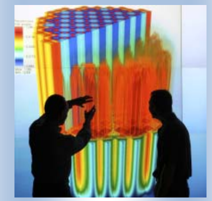
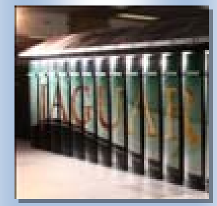
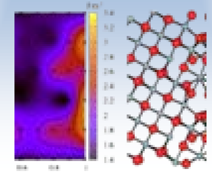






CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

Douglas B. Kothe

Director, CASL
Oak Ridge National Laboratory

Fall Creek Falls
Memphis, TN
Oct 25, 2010

CASL
Consortium for Advanced Simulation of LWRs

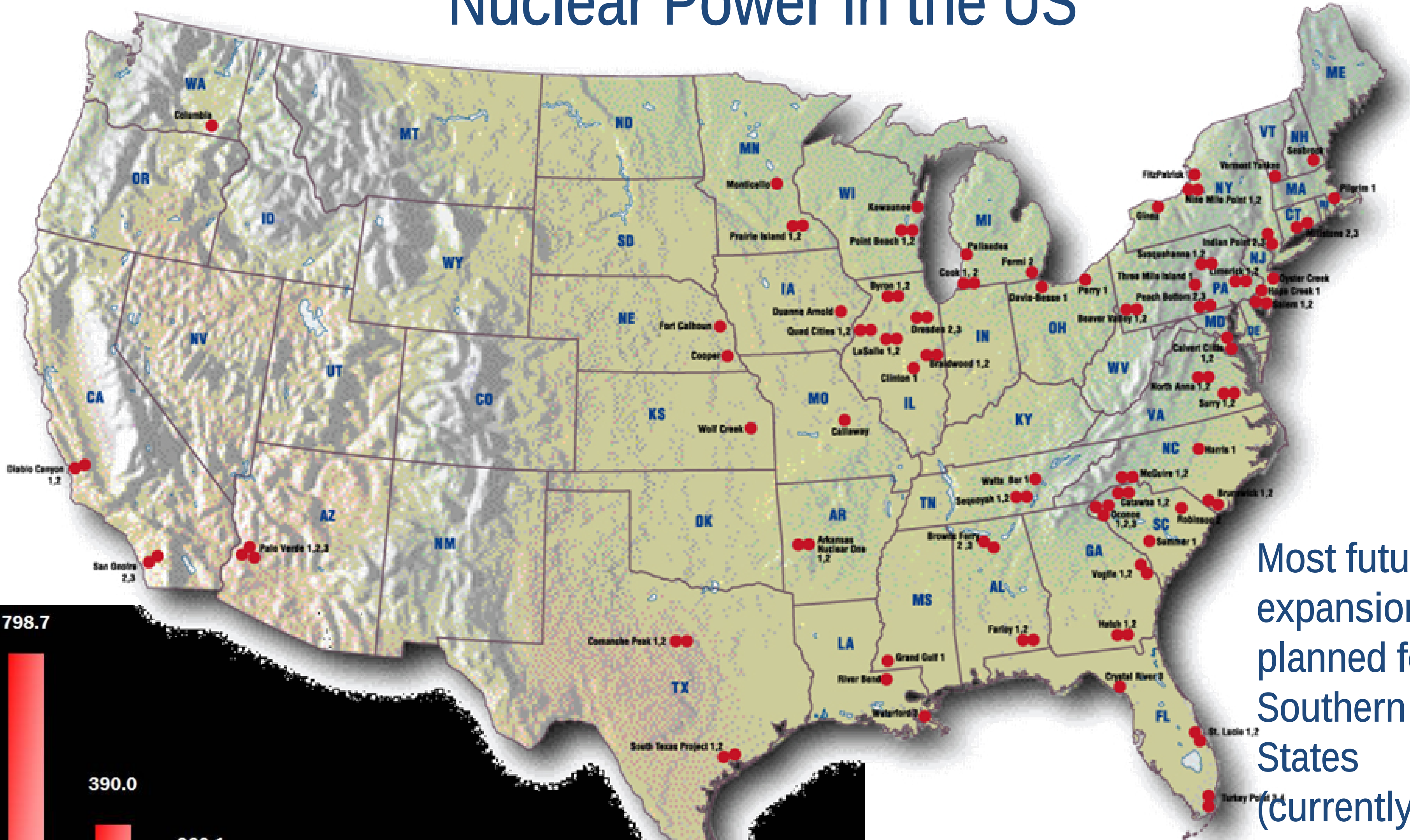
U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Oak Ridge National Laboratory

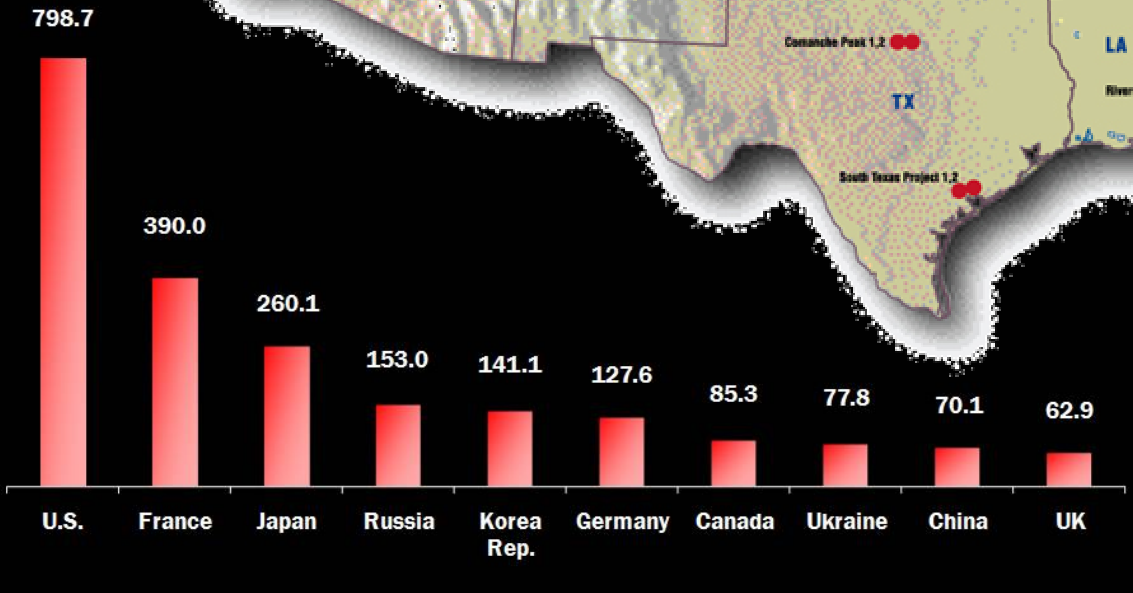
Outline

- 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

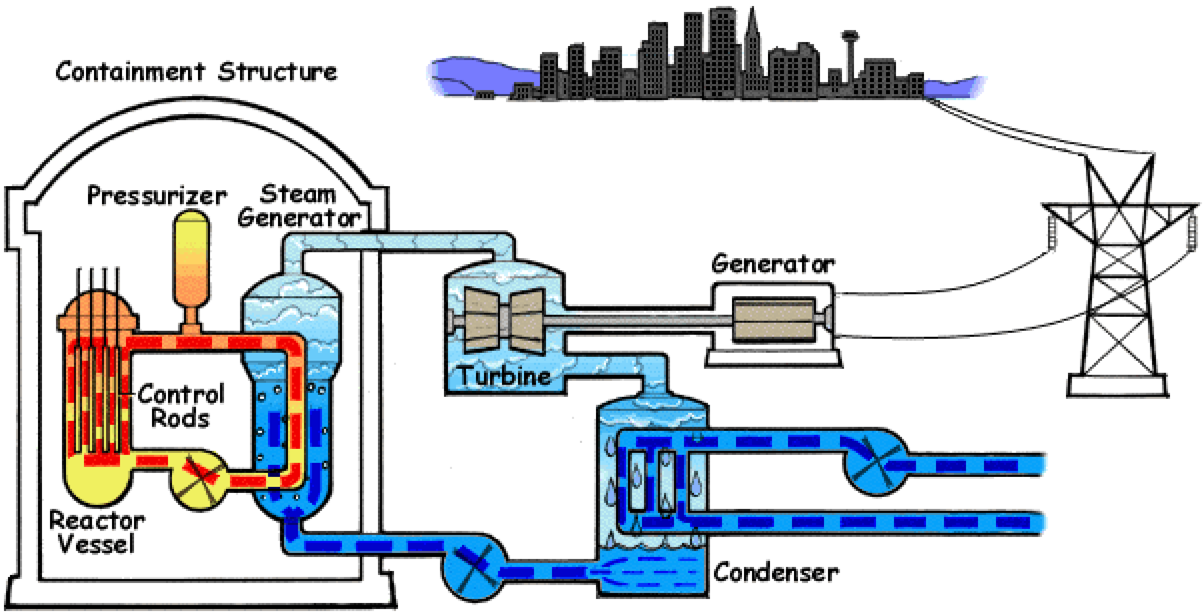


Most future expansion planned for Southern States (currently at 40%)



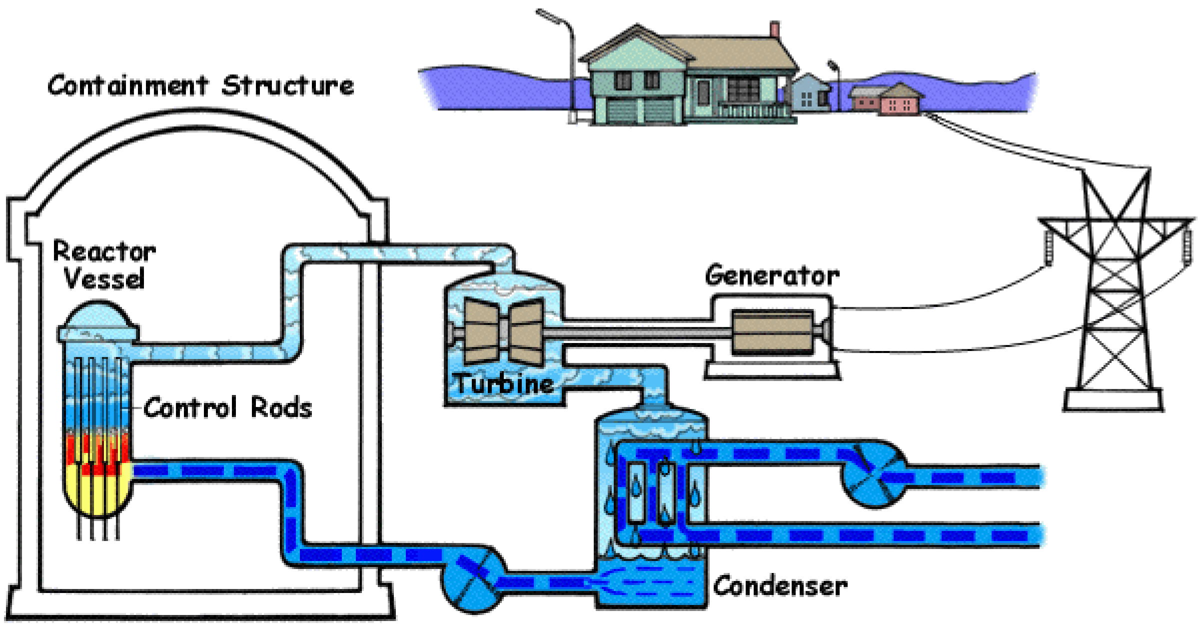
Top 10 Nuclear Generating Countries
2009, Billion kWh
Source: www.nei.org (International Atomic Energy Agency, 5/10)

Common types of Light Water Reactors (LWRs)



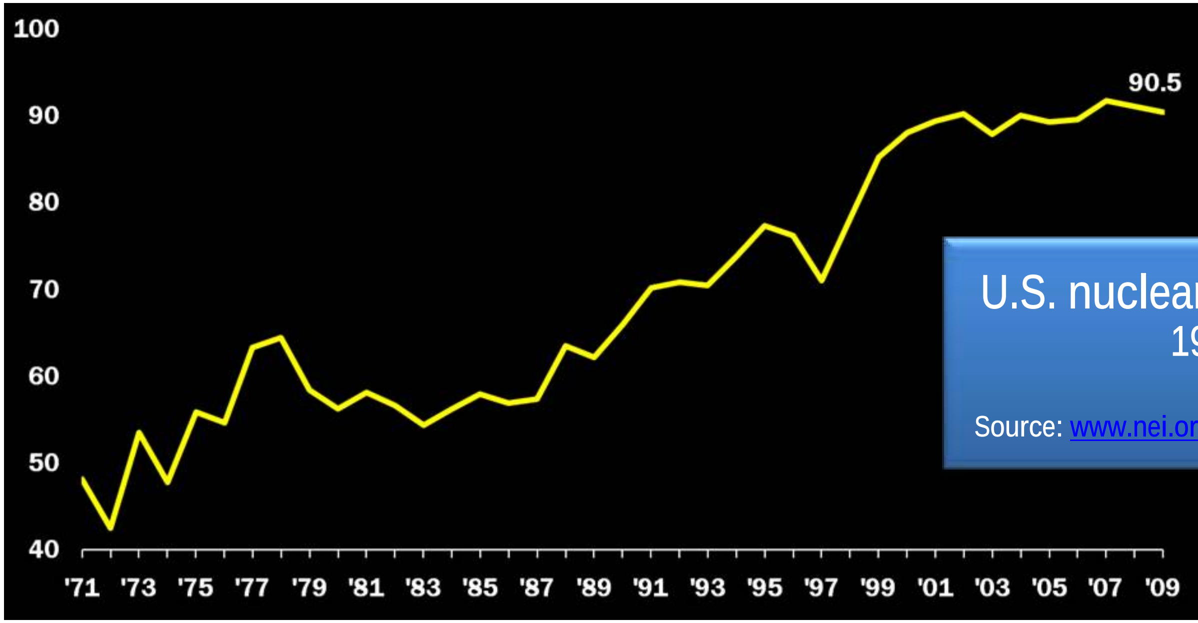
Pressurized Water Reactor (PWR)

Boiling Water Reactor (BWR)



U.S. Nuclear Energy

Increasing cumulative capacity delivering at a high capacity factor

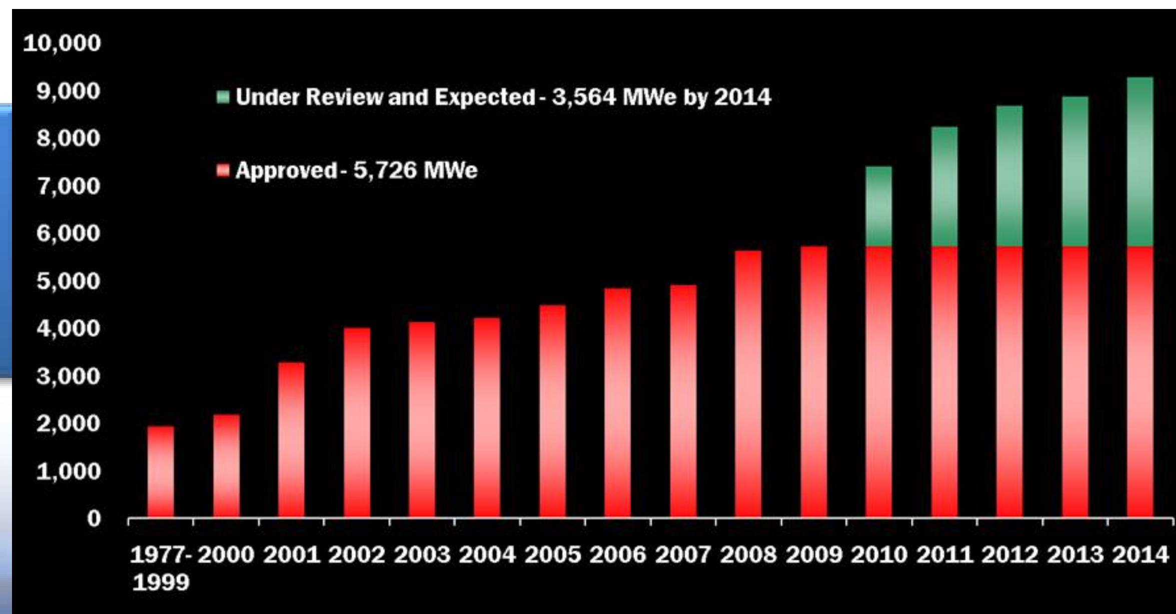


U.S. nuclear industry capacity factors
1971-2009 (percent)

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)



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

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

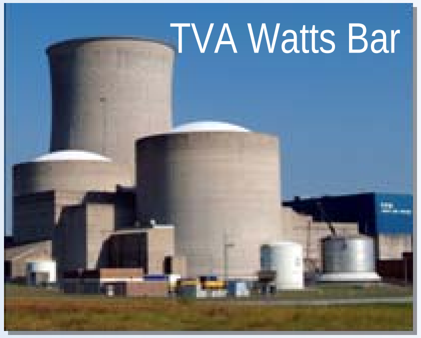
Building on longstanding, productive relationships and collaborations to forge a close, cohesive, and interdependent team that is fully committed to a well-defined plan of action

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 possesses the key elements required for success

ysical reactors	• 3 Westinghouse PWRs at Sequoyah and Watts Bar, operated by TVA
RC engagement	• Existing MOU between NRC Office of Regulatory Research and EPRI • CSO: Develop strategy for NRC engagement; AMA focus area Project 5: Execute strategy
lucation, Training, and Outreach (ETO) Program	• Comprehensive engagement with students, faculty, and practicing scientists, engineers, and regulators • Leverage EPRI's structured technology transfer approach
lidation  ORNL HFIR	• 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
rtual Office, Community, and Computing (VOCC)	• Integration and application of latest and emerging technologies to build an extended "virtual one roof"



Westinghouse CRUD Facility

Reactor performance improvement goals bring benefits and concerns

Can a “Virtual Reactor” be developed to address these performance goals?

ower uprates

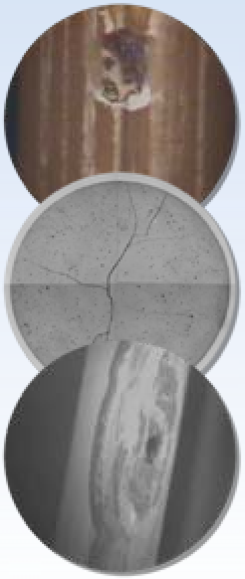
- 5–7 GWe delivered at ~20% of new reactor cost
- Advances in M&S needed to enable further uprates (up to 20 GWe)
- Key concerns:
  - Damage to structures, systems, and components (SSC)
  - Fuel and steam generator integrity
  - Violation of safety limits

Lifetime extension

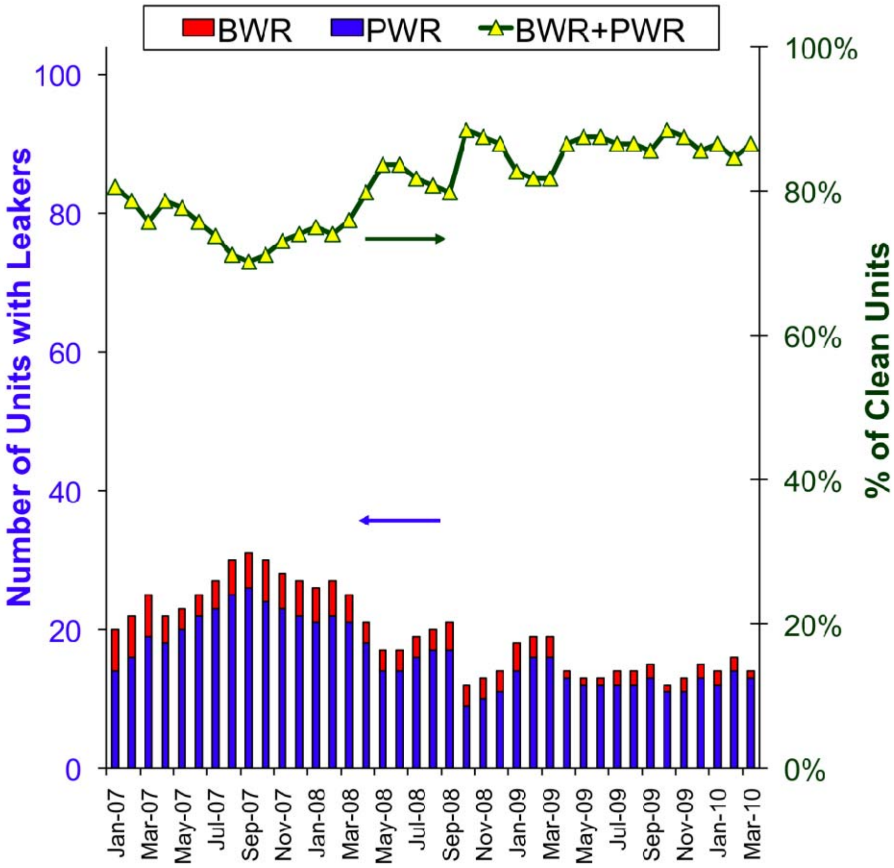
- Reduces cost of electricity
- Essentially expands existing nuclear power fleet
- Requires ability to predict SSC degradation
- Key concerns:
  - Effects of increased radiation and aging on integrity of reactor vessel and internals
  - Ex-vessel performance (effects of aging on containment and piping)

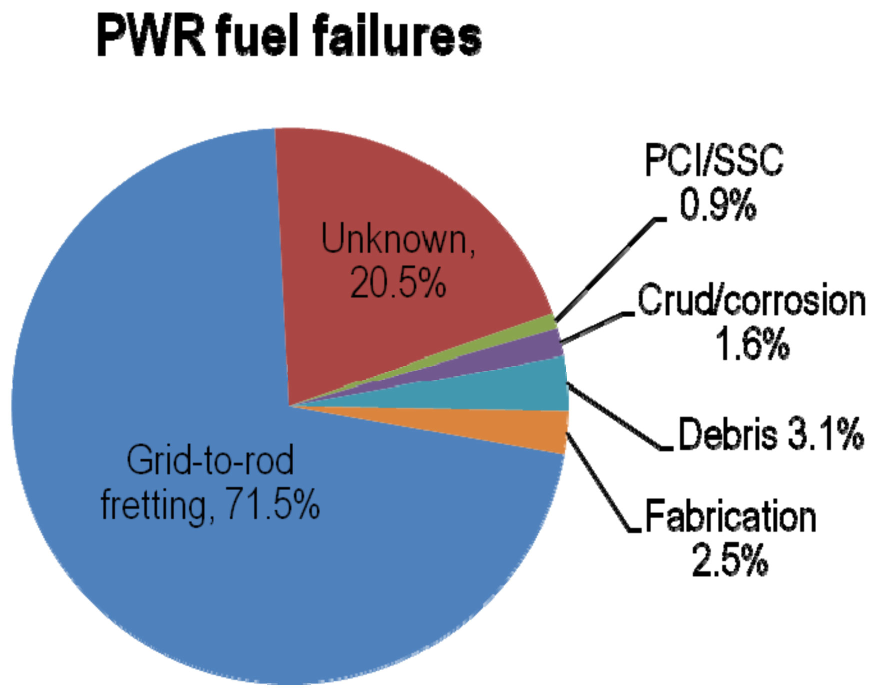
Higher burnup

- 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



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

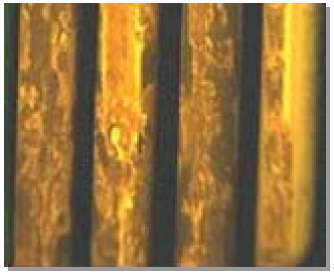




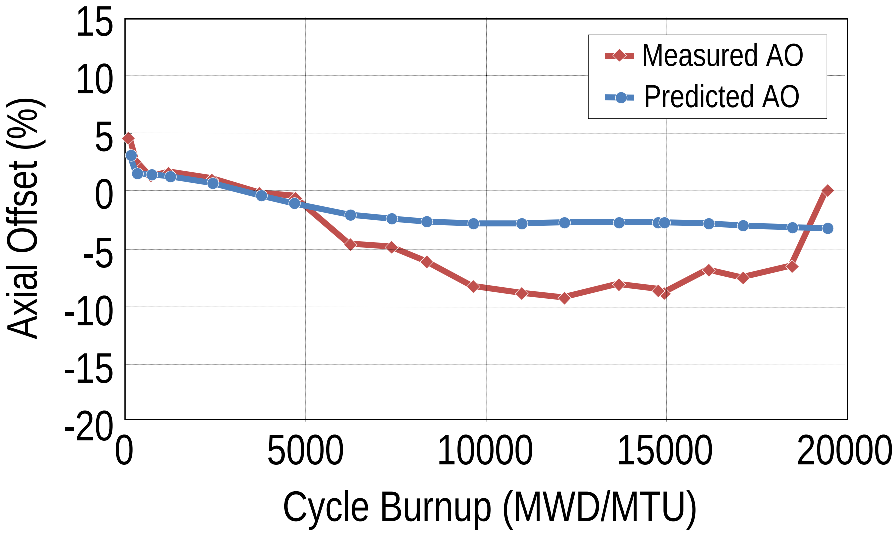
An effective virtual reactor M&S capability will permit proactive evaluation to enable critical performance enhancements

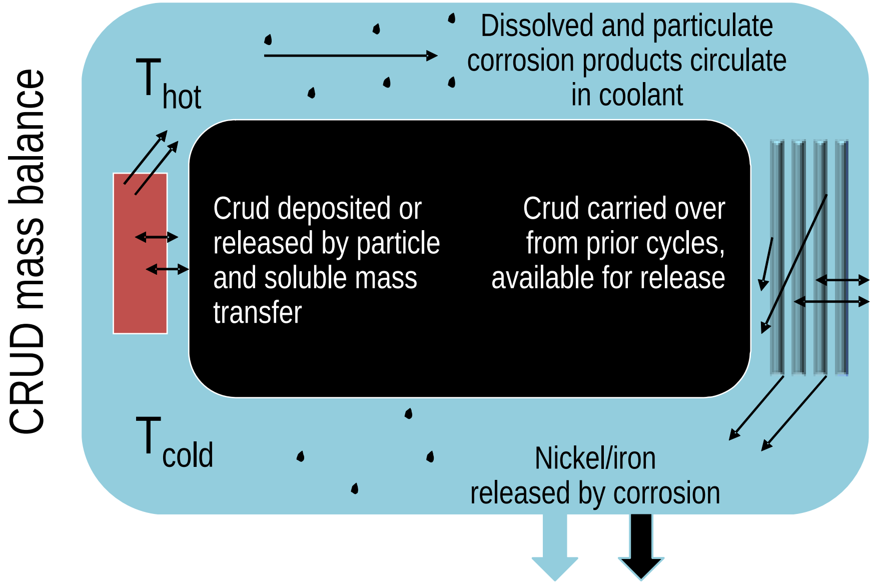
CRUD-induced power shift (CIPS)

- 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

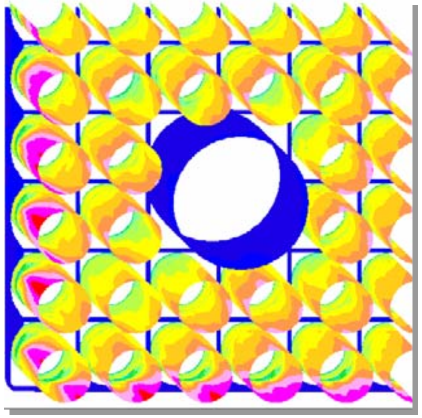


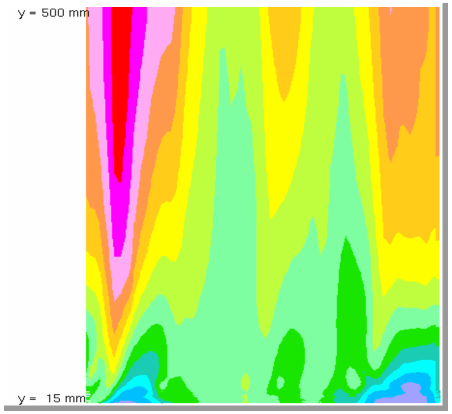


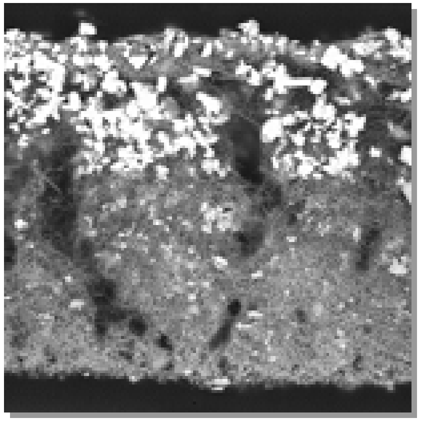
Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth

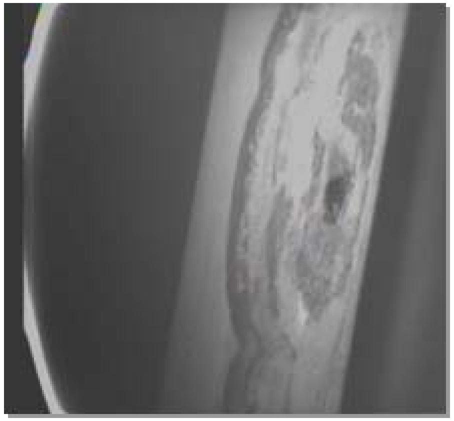
CRUD-induced localized corrosion (CILC)

- 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





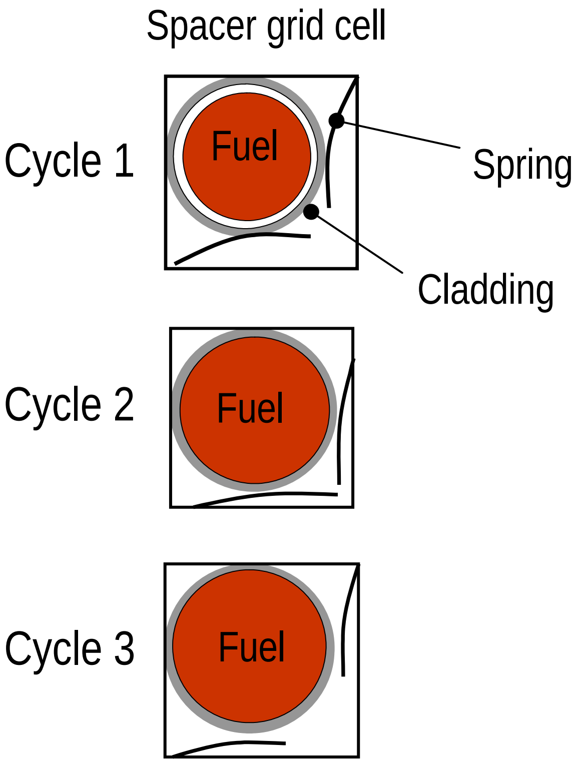




Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

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



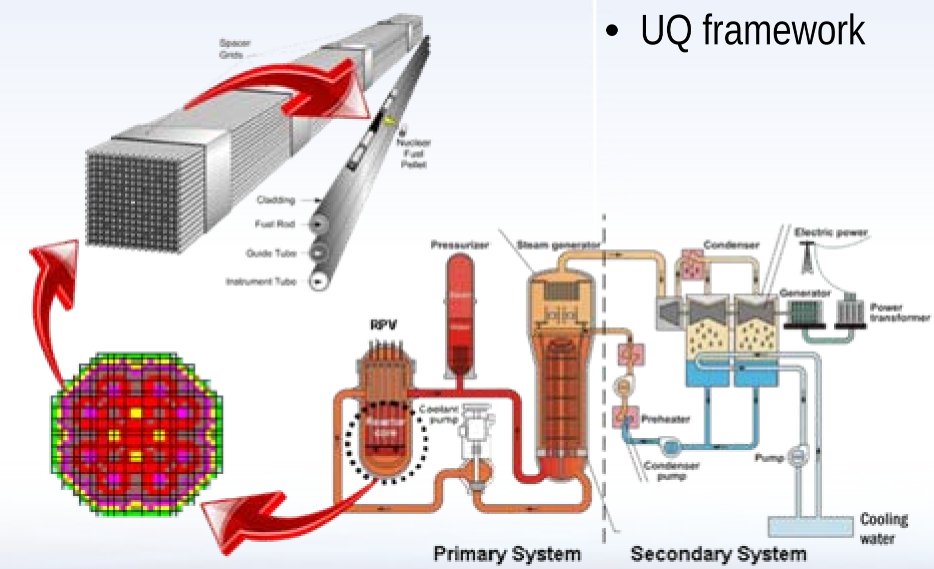
Need: High-fidelity, fluid structural interaction tool
to predict gap, turbulent flow excitation, rod vibration and wear

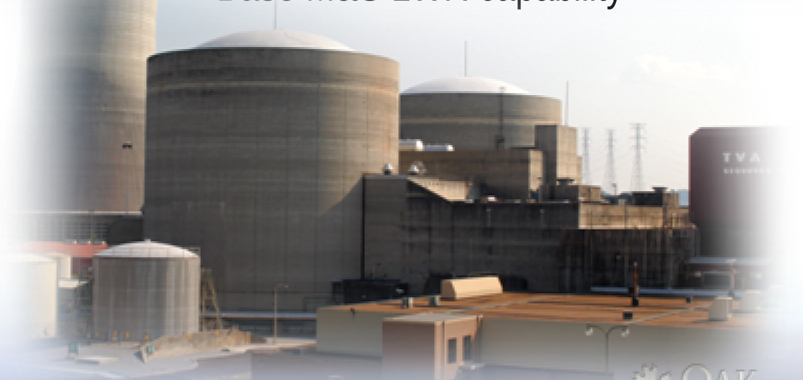
CASL has selected key phenomena limiting reactor performance selected for challenge problems

	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	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

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

Leverage

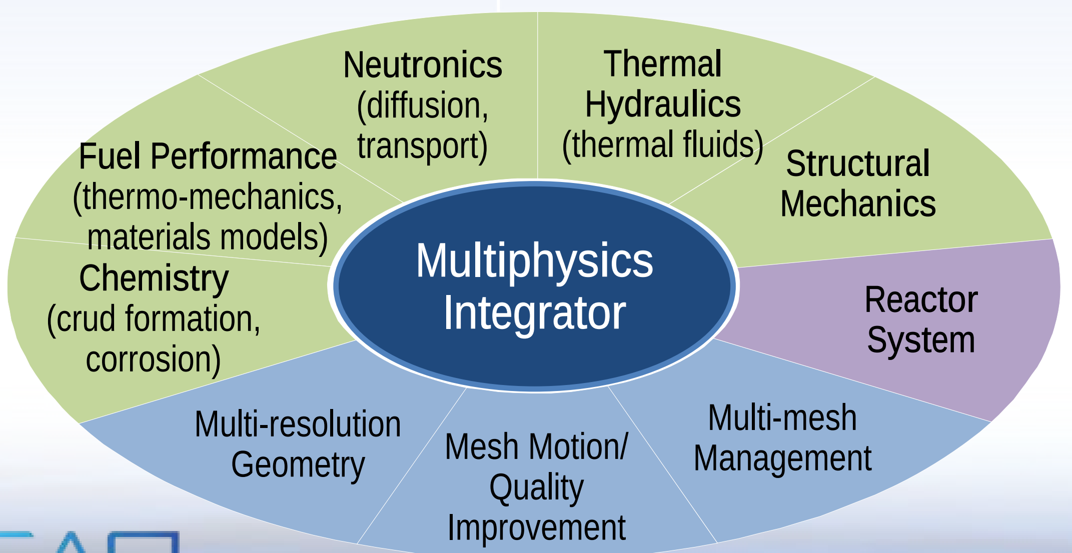
- Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications
- Existing systems and safety analysis simulation tools

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

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

MNM
Models and Numerical Methods

Bill Martin, Lead
Rob Lowrie, Deputy

- Radiation transport
- Thermal hydraulics

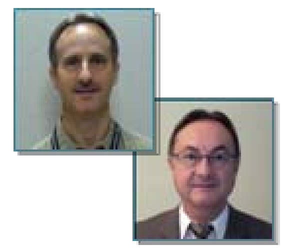
VRI
Virtual Reactor Integration

John Turner, Lead
Randy Summers,
Rich Martineau, Deputiy

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

VUQ
Validation and Uncertainty Quantification

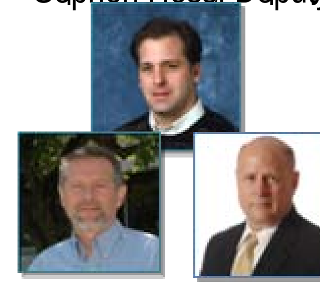
Jim Stewart, Lead
Dan Cacuci, Deputy



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

AMA
Advanced Modeling Applications

Jess Gehin, Lead
Zeses Karoutas, Deputy
Stephen Hess, Deputy



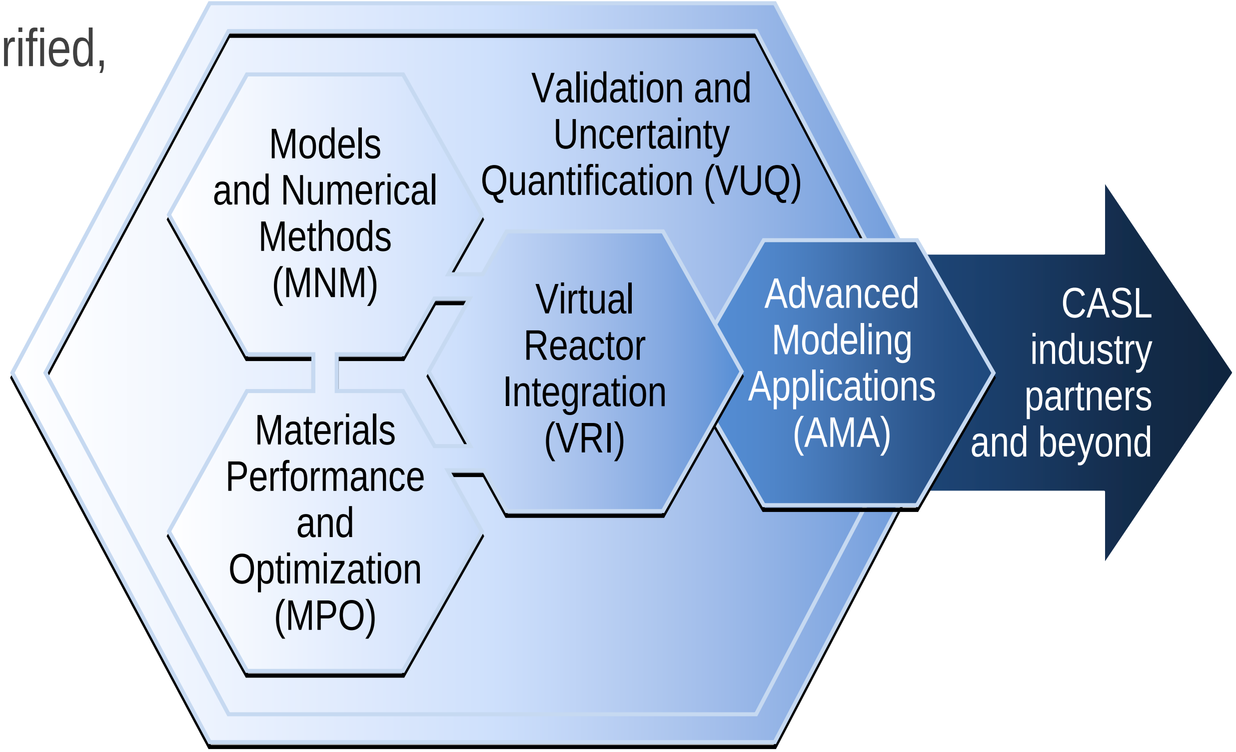
- VR requirements
- VR physical reactor qualification
- Challenge problem application
- VR validation
- NRC engagement

18 integrated and interdependent projects

The Integrated CASL Program

CASL will deliver

- A suite of robust, verified, and usable tools
- Within a common multi-physics environment
- To simulate phenomena within nuclear reactor vessels
- With quantified uncertainties



Virtual Environment for Reactor Analysis (VERA)

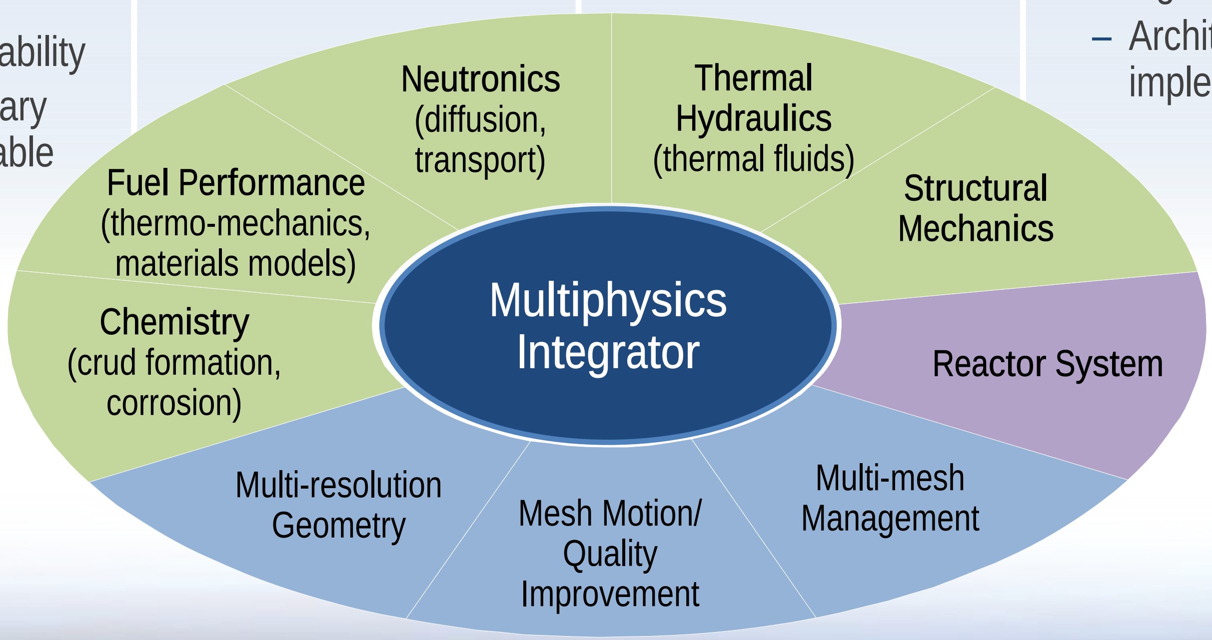
A code system for scalable simulation of nuclear reactor core behavior

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

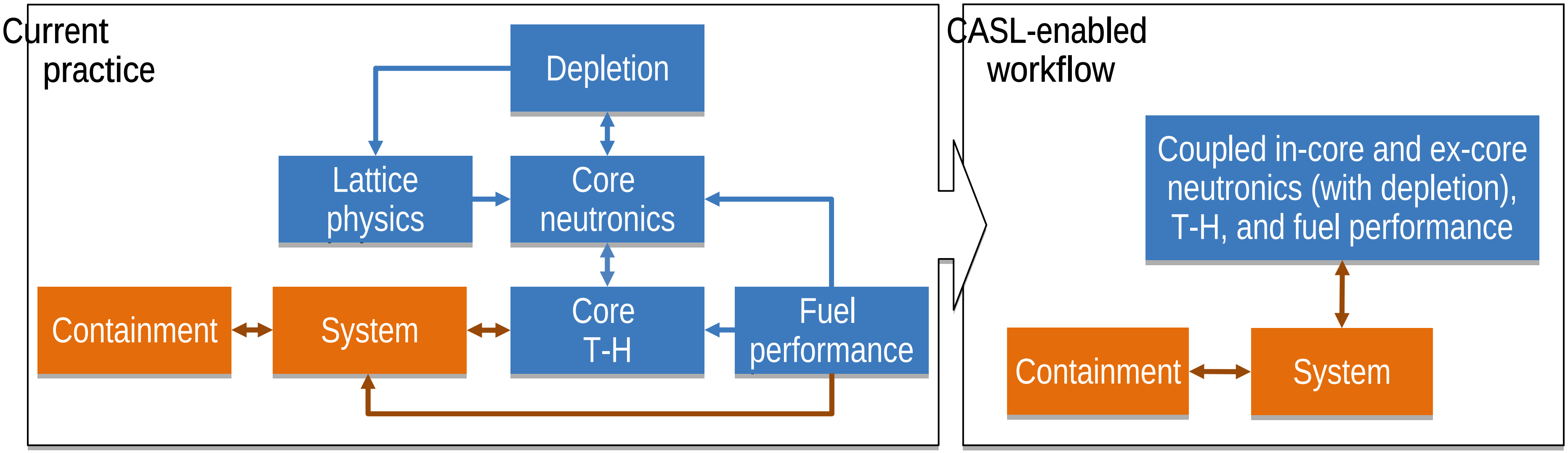
- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

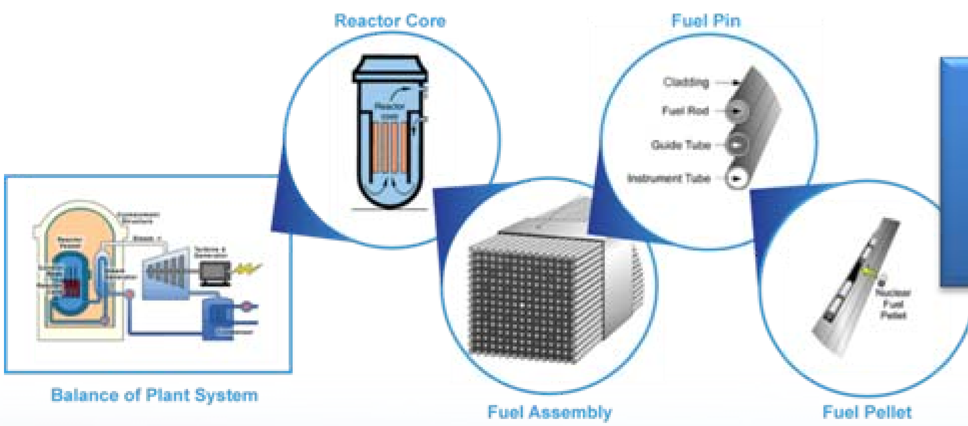
- Development guided by relevant challenge problems
- Broad applicability

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



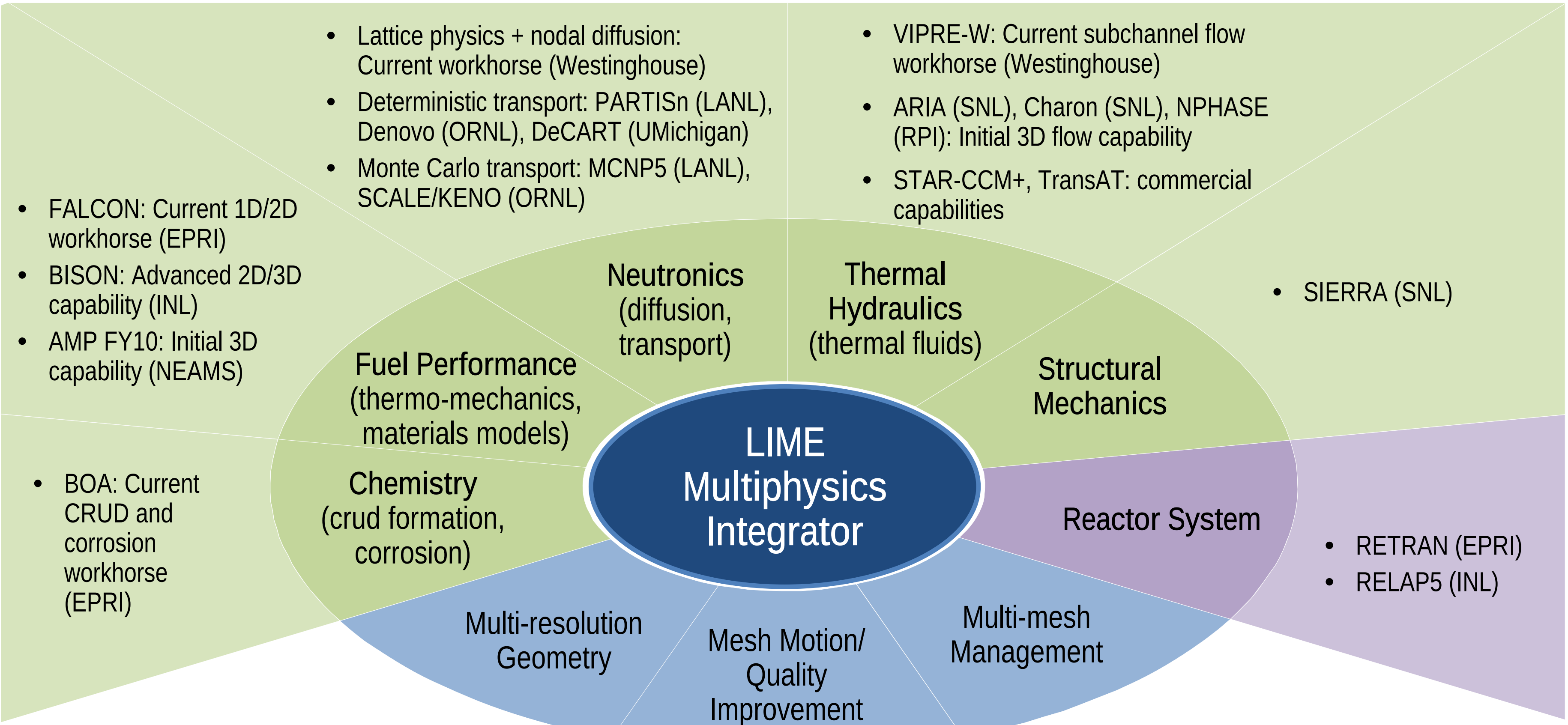
When successful, CASL will enable a new, integrated workflow for design and analysis.





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

Virtual Reactor capability roadmap

Capability	Year 1	Year 2	Year 3	Year 4	Year 5
Neutron Transport	• Full core 3D homogeneous pin cell Sn transport • Full core 2D/1D resolved pin cell MOC transport with T-H coupling	• Full-core 3D homogeneous pin cell Sn transport with T-H coupling	• Full-core 3D pin-resolved transport – both Sn and MOC • Prototype transient 3D transport capability – Sn and/or MOC	• Full-core 3D pin-resolved transport – both Sn and MOC – with T-H coupling • Prototype 3D hybrid Monte Carlo transport	• Transient full-core 3D pin-resolved transport – Sn and/or MOC – with T-H coupling • Full-core 3D hybrid Monte Carlo transport with T-H coupling
Thermal Fluids with Conjugate Heat Transfer	• Subchannel legacy and commercial CFD • Continuum and interface tracking method (ITM) multiphase benchmarks	• Next-generation sub-cooled boiling capability • Subgrid single-phase models informed by ITM	• Next-generation multiphase flow capability • Subgrid multiphase models informed by ITM	• Evaluate multiphase flow capability against benchmarks & exps • Improved numerical methods & coupling	• Refined multiphase flow capability • Targeted methods & coupling advances
Fuel & Clad Performance	• 1.5D legacy capability • Phenomenological models and properties	• Initial fuel mesoscale models for FG release, swelling, µ-structural evolution • Initial corrosion models	• Clad mesoscale µ-structural evolution • Fuel chemistry evolution	• Clad corrosion & refined µ-structural evolution • SCC & fatigue crack propagation	• Full upscale model for fuel/clad performance and life extension predictions
Coolant Chemistry	• Legacy capability	• CRUD source terms and formation and growth model	• Boron uptake in CRUD	• CRUD formation	• CRUD formation & induced corrosion
Structural Thermo Mechanics	• Assess and integrate existing capability with contact	• Loosely coupled structural vibrations • Initial radiation creep & hardening models	• Fully coupled structural vibration for fretting	• Implicit nonlinear fretting models • Improved radiation damage models	• Coupled and formally assessed structural vibration capability
Physics Coupling	• Legacy capabilities coupled via LIME • Subchannel transport & single-phase CFD	• Homogeneous cell transport & CFD • Initial fluid-structure interaction (FSI)	• Improved FSI • Homogeneous cell transport, CFD, fuel, & chemistry	• Pin-resolved transport & CFD	• Full-core transport, CFD, fuel, chemistry, thermo mechanics • Core + physical plant
Validation and Uncertainty Quantification	• DAKOTA interfaced for scoping UQ	• Time-dependent data assimilation for parameters and responses • Model V&V procedures and initial databases	• Sensitivity and UQ capabilities for coupled components • Model V&V procedures and tools for selected modules	• Data assimilation with reduced-order modeling • Model V&V procedures and tools for selected coupled modules	• High-order data assimilation including errors and uncertainties • Model V&V procedures and tools for coupled VERA system of codes

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 Boron uptake and its affect on rod power Crud dryout, clad temp rise, corrosion	High-fidelity CFD, turbulent heat transfer, corrosion chem Coupled CFD & neutronics New models: fundamental R&D and validation data
GTRF	Rod excitation force, natural frequency Rod fatigue vibration and wear	High-resolution CFD-structure interaction & coupling 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 • Physics and material model fidelity • Code verification • Solution verification • Model validation • 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

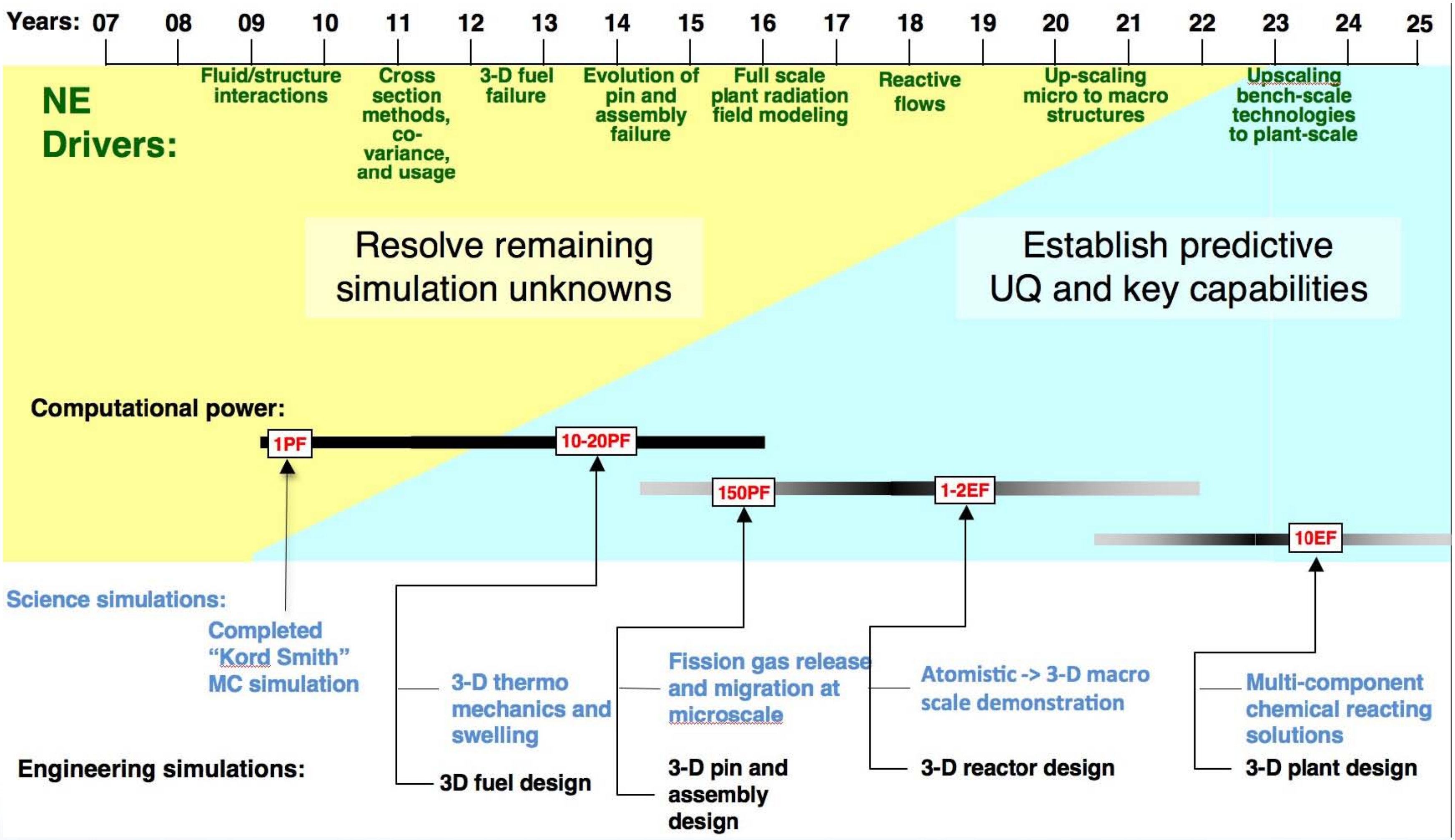
We will annually assess the CASL VR against challenge problems

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

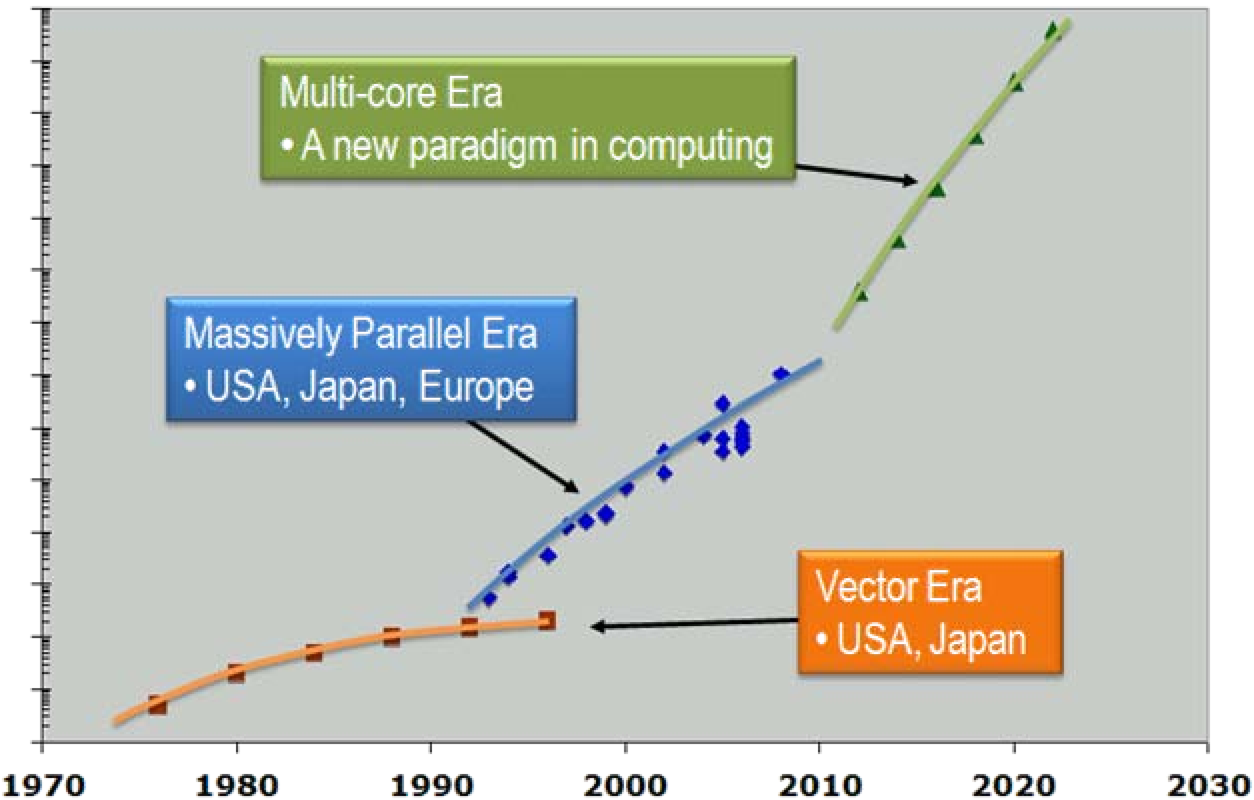
Beyond exascale is needed to regularly perform full core, coupled simulations
We are in the process of quantifying these requirements

Advanced Nuclear Energy Requires Scientific, Computer Science, and Large-Scale Computing Advances



Future large-scale systems present challenges for applications

- Dramatic increases in node parallelism
  - 10 to 100X by 2015
  - 100 to 1000X 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
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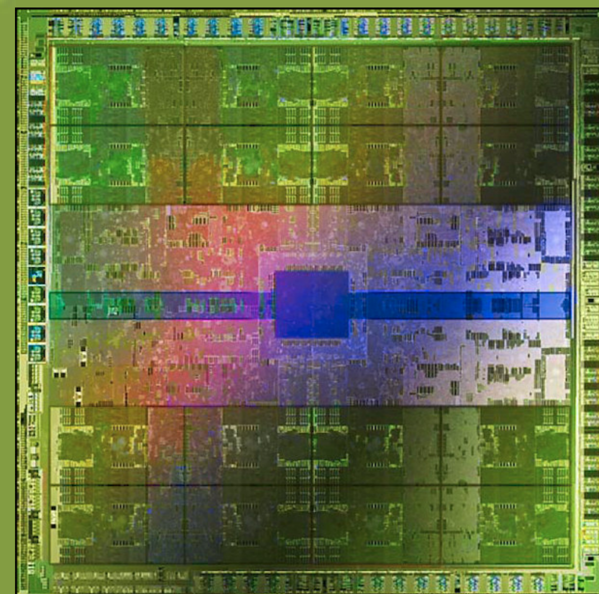
  - Algor that p over
- Expres and dat in appli
  - Progra are curre and in a state of flux

Intel 48-core experimental chip shipping this summer

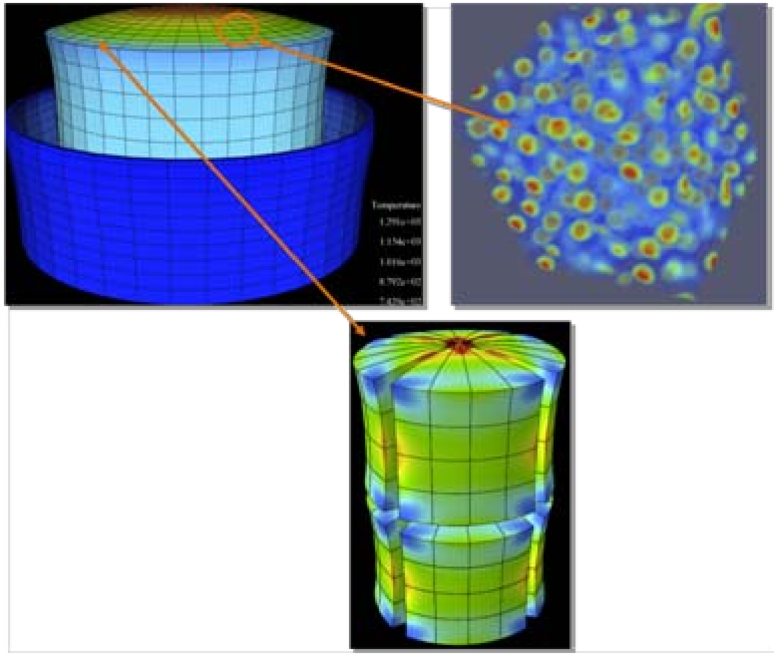


NVIDIA 512-"core" Fermi GPU

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

CASL legacy: what 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?

www.casl.gov or info@casl.gov

Supplemental Material

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
- 05/28/2010: CASL selected

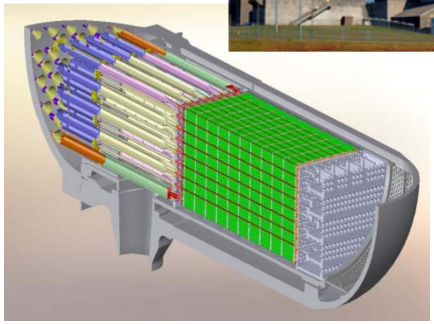
Advanced Modeling Applications

Driving development of VR to support real-world users and applications

Jess Gehin
Zeses Karoutas
Steve Hess

Objectives and Strategies

- Ensure that CASL R&D meets user needs & requirements by setting requirements & assessing VR
- AMA focus area projects:
  - Project 1: Setting VR modeling requirements & assessment
  - Project 2. Performing VR validation
  - Project 3. Performing VR qualification with physical TVA reactor data
  - Project 4. Developing challenge problems & applications
  - Project 5. Supporting NRC engagement
- Relies on CASL's strong industry (W, EPRI, TVA) & national laboratory (ORNL, INL,SNL,LANL) engagement



Requirements Drivers

- AMA is primary connection of CASL R&D with problems to be solved.
- To be successful, AMA needs:
  - Industry input and direction on key limitations to power uprates as limited bychallenge problems
  - Capable VR software with robust, accurate physics models that can be applied in R&D and engineering environments

Outcomes and Impact

- AMA will provide demonstrated applications by industrial partners of CASL capabilities for physical reactors on challenge problems
- Metrics for success include qualification of CASL capabilities with operational data from TVA reactors & successful application to the CASL challenge problems

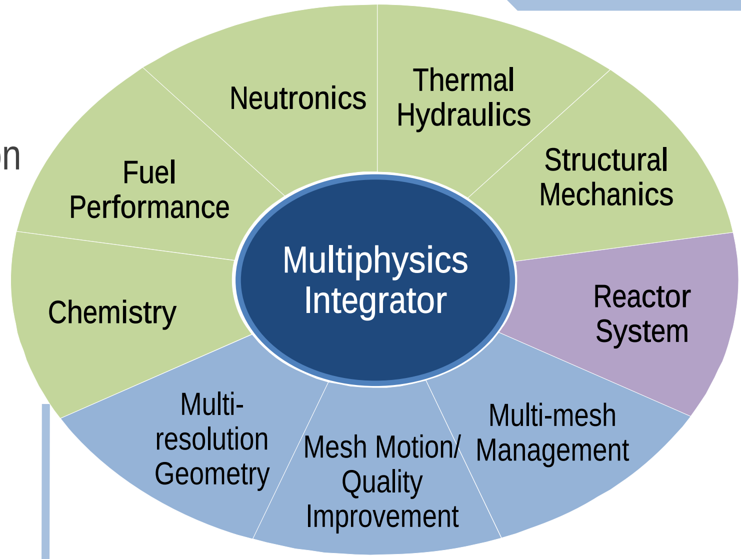
CASL

OAK RIDGE National Laboratory

Virtual Reactor Integration (VRI)

Bridging the gap between research and engineering.

John A. Turner
Randy Summers
Rich Martineau



Objectives and Strategies

- VRI will deliver suite of robust, verified, & usable tools within common multi-physics environment for design & analysis of nuclear reactor cores, with quantified uncertainties.
- VRI focus area projects:
  - VERA: Virtual Environment for Reactor Applications
  - VERA Physics Simulation Suite (PSS)
  - Coupled Mechanics (nuclear fuel performance, assembly dynamics)
- Agile software development processes & partner strengths in large-scale code development are key to meeting VRI challenges

Requirements Drivers

- VRI is conduit between targeted research & engineering analysis
  - guided by current &future simulation and workflow requirements developed with AMA
  - in collaboration with VUQ on improved tools & methodologies for quantification of uncertainties,
  - research, development,& Integration of advanced capabilities with the MPO and MNM focus areas.
- VRI depends on several external programs such as DOE/NE NEAMS for key capabilities

Outcomes and Impact

- VRI will deliver environment described above, portions of which will be openly-available.
- VRI success can be measured by
  - downloads of open portion(s) of VERA
  - measurable use of VERA by industry partners in understanding & mitigating key issues
- VRI success will transform industry analysis, bringing tightly-coupled, high-fidelity simulation into daily engineering workflows.

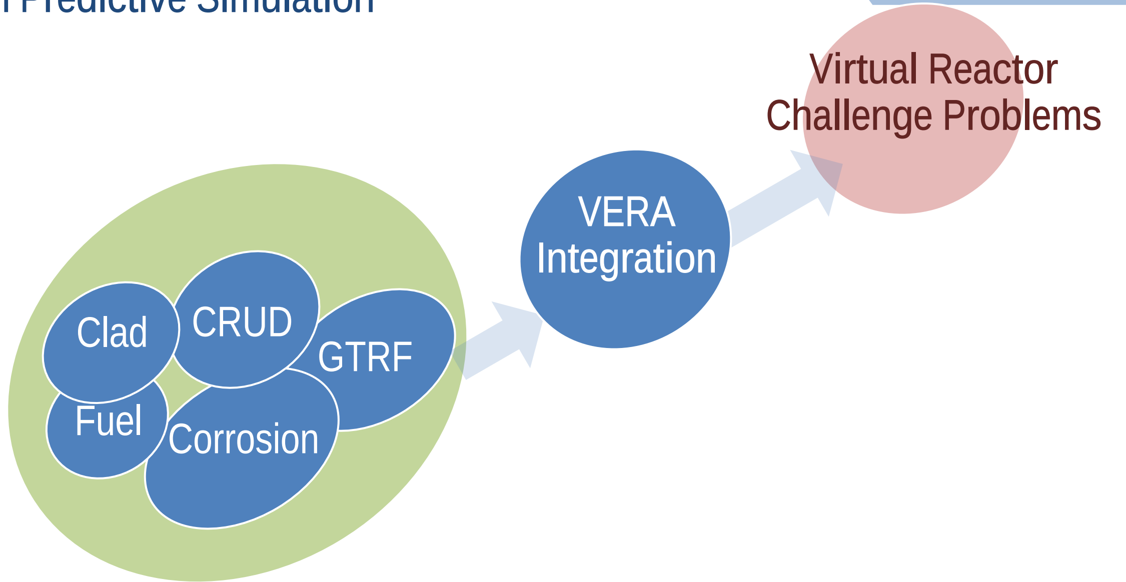
Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

Chris Stanek
Brian Wirth
Sid Yip

Objectives and Strategies

- Initial focus: Provide physics-based materials models of CRUD, GTRF and PCI for 3D, multi-physics, virtual reactor simulator
- Improved physics and chemistry insight delivered via constitutive relations
- MPO focus area projects: 6 as indicated by =>
- MPO is comprised a diverse group of computational materials scientists with a wide range of capabilities



Requirements Drivers

- MPO enables solutions to CASL challenge problems by delivering a multiphysics, multiscale materials M&S capability to the CASL virtual reactor
- What does MPO need to be successful?
  - Industrial guidance for problem definition
  - Experimental data, both full scale reactor tests and unit mechanisms
  - External program leverage, e.g. EFRCs, FCRD, etc.

Outcomes and Impact

- Initial focus: Predictive models of fuel failure, that quantitatively define operating margins & lifetime limits
- Longer term focus: Predictive models for internals integrity and advanced fuel forms
- Validated predictions of materials performance
- Support enabling power uprates, lifetime extension & higher fuel burnup as relates to fuel & structural materials performance.

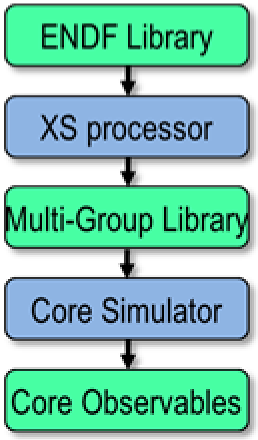
Modeling & Numerical Methods

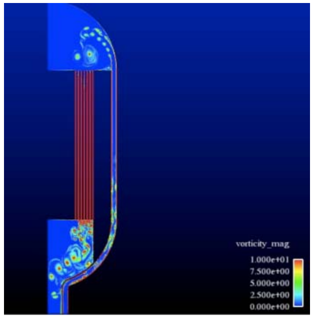
Delivering state-of-the-art radiation transport & T-H simulation tools to VERA

Bill R. Martin
Robert B. Lowrie

Objectives and Strategies

- Deliver next-generation, non-proprietary, scalable transport & T-H simulation tools to VERA, interfaced with the latest VUQ technologies
- Accommodate tight coupling with other physics: conjugate heat transfer, structural mechanics (GTRF), neutronics, etc.
- MNM focus area projects:
  - Project 1. Transport: Pursue 3 transport methodologies to achieve 3D pin-resolved transport for down selection, benchmarking & advanced transport; &, eliminate key currently existing approximations
  - Project 2. T-H: CFD development that complements capability in existing commercial codes;&, generate and incorporate Interface Treatment Method (ITM) results & experimental data into CFD subgrid models
- CASL team has vast experience with existing commercial and research tools, and leverages experience and funding from DOE-NE, Office of Science & NNSA





Requirements Drivers

- Accommodate tight coupling to CFD (including conjugate heat transfer), structural analysis, neutronics & fuel performance models
- Effort needed to attain mesh & physics fidelity required for detailed investigation of CASL Challenge Problems
- Algorithms must be scalable to take advantage of leadership class computing.
- Leveraging of NE, Office of Science, and NNSA funding is required to achieve goals

Outcomes and Impact

- MNM capabilities will contribute to
  - Meeting early CRUD and GTRF milestones
  - Coupled neutronic, CFD, structural, and materials performance capability
- VVERA will have multiple 3D "transport" capabilities on Day 1
- VERA will have latest CFD capability: both single- and multiphase, state-of-the-art subgrid models, coupled with & targeted towards specific reactor physics, running on the latest computer architectures.
- Primary success metric: Using the capabilities developed to gain new insight into the CASL Challenge Problems

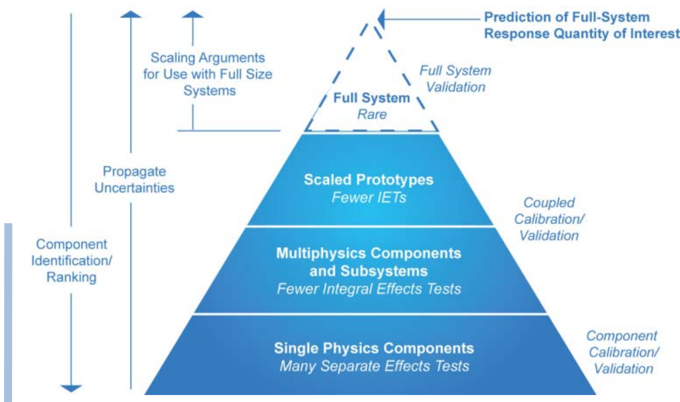
Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive M&S capabilities

Jim Stewart (SNL)
Dan Cacuci (NCSU)

Objectives and Strategies

- VUQ is dedicated to developing overall V&V approach
- VUQ *focus area projects:*
  - Project 1: Verification, Validation, & Calibration through Data Assimilation
  - Project 2: Sensitivity Analysis & Uncertainty Quantification
- VUQ has an experienced team across each of these areas
  - Mathematical foundations
  - Software (e.g. SNL's DAKOTA, Trilinos, and Encore toolkits)
  - Programs (e.g., NEAMS, LWRS, NEUP, ASC V&V)



Requirements Drivers

- V&V & UQ methodologies & tools are needed by every Focus Area
- VUQ is the CASL "integrator;" we need:
  - Access to software & underlying math models
  - Validation data (at all physical scales)
  - Partnerships with other Focus Areas to implement uniform VUQ practices

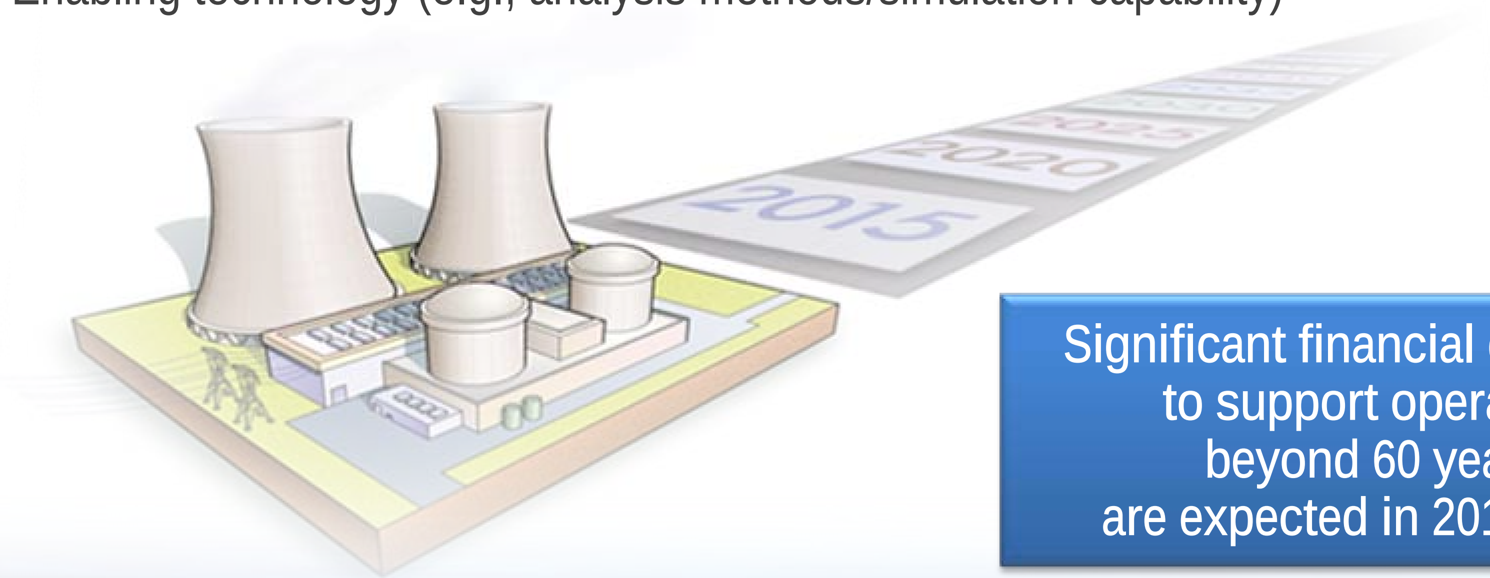
Outcomes and Impact

- Continuous evolution towards transformational, predictive M&S
- Capability to quantify & reduce uncertainties for the CASL challenge problems
- Ability to predict *with confidence* scenarios for which experimental data is not directly available
- Framework and tools to accomplish software V&V

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

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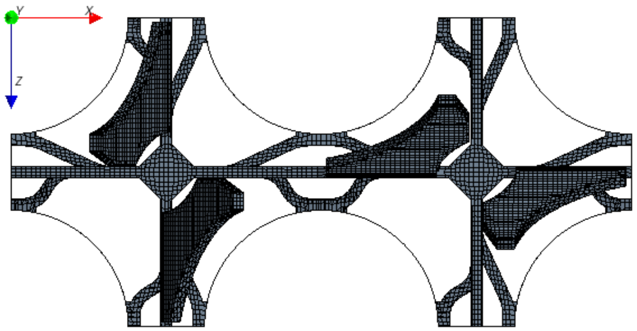
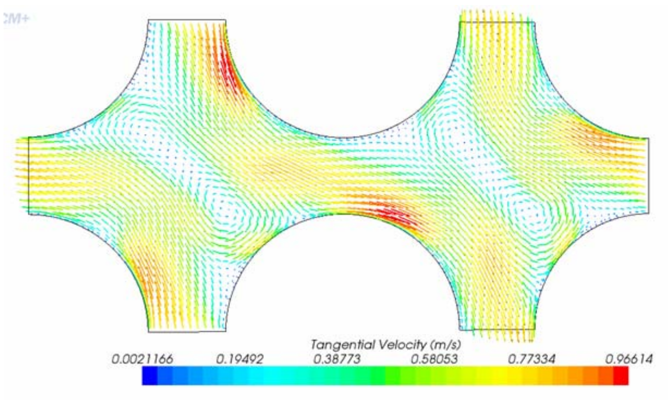
CASL Senior Leadership

CASL Technical Leadership

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

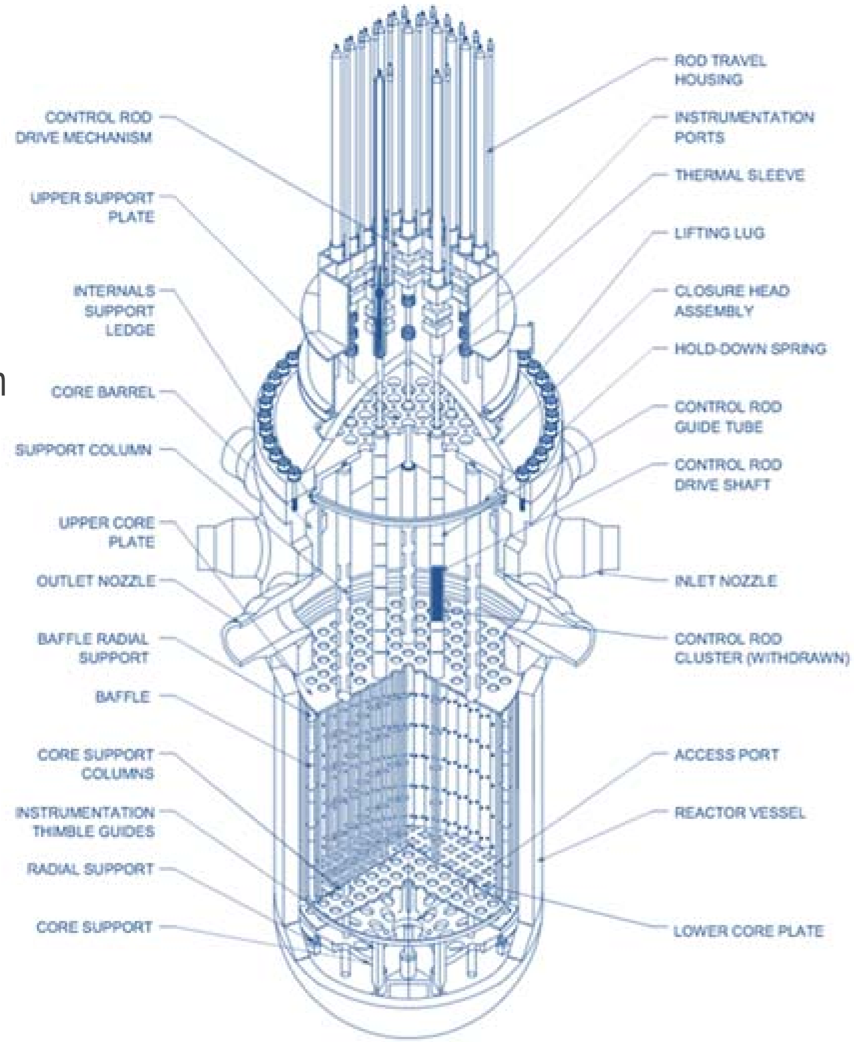




Need: High-fidelity modeling of complex flow and heat transfer for all pins in core downstream of spacer grids

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

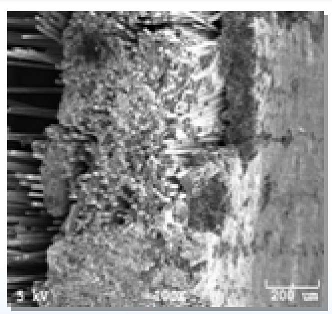


Need: High-fidelity tool to predict temperatures, stresses, and material performance (fatigue and cracking) over long-term operation

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

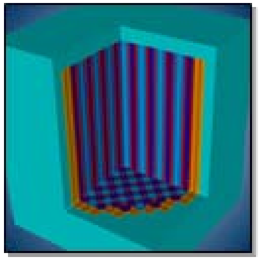
Challenge Problem	Description	Relevance
CRUD	CIPS: Deviation in axial power shape caused by CRUD deposition in high power density regions with subcooled boiling. CILC: Clad corrosion and failure due to CRUD deposition	Power uprates yield higher power density and an increased potential for CRUD growth, 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

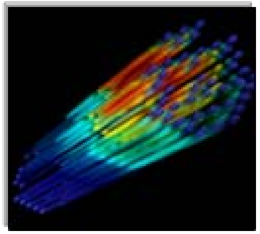
A Virtual Reactor developed and successfully applied to key challenge problems benefits the nuclear industry

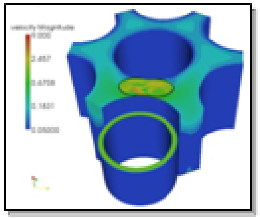
Challenge Problem	Description	Relevance
LOCA (Safety)	Numerous fuel failure modes resulting in fission product release and coolable geometry degradation	Realistic LOCA analyses (10 CFR 50.46) can enable power uprates that would not have been achievable with previously licensed evaluation models
RIA (Safety)	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

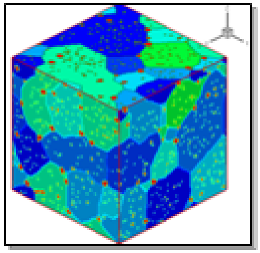
The CASL VR has a mature starting point

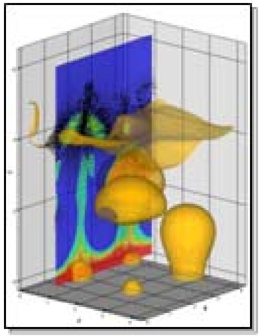
- Building on existing capability to deliver versatile tools
  - Initial focus on PWRs
  - Extensible to other reactor types
- Implemented as a component-based architecture integrating current and legacy workflows and capabilities
  - **Includes tools used to design and license the U.S. PWR fleet**
- 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





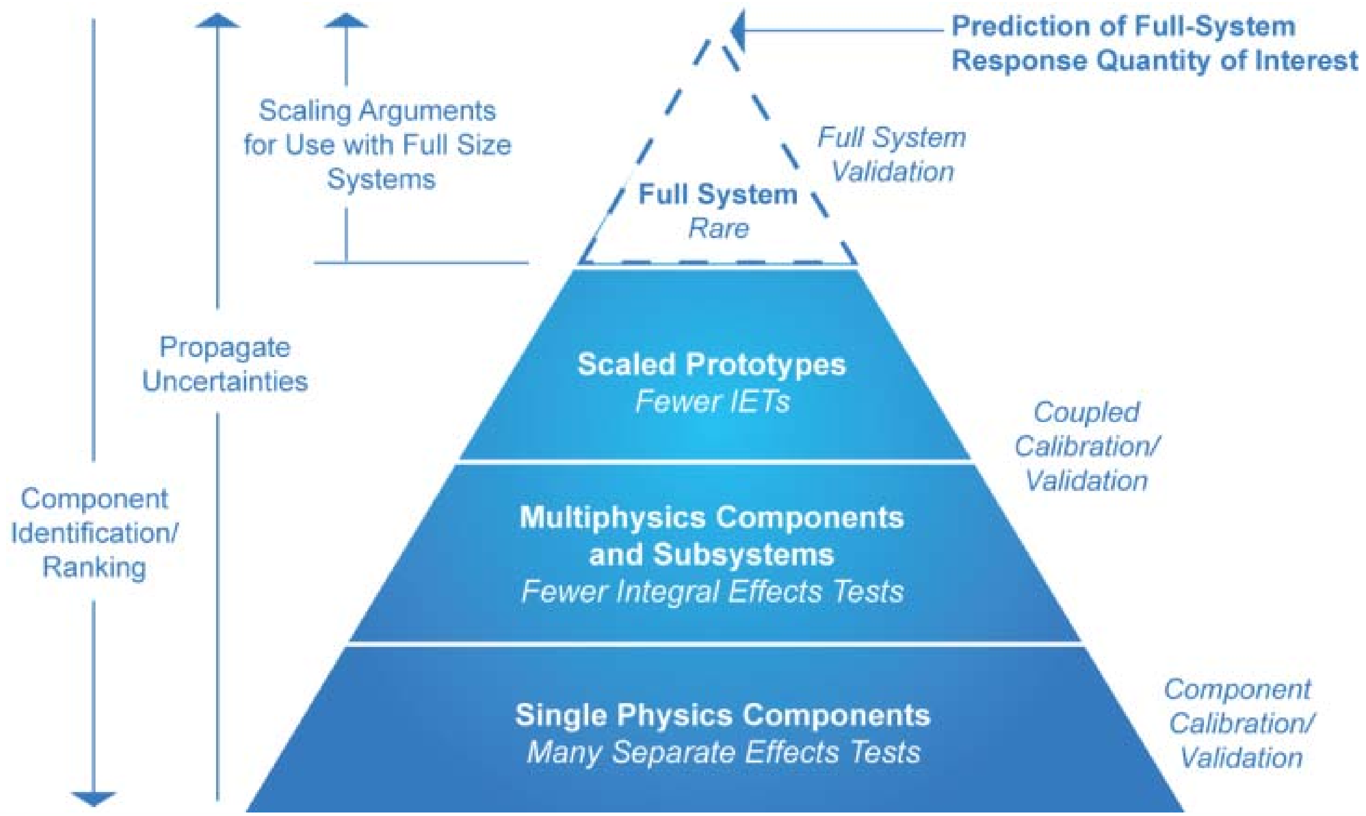






Denovo HPC Transport

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

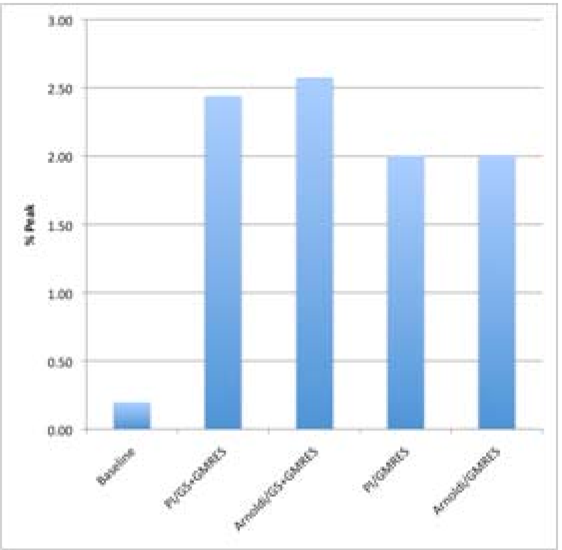


AMA

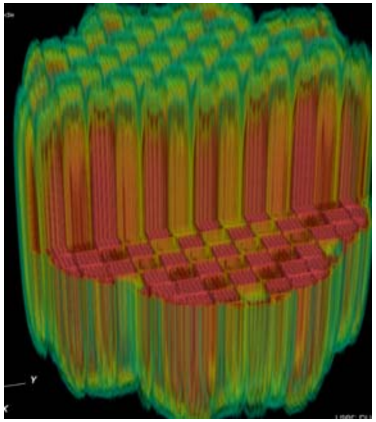
VRI

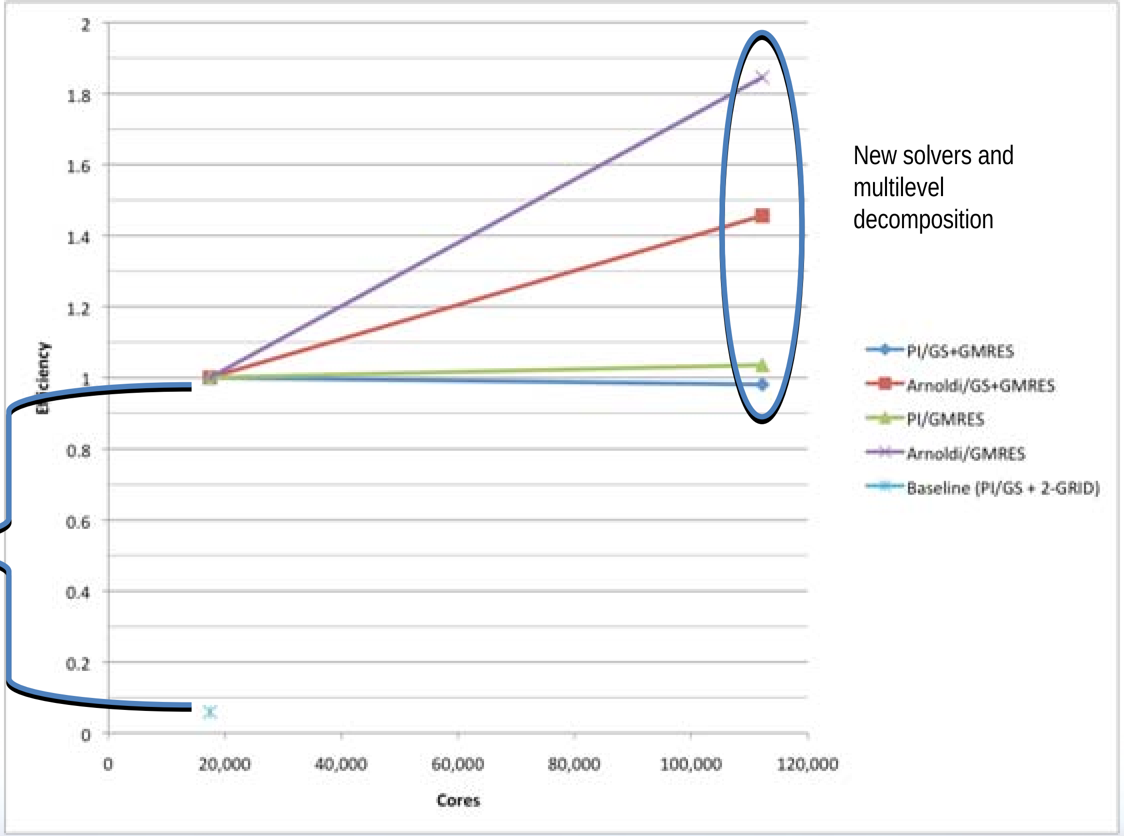
MPO
+
MNM

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)

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

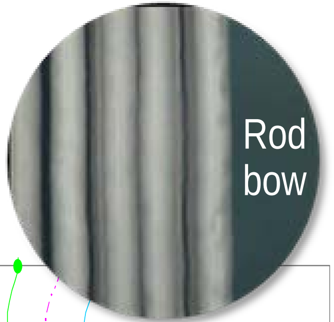
Safety	Operating	Design
• DNB safety limit • Reactivity coefficients • Shutdown margin • Enrichment • Internal gas pressure • PCMI • RIA fragmentation • Non-LOCA runaway oxidation • LOCA: PCT, oxidation, H release, long-term cooling • Seismic loads • Holddown force • Criticality	• DNB operating limit • 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

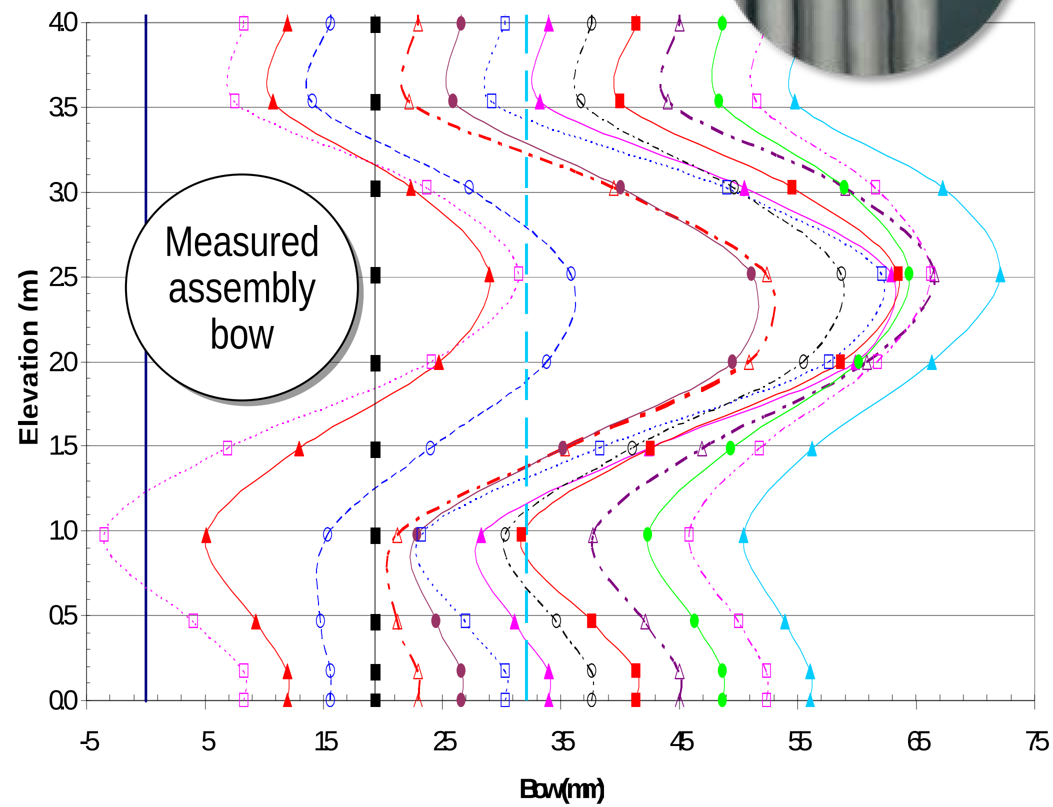
Source: *Fuel Safety Criteria in NEA Member Countries,* NEA/CSNI/R(2003)10

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





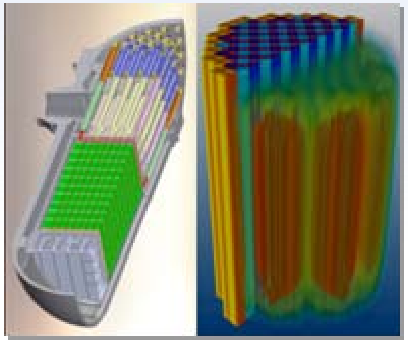
Can an advanced "Virtual Reactor" be developed and applied to proactively address critical performance goals for nuclear power?

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



Science-Based Nuclear Energy Systems Enabled by Advanced M&S at the Extreme Scale

Exascale workshop concluded that 4 areas have high priorities

- Integrated Performance and Safety Codes
  - Reactor core and safety simulations, nuclear fuel performance simulations, separations and safeguard simulations, waste forms and repository simulations, materials simulations
- Material Behaviors
  - Understanding the behavior of the materials in existing reactors that have been exposed to hostile conditions. This area also considers how to create advanced materials that can be part of future systems
- V&V and UQ
  - Improve the confidence users have in simulations' predictive responses and our understanding of prediction uncertainties in simulations.
- Systems Integration
  - Robust energy system analysis capability is critical to providing sound analysis of important policy decisions