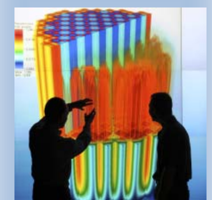
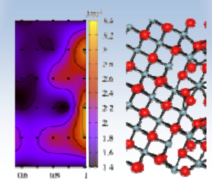



# CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

Douglas B. Kothe

Director, CASL
Oak Ridge National Laboratory

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Oak Ridge National Laboratory

# 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

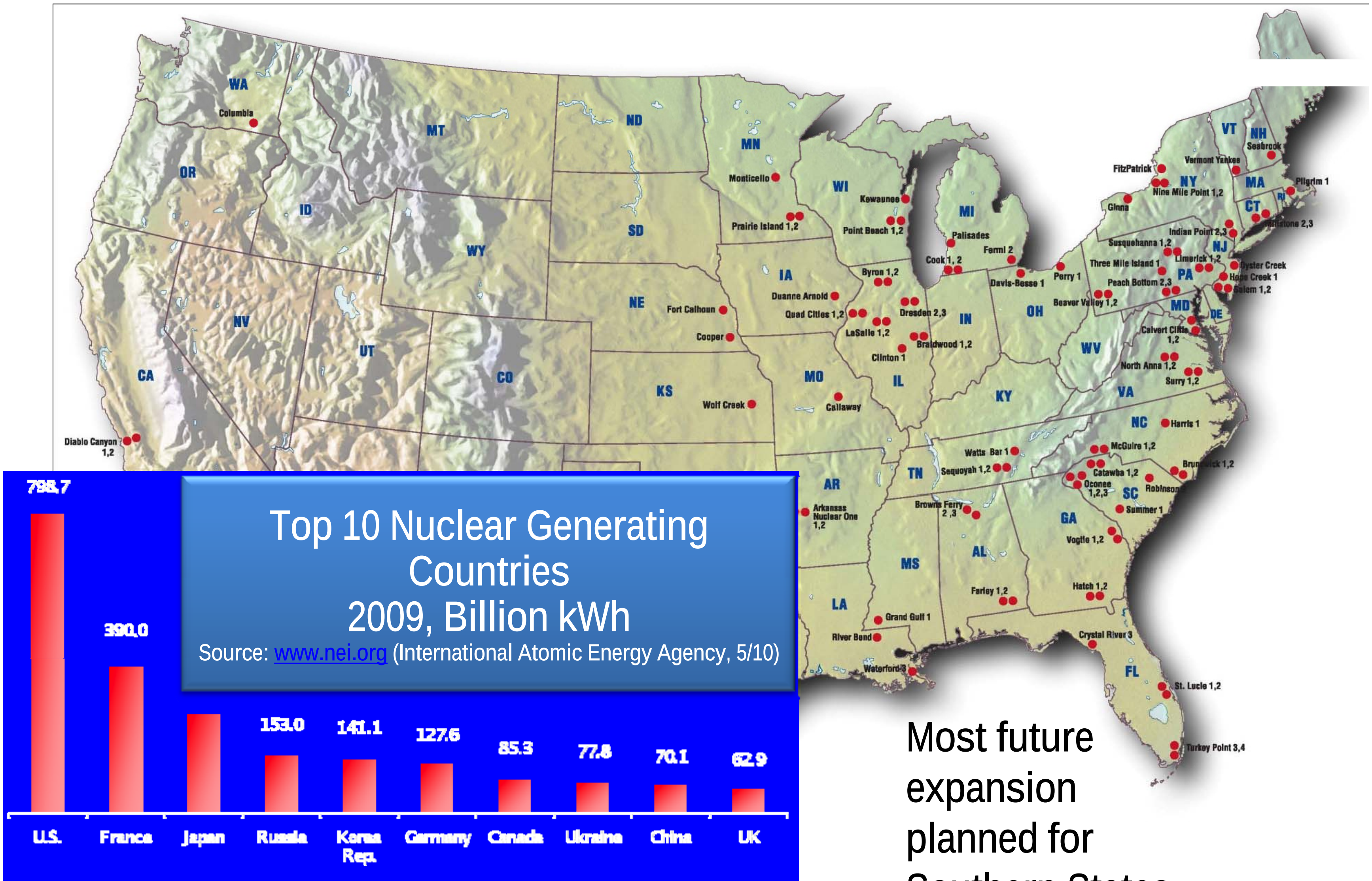
## Individual contributors

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

# Outline

- Current Light Water Reactor (LWR) experience operational challenges
- Modeling and simulation (M&S) *challenge problems* that drive development of "virtual reactor" (VR) for LWRs
- How and why CASL – A DOE Energy Innovation Hub for M&S of Nuclear Reactors – can make a difference in the short and long term

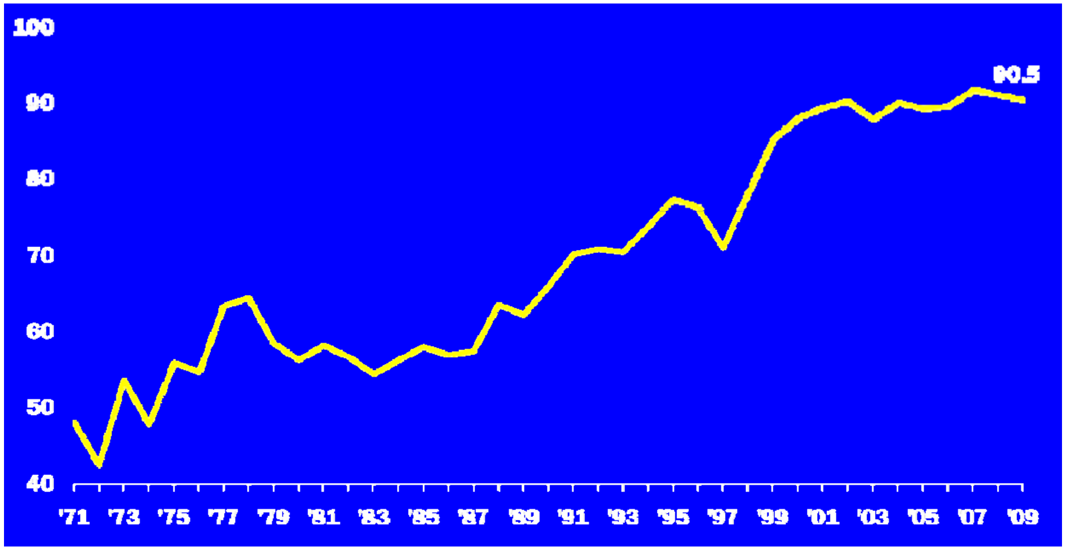
# Nuclear Power in the US




Most future expansion planned for Southern States

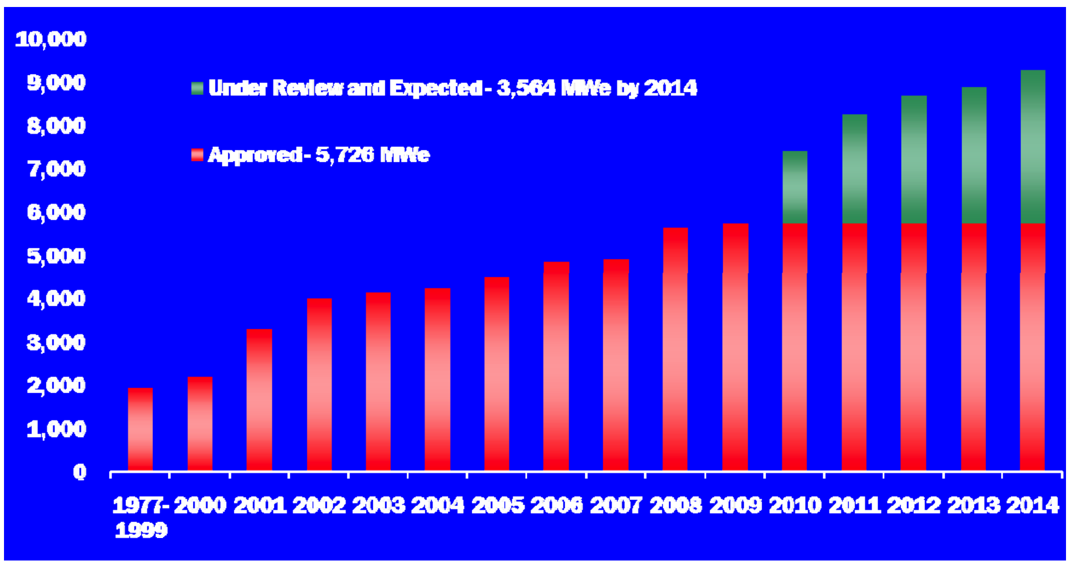
# U.S. Nuclear Energy

## Increasing cumulative capacity delivering at a high capacity factor




U.S. nuclear industry capacity factors, 1971-2009 (percent)

Source: www.nei.org (Energy Information Administration, 5/10)




Cumulative Capacity Additions at U.S. Nuclear Facilities 1977-2014

Source: www.nei.org (Nuclear Regulatory Commission, 6/10)

# There are numerous safety, operating, and design aspects to consider for nuclear reactors

| Safety | Operating | Design |
|---|---|---|
| • DNB safety limit<br>• Reactivity coefficients<br>• Shutdown margin<br>• Enrichment<br>• Internal gas pressure<br>• PCMI<br>• RIA fragmentation<br>• Non-LOCA runaway oxidation<br>• LOCA: PCT, oxidation, H release, long-term cooling<br>• Seismic loads<br>• Holddown force<br>• Criticality | • DNB operating limit<br>• LHGR limit<br>• PCI<br>• Coolant activity<br>• Gap activity<br>• Source term<br>• Control rod drop time<br>• RIA fuel failure limit | • Crud deposition<br>• Stress/strain/fatigue<br>• Oxidation<br>• Hydride concentration<br>• Transport loads<br>• Fretting wear<br>• Clad diameter increase<br>• Cladding elongation<br>• Radial peaking factor<br>• 3D peaking factor<br>• Cladding stability |

Source: *Fuel Safety Criteria in NEA Member Countries,* NEA/CSNI/R(2003)10

# Critical elements for integration of Modeling and Simulation (M&S) into nuclear energy decisions

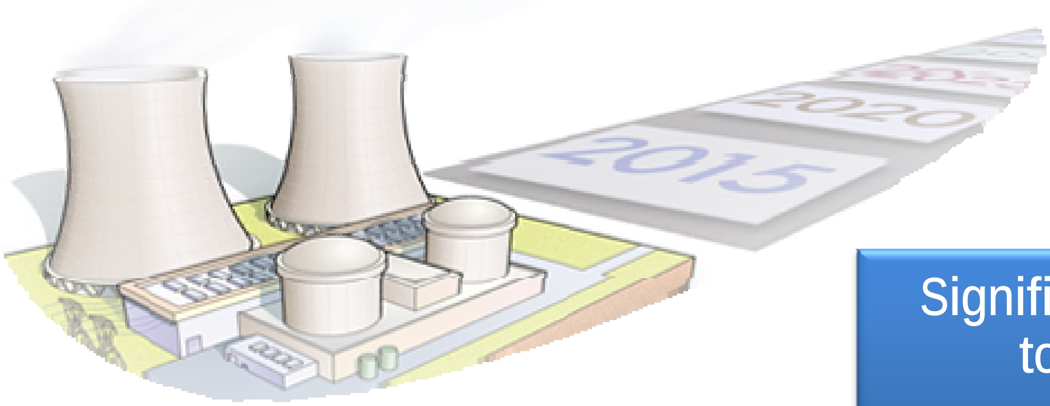
| | |
|---|---|
| Acceptance by user community | • Address real problems in a manner that is more cost-effective than current technology<br>• Meet needs of utility owner-operators, reactor vendors, fuel suppliers, engineering providers, and national laboratories |
| Acceptance by regulatory authority | • Address issues that could impact public safety<br>• Deliver accurate and verifiable results |
| Acceptance of outcomes by public | • Provide outcomes that ensure high levels of plant safety and performance |

**A team pursuing transformational nuclear computational science must have unique capabilities for identifying, understanding, and solving nuclear reactor safety and performance issues**

# Life extension driven by economic decision on ability to continue to operate the plant

Key technical elements for basis of license renewal and life extension:

- Identify and quantify potential “life limiting” issues
- Structures, systems, and components aging and life-cycle management
- Opportunities for modernization and power uprates
- Enabling technology (e.g., analysis methods/simulation capability)




Significant financial decisions to support operation beyond 60 years are expected in 2014–2019

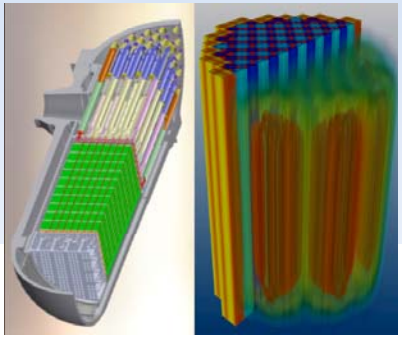
# Can an advanced “Virtual Reactor” be developed and applied to proactively address critical performance goals for nuclear power?

**1** Reduce capital and operating costs per unit energy by:

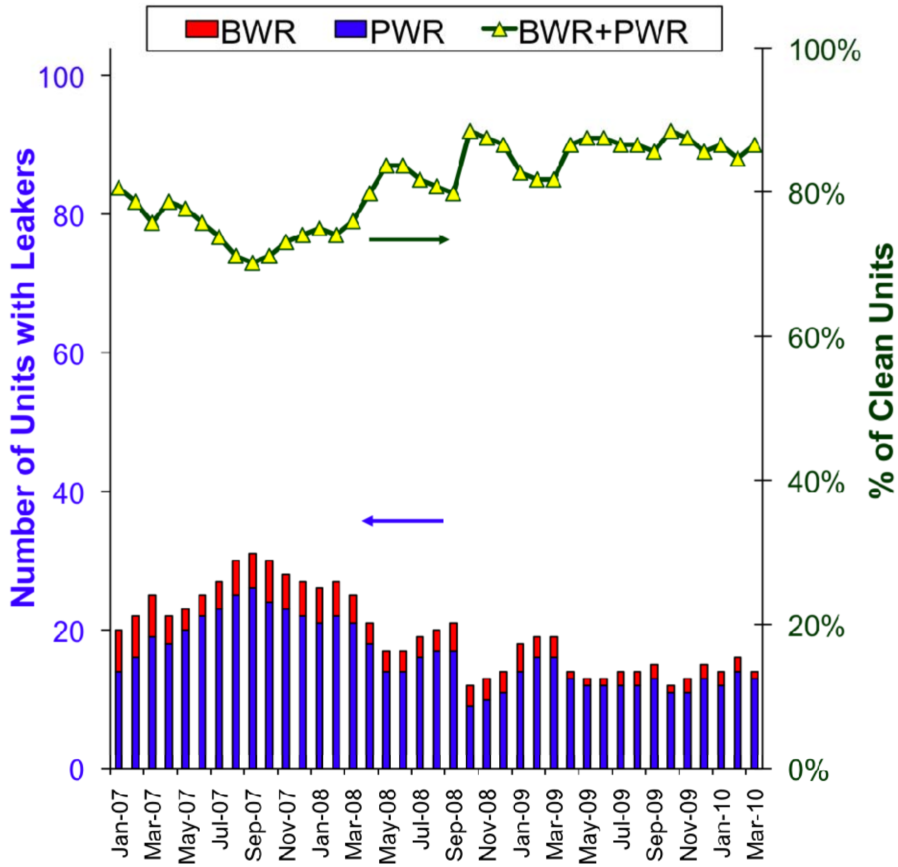
- Power uprates
- Lifetime extension

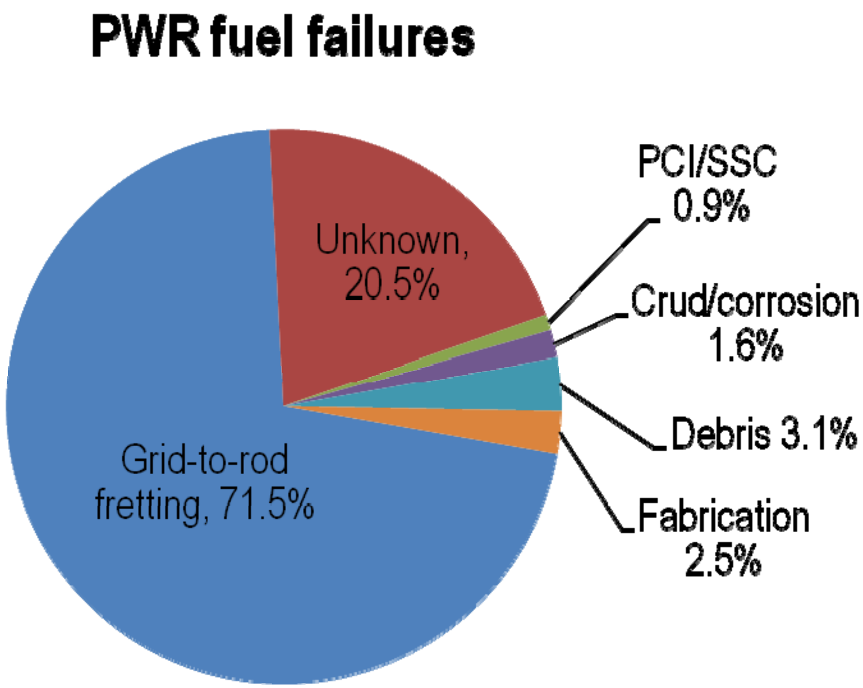
**2** Reduce nuclear waste volume generated by enabling higher fuel burnups

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



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

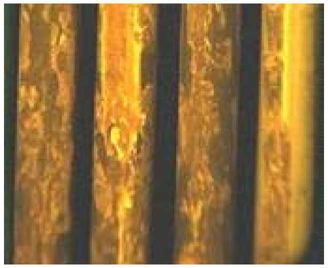


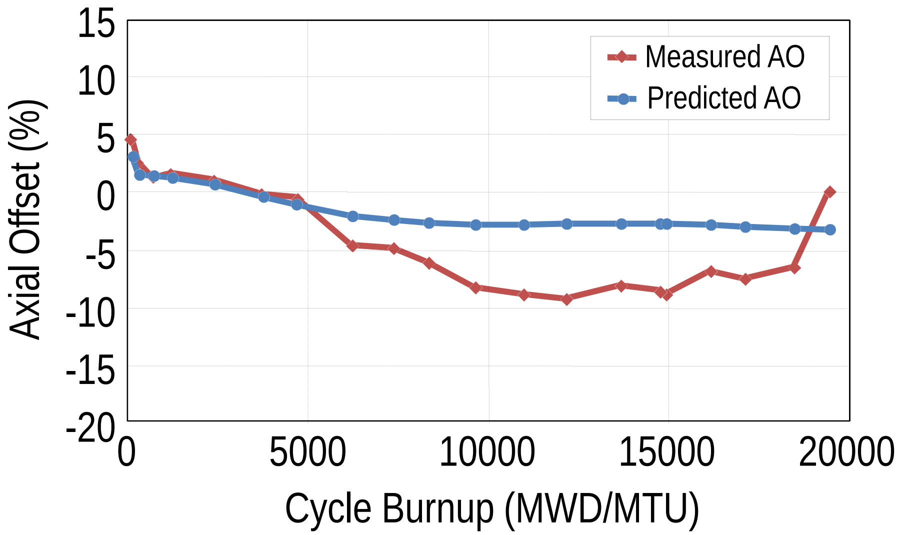

An effective virtual reactor M&S capability will permit proactive evaluation to enable critical performance enhancements

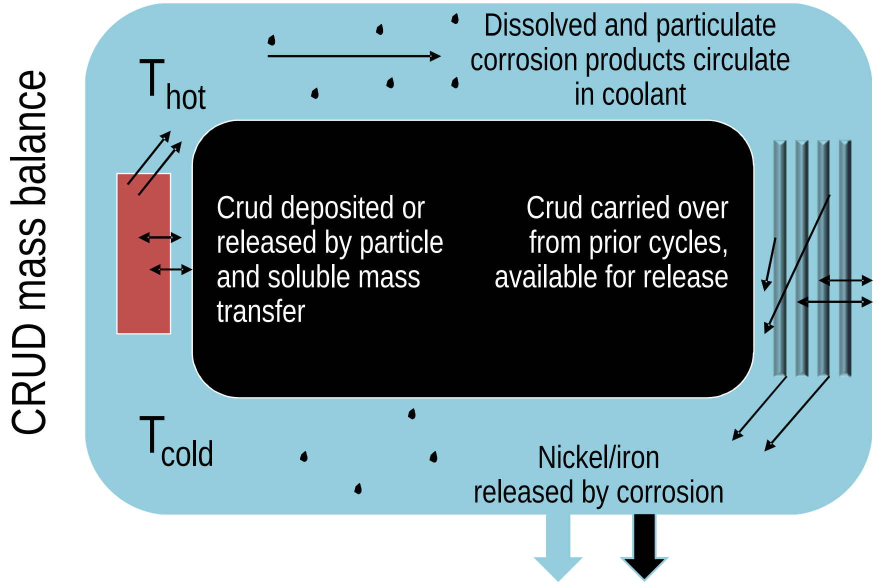
# CRUD-induced power shift (CIPS)

- 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

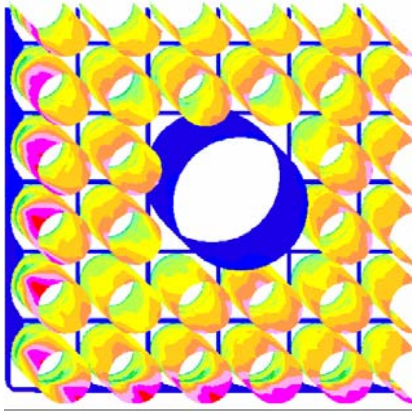


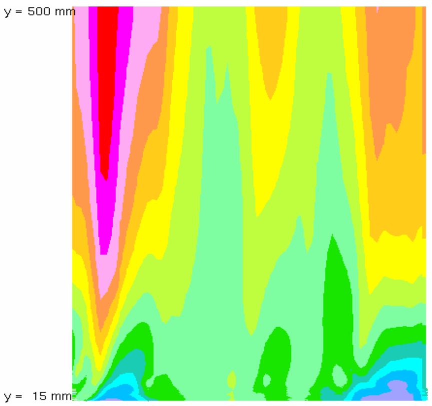



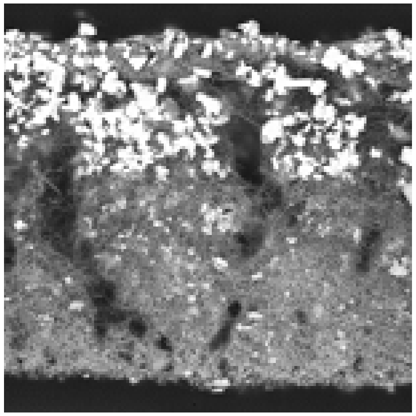

**Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth**

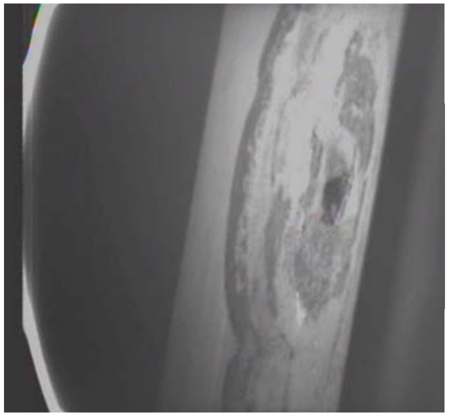
# CRUD-induced localized corrosion (CILC)

- 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





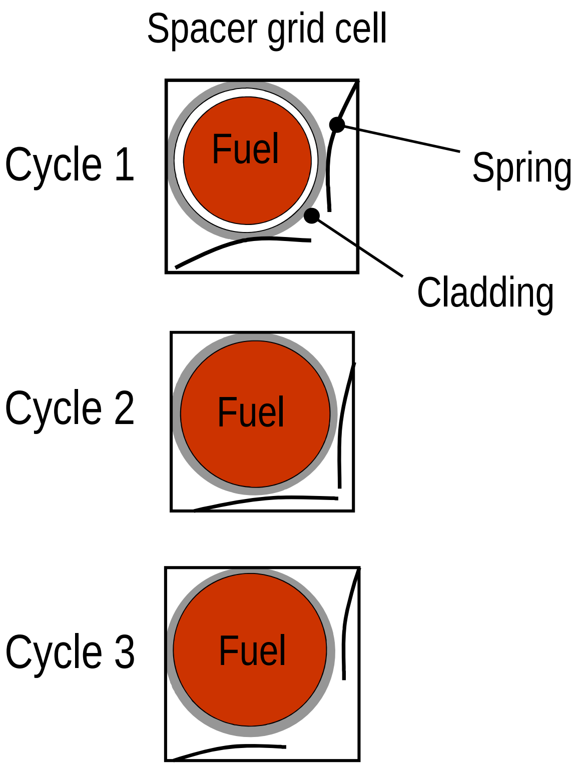





Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

# 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

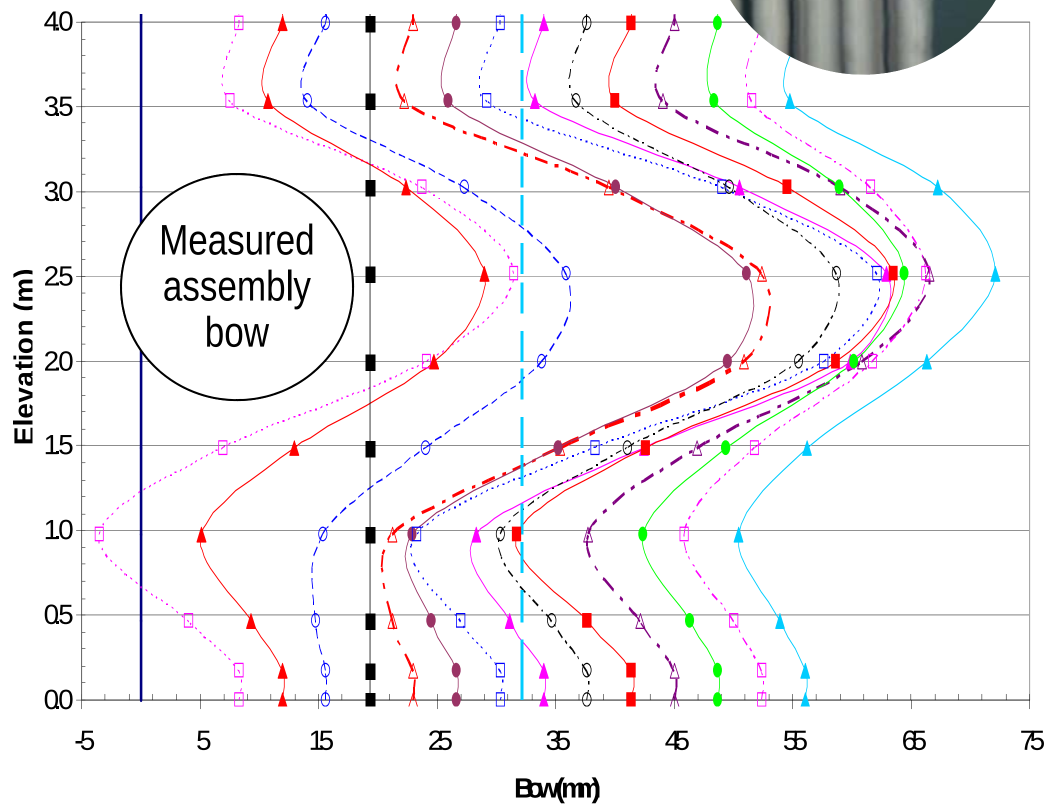


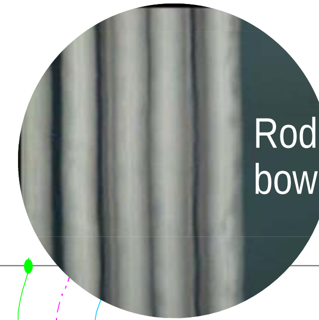

Need: High-fidelity, fluid structural interaction tool
to predict gap, turbulent flow excitation, rod vibration and wear

# 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

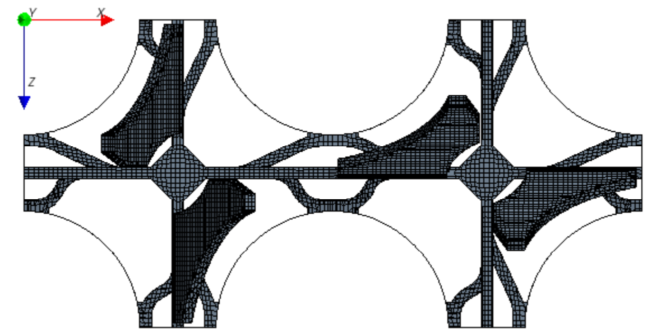
**Need: Tool to predict distortion and impact on power distributions and safety analyses**

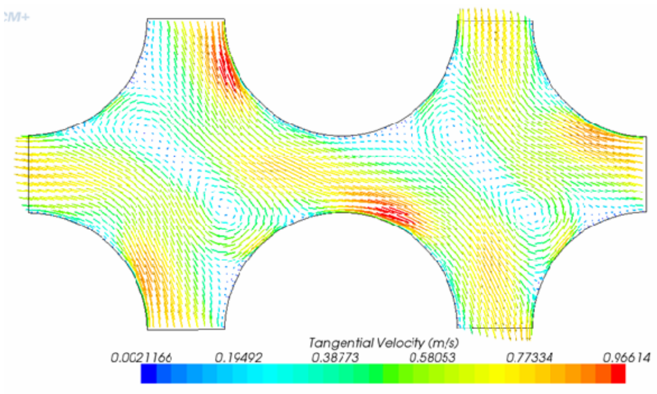


# Departure from nucleate boiling (DNB)

- 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

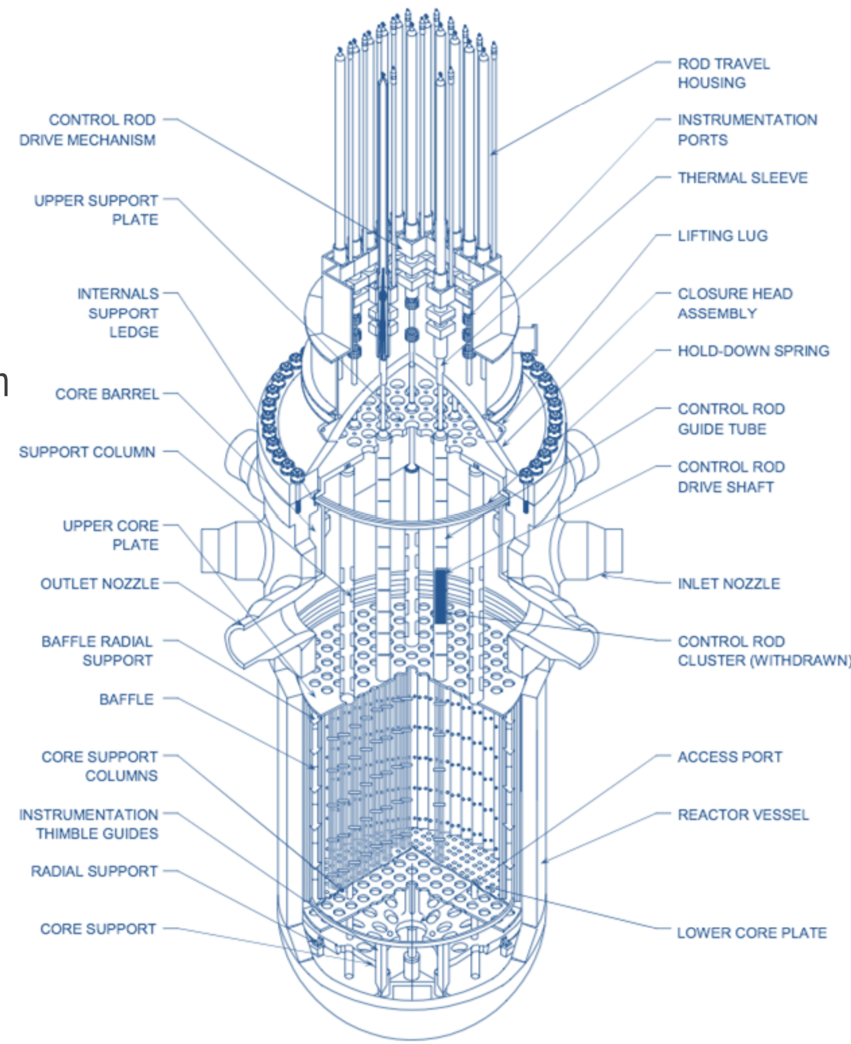





**Need: High-fidelity modeling of complex flow and heat transfer for all pins in core downstream of spacer grids**

# Reactor vessel and internals integrity

- Reactor vessel:
  - Radiation damage results in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses with safety injection system
  - Increased power rating and lifetime both increase radiation damage to the vessel
  - Low leakage loading patterns and proposed revised NRC rule indicate that expected vessel lifetime > 80 years for most PWRs
- Internals:
  - Damage can be caused by thermal fatigue, mechanical fatigue, radiation damage, and SCC
  - Replacement cost of internals is high, making lifetime extension less economically attractive

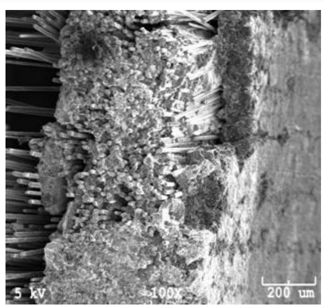



**Need: High-fidelity tool to predict temperatures, stresses, and material performance (fatigue and cracking) over long-term operation**

# New materials and fuel concepts for transformational performance improvement

- SiC cladding
  - Enrichment savings due to lower cross section
  - Uprate capability
  - Insensitive to dryout or DNB (operational capability: >1900°C)
  - Immunity to fretting failure
  - Simplification of safety systems

**Ongoing DOE Project with 5 CASL partners leading: WEC, EPRI, MIT, INL, ORNL**



- UN fuel
  - Higher U-235 loadings than $UO_2$ without increase in U-235 enrichment
  - Much higher thermal conductivity and increased thermal output capability (upratings)
  - Cooler fuel and lower fission gas release
  - Improved accident and transient performance

**Need: New materials models and methods to evaluate performance of advanced fuel designs**

# A Virtual Reactor developed and successfully applied to key challenge problems benefits the nuclear industry

| Challenge Problem | Description | Relevance |
|---|---|---|
| CRUD | CIPS: Deviation in axial power shape caused by CRUD deposition in high power density regions with subcooled boiling. CILC: Clad corrosion and failure due to CRUD deposition | Power uprates yield higher power density and an increased potential for CRUD growth, axial power offsets, and clad failures |
| GTRF | Clad failure due to flow vibration-induced rod-spring interactions amplified by irradiation-induced grid spacer growth and spring relaxation | Power uprates and burnup increase potential for fretting failures, the leading cause of fuel failures in PWRs |
| Internals Lifetime (LE) | Damage to internals packages caused by thermal fatigue, mechanical fatigue, radiation damage, and stress corrosion cracking. | Replacement cost of internals is high, making lifetime extension less economically attractive |
| DNB (Safety) | Local clad surface dryout causing dramatic reduction in heat transfer capability during certain accident transients (e.g., overpower and low coolant flow) | Power uprates require improved quantification of margins for DNB limits |
| FAD | Distortion or component structural failure due to excessive axial forces caused by radiation-induced swelling | Power uprates and increased burnups may increase fuel distortions and alter core power distributions and fuel handling scenarios |
| Advanced Fuel Forms (AF, Safety, GTRF) | Examination of new cladding material, fuel material, and fuel pin geometries. | New fuel forms will enable power uprates, higher fuel burnups, and lower fuel cycle costs than can be achieved by incremental modifications of current fuel forms, i.e., zirconium alloy cladding, $UO_2$ fuel pellet, and cylindrical geometry |

# A Virtual Reactor developed and successfully applied to key challenge problems benefits the nuclear industry

| Challenge Problem | Description | Relevance |
|---|---|---|
| LOCA (Safety) | Numerous fuel failure modes resulting in fission product release and coolable geometry degradation | Realistic LOCA analyses (10 CFR 50.46) can enable power uprates that would not have been achievable with previously licensed evaluation models |
| RIA (Safety) | Clad failure due to rapid heating of the pellet, leading to pellet disintegration caused by the rim effect | Higher fuel burnup increases rim effect; power uprates may lead to increased energy during RIA. Currently not limiting but may change with further test data (e.g., CABRI) |
| PCI (Safety, AF) | Clad failure due to radiation-induced fuel rod/cladding contact from stress corrosion cracking and fuel defects | Power uprates and increased burnups increase fuel/clad contact and the likelihood for fuel failures. Currently only limits power ramp rates during normal operation, which are infrequent |
| Reactor Vessel Lifetime (LE) | Radiation damage resulting in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses with Safety Injection System (SIS). | Increased power rating and lifetime both increase radiation damage to the vessel. Low leakage loading patterns and proposed revised NRC rule indicate that expected vessel lifetime exceeds 80 years for most PWRs |

# CASL has selected key phenomena limiting reactor performance selected for challenge problems

| | Power uprate | High burnup | Life extension |
|---|---|---|---|
| Operational | | | |
| 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 | | | |
| 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 | × | | × |

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

## Leverage

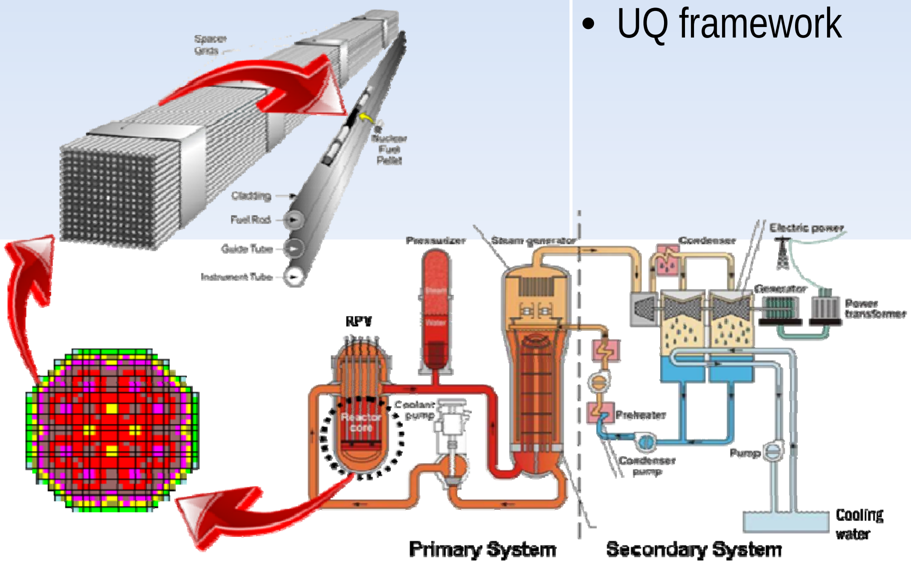
- Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications
- Existing systems and safety analysis simulation tools

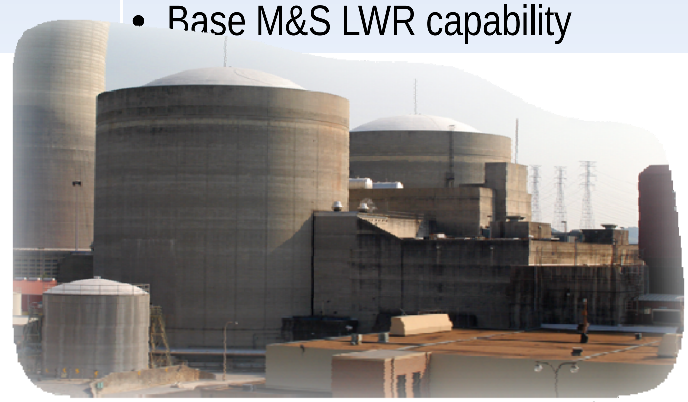
## Develop

- 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

## Deliver

- 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 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
Brian Wirth, Deputy

**MNM**
**Models and Numerical Methods**
Bill Martin, Lead
Rob Lowrie, Deputy

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

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

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

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

**MNM**
- Radiation transport
- Thermal hydraulics

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

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

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

18 integrated and interdependent projects

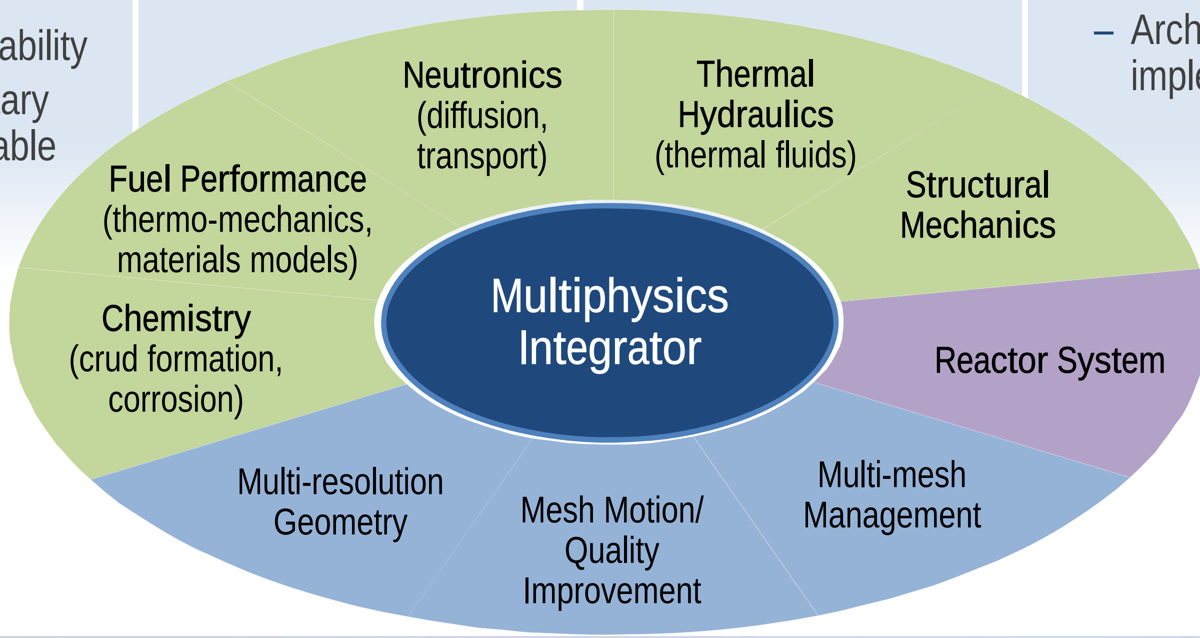
# The CASL Virtual Reactor:
# A code system for scalable simulation of nuclear reactor core behavior

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

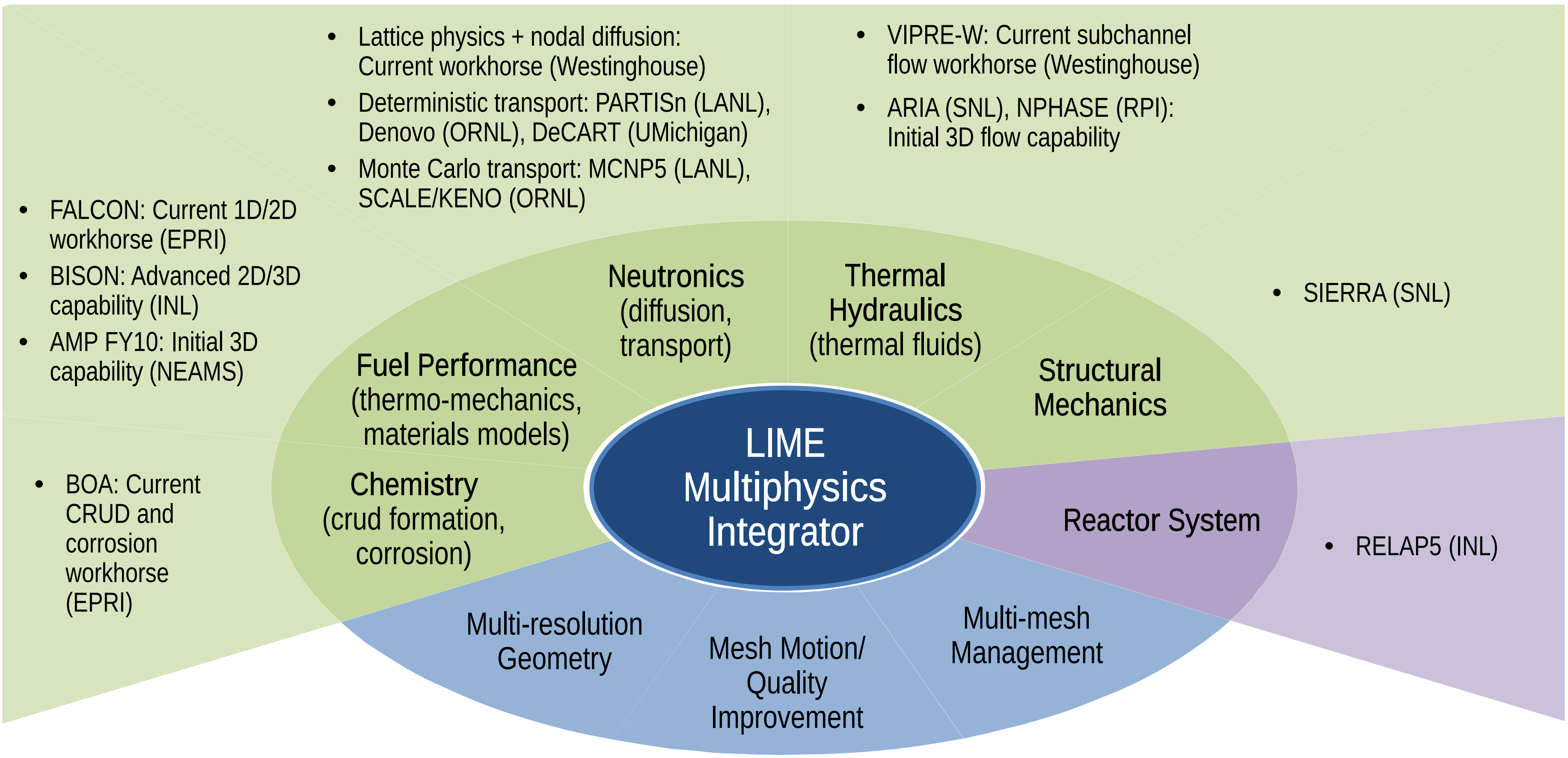
- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

- 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



# The CASL VR builds on a foundation of mature, validated, and widely used software




- CASL developers have delivered code for production (not just research)
  - ORNL and LANL codes account for almost 80% of RSICC distributions since 2005

# VR development is driven by requirements of annual L1 milestones

| CRUD, GTRF | CRUD, GTRF | CRUD, GTRF, Safety, OR | CRUD, GTRF, LE | CRUD, GTRF, LE, Safety, OR, AF |
|---|---|---|---|---|
| Initial core simulation using coupled tools and models | Detailed phenomena modeling in fully coupled VR | Assembly simulation with rod fretting and upscaled material models | Initial predictive reactor modeling in coupled VR | Predictive reactor simulation coupled to physical plant |

FY10 → FY11 → FY12 → FY13 → FY14 → FY15

# Capabilities are developed and integrated collaboratively with Focus Areas and external projects

| CRUD, GTRF | CRUD, GTRF | CRUD, GTRF, Safety, OR | CRUD, GTRF, LE | CRUD, GTRF, LE, Safety, OR, AF |
|---|---|---|---|---|
| • Improved coupling of existing tools | • Chemistry: BOA<br>• Initial sub-cooled boiling model<br>• Transient single-phase CFD | • Improved chemistry<br>• Initial FSI<br>• Transient multiphase CFD<br>• Pin-resolved transport | • Coupled transport, flow, chemistry<br>• Materials damage models<br>• Tightly-coupled FSI<br>• Initial hybrid transport | • Improved materials and chemistry models<br>• Hybrid transport<br>• Improved coupling<br>• Performance, scalability |

FY10 FY11 FY12 FY13 FY14 FY15

# VR development cycle is planned around major releases for L1 simulations

**CRUD, GTRF**
- Improved coupling of existing tools

**CRUD, GTRF**
- Chemistry: BOA
- Initial sub-cooled boiling model
- Transient single-phase CFD

**CRUD, GTRF, Safety, OR**
- Improved chemistry
- Initial FSI
- Transient multiphase CFD
- Pin-resolved transport

**CRUD, GTRF, LE**
- Coupled transport, flow, chemistry
- Materials damage models
- Tightly-coupled FSI
- Initial hybrid transport

**CRUD, GTRF, LE, Safety, OR, AF**
- Improved materials and chemistry models
- Hybrid transport
- Improved coupling
- Performance, scalability

FY10 FY11 FY12 FY13 FY14 FY15

**Q4**
- Requirements
- New feature development

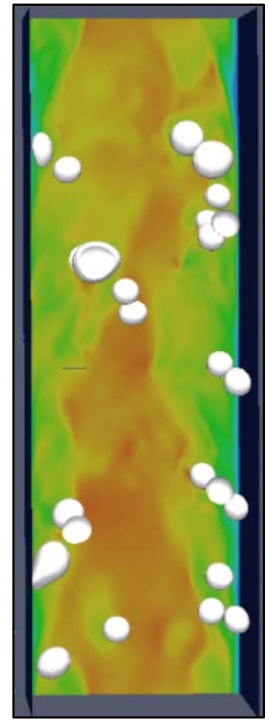
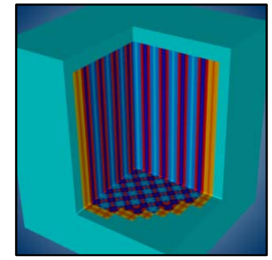
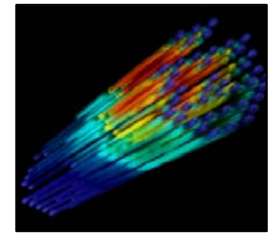
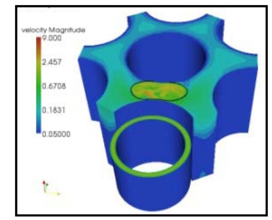
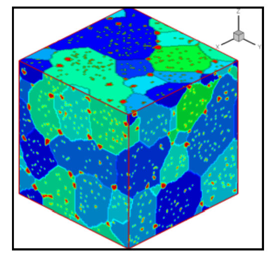
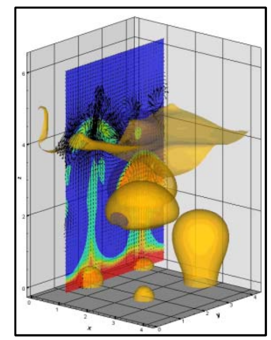
**Q1**
- Integration
- Performance

**Q2**
- Feature-frozen beta release
- AMA begins L1 scoping

**Q3**
- Major release for L1 simulations and assessment

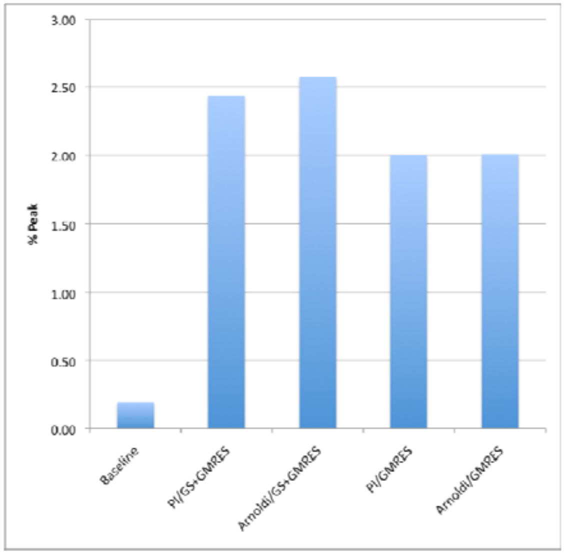
# The CASL VR has a mature starting point

- Building on existing capability to deliver versatile tools
  - Initial focus on PWRs
  - Extensible to other reactor types
- Implemented as a component-based architecture integrating current and legacy workflows and capabilities
  - **Includes tools used to design and license the U.S. PWR fleet**
- An evolving state-of-the-art software design and ecosystem
  - Designed to exploit advanced computing platforms
  - Full coupling of all relevant physical processes
  - Integrated high-fidelity CFD, transport, and mechanics incorporated into the workflows of designers
  - Advanced methods for understanding sensitivities and propagating uncertainties

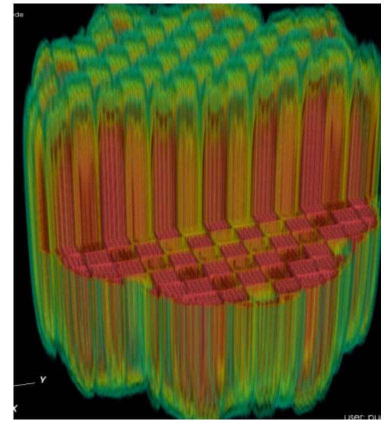







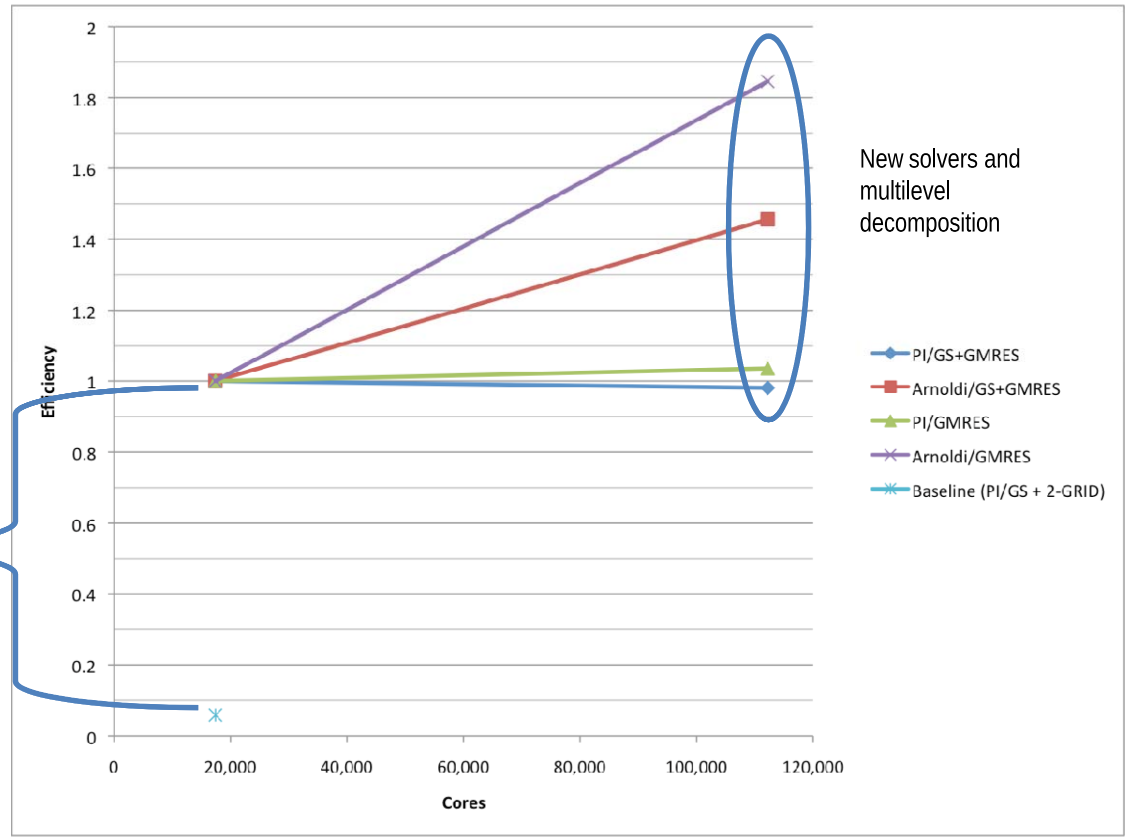
# Denovo HPC Transport

# Denovo Parallel Performance




Factor of 10x increase in peak efficiency gained through Joule project + ASCR OLCF-3 project work






Optimizations made during first part of 2010 Joule project (sweep-ordering)

# CASL Challenge Problems Possess Uncertainties

## That can be reduced via model improvements & leadership-class systems

| Challenge Problem | Uncertainty | Principal Source of Improvement |
|---|---|---|
| CRUD | Crud concentration, deposition, thickness<br>Boron uptake and its affect on rod power<br>Crud dryout, clad temp rise, corrosion | High-fidelity CFD, turbulent heat transfer, corrosion chem<br>Coupled CFD & neutronics<br>New models: fundamental R&D and validation data |
| GTRF | Rod excitation force, natural frequency<br>Rod fatigue vibration and wear | High-resolution CFD-structure interaction & coupling<br>Grid/clad interaction, fatigue, stress building, cracking |
| PCI (Pellet Clad Interaction) | Pellet / clad stresses and cracking | High-fidelity coupled CFD / neutronics / fuel performance |
| DNB (Safety) | Location of hot channel | Minimum DNB prediction: coupled CFD / neutronics |
| FAD | Fuel assembly bow | High-resolution coupled CFD / structure / neutronics for vs fluence & power history |

# The Predictive Capability Maturity Model (PCMM) will be used to measure the progress of VR development

- Developed for modeling and simulation efforts based on similar assessment models for other areas such as NASA's Technical Readiness Levels and Carnegie Mellon's Capability Maturity Model
- Measures process maturity by objectively assessing technical elements

| Technical elements |
|---|
| • Representation and geometric fidelity<br>• Physics and material model fidelity<br>• Code verification<br>• Solution verification<br>• Model validation<br>• Uncertainty quantification and sensitivity analysis |

| Maturity level | Assessment of completeness / characterization | Evidence of maturity |
|---|---|---|
| Level 0 | Little or no assessment | Individual judgment and experience |
| Level 1 | Informal assessment | Some evidence of maturity |
| Level 2 | Some formal assessment, some internal peer review | Significant evidence of maturity |
| Level 3 | Formal assessment, essentially all by independent peer review | Detailed and complete evidence of maturity |

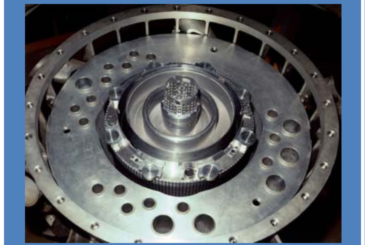
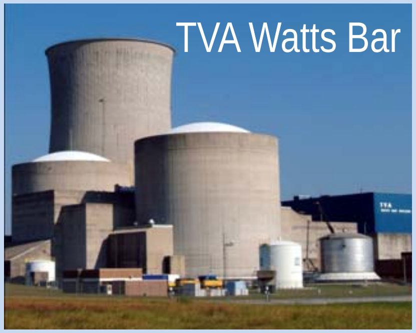
**We will annually assess the CASL VR against challenge problems**

# In-core Nuclear Reactor Computational Requirements

- Neutronics (steady state)
  - Assembly (lattice), full core, vessel
- Thermal hydraulics (steady state and transient)
  - Assembly (subchannel / multiphase, CFD / single & multiphase)
  - Full core (subchannel / single & multiphase, CFD / single & multiphase)
  - Vessel (CFD / single & multiphase)
- Coupled neutronics and thermal hydraulics (steady state)
- Coupled thermal hydraulics and mechanics
- Coupled neutronics, thermal hydraulics, mechanics
- Add detailed fuel performance to all the above

Beyond exascale is needed to regularly perform full core, coupled simulations
We are in the process of quantifying these requirements

# CASL possesses the 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<br>• 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<br>• Leverage EPRI's structured technology transfer approach |
| Validation<br><br>ORNL HFIR | • One entire focus area dedicated to validation and UQ<br>• Extensive reactor design information and test and operational data<br>• 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<br><br>TVA Watts Bar<br><br>Westinghouse CRUD Facility |
| Virtual Office, Community, and Computing (VOCC) | • Integration and application of latest and emerging technologies to build an extended "virtual one roof" |

# Questions?

www.casl.gov or info@casl.gov