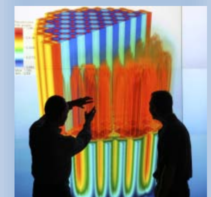
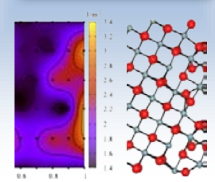




CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

John A. Turner

Virtual Reactor Integration Focus Area Lead, CASL
Group Leader, Computational Engineering & Energy Sciences
Computer Science & Mathematics Division
Oak Ridge National Laboratory

Presentation to the
37th HPC User Forum
Seattle, WA
14 September 2010

Consortium for Advanced Simulation of LWRs

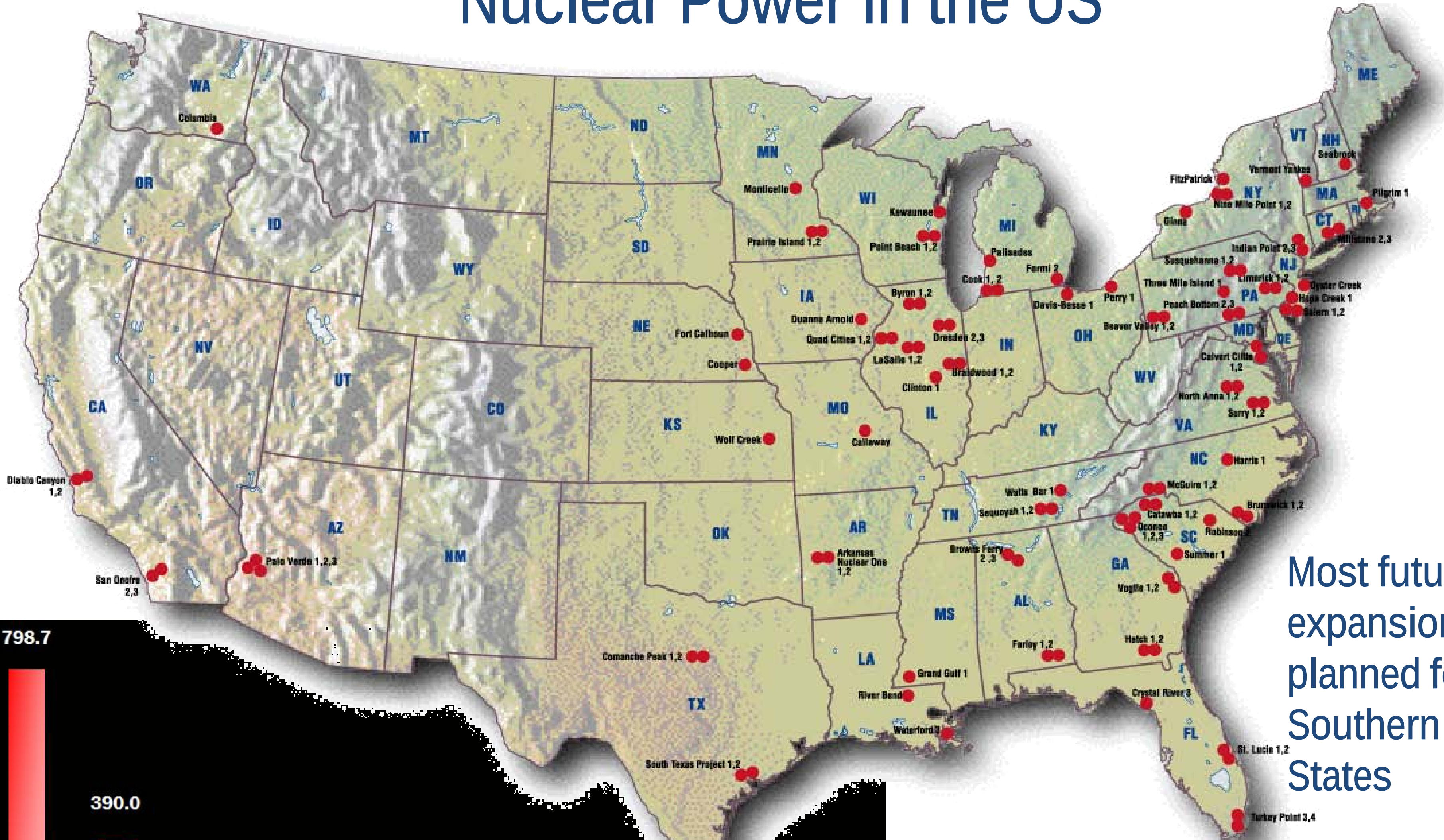
U.S. DEPARTMENT OF ENERGY | Nuclear Energy

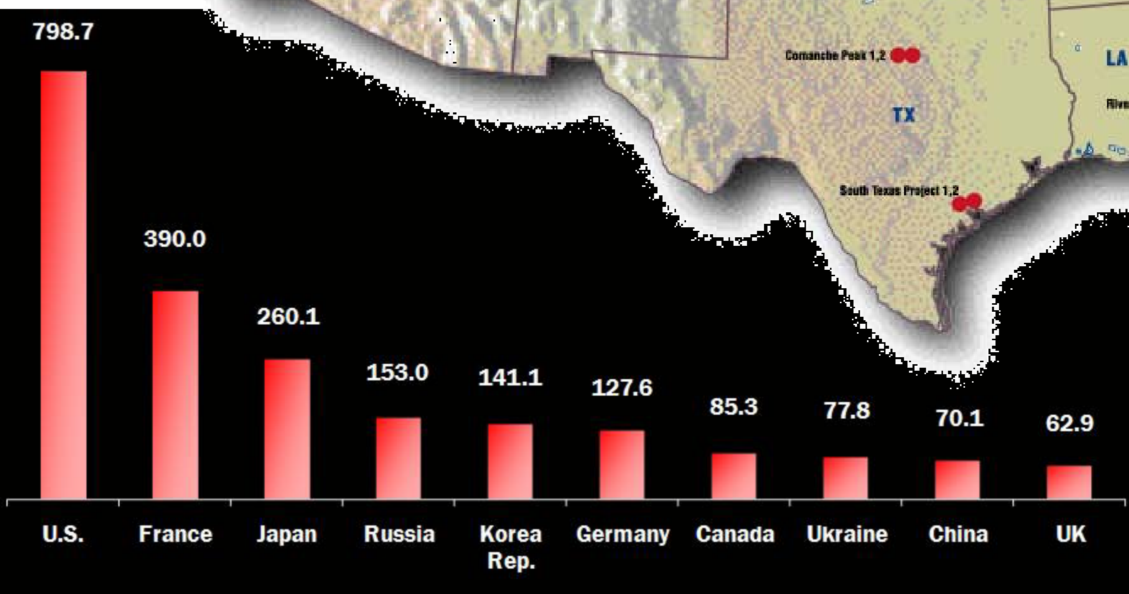
Oak Ridge National Laboratory

Outline

- Nuclear energy in the U.S.
- Light Water Reactor (LWR) operational challenges
- DOE Energy Innovation Hubs (EIH)
  - EIH for Modeling and Simulation of Nuclear Reactors
- The Consortium for Advanced Simulation of LWRs (CASL)
  - Vision, Scope, Organization, Plans, Challenges

Nuclear Power in the US

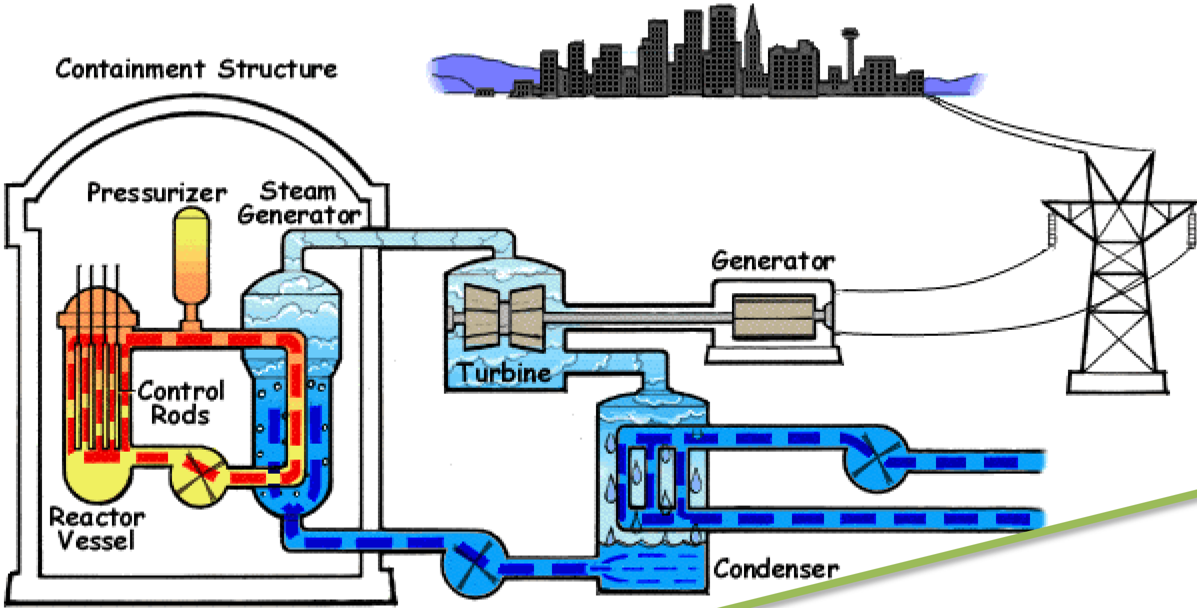




Most future expansion planned for Southern States

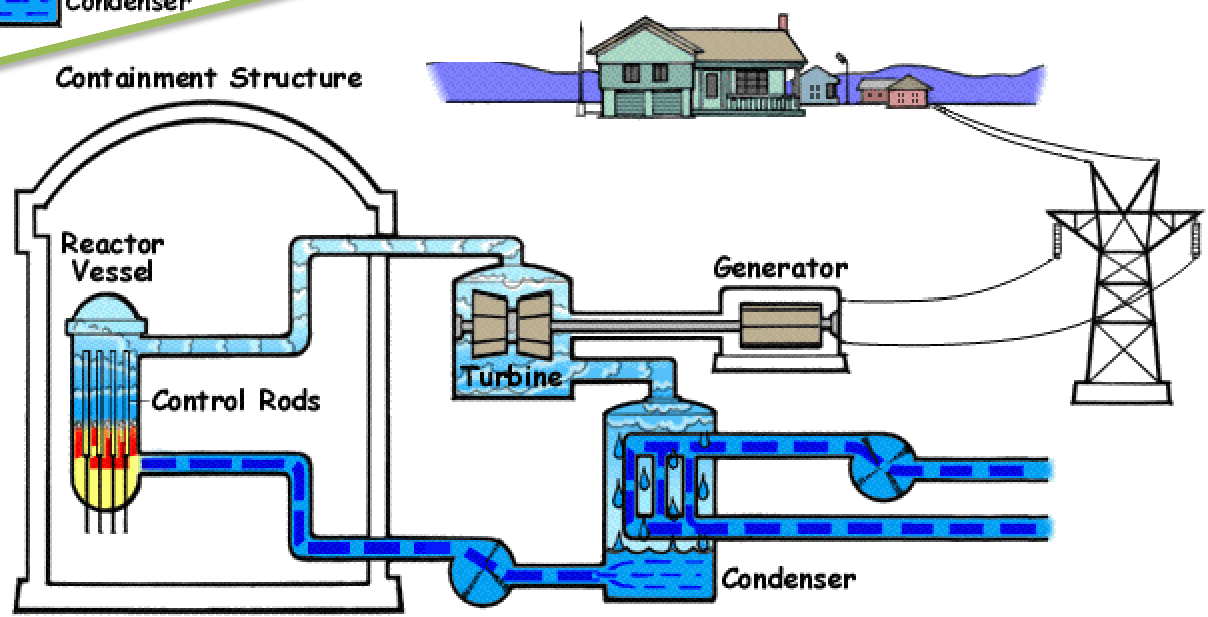
Top 10 Nuclear Generating Countries
2009, Billion kWh
Source: www.nei.org (International Atomic Energy Agency, 5/10)

Common types of Light Water Reactors (LWRs)



Pressurized Water Reactor (PWR)

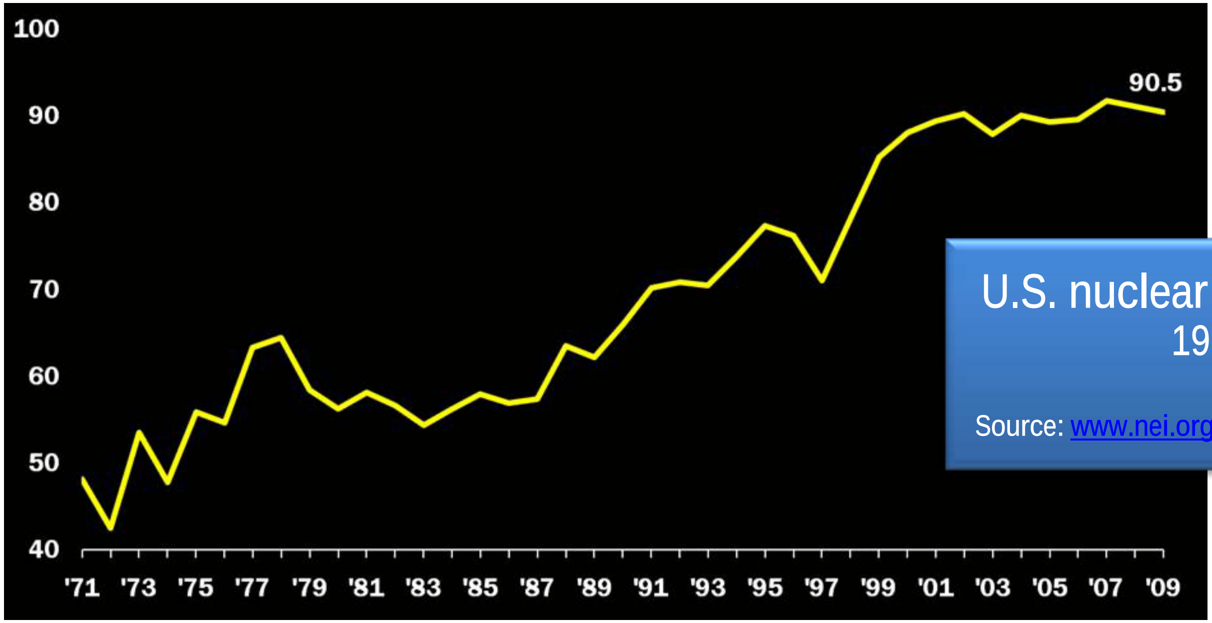
Boiling Water Reactor (BWR)



http://www.nrc.gov/reading-rm/basic-ref/students/animated-pwr.html
http://www.nrc.gov/reading-rm/basic-ref/students/animated-bwr.html

U.S. Nuclear Energy

Increasing cumulative capacity delivering at a high capacity factor

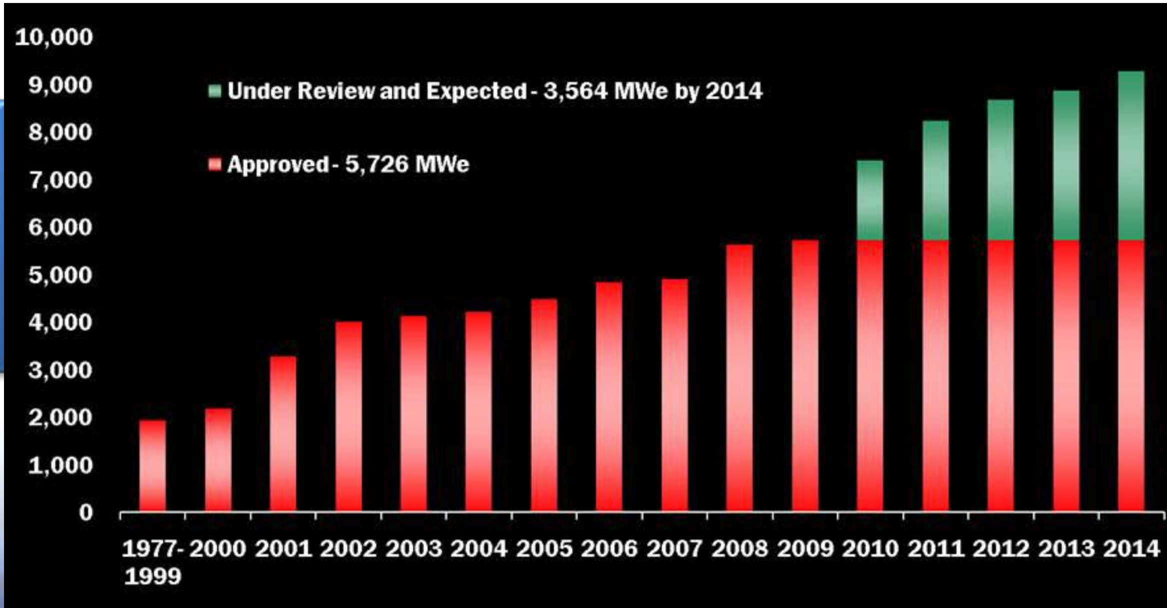


U.S. nuclear industry capacity factors
1971-2009 (percent)

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

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:

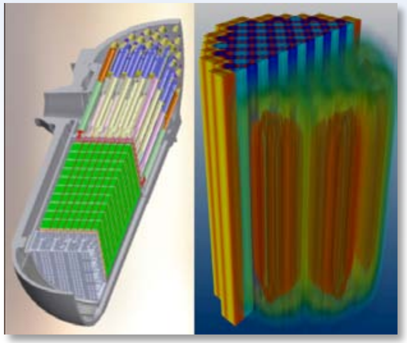
- Power uprates
- Lifetime extension

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



Each reactor performance improvement goal brings benefits and concerns

Power uprates

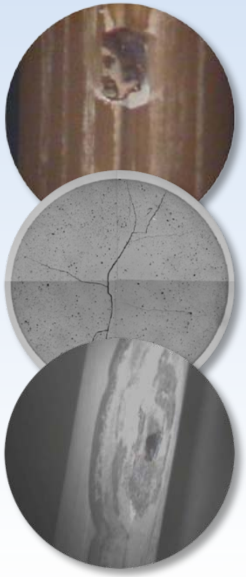
- 5–7 GWe delivered at ~20% of new reactor cost
- Advances in M&S needed to enable further uprates (up to 20 GWe)
- Key concerns:
  - Damage to structures, systems, and components (SSC)
  - Fuel and steam generator integrity
  - Violation of safety limits

Lifetime extension

- 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)

Higher burnup

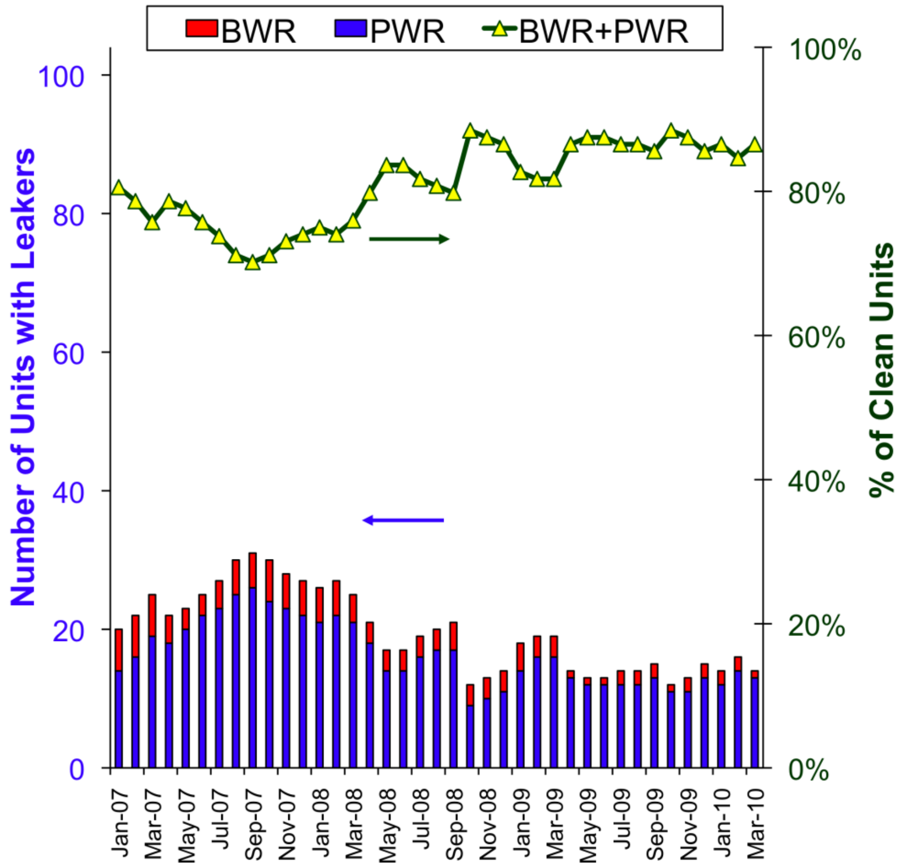
- Supports reduction in amount of used nuclear fuel
- Supports uprates by avoiding need for additional fuel
- Key concerns:
  - Cladding integrity
  - Fretting
  - Corrosion/ CRUD
  - Hydriding
  - Creep
  - Fuel-cladding mechanical interactions

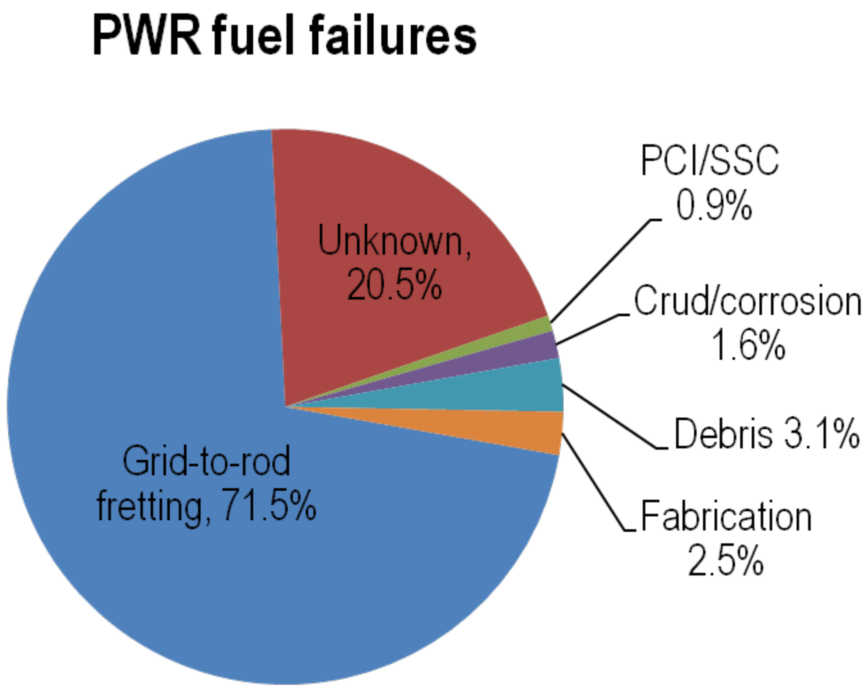


Key phenomena limiting reactor performance can be categorized and prioritized.

	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	×		×

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





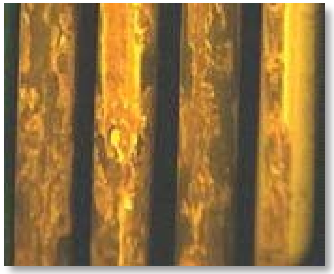
An effective virtual reactor M&S capability will permit proactive evaluation to enable critical performance enhancements

CASL

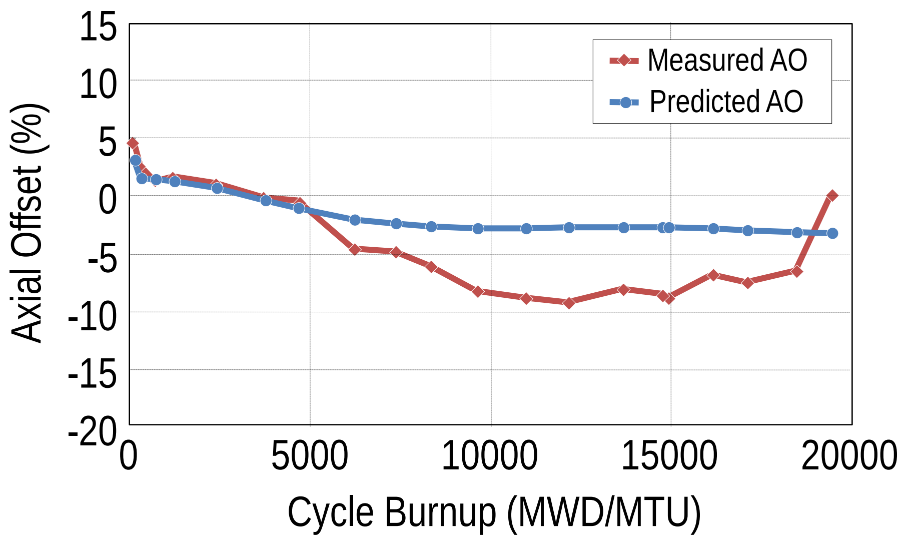
Oak Ridge National Laboratory

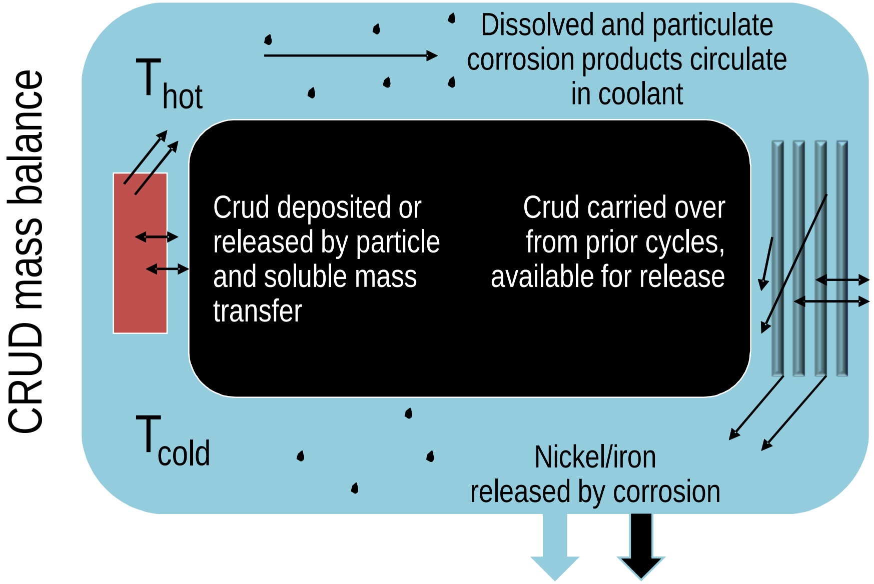
CRUD-induced power shift (CIPS)

- 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

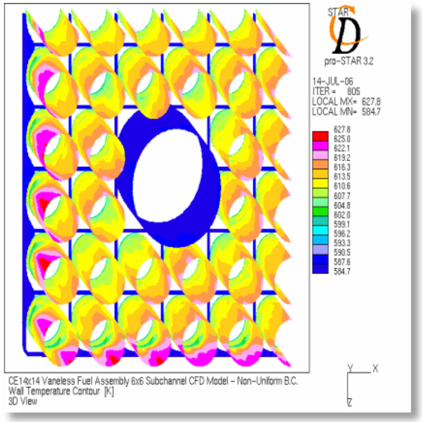


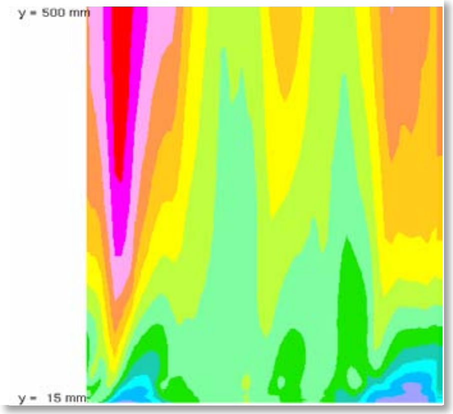


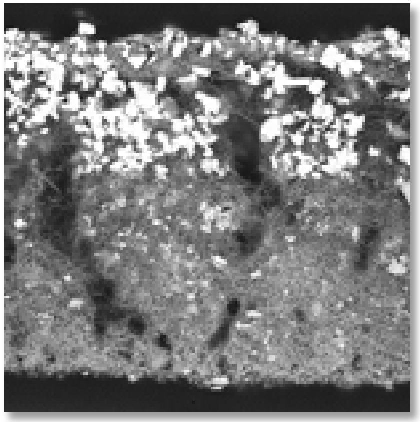
Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth

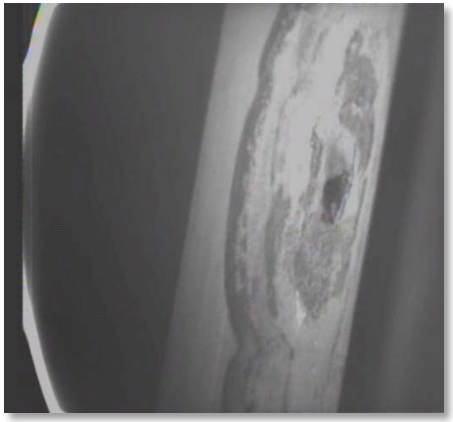
CRUD-induced localized corrosion (CILC)

- 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





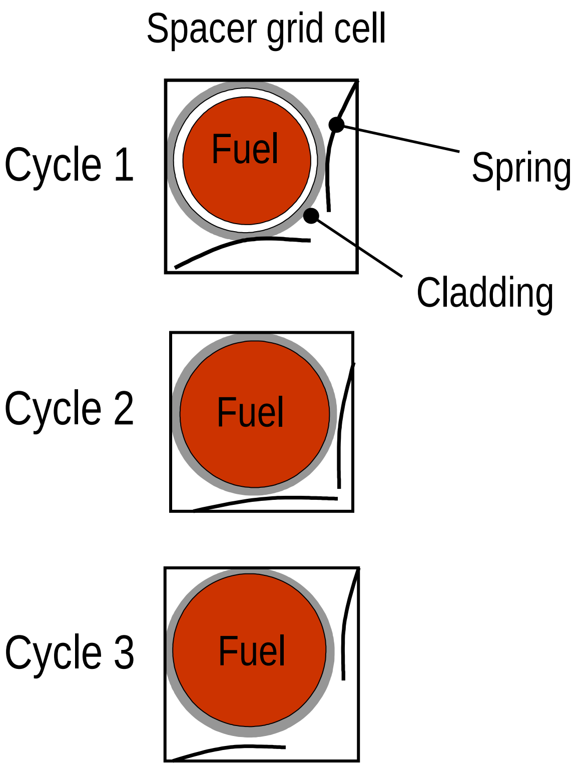




Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

Grid-to-rod fretting failure (GTRF)

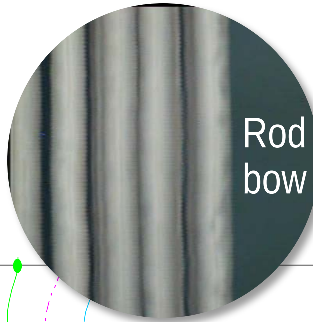
- Clad failure can occur as the result of rod-spring interactions
  - Induced by flow vibration
  - Amplified by irradiation-induced grid spacer growth and spring relaxation
- Power uprates and burnup increase potential for fretting failures
  - Leading cause of fuel failures in PWRs

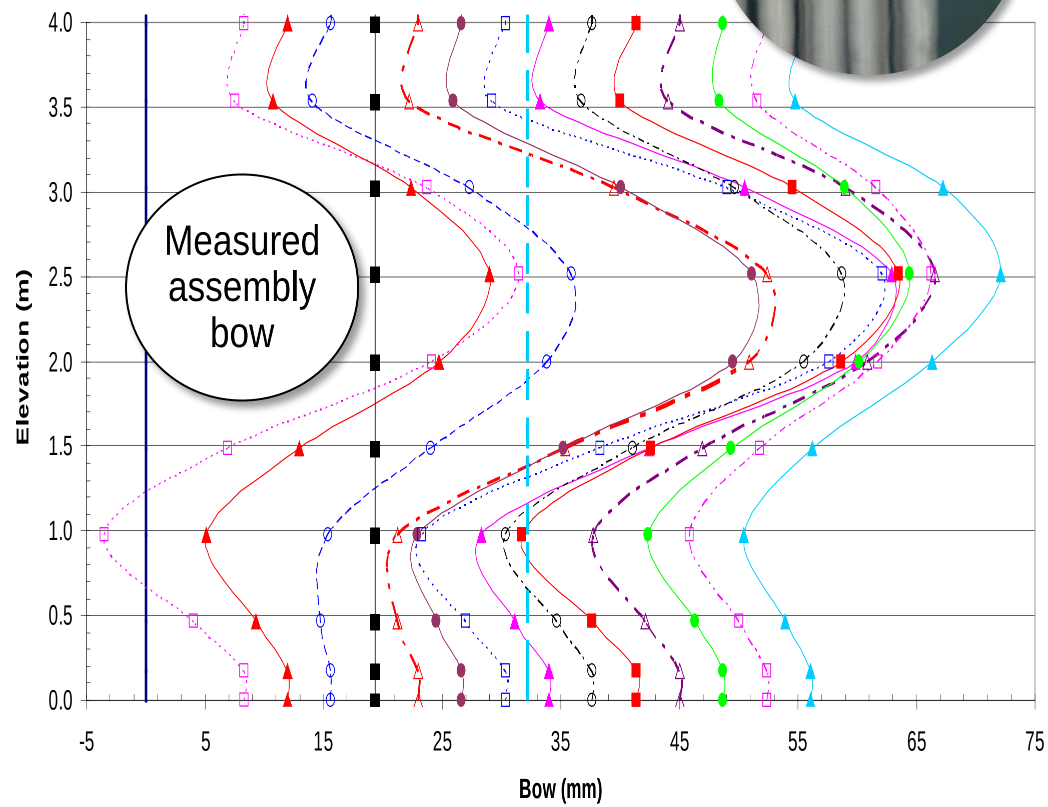


Need: High-fidelity, fluid structural interaction tool to predict gap, turbulent flow excitation, rod vibration and wear

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

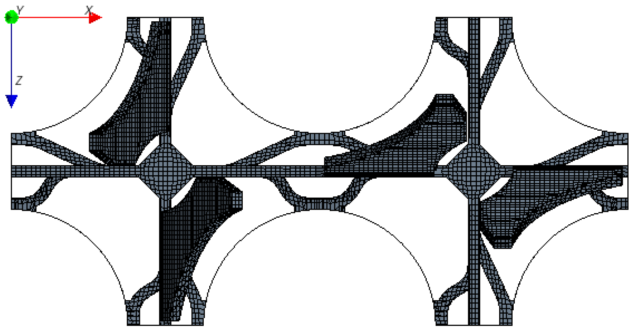


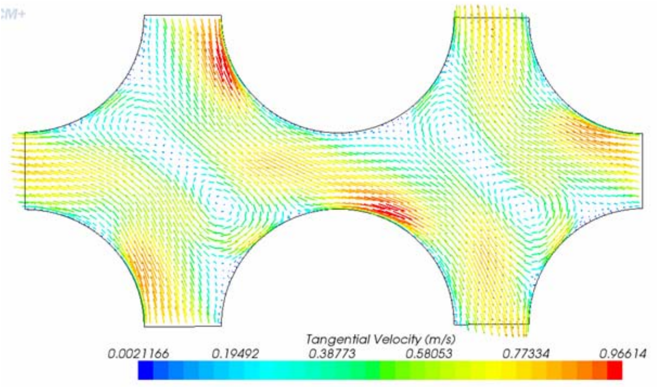


Need: Tool to predict distortion and impact on power distributions and safety analyses

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

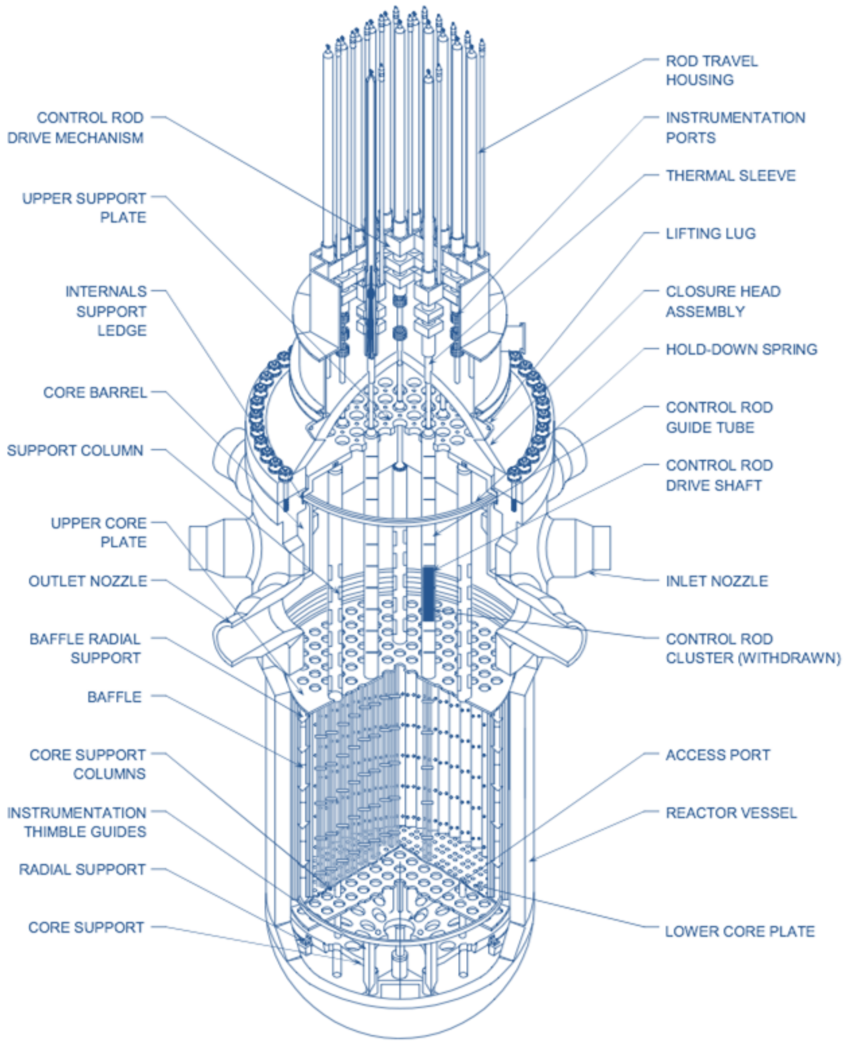




Need: High-fidelity modeling of complex flow and heat transfer for all pins in core downstream of spacer grids

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

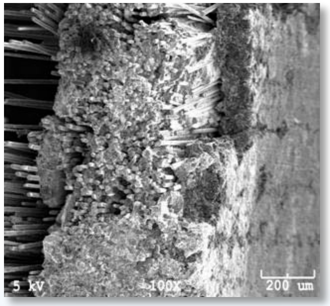


Need: High-fidelity tool to predict temperatures, stresses, and material performance (fatigue and cracking) over long-term operation

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

What is a DOE Energy Innovation Hub?

- modeled after research entities likes the Manhattan Project (nuclear weapons), Lincoln Lab at MIT (radar), and AT&T Bell Labs (transistor)
  - highly-integrated and collaborative teams working to solve priority technology challenges
  - focus on a single topic, and span the spectrum from basic research through engineering development to partnering with industry in commercialization
  - bring together expertise across the R&D enterprise (gov, academia, industry, non-profits) to become a world-leading center in its topical area
- target problems in areas presenting the most critical barriers to achieving national climate and energy goals
  - problems that have proven the most resistant to solution via the normal R&D enterprise
- 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

DOE Energy Innovation Hub for NE M&S Timeline

- 04/06/2009: Secretary Chu proposes 8 Energy Innovation Hubs
  - “mini-Bell Labs” focused on tough problems relevant to energy
  - $25M per yr for 5 years, with possible 5-yr extension
- 06/25/2009: House bill does not approve any of the 8 proposed Hubs
  - provides $35M in Basic Energy Sciences for the Secretary to select one Hub
- 07/09/2009: Senate approves 3 of the 8 proposed hubs, but at $22M
  - Fuels from sunlight (in EERE)
  - Energy efficient building systems (in EERE)
  - Modeling and simulation (in NE)
- 07/22/2009: Johnson memo providing more detail on Hubs
- 10/01/2009: Final bill out of conference matches Senate bill
- 12/07/2009: Informational workshop
- 01/20/2010: FOA released
- 03/08/2010: proposals due (originally 3/1/10)
- 04/23/2010: CASL site visit at ORNL
- 05/27/2010: CASL selected

The Consortium for Advanced Simulation of Light Water Reactors (CASL)

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

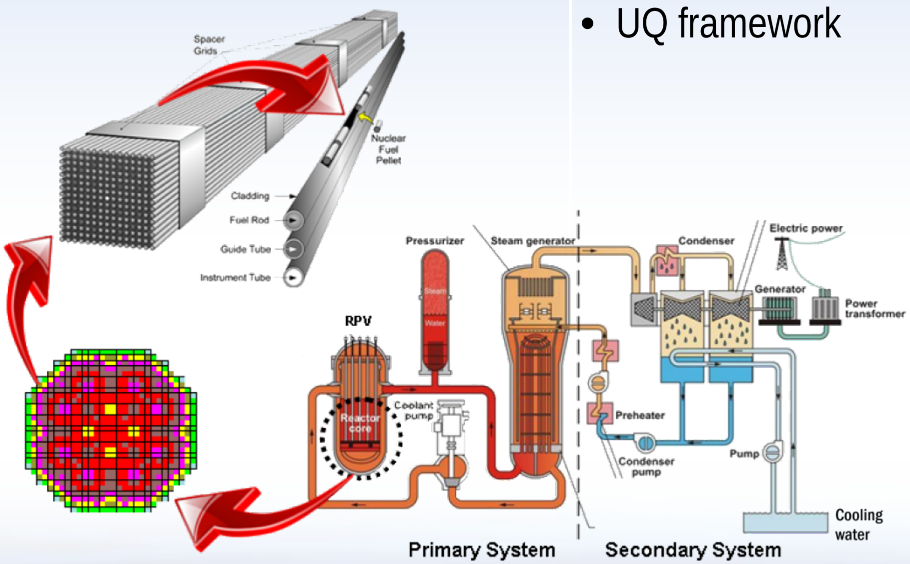
University of Tennessee

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

Oak Ridge National Laboratory

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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)
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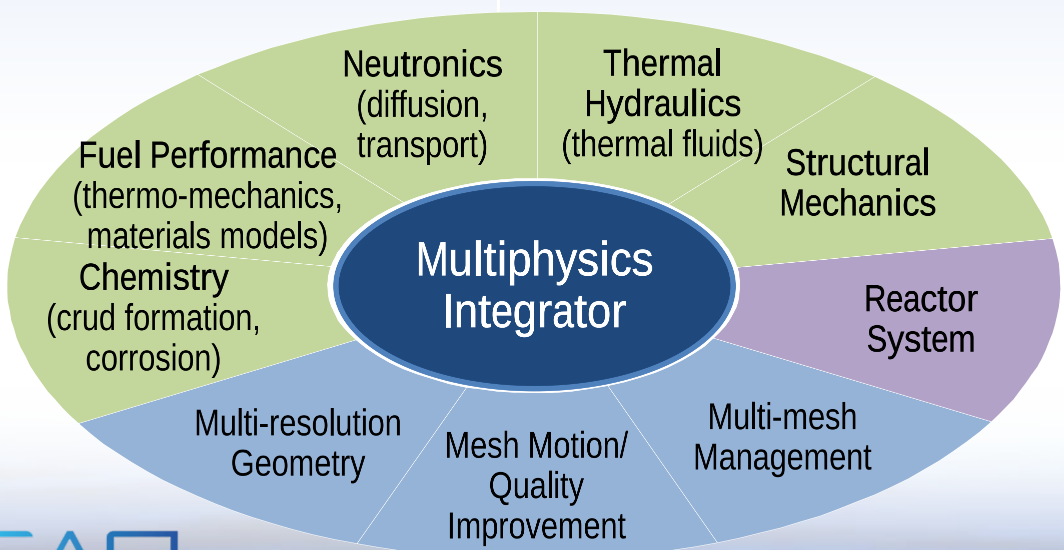

CASL scope: Develop and apply the VR to assess fuel design, operation, and safety criteria

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 Organization

- **Board of Directors**
  Ernest Moniz, Chairman
- **U.S. Department of Energy**

- **Director:** Doug Kothe
  Deputy: Ronaldo Szilard
  Chief Scientist: Paul Turinsky
  Chief Strategy Officer: Mario Carelli
  - **Project Management**
    Jeff Banta
  - **Partnership/Alliance Management**
    Jeff Cornett
  - **Operations**
    Becky Verastegui
  - **Materials Performance and Optimization**
    Chris Stanek
    Sid Yip
    Brian Wirth
  - **Models and Numerical Methods**
    Bill Martin
    Rob Lowrie
  - **Virtual Reactor Integration**
    John Turner
    Randy Summers
    Rich Martineau
  - **Validation and Uncertainty Quantification**
    Jim Stewart
    Dan Cacuci
  - **Advanced Modeling Applications**
    Jess Gehin
    Zeses Karoutas

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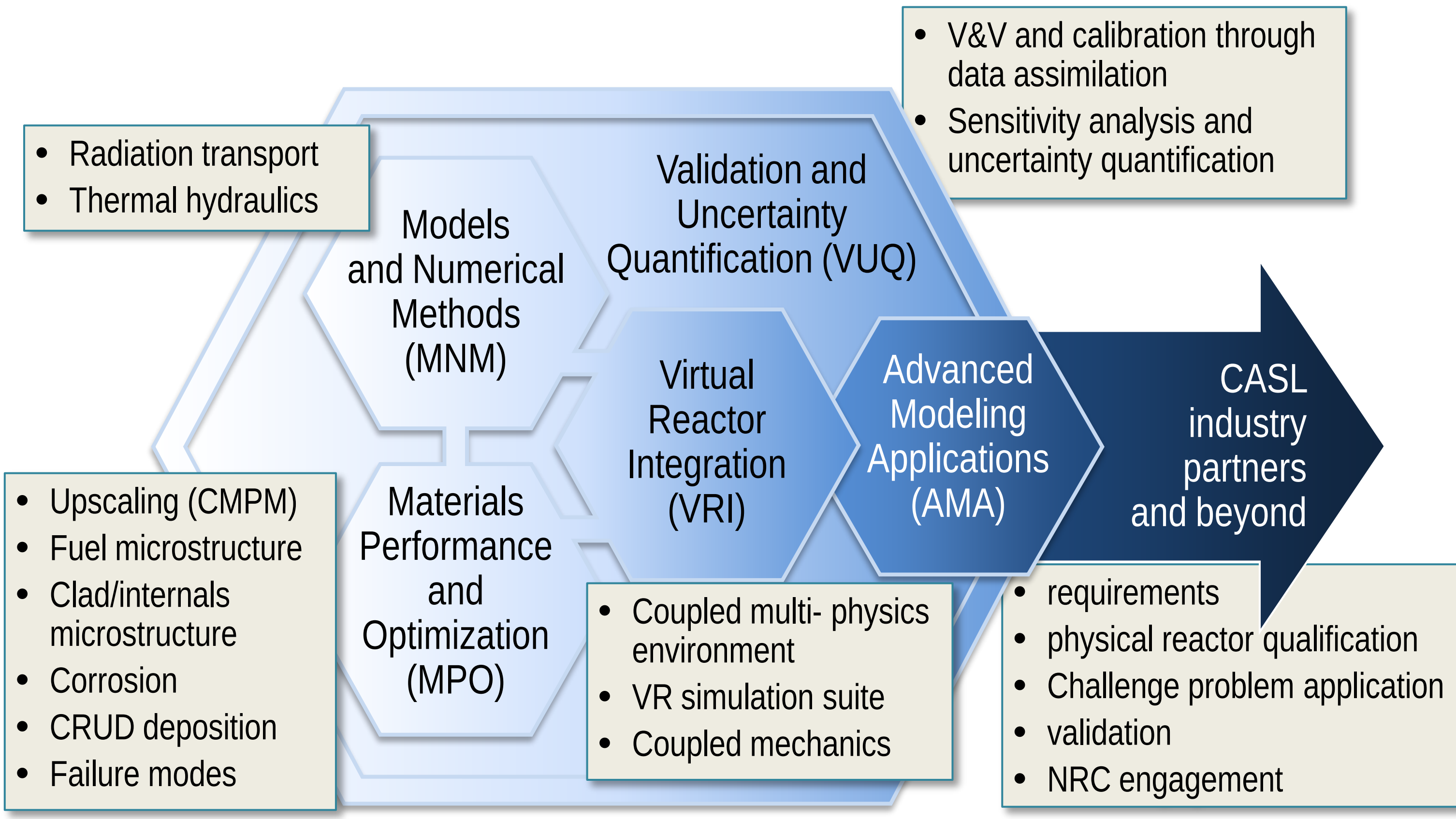
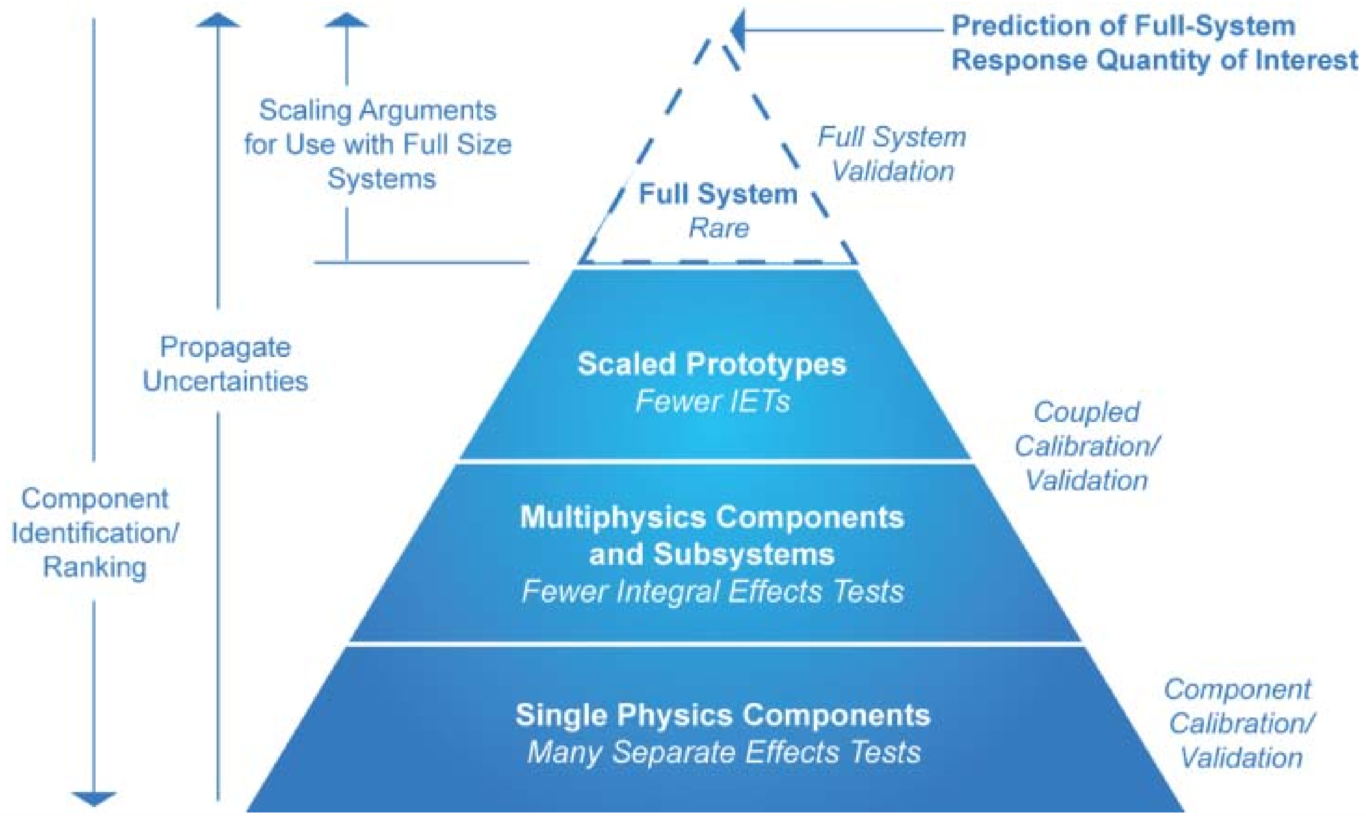
- Commercialization
  Jeff Cornett, Chairman
- Communications, Policy, and Economic Development
  Ken Nemeth, Chairman

CASL Technical Focus Areas



All Focus Areas span institutions (labs, universities, industry)

The validation hierarchy integrates all CASL Focus Areas, executed in a bottom-up and top-down way



AMA

VRI

MPO
+
MNM

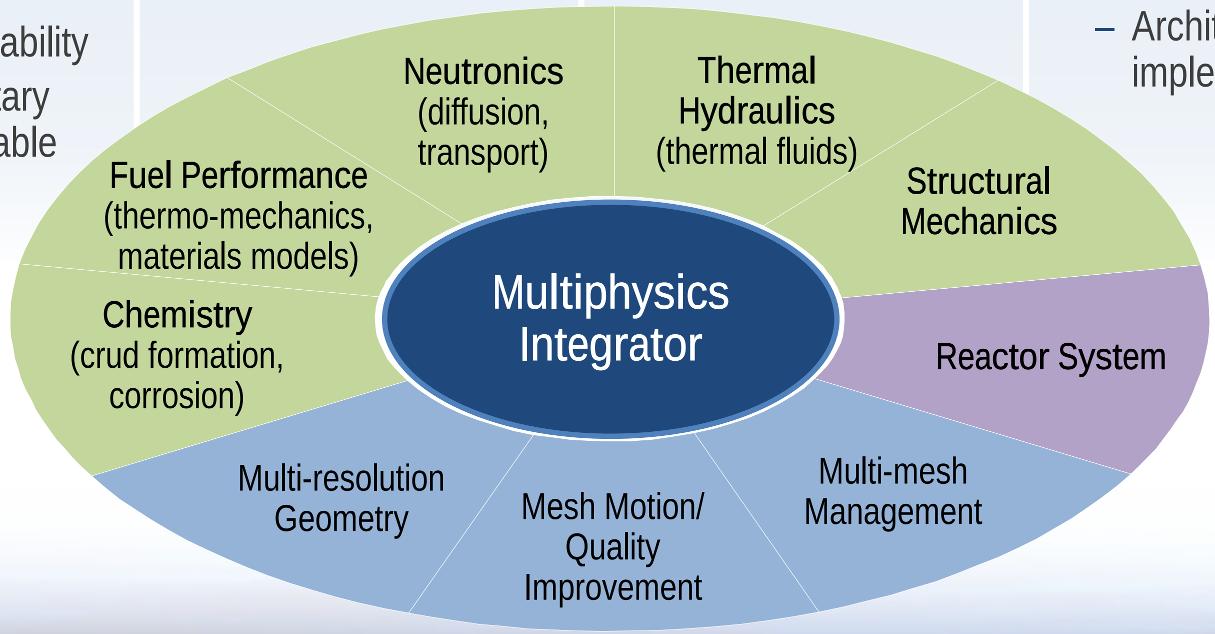
Virtual Environment for Reactor Analysis (VERA)
A code system for scalable simulation of nuclear reactor core behavior

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

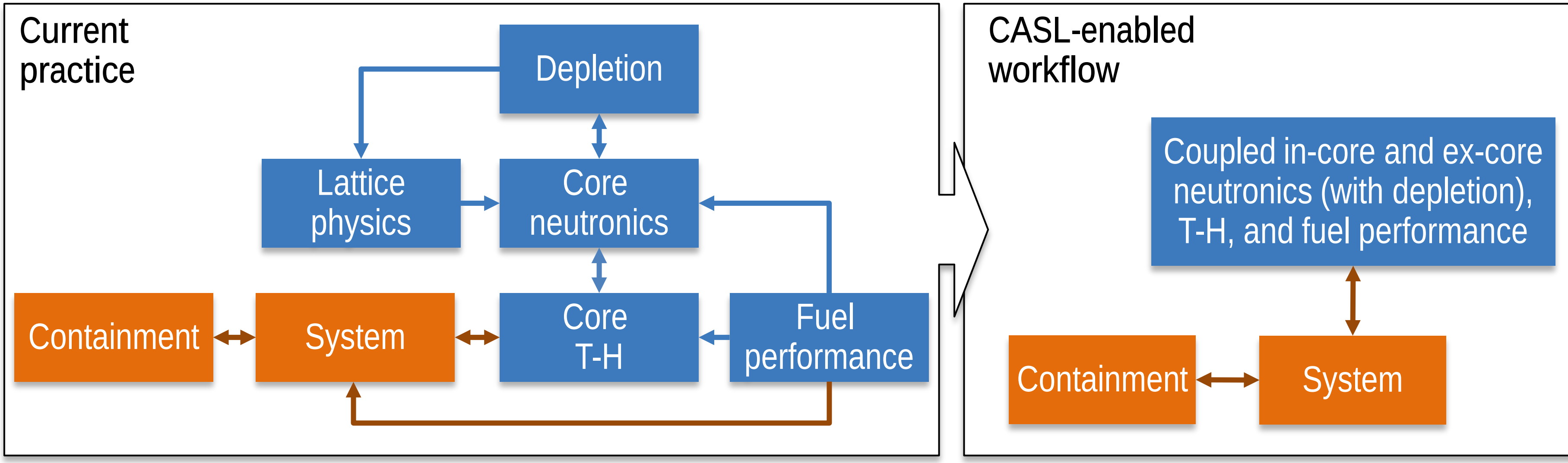
- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

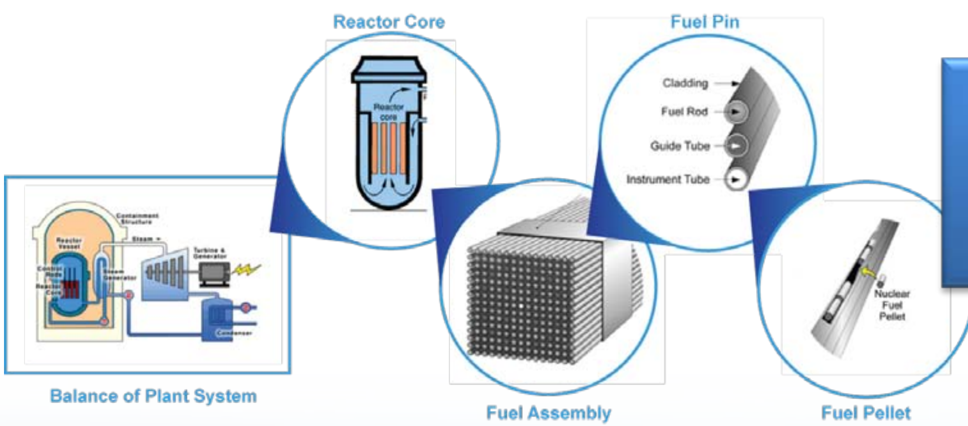
- Development guided by relevant challenge problems
- Broad applicability

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



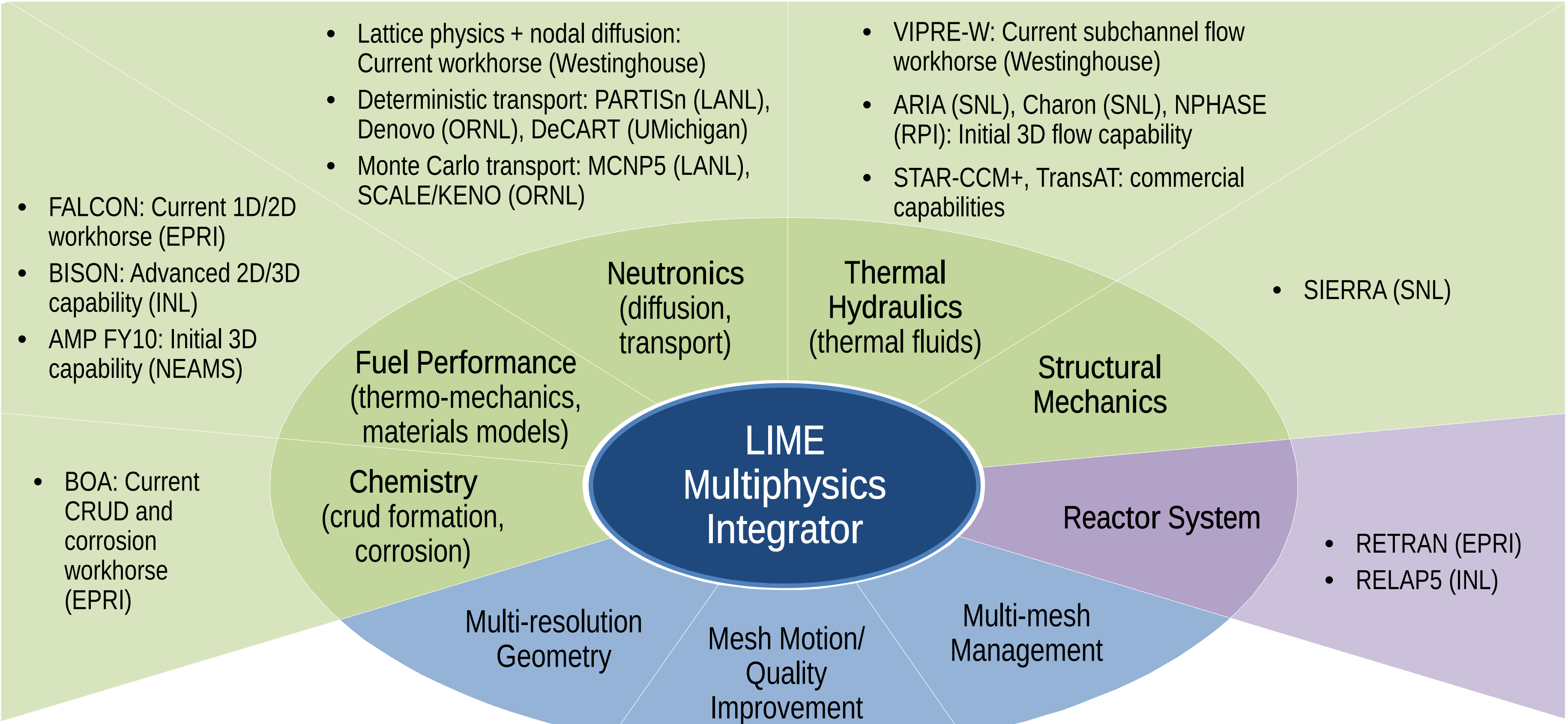
When successful, CASL will enable a new, integrated workflow for design and analysis.





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

The VERA Physics Simulation Suite builds on a foundation of mature, validated, and widely used software.



LIME

- Sandia National Laboratories
  - Lightweight Integrating Multiphysics Environment

RAVE

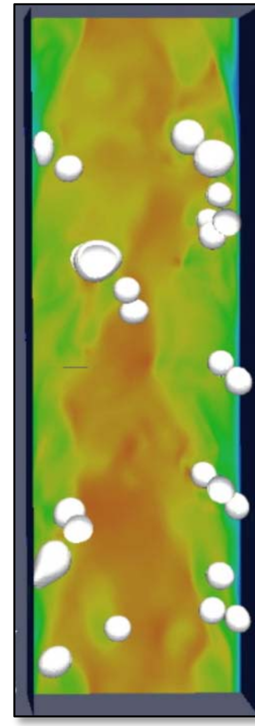
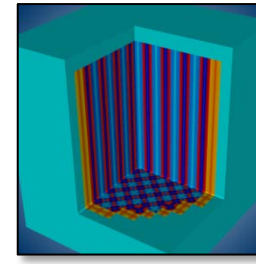
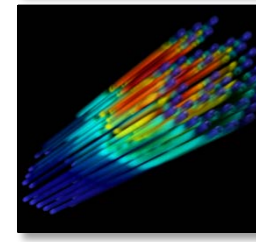
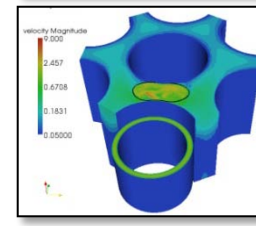
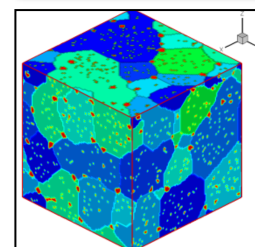
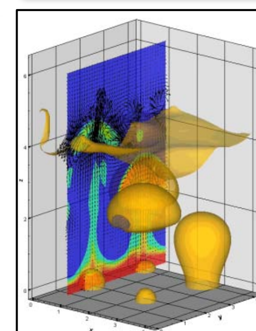
- Westinghouse suite of integrated capabilities
  - RETRAN
  - VIPRE-W
  - PARAGON / ANC

Numerical Nuclear Reactor

- Univ. of Michigan
  - STAR-CD
  - DeCART

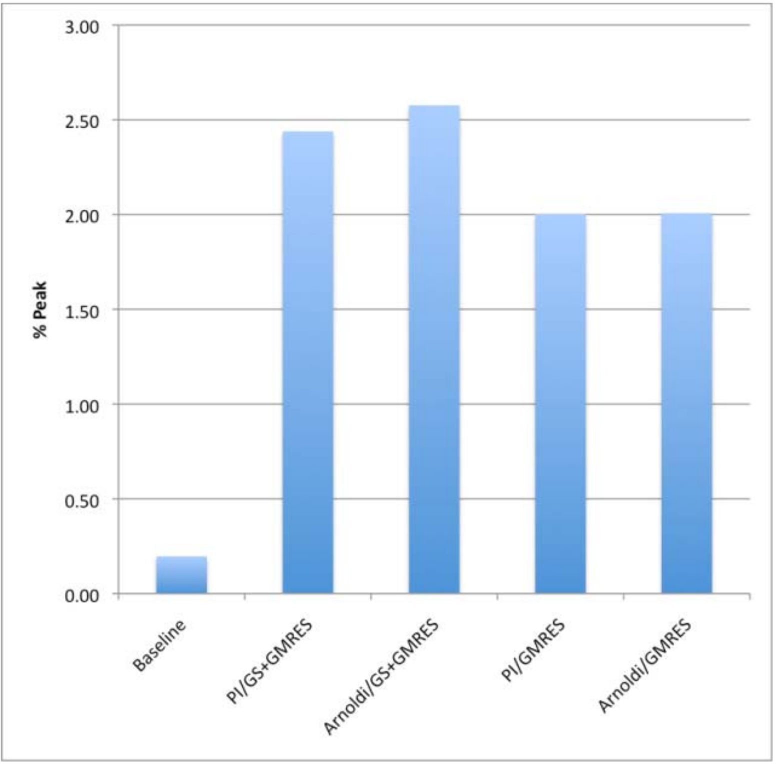
The CASL VR has a mature starting point

- 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

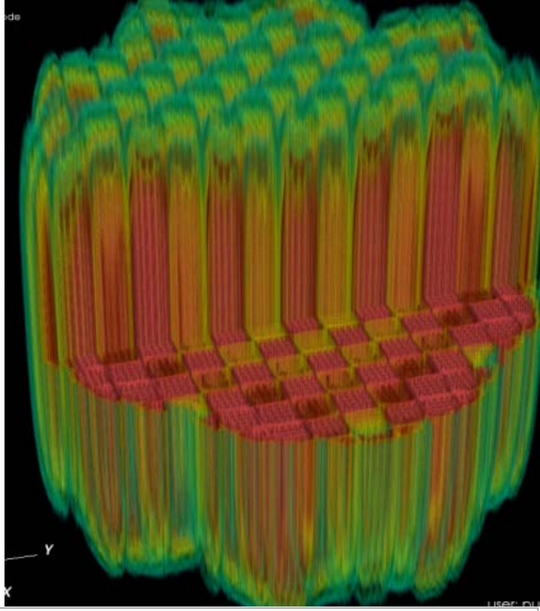







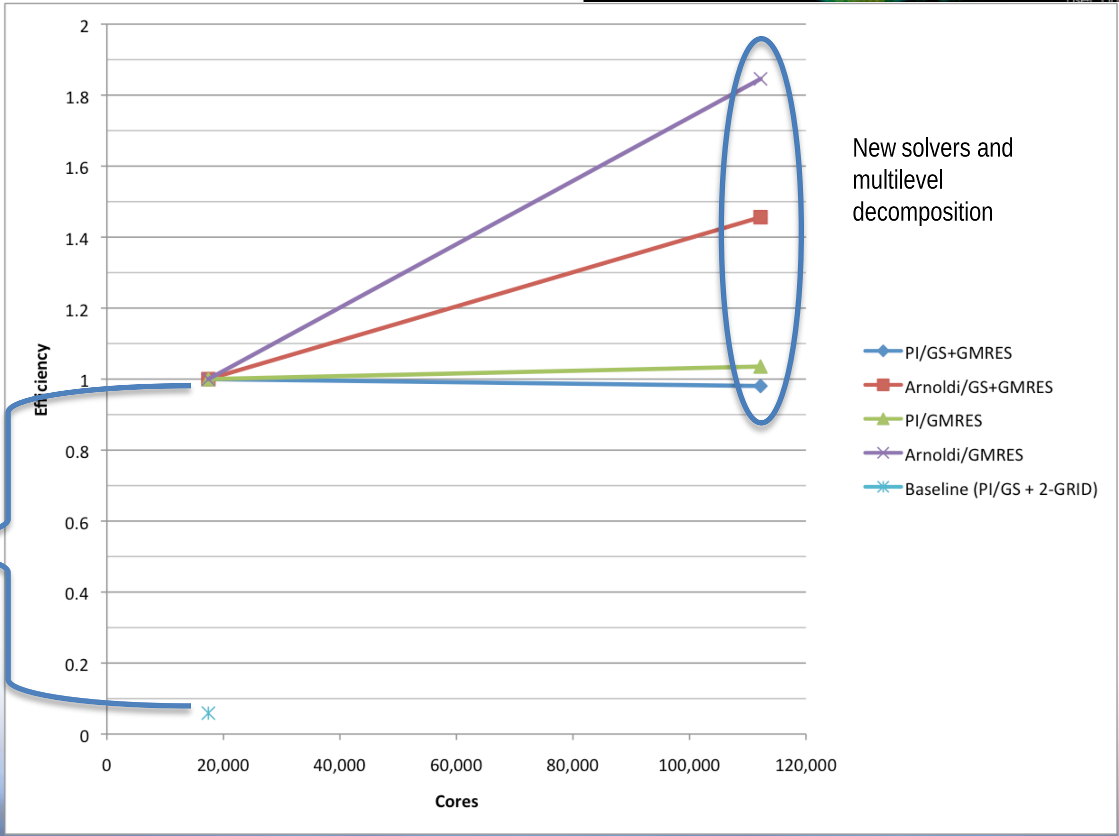
Denovo HPC Transport

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

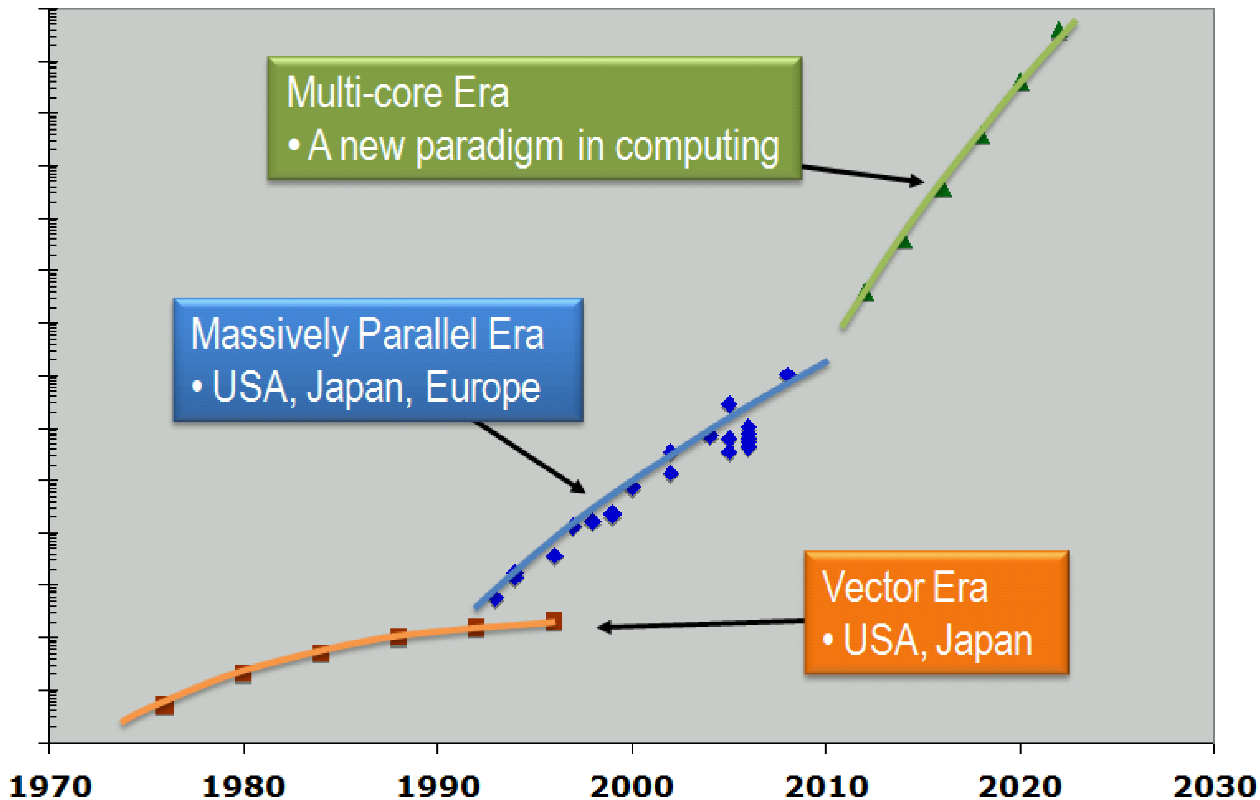
In-core Nuclear Reactor Computational Requirements

- 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

Future large-scale systems present challenges for applications

- Dramatic increases in node parallelism
  - 10 to 100× by 2015
  - 100 to 1000× by 2018
- Increase in system size contributes to lower mean time to interrupt (MTTI)
- Dealing with multiple additional levels of memory hierarchy
  - Algorithms and implementations that prioritize data movement over compute cycles
- Expressing this parallelism and data movement in applications
  - Programming models and tools are currently immature and in a state of flux

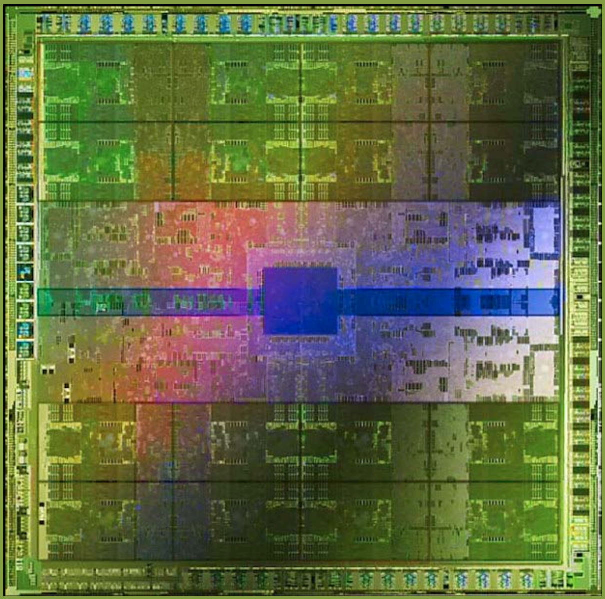


Exascale Initiative Steering Committee

Future ~~large-scale~~ desktop systems present challenges for applications

- Node parallelism increases
  - 10 to 1
  - 100 t
- Increas contribu to interr
- Dealing levels o
  - Algor that p over
- Express and dat in appli
  - Progra are curre and in a state of flux

Intel 48-core experimental chip shipping this summer

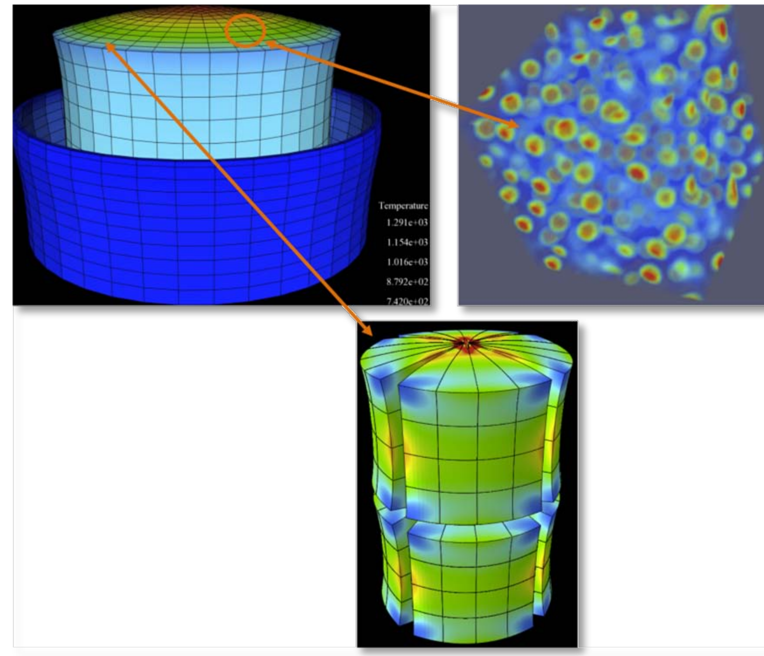


NVIDIA 512-"core" Fermi GPU

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

CASL legacy: what will we leave behind?

A preeminent computational science institute for nuclear energy



- VERA: 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?

www.casl.gov or info@casl.gov