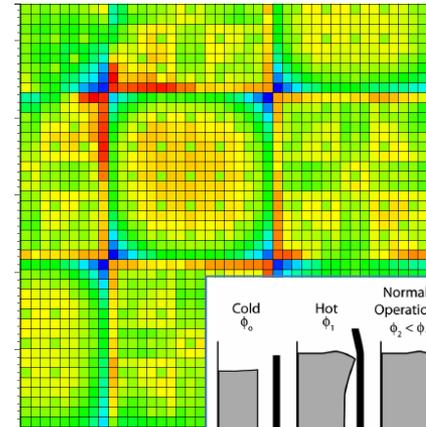
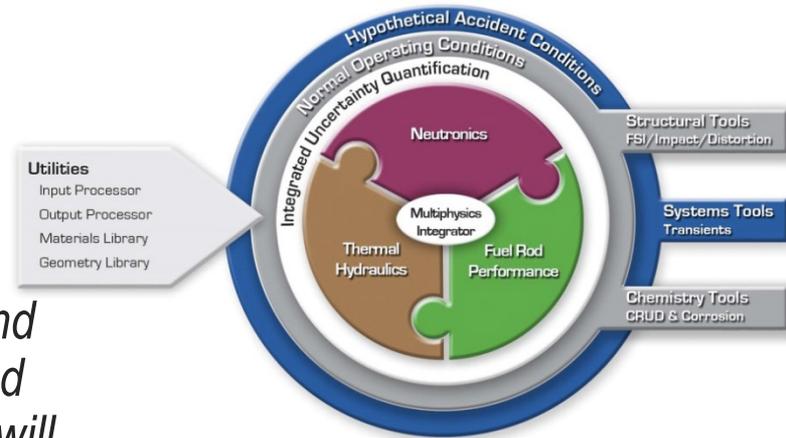


## Materials Performance and Optimization



# CASL Test Stands: From Plan to Execution

- Early deployment into industrial environment for rapid and enhanced testing, use, and ultimate adoption of VERA to support real-world LWR applications
- Excerpt from 2010 Proposal: “... *interactive VR ‘test stands’ will be set up to provide industry-led design and analysis teams with opportunities to test, evaluate, and begin to apply the VR. ... A beta version(s) of the VR will be applied and compared with the reference case and plant data. The VR will also be measured against all the challenge problems ...*”
- Status of initial deployment to core industry partners
  - WEC: Deployment scheduled Jun 2013; focus on VERA simulation of AP1000 first core startup
  - EPRI: Deployment planned for Dec 2013; new EPRI computing capabilities will be utilized to test VERA fuel (Peregrine) performance applications
  - TVA: Deployment planned for Spring/Summer 2014; focus currently under discussion



# CASL at Year 3



- ✓ First VERA Test Stand deployed to industry for application to WEC Gen III AP1000 design (4 now under construction in US)
- ✓ First and successful comparison against operational reactor data (Watts Bar 1 zero power physics tests)
- ✓ Challenge Problem solution metrics and VERA products defined and driving development and application to real operational PWR core scenarios
- ✓ VERA: multi-physics integrator functional for coupling multiple applications (neutronics, T-H, fuel, CRUD, UQ) to address feedback effects not currently reflected in the industry analytical approach
- ✓ VERA: baseline industry physics capabilities integrated to demonstrate increased fidelity of the coupled approach for a direct industry comparison point.
- ✓ VERA-CS: progressed thru 6 (almost 7) core physics benchmark problems required for real industry use
- ✓ Continued targeted development of advanced simulation components: UQ, neutron transport, multiphase CFD, CRUD deposition/corrosion, fuel performance, structural dynamics

## Scientific Output thru Jun 2013

- 81+ journal articles
- 328 conference papers
- 28 technical reports
- 51+ invited talks
- 382 milestone reports
- 216 programmatic reports

# Questions?

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