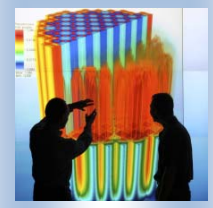
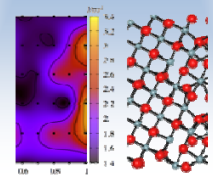




CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

Doug Kothe
Director, CASL

Director of Science, Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory

Consortium for Advanced Simulation of LWRs

SciDAC 2010
July 12, 2010 Chattanooga, TN

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Outline

- The DOE Energy Innovation Hub for modeling and simulation (M&S) of nuclear reactors: background
- CASL mission, vision, objectives, execution plan
- CASL interfaces and science program
- Path forward

What is a DOE Energy Innovation Hub?
(as documented)

- Target problems in areas presenting the most critical barriers to achieving national climate and energy goals that have heretofore proven the most resistant to solution via the normal R&D enterprise
- Represent a new structure, modeled after research entities likes the Manhattan Project (nuclear weapons), Lincoln Lab at MIT (radar), and AT&T Bell Labs (transistor)
- Consistent with Brookings Institution's recommendations for "Energy Discovery-Innovation Institutes" (early 2009)
  - "…new research paradigms are necessary, we believe, that better leverage the unique capacity of America's research" - Dr. Jim Duderstadt, President Emeritus, University of Michigan
- Focuses on a single topic, with work spanning the gamut, from basic research through engineering development to partnering with industry in commercialization
- Large, highly integrated and collaborative creative teams working to solve priority technology challenges
  - Brings together the top talent across the R&D enterprise (gov, academia, industry, non-profits) to become a world-leading R&D center in its topical area

Attributes Sought by DOE for the Energy Innovation Hub for M&S of Nuclear Reactors

- Utilize existing advanced M&S capabilities developed in other programs within DOE and other agencies
- Apply them through a new multi-physics environment and develop capabilities as appropriate
- Adapt the new tools into the current and future culture of nuclear engineers and produce a multi-physics environment to be used by a wide range of practitioners to conduct predictive simulations
- Have a clear mission that focuses and drives R&D
- Use data from a real physical operation reactor to validate the virtual reactor
- Lead organization with strong scientific leadership and a clearly defined central location (“one roof” plan)

The CASL Team: A unique lab-university-industry partnership

Core partners

Oak Ridge National Laboratory

Electric Power Research Institute

Idaho National Laboratory

Los Alamos National Laboratory

Massachusetts Institute of Technology

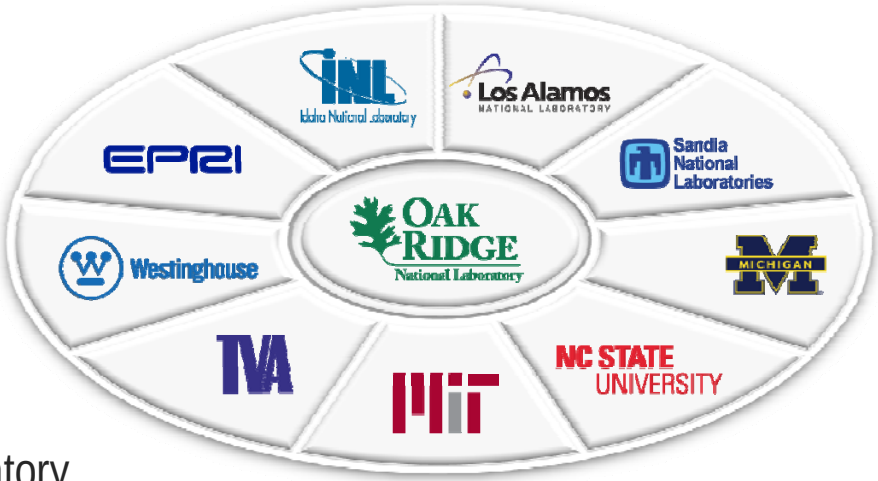
North Carolina State University

Sandia National Laboratories

Tennessee Valley Authority

University of Michigan

Westinghouse Electric Company



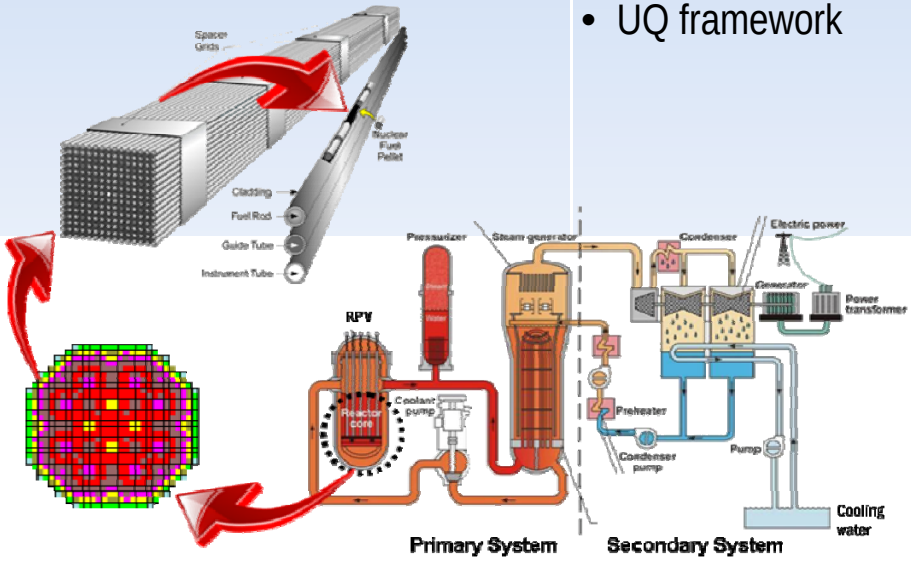
Building on longstanding, productive relationships and collaborations to forge a close, cohesive, and interdependent team that is fully committed to a well-defined plan of action

Individual contributors

ASCOMP GmbH
CD-adapco, Inc.
City University of New York
Florida State University
Imperial College London
Rensselaer Polytechnic Institute
Southern States Energy Board
Texas A&M University
University of Florida
University of Tennessee
University of Wisconsin
Worcester Polytechnic Institute

CASL vision: Create a virtual reactor (VR) for *predictive* simulation of LWRs

Leverage	Develop	Deliver
• Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications • Existing systems and safety analysis simulation tools	• New requirements-driven physical models • Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy • Improved systems and safety analysis tools • UQ framework	• An unprecedented predictive simulation tool for simulation of physical reactors • Architected for platform portability ranging from desktops to DOE's leadership-class and advanced architecture systems (large user base) • Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors • Base M&S LWR capability



CASL mission: Develop and apply the VR to address 3 critical performance goals for nuclear power

1

Reduce capital and operating costs per unit energy by:

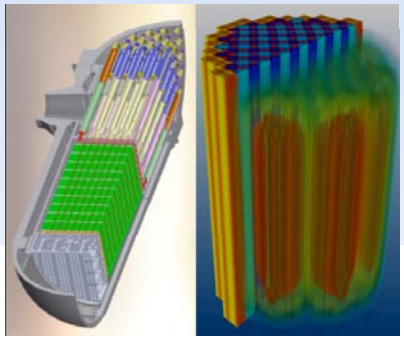
- Power uprates
- Lifetime extension

2

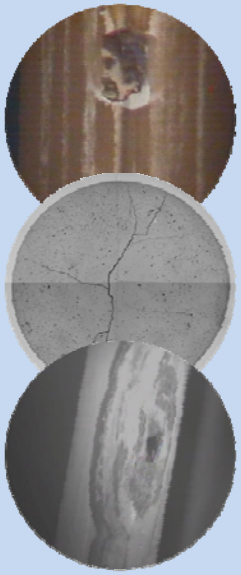
Reduce nuclear waste volume generated by enabling higher fuel burnups

3

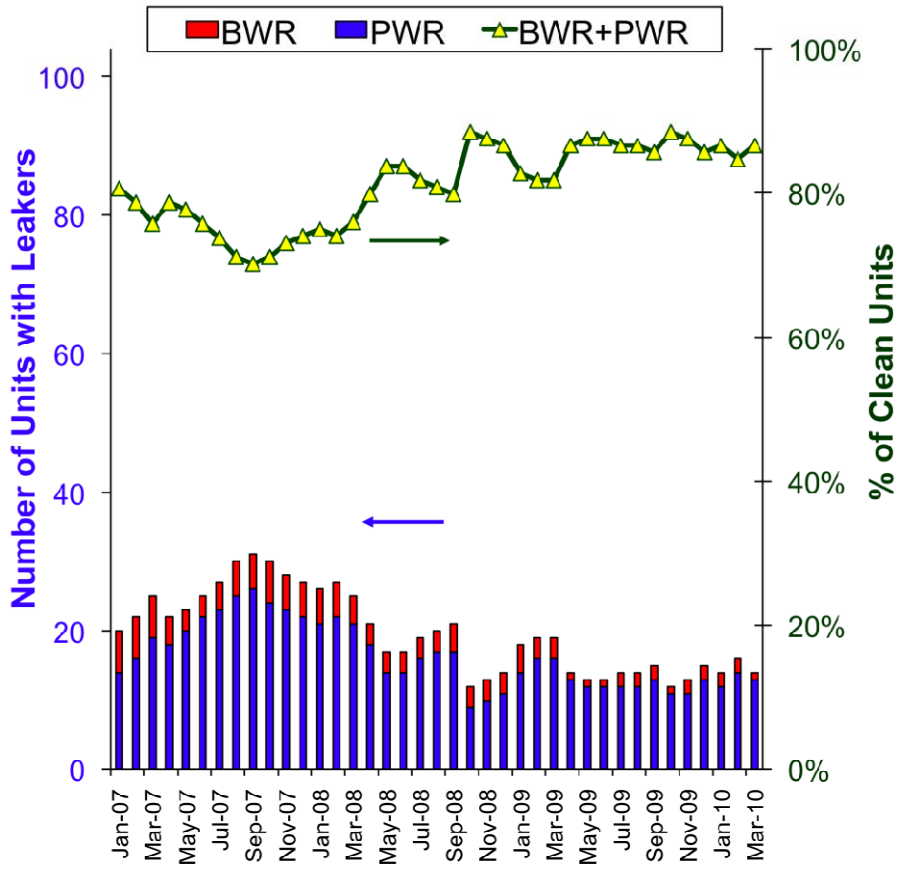
Enhance nuclear safety by enabling high-fidelity predictive capability for component and system performance from beginning of life through failure

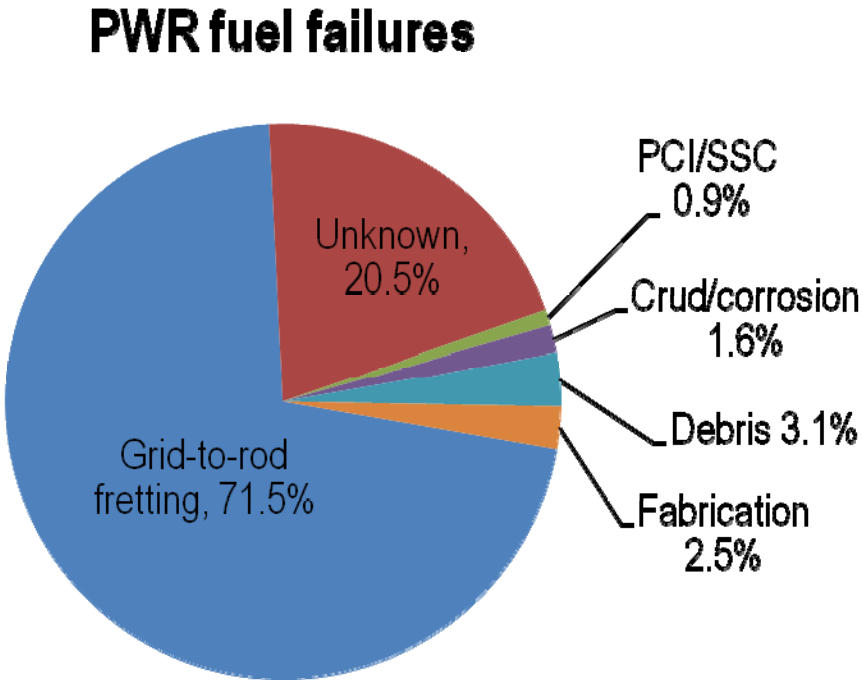


Each reactor performance improvement goal brings benefits and concerns

Power uprates	Lifetime extension	Higher burnup
• 5–7 GWe delivered at ~20% of new reactor cost • Advances in M&S needed to enable further uprates (up to 20 GWe) • Key concerns: – Damage to structures, systems, and components (SSC) – Fuel and steam generator integrity – Violation of safety limits	• Reduces cost of electricity • Essentially expands existing nuclear power fleet • Requires ability to predict SSC degradation • Key concerns: – Effects of increased radiation and aging on integrity of reactor vessel and internals – Ex-vessel performance (effects of aging on containment and piping)	• Supports reduction in amount of used nuclear fuel • Supports uprates by avoiding need for additional fuel • Key concerns: – Cladding integrity – Fretting – Corrosion/ CRUD – Hydriding – Creep – Fuel-cladding mechanical interactions 

Current fuel performance issues provide insights for further power uprates and increased fuel burnups



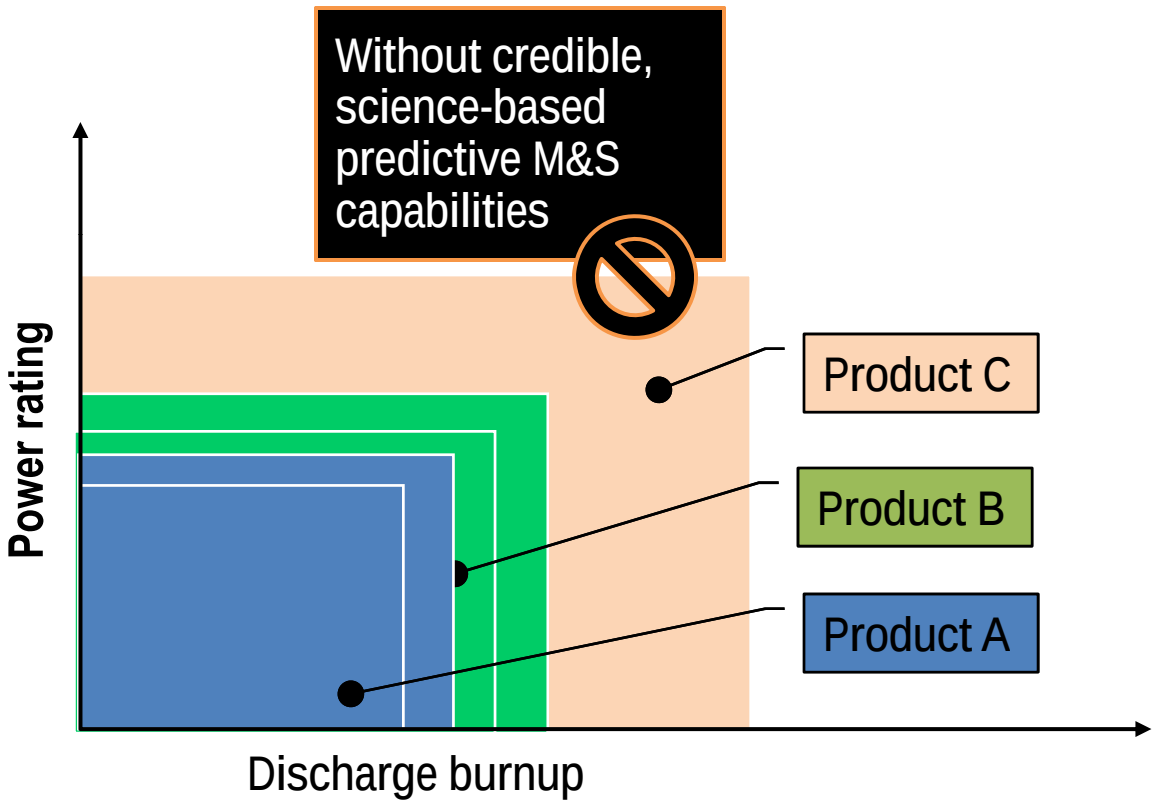


CASL VR M&S capability will permit proactive evaluation to enable critical performance enhancements

CASL targets key limiting phenomena that are barriers to improved reactor performance

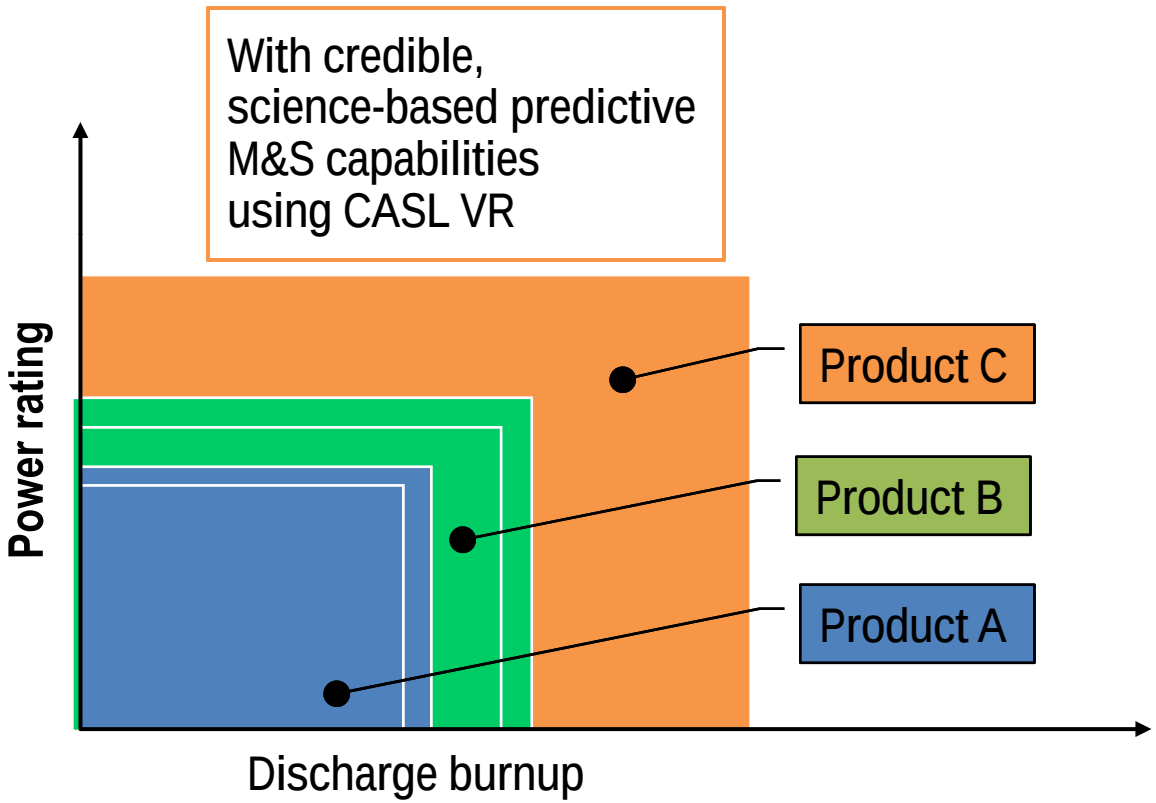
	Power uprate	High burnup	Life extension
Operational "Challenge Problems"			
CRUD-Induced Power Shift (CIPS)	×	×	
CRUD-Induced Localized Corrosion (CILC)	×	×	
Grid-to-Rod Fretting Failure (GTRF)		×	
Pellet Clad Interaction (PCI)	×	×	
Fuel Assembly Distortion (FAD)	×	×	
Safety "Challenge Problems"			
Departure from Nucleate Boiling (DNB)	×		
Cladding Integrity during Loss of Coolant Accidents (LOCA)	×	×	
Cladding Integrity during Reactivity Insertion Accidents (RIA)	×	×	
Reactor Vessel Integrity	×		×
Reactor Internals Integrity	×		×

Current M&S capability
Limited by demonstration basis used for validation



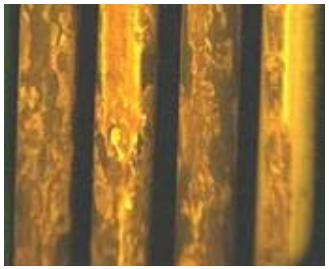
CASL science objective

Enabling stretched performance of current products and more timely introduction of new enhanced products

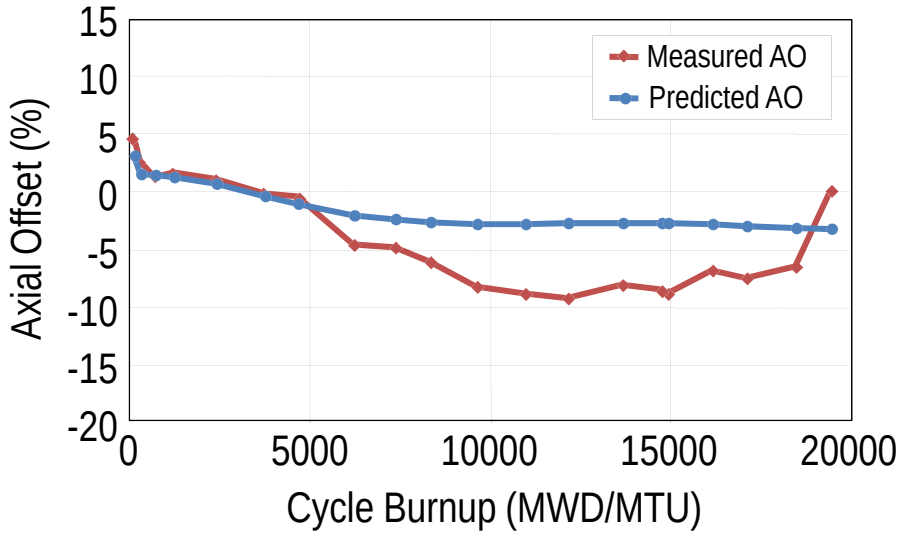


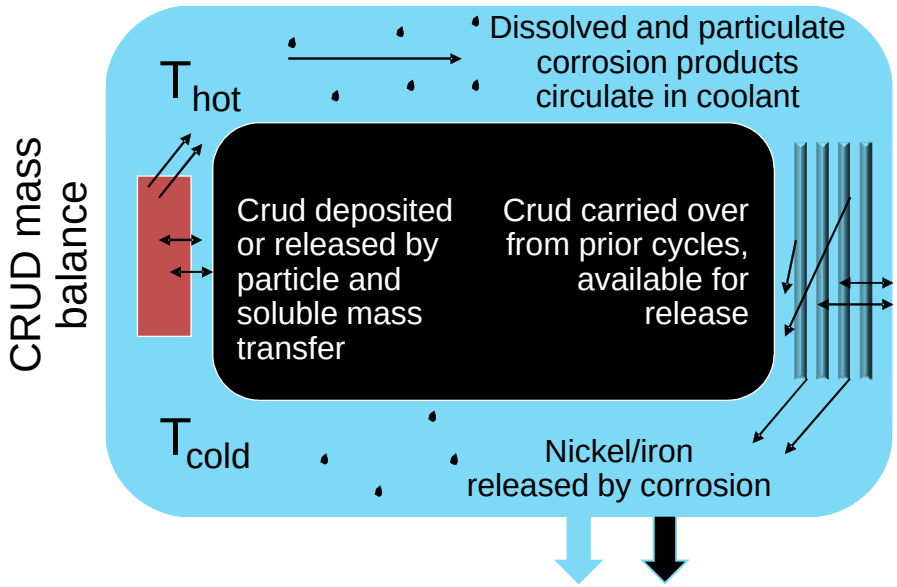
CRUD-induced power shift (CIPS)

- Deviation in axial power shape
  - Cause: Boron uptake in CRUD deposits in high power density regions with subcooled boiling
  - Affects fuel management and thermal margin in many plants
- Power uprates will increase potential for CRUD growth



CRUD deposits

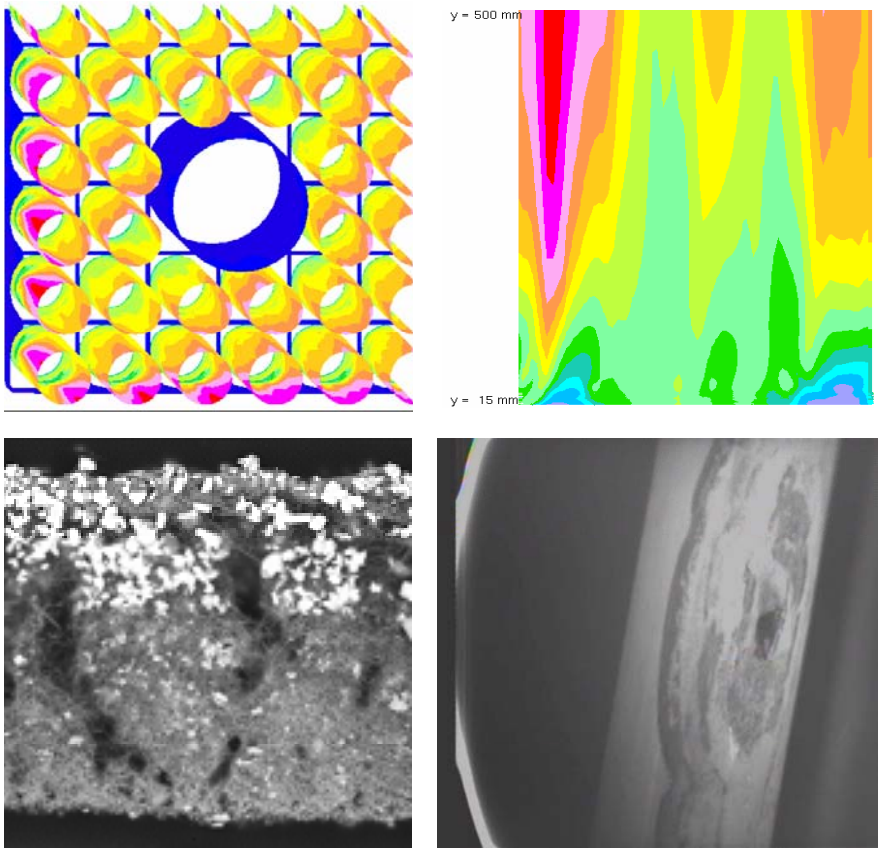




Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth

CRUD-induced localized corrosion (CILC)

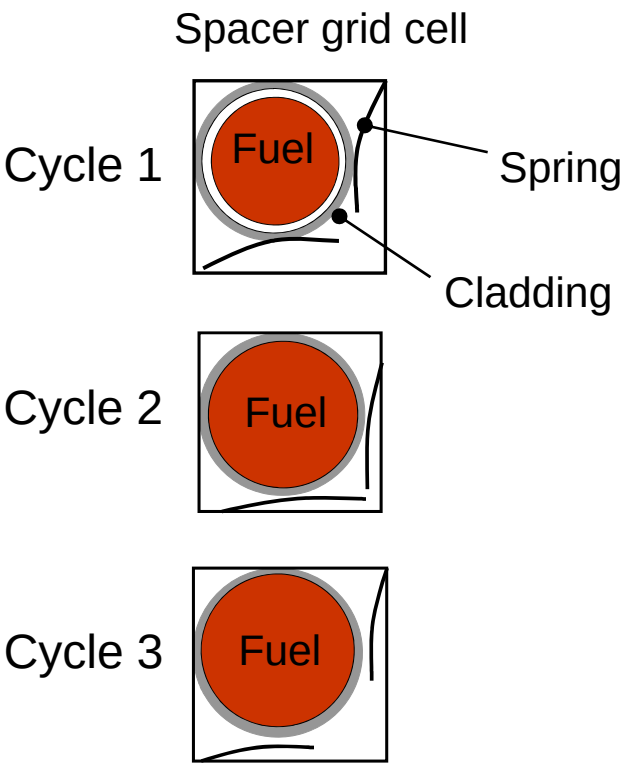
- Hot spots on fuel
  lead to localized boiling
- Excessive boiling with high
  CRUD concentration in coolant
  can lead to thick CRUD deposits,
  CRUD dryout,
  and accelerated corrosion
- Result: Fuel leaker



Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

Grid-to-rod fretting failure (GTRF)

- Clad failure can occur as the result of rod-spring interactions
  - Induced by flow vibration
  - Amplified by irradiation-induced grid spacer growth and spring relaxation
- Power uprates and burnup increase potential for fretting failures
  - Leading cause of fuel failures in PWRs

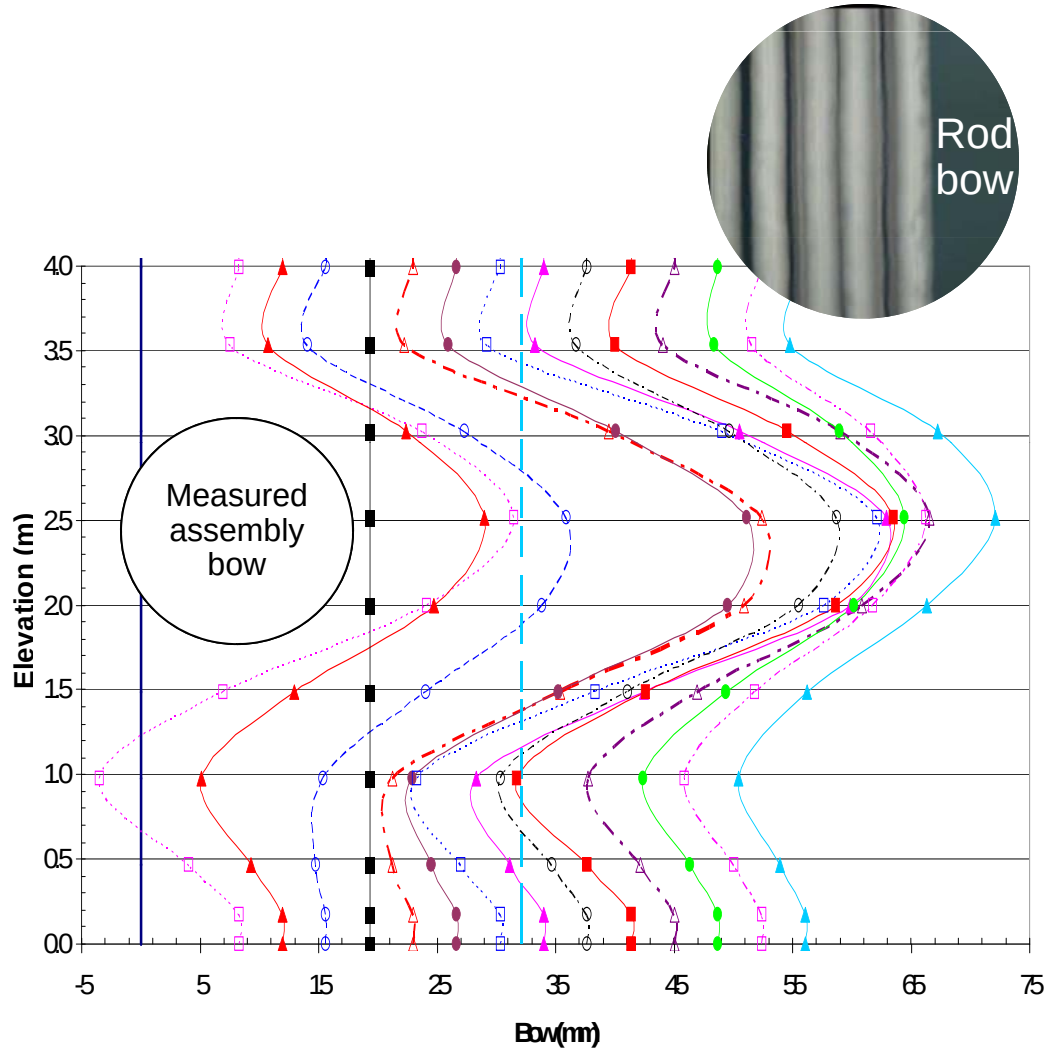


Need: High-fidelity, fluid structural interaction tool to predict gap, turbulent flow excitation, rod vibration and wear

Fuel assembly distortion (FAD)

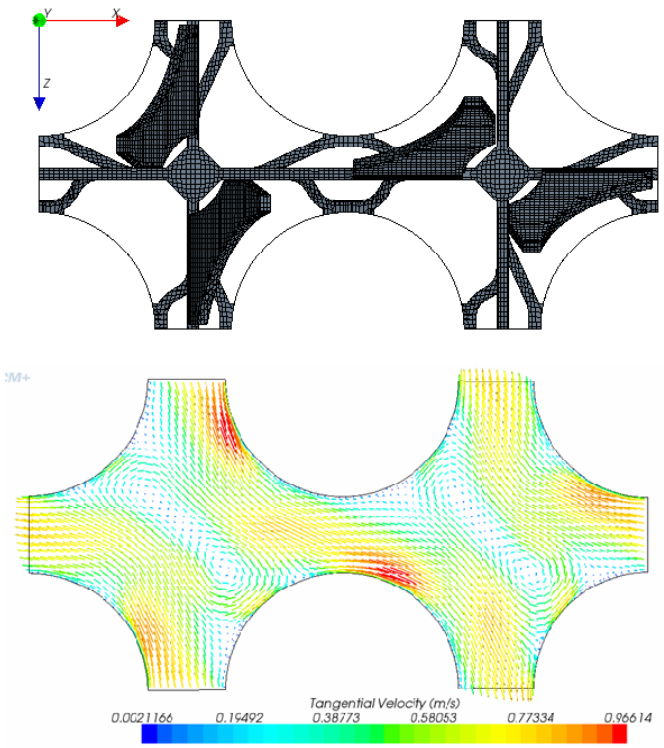
- Excessive axial forces caused by radiation-induced swelling lead to distortion or structural failure
- Power uprates and increased burnups:
  - May increase fuel distortions
  - May alter core power distributions, fuel handling scenarios, control rod insertability, and plant operation

Need: Tool to predict distortion and impact on power distributions and safety analyses



Departure from nucleate boiling (DNB)

- Local clad surface dryout causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow)
- Current limitations:
  - Absence of detailed pin modeling in TH methods results in conservative analysis
  - Detailed flow patterns and mixing not explicitly modeled in single- and two-phase flow downstream of spacer grids
- Power uprates require improved quantification of margins for DNB or dryout limits



Need: High-fidelity modeling of complex flow and heat transfer for all pins in core downstream of spacer grids

A comprehensive set of milestones is defined to drive solution of the challenge problems

Industry challenges and needs

Challenge problems

L1 Milestones in 6 challenge categories

- CRUD
- Grid-to-rod fretting (GTRF)/ fuel assembly distortion (FAD)
- Operational reactor
- Safety
- Lifetime extension
- Advanced fuels

L2 Milestones
Discipline-oriented focus areas

L3 Milestones
Projects

Year	VR Capability	L1 Milestone Category	L1 Milestone
1	Initial core simulation using coupled tools and models	CRUD	Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate quantities relevant to CRUD initiation and growth
		GTRF/FAD	Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting
2	Detailed phenomena modeling in fully coupled VR	CRUD	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness
		GTRF/FAD	Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration
3	Assembly simulation with rod fretting and upscaled materials models	CRUD	Model boron uptake from reactor coolant into CRUD on fuel rods
		GTRF/FAD	Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods
		Safety	Initial modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		OR	Initial modeling of reactor operation, qualify with operational data
4	Initial predictive reactor modeling in coupled VR	CRUD	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape
		GTRF/FAD	Calculate fuel rod material wear resulting from GTRF
			Model reactor vessel fluence and material [illegible]

CASL scope: Develop and apply the VR to assess fuel design, operation, and safety criteria

Near-term priorities (years 1–5)

- Deliver improved predictive simulation of PWR core, internals, and vessel
  - Couple VR to evolving out-of-vessel simulation capability
  - Maintain applicability to other NPP types
- Execute work in 5 technical focus areas to:
  - Equip the VR with necessary physical models and multiphysics integrators
  - Build the VR with a comprehensive, usable, and extensible software system
  - Validate and assess the VR models with self-consistent quantified uncertainties

Longer-term priorities (years 6–10)

- Expand activities to include structures, systems, and components beyond the reactor vessel
- Established a focused effort on BWRs and SMRs
- Continue focus on delivering a useful VR to:
  - Reactor designers
  - NPP operators
  - Nuclear regulators
  - New generation of nuclear energy professionals

Focus on challenge problem solutions

CASL's technical focus areas will execute the plan

MPO
Materials Performance and Optimization
Chris Stanek, Lead
Sid Yip, Deputy

- Upscaling (CMPM)
- Fuel microstructure
- Clad/internals microstructure
- Corrosion
- CRUD deposition
- Failure modes

MNM
Models and Numerical Methods
Bill Martin, Lead
Ed Dendy, Deputy

- Radiation transport
- Thermal hydraulics

VRI
Virtual Reactor Integration
John Turner, Lead
Randy Summers,
Rich Martineau, Deputies

- Coupled multi- physics environment
- VR simulation suite
- Coupled mechanics

VUQ
Validation and Uncertainty Quantification
Jim Stewart, Lead
Dan Cacuci, Deputy

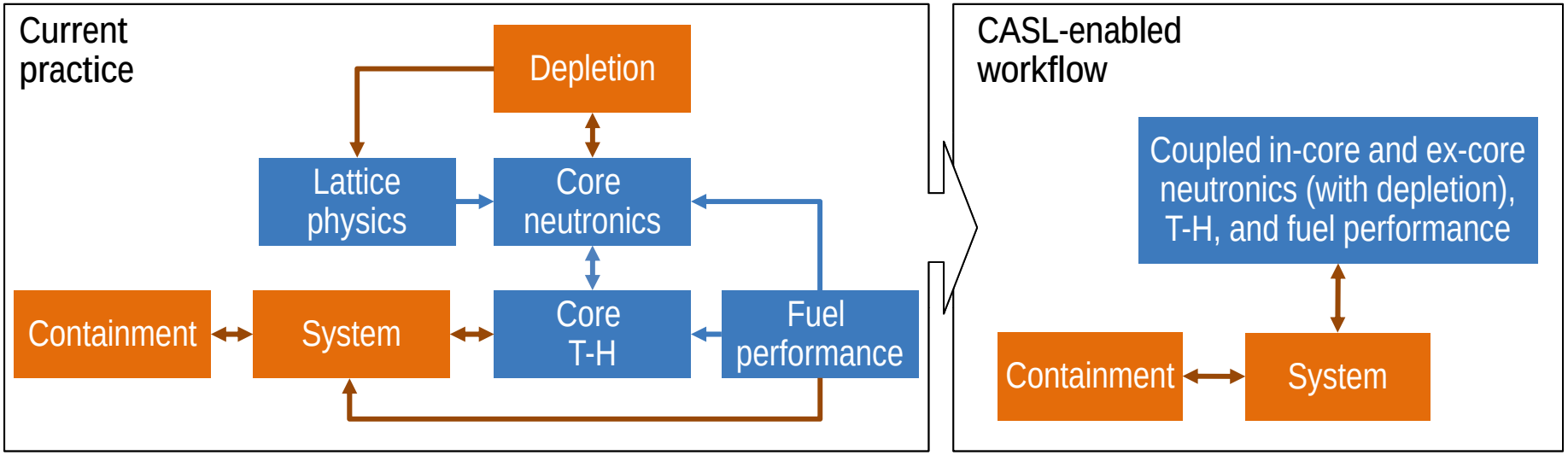
- V&V and calibration through data assimilation
- Sensitivity analysis and uncertainty quantification

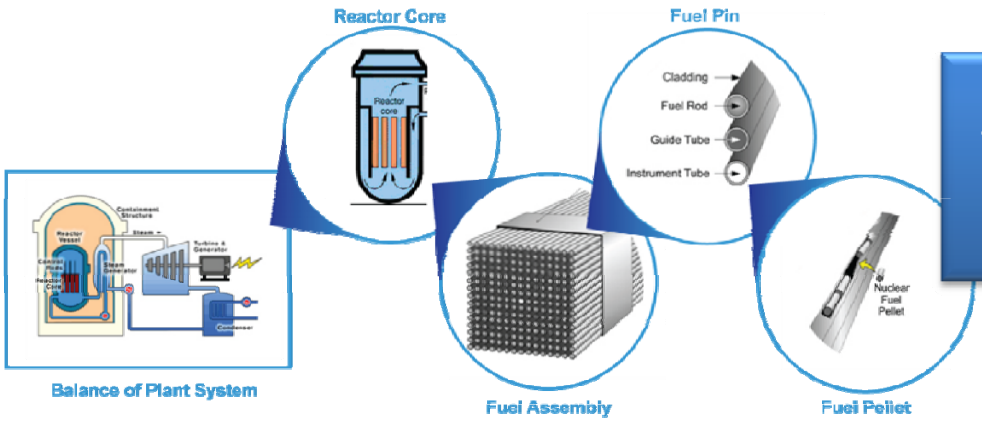
AMA
Advanced Modeling Applications
Jess Gehin, Lead
Zeses Karoutas, Deputy

- VR requirements
- VR physical reactor qualification
- Challenge problem application
- VR validation
- NRC engagement

18 integrated and interdependent projects

The CASL Virtual Reactor is at the heart of the plan and is the science and technology integrator





Suite of advanced yet usable M&S tools and methods, integrated within a common software infrastructure for predictive simulation of LWRs

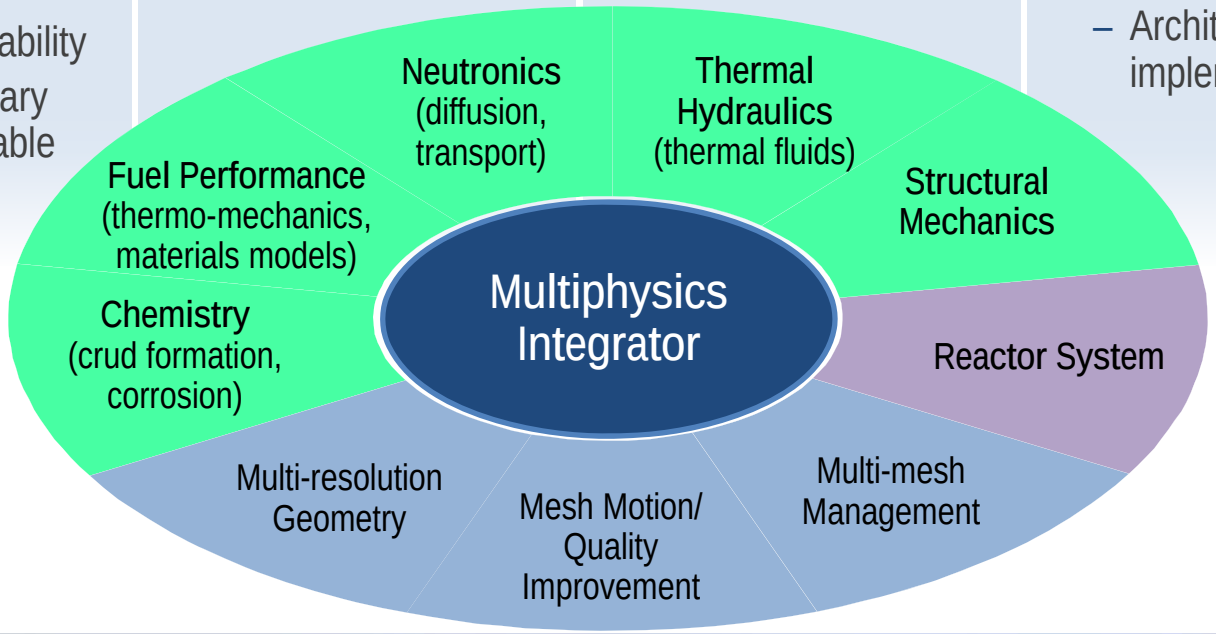
The CASL Virtual Reactor:
A code system for scalable simulation of nuclear reactor core behavior

- Flexible coupling of physics components
- Toolkit of components
  - Not a single executable
  - Both legacy and new capability
  - Both proprietary and distributable

- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

- Development guided by relevant challenge problems
- Broad applicability

- Scalable from high-end workstation to existing and future HPC platforms
  - Diversity of models, approximations, algorithms
  - Architecture-aware implementations



desktop

Future large-scale systems present challenges for applications

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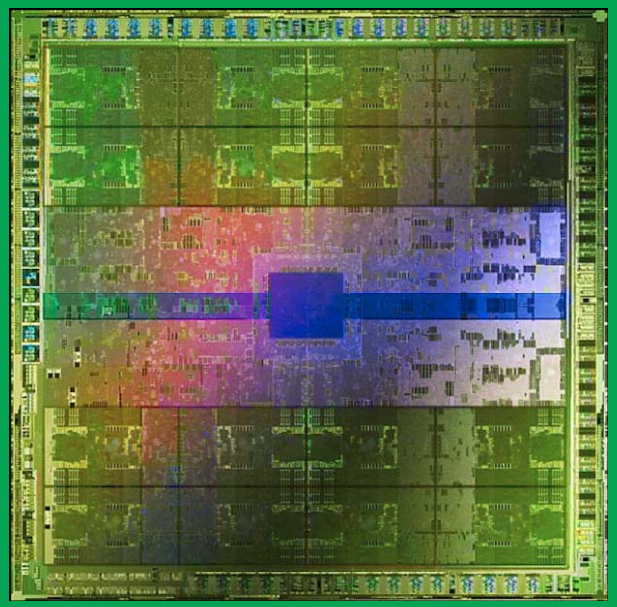
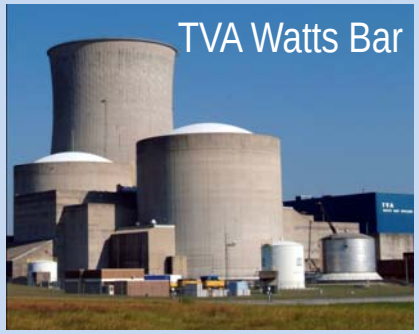
Intel 48-core experimental chip shipping this summer



NVIDIA 512-"core" Fermi GPU

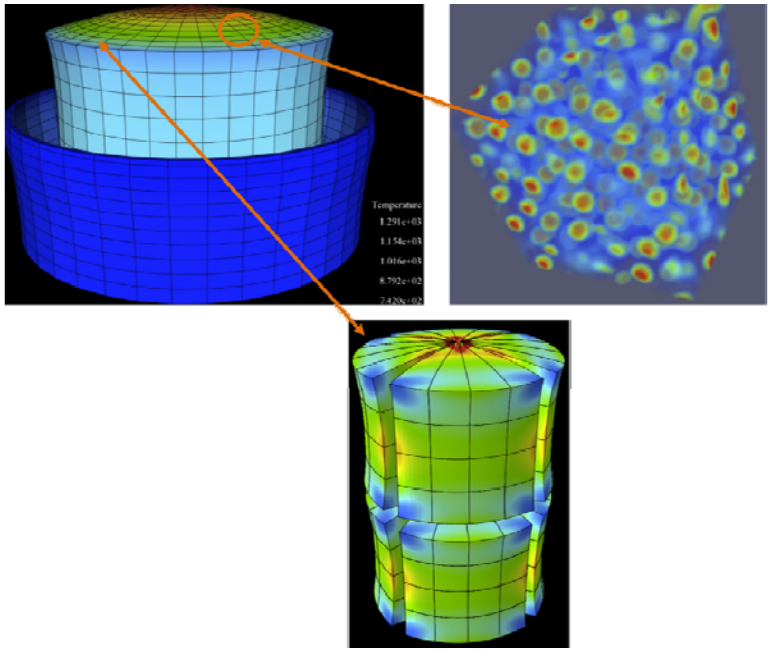
Over the life of CASL, these challenges will become increasingly significant at the desktop level

Other key elements required for success

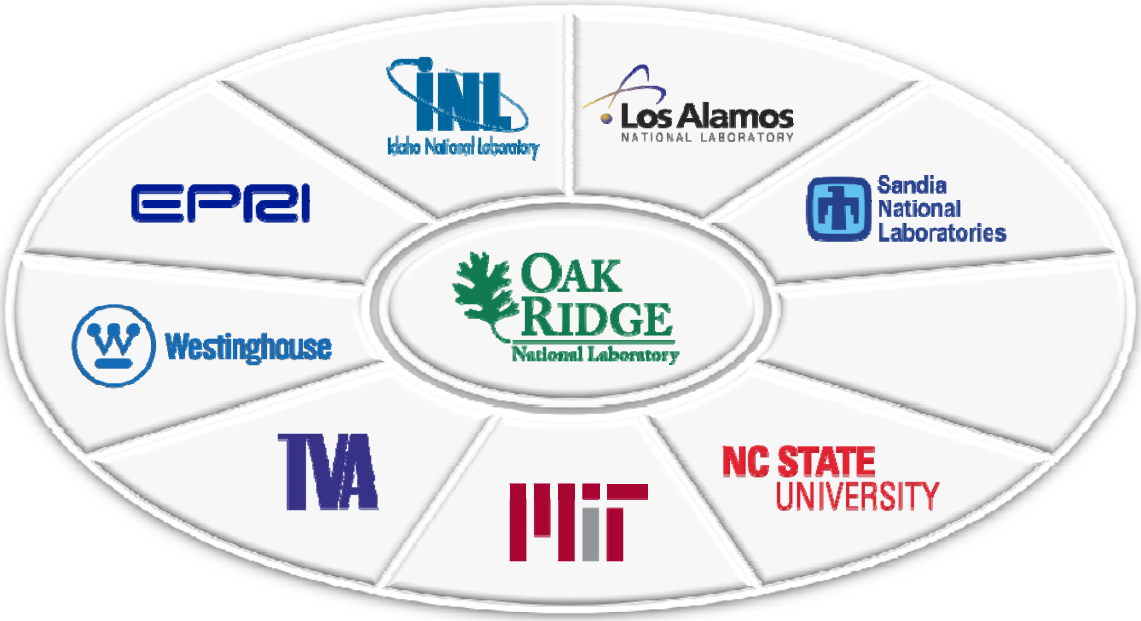
Physical reactors	• 3 Westinghouse PWRs at Sequoyah and Watts Bar, operated by TVA
NRC engagement	• Existing MOU between NRC Office of Regulatory Research and EPRI • CSO: Develop strategy for NRC engagement; AMA focus area Project 5: Execute strategy
Education, Training, and Outreach (ETO) Program	• Comprehensive engagement with students, faculty, and practicing scientists, engineers, and regulators • Leverage EPRI's structured technology transfer approach
Validation ORNL HFIR INL ATR	• One entire focus area dedicated to validation and UQ • Extensive reactor design information and test and operational data • Data validation needs and sources identified: Integral and separate-effects tests, PIE of used fuels, plant and in-core diagnostics, in- and out-of-pile testing of prototypic fuels  TVA Watts Bar Westinghouse CRUD Facility
Virtual Office, Community, and Computing (VOCC)	• Integration and application of latest and emerging technologies to build an extended "virtual one roof"

CASL legacy: what do we leave “behind”?

A preeminent computational science institute for nuclear energy



- CASL VR: Advanced M&S environment for predictive simulation of LWRs
  - Operating on current and future leadership-class computers
  - Deployed by industry (software “test stands” at EPRI and Westinghouse)
- Advanced M&S capabilities:
  - Advances in HPC algorithms and methods
  - Validated tools for advancing reactor design
- Fundamental science advances documented in peer-reviewed publications
- Innovations that contribute to U.S. economic competitiveness
- Highly skilled work force with education and training needed:
  - To sustain and enhance today’s nuclear power plants
  - To deliver next-generation systems

Questions

contact@casl.gov; www.casl.gov