CASL: The Consortium for Advanced Simulation of Light Water Reactors

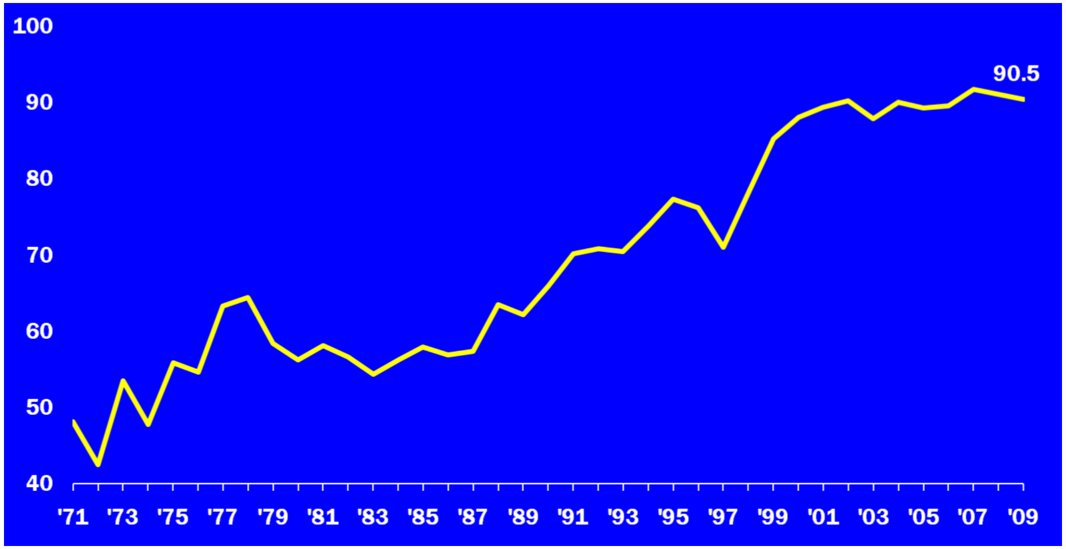
A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

CASL Project Summary Slides
August 1, 2011

CASL-U-2011-0137-000

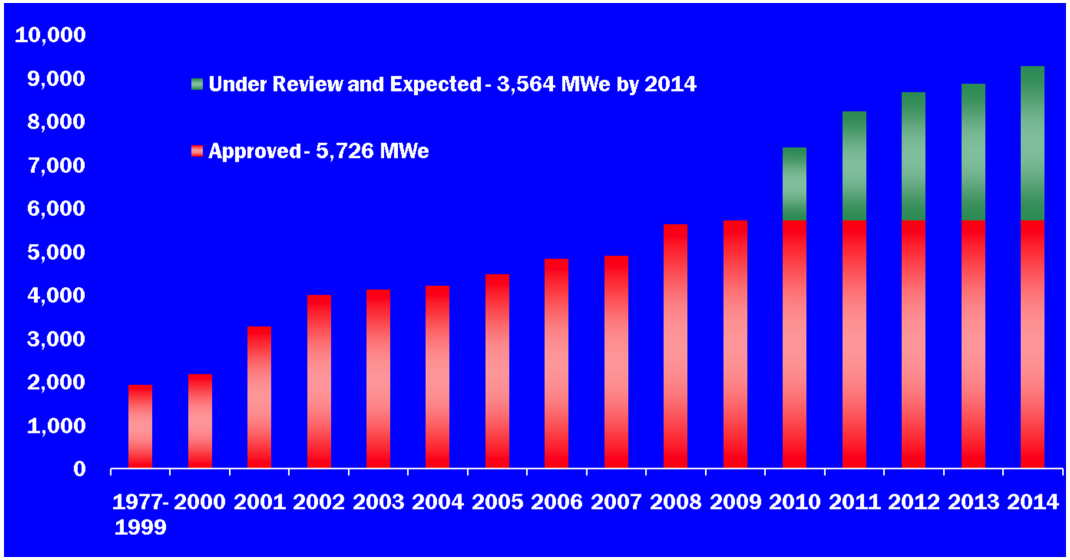
U.S. Nuclear Energy

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)

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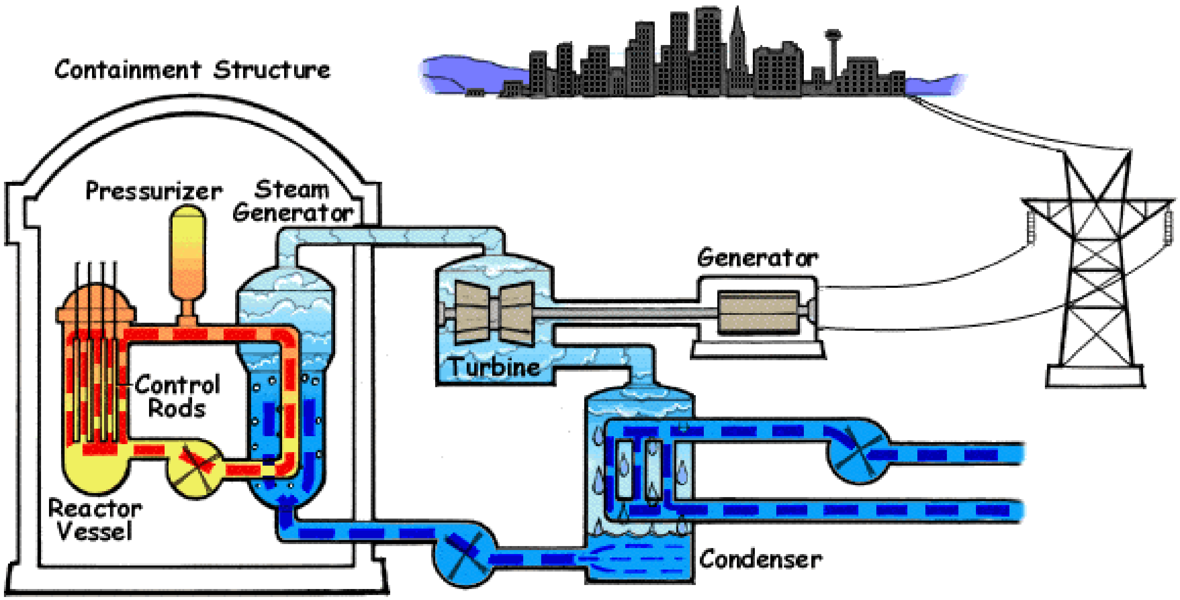
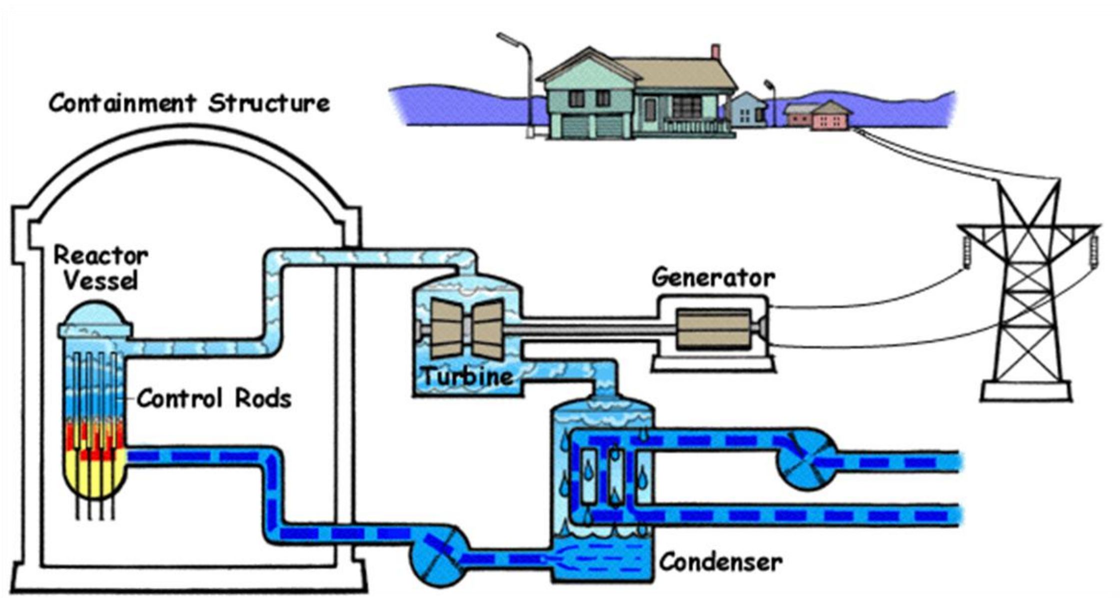
Common types of Light Water Reactors (LWRs)



Pressurized Water Reactor (PWR)



Boiling Water Reactor (BWR)

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

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

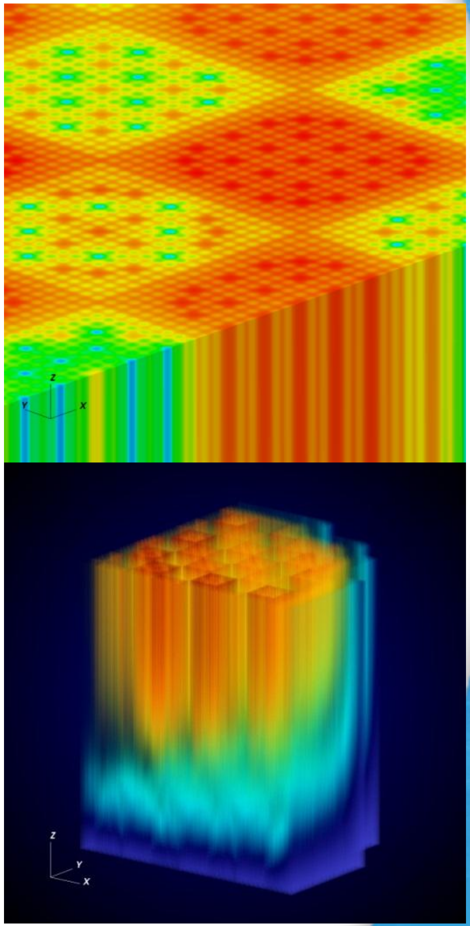
Source: *Fuel Safety Criteria in NEA Member Countries,* NEA/CSNI/R(2003)10

What is a DOE Energy Innovation Hub?

- 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
- Focus 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
  - Bring 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 Modeling & Simulation of Nuclear Reactors

- **Utilize existing** advanced modeling and simulation 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 real physical operation reactors to validate** the virtual reactor
- Lead organization with **strong scientific leadership** and a clearly defined central location (“one roof” plan)



The Consortium for Advanced Simulation of Light Water Reactors

Core partners

Oak Ridge National Laboratory, HQ

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

Individual contributors

Anatech
ASCOMP GmbH
CD-adapco, Inc.
City University of New York
Core Physics
Florida State University
Imperial College London
Notre Dame University
Pacific Northwest National Laboratory
Rensselaer Polytechnic Institute
Southern States Energy Board
Texas A&M University
University of Florida
University of Tennessee
University of Wisconsin

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

DOE Energy Innovation Hub Timeline for CASL

- 04/06/2009: Secretary Chu proposes 8 Energy Innovation Hubs
  - "mini-Bell Labs" focused on tough problems relevant to energy
  - $25M per year for 5 years, with possible 5-year extension
- 06/25/2009: House does not approve the 8 proposed Hubs
- 07/09/2009: Senate approves 3 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: Funding Opportunity Announcement released
- 03/08/2010: Proposals due (originally 3/1/10)
- 04/23/2010: CASL site visit at ORNL
- 05/28/2010: CASL selected
- 07/01/2010: Formal start date

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:

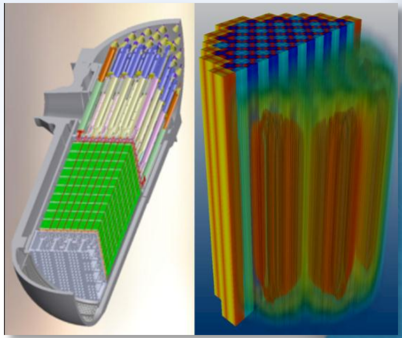
- Power uprates
- Lifetime extension

2

Reduce nuclear waste volume generated by enabling higher fuel burnups

3

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



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Each reactor performance improvement goal brings benefits and concerns

Power uprates

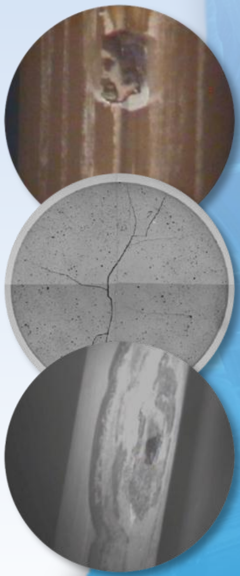
- 5–7 GWe delivered at ~20% of new reactor cost
- Advances in M&S needed to enable further uprates (up to 20 GWe)
- **Key concerns:**
  - Damage to structures, systems, and components (SSC)
  - Fuel and steam generator integrity
  - Violation of safety limits

Lifetime extension

- Reduces cost of electricity
- Essentially expands existing nuclear power fleet
- Requires ability to predict structures, systems, and components aging and life-cycle management
- **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)
  - Significant financial decisions to support operation beyond 60 years must be made in ~5 yrs

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



CASL scope: Develop and apply the “Virtual Reactor” 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

Key Challenge Problems Limiting Reactor Performance

	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	×		×

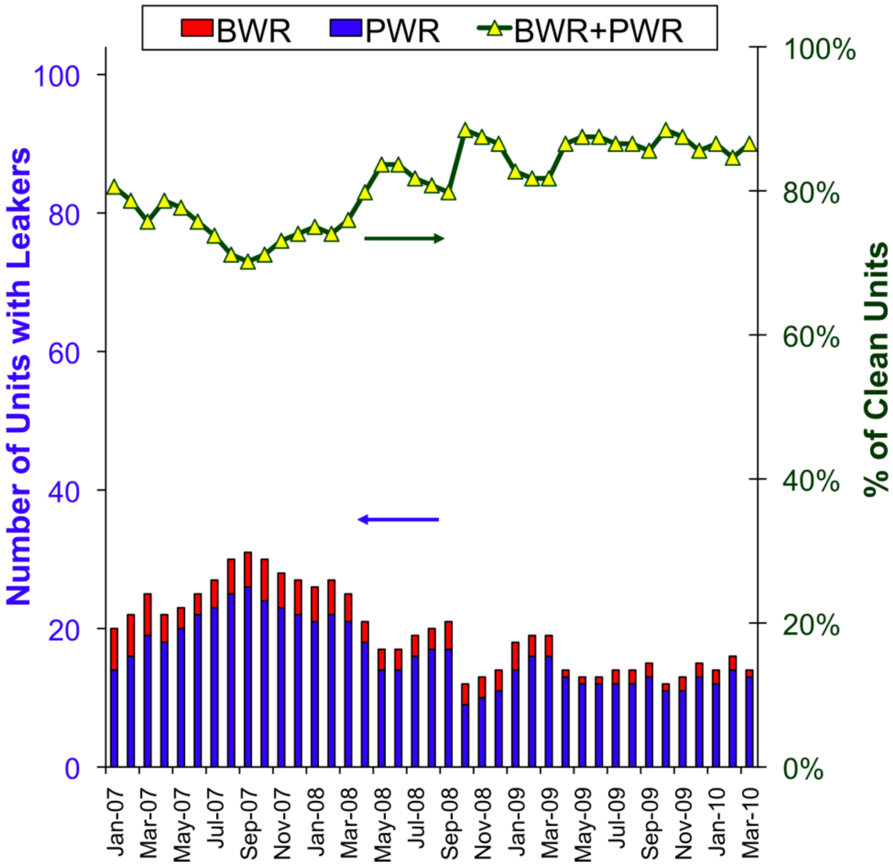
CASL Challenge Problems Drive the Virtual Reactor

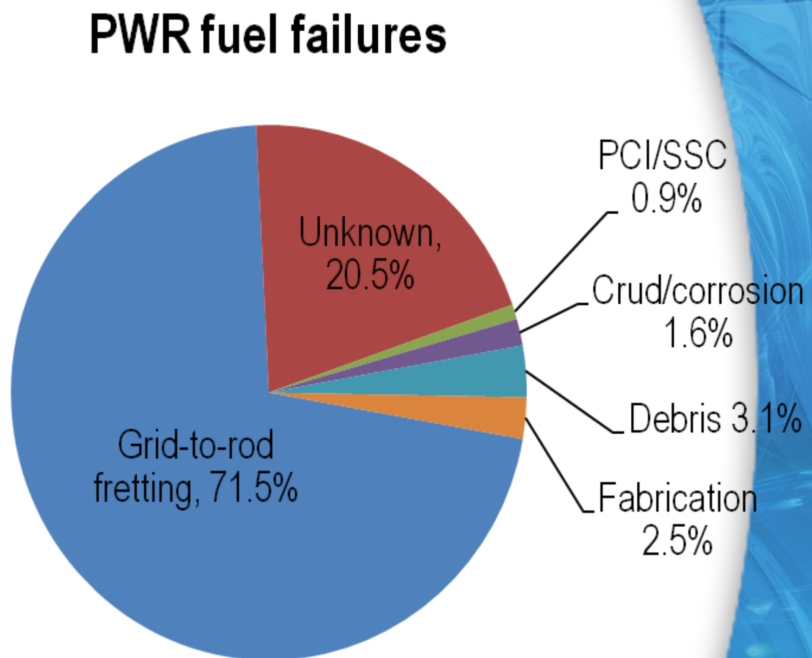
Challenge Problem	Description	Relevance
CRUD	CIPS: Deviation in axial power shape caused by CRUD deposition in high power density regions with subcooled boiling. CILC: Clad corrosion and failure due to CRUD deposition	Power uprates require higher power density with increased potential for CRUD growth, 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	Currently the leading cause of fuel failures in PWRs; power uprates and burnup can further increase potential for fretting failures
RPV Internals Lifetime (Life Extension)	Damage to RPV internal components 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 extended power uprates, higher fuel burnups, and lower fuel cycle costs than can be achieved by incremental modifications of current fuel forms

CASL Challenge Problems Drive the Virtual Reactor Development and Application

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 release 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
Reactor Vessel Lifetime (Life Extension)	Radiation damage resulting in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses during Safety Injection System (SIS) operation	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

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

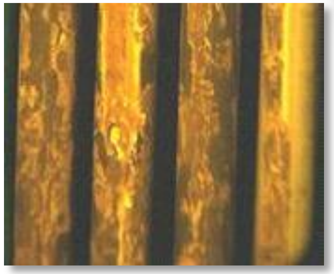




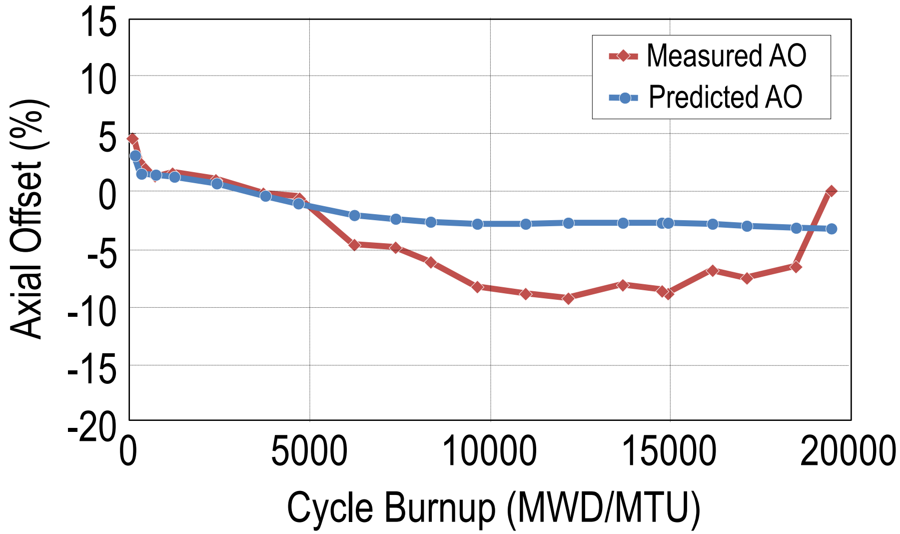
An effective virtual reactor M&S capability will permit proactive evaluation to enable critical performance enhancements

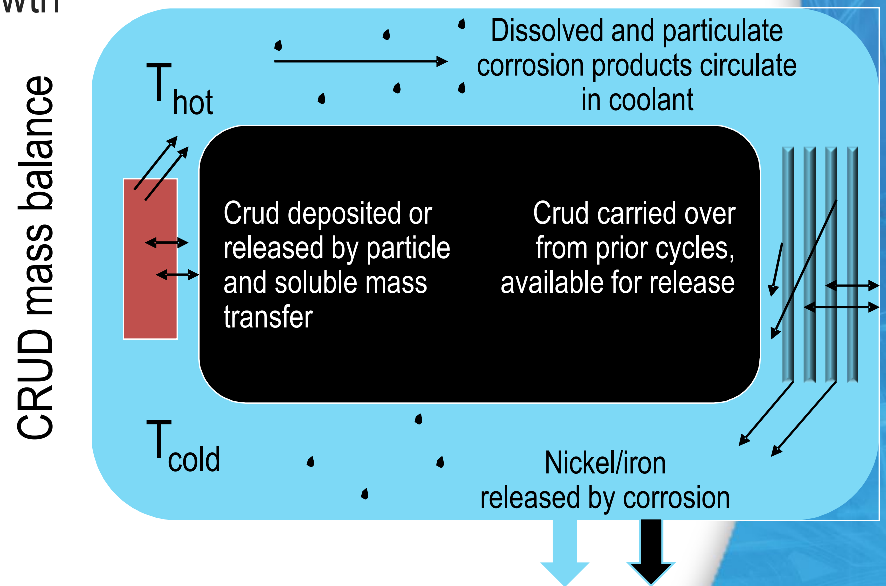
CRUD-induced power shift (CIPS)

- 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

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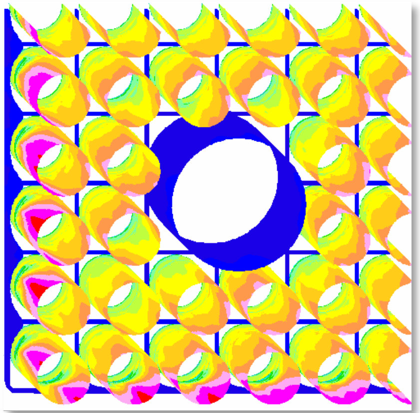
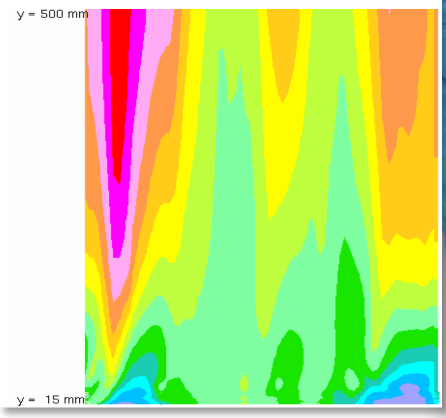
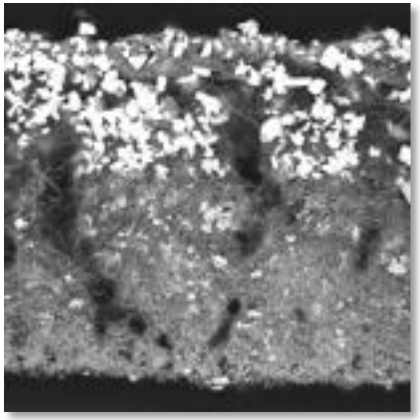
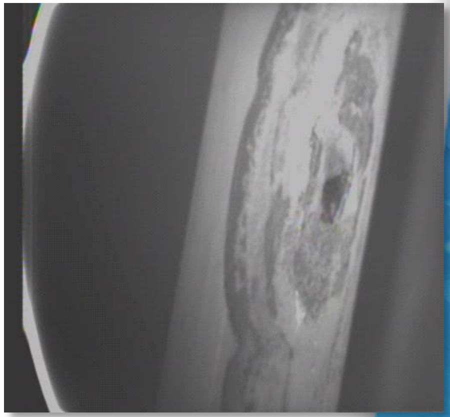
CRUD-induced localized corrosion (CILC)

- 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





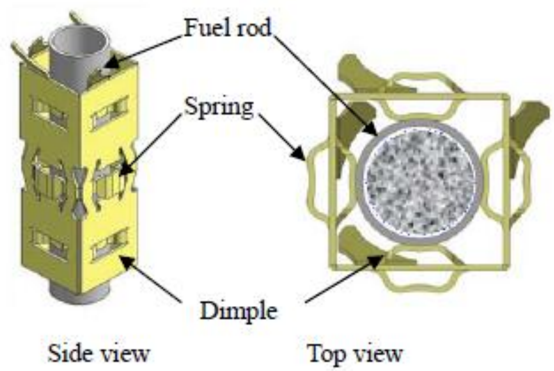


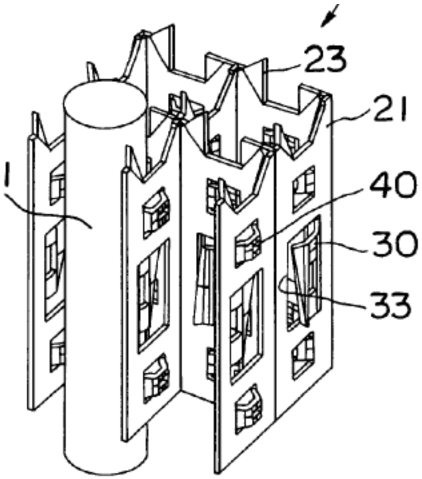


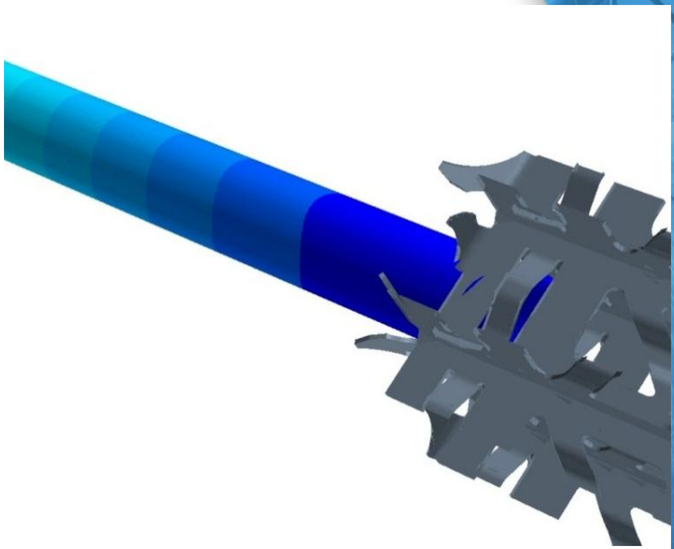
Need: High-fidelity, high-resolution capability to predict hot spots, localized crud thickness, and corrosion

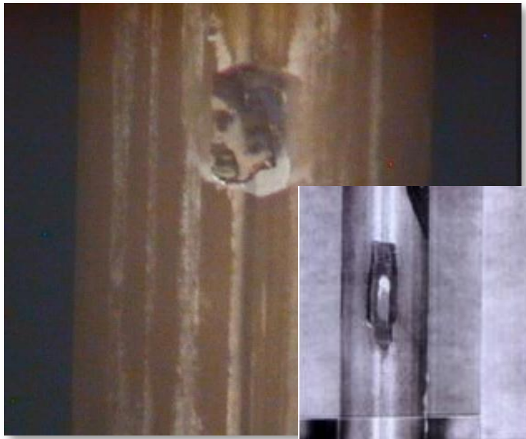
Grid-to-Rod-Fretting (GTRF)

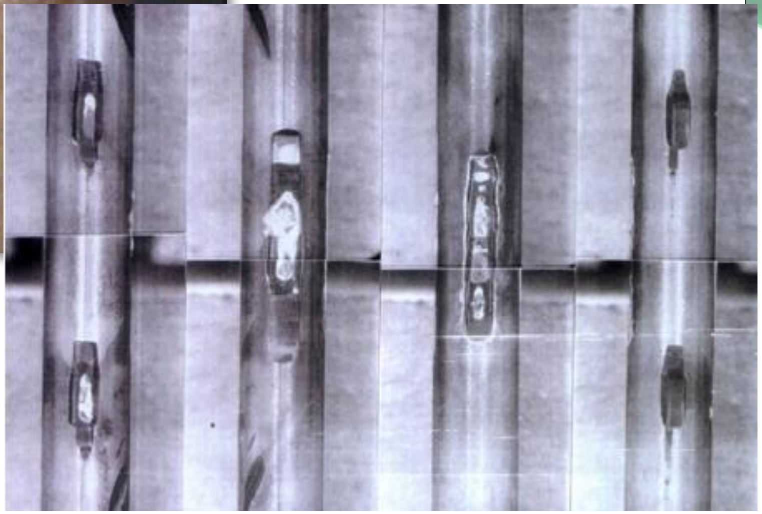
Spacer Grid with Springs/Dimples

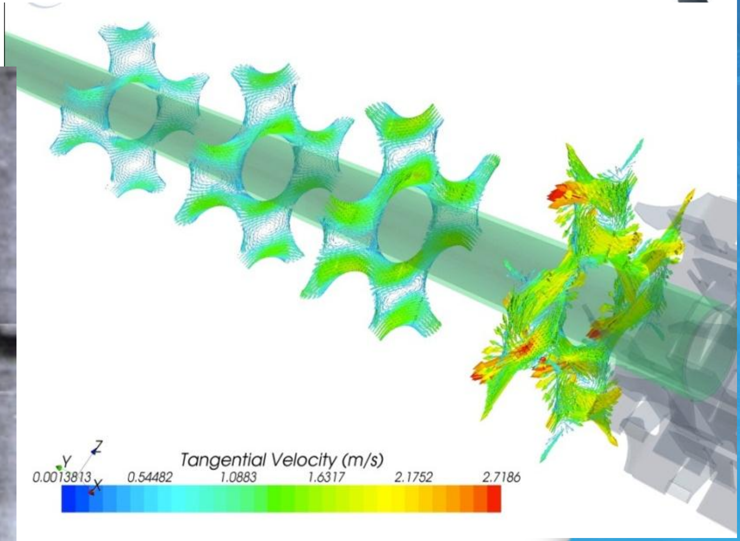












CASL's "one roof" approach

Single primary physical address	Strong, motivated, unified management team	Milestone-driven plan
• Extended and enhanced by a "virtual one roof" approach • New facility at ORNL, designed to provide highly collaborative work space • Virtual Office, Community, and Computing (VOCC) Project – Integration of best current and emerging technologies for collaboration to build an extended "virtual one roof"	• Monthly "collocation weeks" drive regular residency at CASL HQ (ORNL) • Practiced and proven in R&D program management • FAs: Lead + Deputy Lead – Broad coverage of science and engineering – Enables higher CASL residency for each FA leadership team	• Executed by multidisciplinary teams – 10 core institutions – Individual contributors with specialized knowledge and skills • Establishes annual commitments and reports quarterly progress • Drives collocation requirements

CASL's "virtual one roof" approach delivers maximum value

- Structured to ensure integration:
  - Coherent vision, clear goal, and well-defined milestones
  - Leadership by a strong and centralized management team
  - Processes to ensure well-informed and timely decision-making and program integration
- Utilization of existing infrastructure and equipment at partner institutions
  - Provide for close engagement of top talent
  - Accommodate academic and industry residency commitments
  - Enable leveraging of partner infrastructure and facility resources

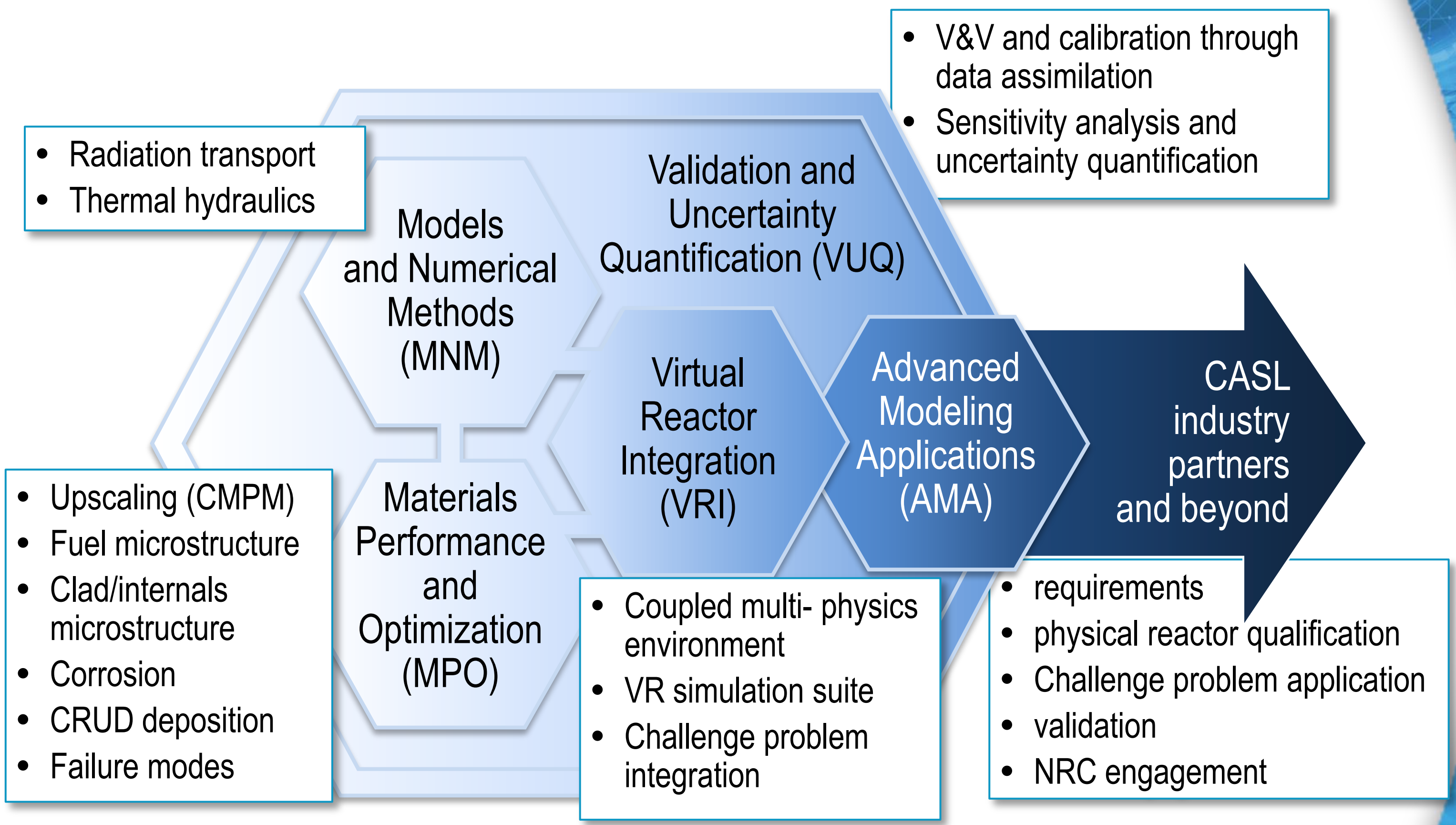
Ready access to exceptional and experienced leaders in science, engineering, applications, and design

CASL Collaboration and Ideation (C&I)

- Create a state-of-the-art scientific collaboration space to support the cognitive convergence of the best scientists, engineers, and industrialists available under “one-virtual-roof”
  - Understand CASL’s C&I needs
  - Evaluate existing and new tools and capabilities; make recommendations
  - Identify paths for R&D of technology gaps
- Our virtual one-roof efforts include
  - *Synchronous Communication*: Immersive Telepresence & video desktop collaboration
  - *Online collaboration tools*: Webex, ReadyTalk, EVO, Live Meeting
  - *Sharing data between electronic venues*: Conduit, CAVELIB, Chromium, Visit, etc.
  - *Connectivity to HPC resources*: democratization to all CASL partners
  - *Assist in human-computer interaction design for CASL end user*: standardize design and interaction

Problem solving at the speed of human insight

CASL Technical Focus Areas



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

Advanced Modeling Application (AMA) Focus Area

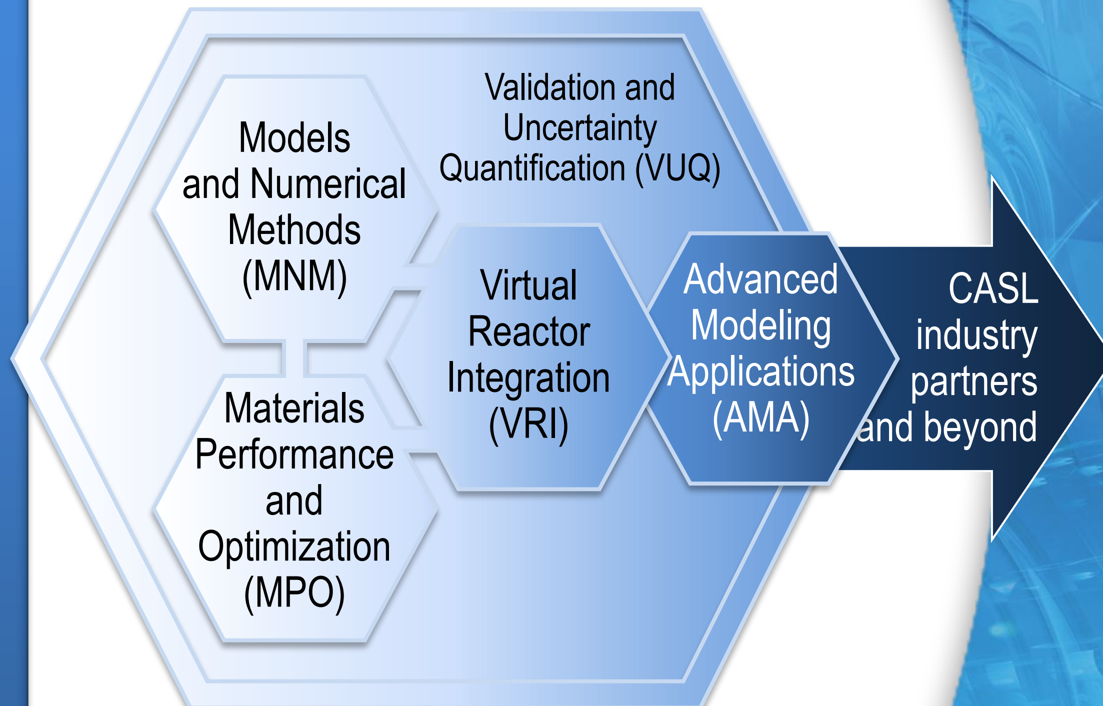
Driving development of VR to support real-world users and applications

Objectives:

Ensure that CASL VR meets user needs and requirements by setting requirements and assessing VR

Support development of VR that meets user needs by directly engaging users in:

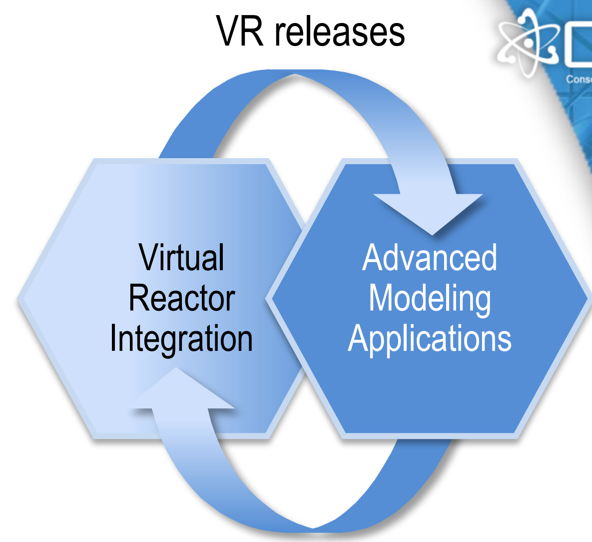
- Setting VR modeling requirements and assessment
- Performing VR validation
- Performing VR qualification with physical TVA reactor data
- Developing challenge problems and applications
- Supporting NRC engagement



AMA drives the VR development to meet the application needs to support industry applications for power uprates and life extension

AMA has strong connection to VRI and industry use of VR

- Enabling strong AMA/VRI collaboration, as needed for successful VR development:
  - Leadership co-location at CASL
  - Interaction with VRI via weekly meetings, code evaluation meetings, and day-to-day interactions at CASL
- Supporting demonstration in engineering environment
  - Key elements of AMA located on application/use site “test stands”
  - Coordination with CASL via on-line meetings, video conference, and project-specific messaging rooms
  - Physical reactor applications at TVA’s Watts Bar and Sequoyah nuclear plants



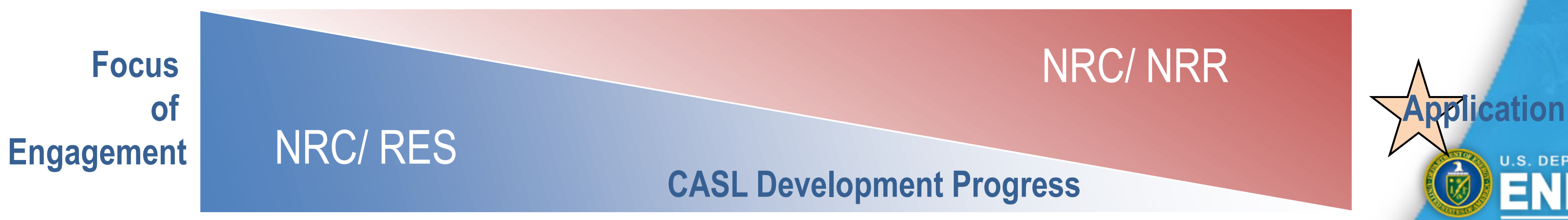
VR requirements and priorities
VR assessment of capabilities
VR qualification with physical reactor data and validation

Industry test stands

Westinghouse	EPRI
• Pittsburgh: Reload engineering and advanced fuels • Columbia: Fuel performance	• Charlotte: Industry interface • Palo Alto: Fuel management research

NRC Engagement - Overview

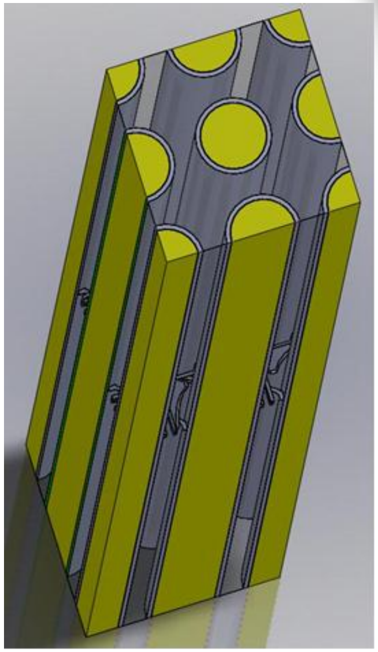
- **Final Objective: Inform, discuss, and exchange information with NRC Staff on CASL activities, approaches, and developments leading to NRC approval/licensing of applications using CASL developed methodology**
  - Familiarize NRC with CASL R&D and use of advanced M&S for nuclear reactors
  - Seek feedback and exchange on scope of work, developments, and approaches
- **Approach: Engage with RES and NRR**
  - RES: Interface in development of new M&S capabilities
    - Allow for review and technical feedback on CASL developments
    - Provide for exchange on V&V plans and results – a key issue of interest to NRC
  - NRR: Interface in the approval of new M&S capabilities
    - Keep NRR informed of progress and include in interaction process with RES
    - WEC, as the CASL vendor partner, will submit CASL-developed methods and coordinate interactions with NRR
    - Timing of this activity based on progress with RES and the viability of CASL capabilities to support physical reactors

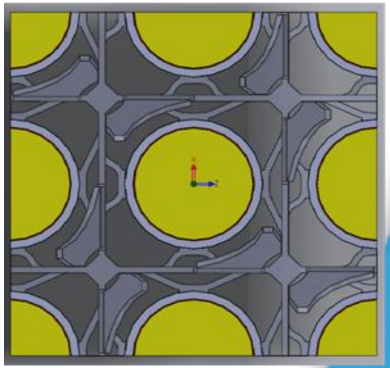


We Plan to Develop Advanced Tools as Guided by a Systematic Scale Up

From pellet to pin to 3x3 pin to pin fuel assembly to fuel assembly array to full core

- An appropriate plan for modeling, mesh mapping, and scale up will be developed for each challenge problem to provide a defined pathway to address the challenge problem and validate the solution.
- A suggested sequence for scale-up to demonstrate and validate challenge problem solution is the following:
  - Reduced pin geometry array standard test bench,
  - Full pin geometry array (for comparison to experimental test data such as VIPRE, Nestor, etc.),
  - Pin fuel assembly, fuel assembly array,
  - ¼ core geometry, full core geometry (with asymmetries)
- Define a 3x3 pin bench CFD/Neutronics model with 3D fuel rod where different multi-physics models can be developed and compared to available test data/validation problems
  - Crud, Corrosion, PCI, Rod Vibration & Fluid Structural Interaction, GTRF, PCI, Hydrogen, Primary Hydriding, DNB, Axial/Radial Growth
- Obtain validation data to support new model development





CASL is Integrating and Coupling Existing M&S Capabilities to Establish Challenge Problem Baselines

CASL-developed capabilities will be measured relative to this baseline

Fuel Perfomance (FP)

Baseline: link element of FP code to VIPRE-W

- Evaluate fuel temp, RIP, Corrosion Stress, Strain, Hydrogen, Growth, PCI
- Hot Cell, PIE, Halden, Stiudsvik data

CRUD / Corrosion

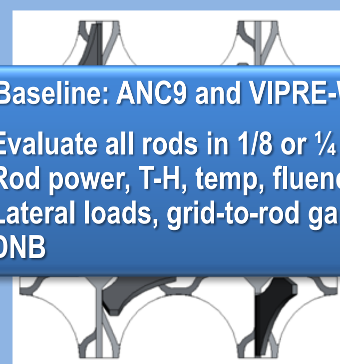
Baseline: link BOA to ANC9 and VIPRE-W

- Evaluate crud thk, boron uptake, clad corroion, CIPS, CILC
- WALT loop, PIE, Halden PIV, LDV, Nester , PSBT, MIT, Data

Baseline: link RETRAN, then RELAP5

•Evaluate DNB, RIA , LOCA
•CHF, CABRI, FLECHT, APEX, NSRR, Halden Data

Neutronics /CFD



Baseline: ANC9 and VIPRE-W

- Evaluate all rods in 1/8 or ¼ core
- Rod power, T-H, temp, fluence
- Lateral loads, grid-to-rod gap
- DNB

Advanced Materials

Link to 3D FEA Fuel Rod

•Evaluate fuel temp, RIP, Corrosion Stress, Strain, Hydrogen, Growth, PCI
•HFIR, Data

Fuel Assembly Distortion (FAD)

Baseline: link fuel bow tool to ANC9

- Evaluate assembly bow and impact on power and TH
- PIE Data

Grid to Rod Fretting (GTRF)

Baseline: link rod vibration tool to VIPRE-W

- Evaluate grid to rod gap, rod vibration & wear
- Westinghouse Labs, PIE

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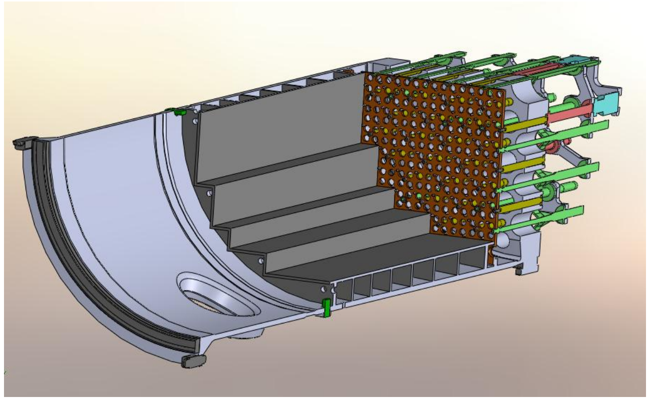
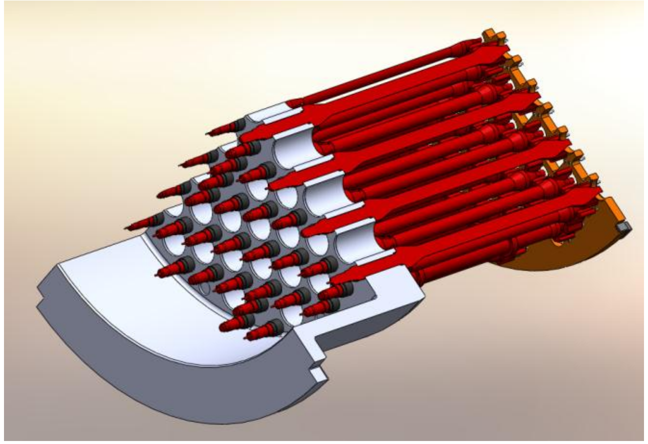
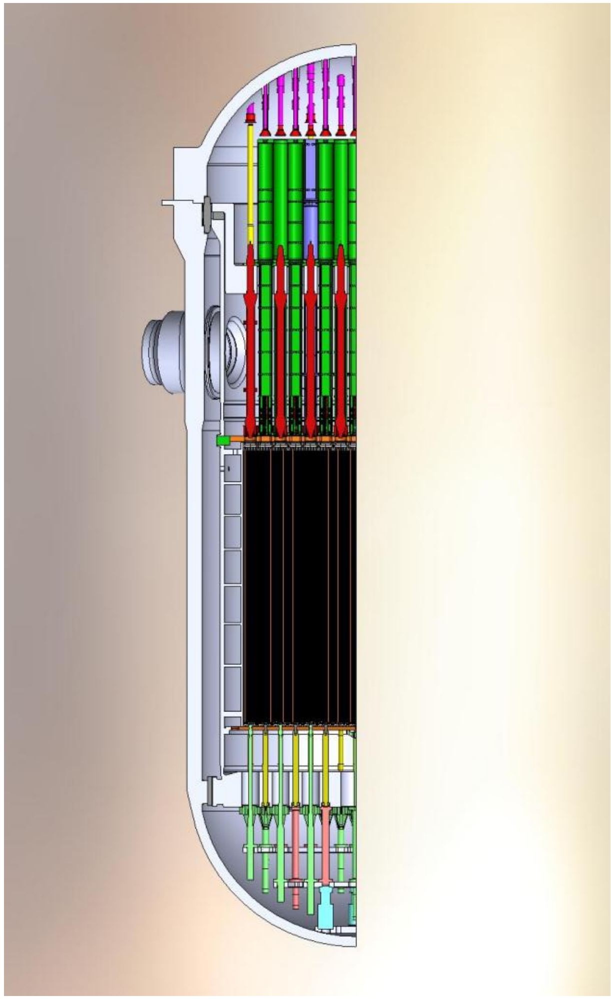
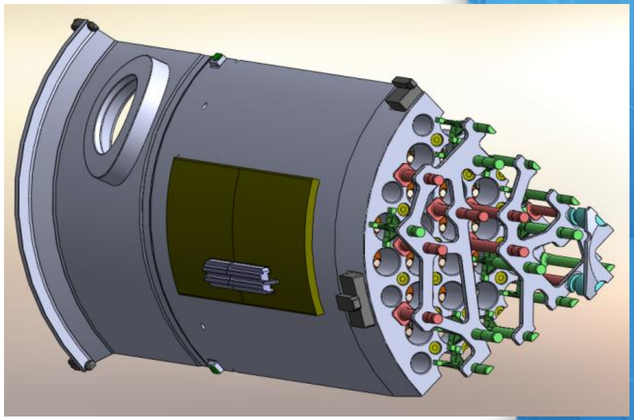
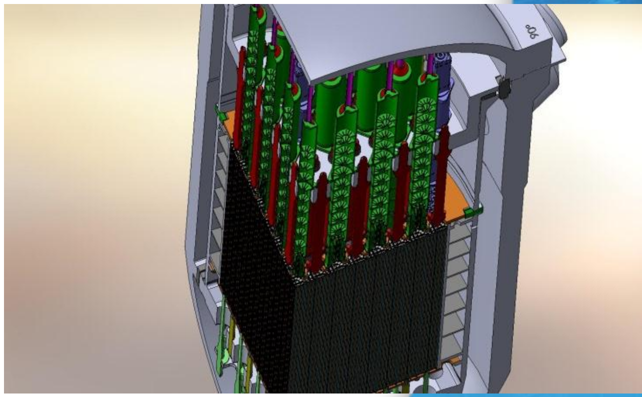
TVA Plant Model Development is Underway







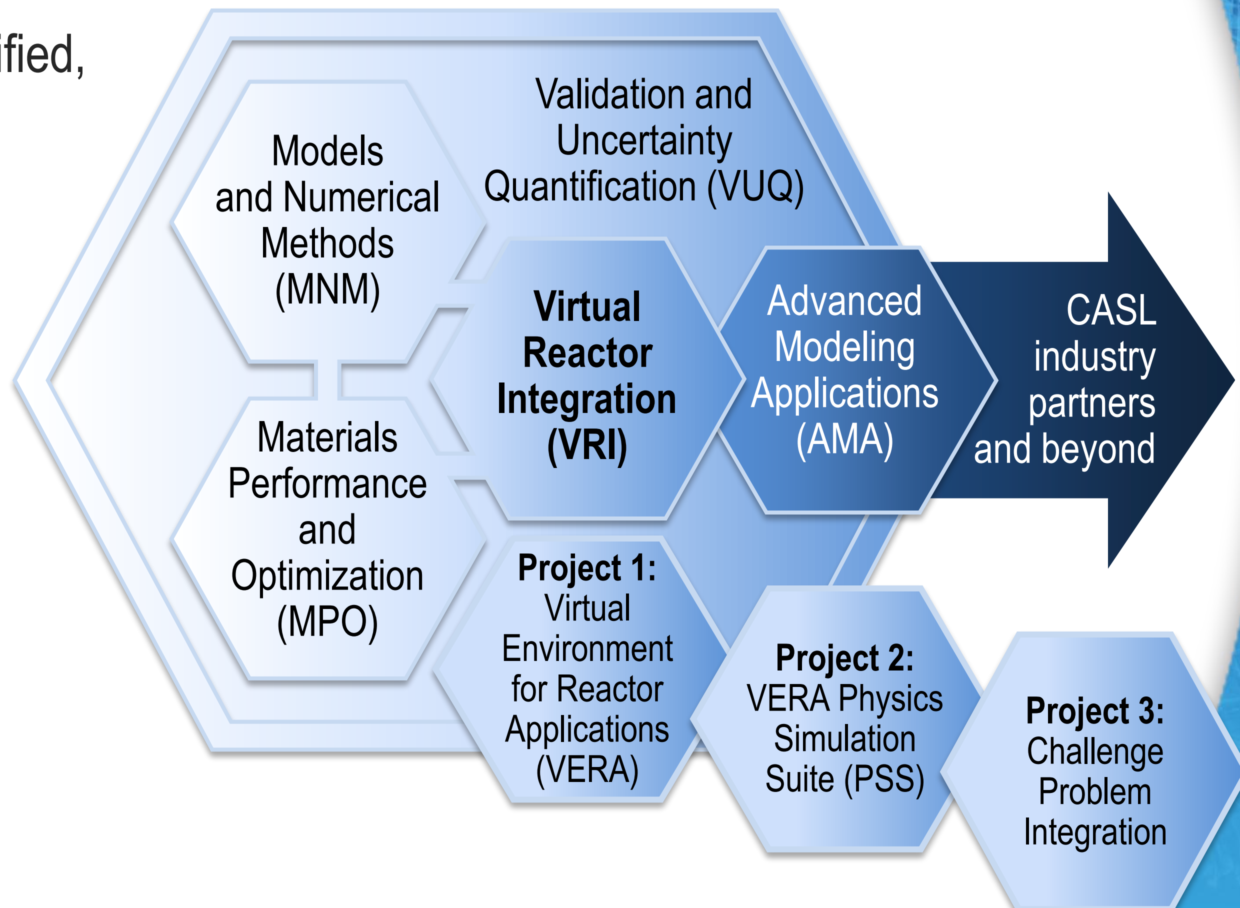




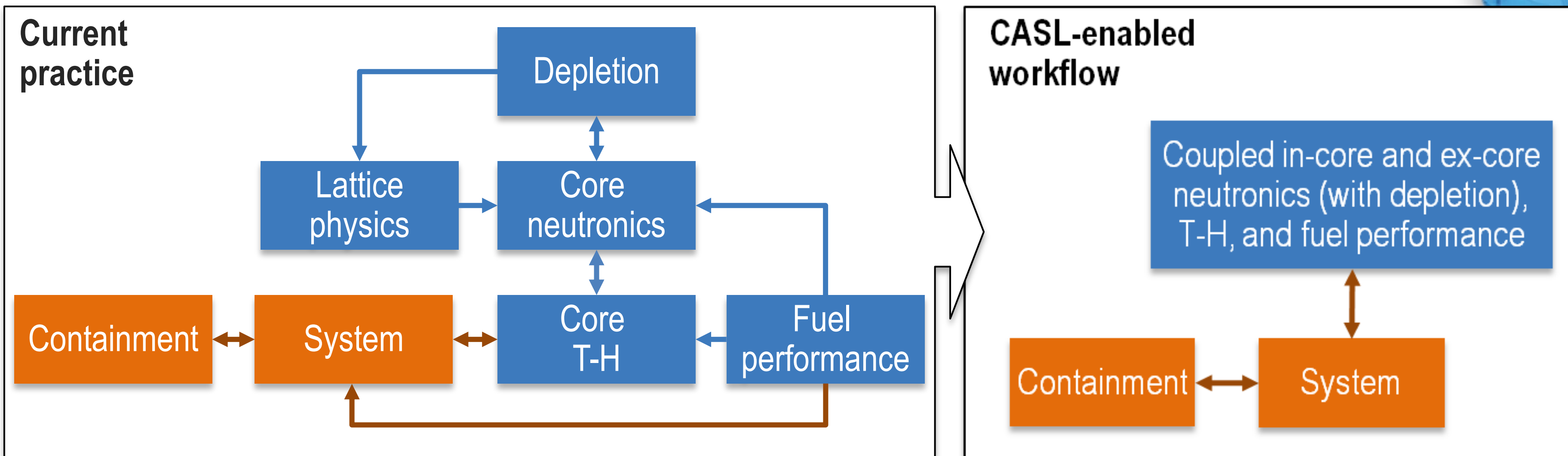
The Virtual Reactor Integration Focus Area is the conduit between science and design/engineering

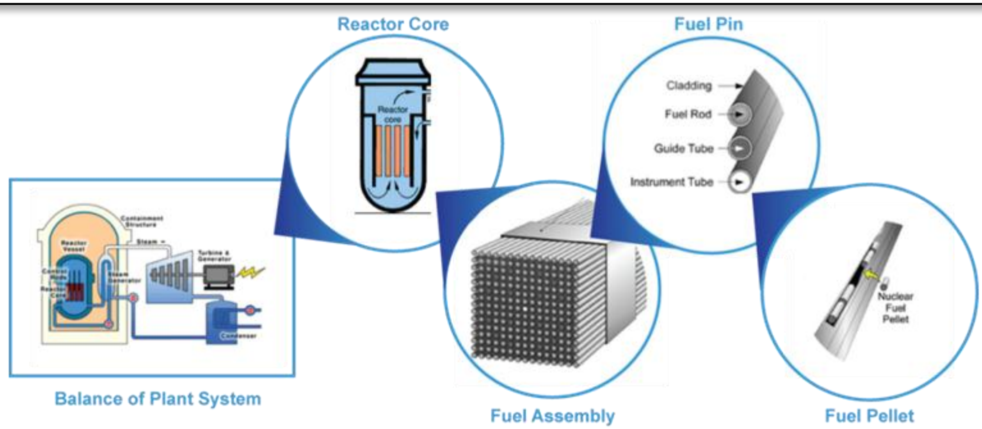
VRI will deliver

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



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





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

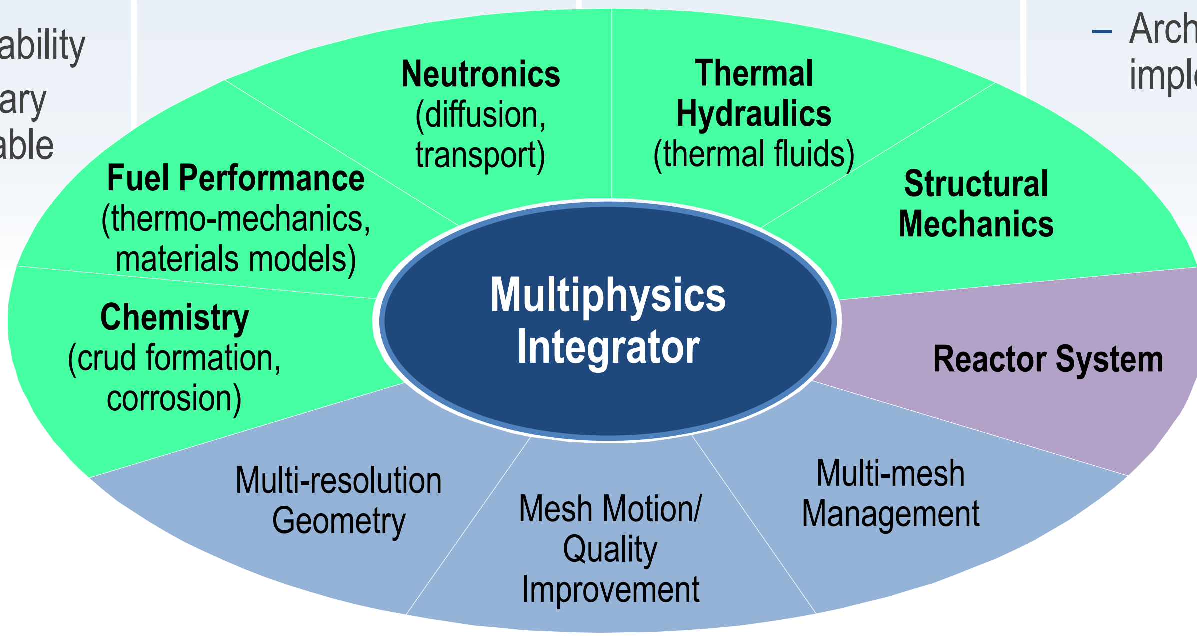
Virtual Environment for Reactor Analysis (VERA)
A code system for scalable simulation of nuclear reactor core behavior

- 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



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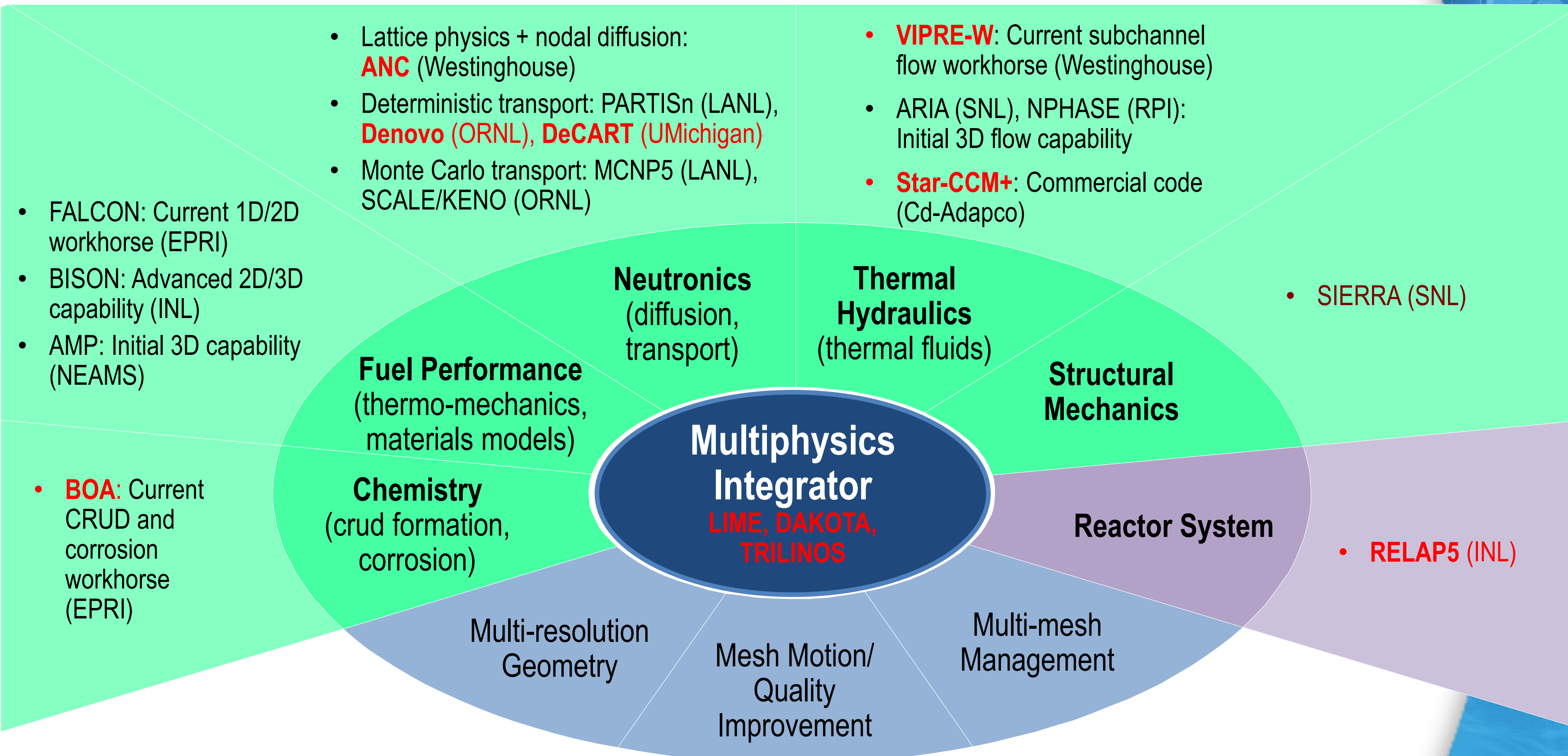
VERA builds on a foundation of mature, validated, and widely used software



VERA Version 1.0 release L2 milestone achieved on time on Mar 31, 2011

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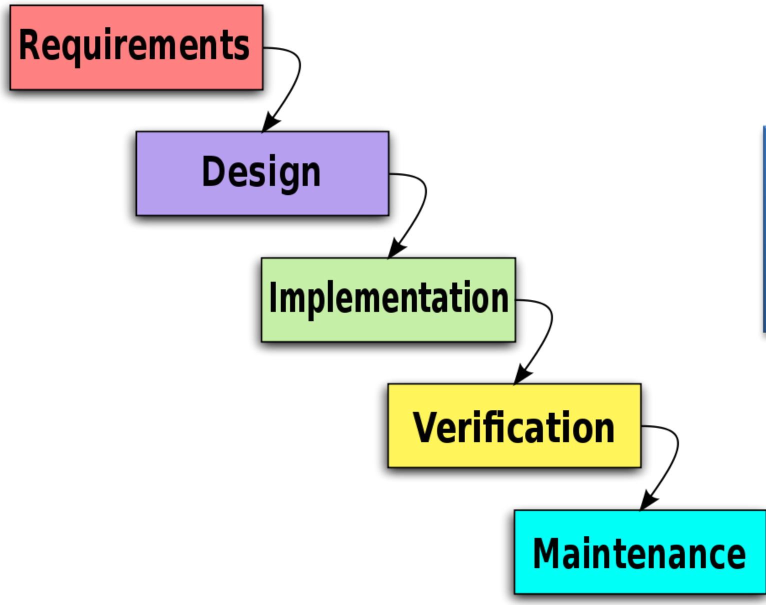
CASL is using Agile software development processes

- software development processes:
  - processes, practices and activities that drive software development
  - customer interactions (e.g. requirements gathering)
  - contract models
  - planning, day-to-day coordination, releases, etc.



Traditional waterfall approach is unable to accommodate changing requirements and research-driven projects.

CASL is using Agile software development processes

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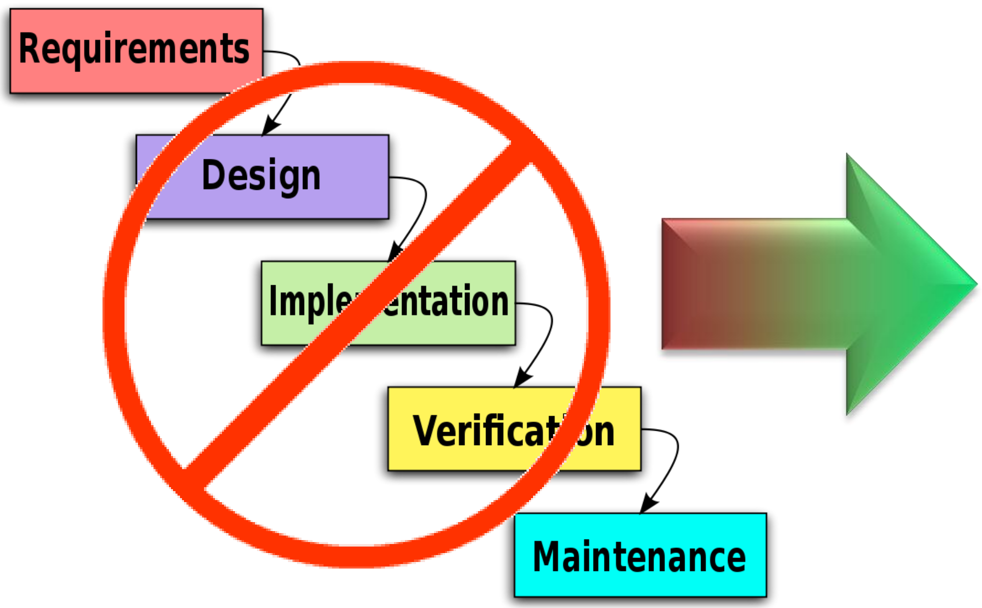
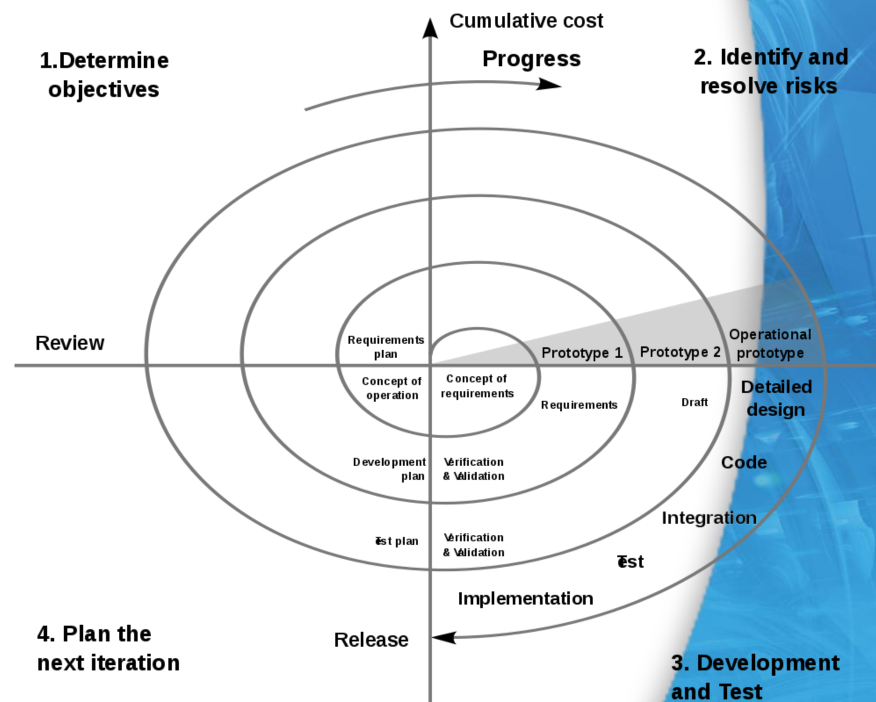




Agile methods fix Time (fixed iterations, fixed releases) and Effort (fixed team size) and vary Scope (functionality) based on iterative feedback.

Virtual Reactor (VERA) 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 (Sn, MOC) transport • Initial transient 3D (Sn, MOC) transport capability	• Full-core 3D pin-resolved (Sn, MOC) transport with T-H coupling • Initial 3D hybrid MC transport	• Transient full-core 3D pin-resolved (Sn, MOC) transport with T-H coupling • Full-core 3D hybrid MC transport with T-H coupling
Thermal Fluids with Conjugate Heat Transfer	• Subchannel legacy and commercial CFD • Continuum & 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 • Improved numerical methods & coupling	• Refined multiphase flow capability • Targeted methods & coupling advances
Fuel & Clad Performance	• 1.5D legacy capability • Phenomenological models & 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 performance and life extension predictions
Coolant Chemistry	• Legacy capability	• CRUD source terms & growth model	• Boron uptake in CRUD	• CRUD formation	• CRUD formation & induced corrosion
Structural Thermo Mechanics	• Assess and integrate existing capability	• Loosely coupled structural vibrations • Initial radiation creep & hardening models	• Fully coupled structural vibration for fretting	• Implicit nonlinear fretting • Improved radiation damage models	• Formally assessed structural vibration capability
Physics Coupling	• Legacy coupled via LIME • Subchannel transport & single-phase CFD	• Homogeneous cell transport & CFD • Initial FSI	• Improved FSI • Homogeneous cell transport, CFD, fuel, & chemistry	• Pin-resolved transport & CFD	• Full-core transport, CFD, fuel, chemistry, mechanics • Core + physical plant
Validation and Uncertainty Quantification	• DAKOTA for scoping UQ	• Time-dependent DA for parameters and responses • Model V&V procedures and initial databases	• Sensitivity and UQ for coupled components • Model V&V tools for selected modules	• DA with reduced-order modeling • Model V&V tools for selected coupled modules	• High-order DA including errors and uncertainties • Model V&V tools for coupled VERA system

MPO objective: *Deliver materials physics-based constitutive models to the virtual reactor for CASL challenge problems*

Near term effort

Incorporate available, engineering-scale fuel/clad/corrosion constitutive models into 3-D, high resolution coupled physics simulation capability (interfaced with virtual reactor);

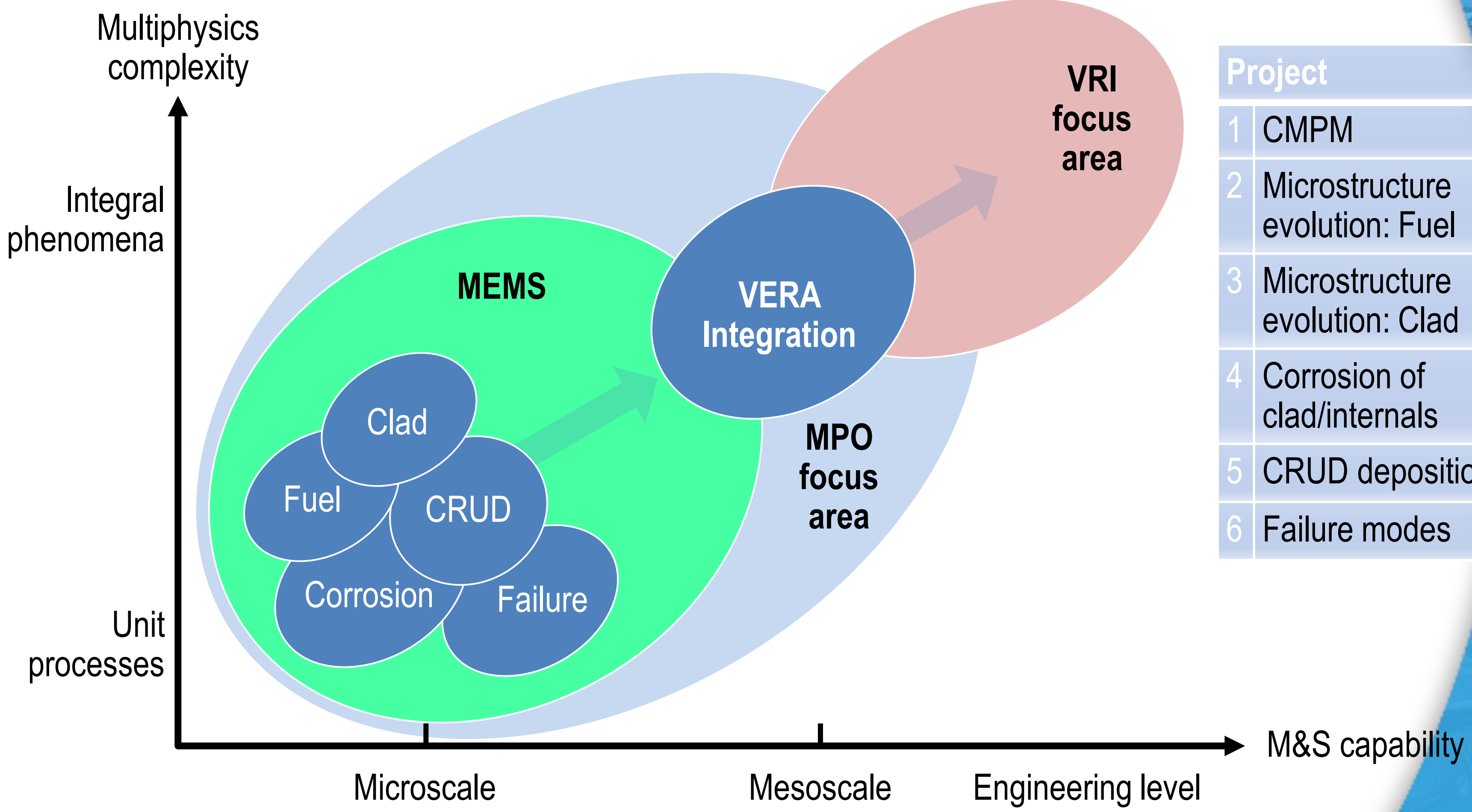
Initiate a series of microscale activities to provide mechanistic/physical insight into complex degradation phenomena corresponding to challenge problems: PCI, GTRF and CRUD

Intermediate and out-year effort

Microscale models will be used to refine physics-based constitutive relations that can address coupled environments of T, stress, reactivity, radiation, etc.

Improved constitutive models are then utilized by the virtual reactor for fully coupled neutronics, CFD, thermal hydraulics simulations of fuel behavior.

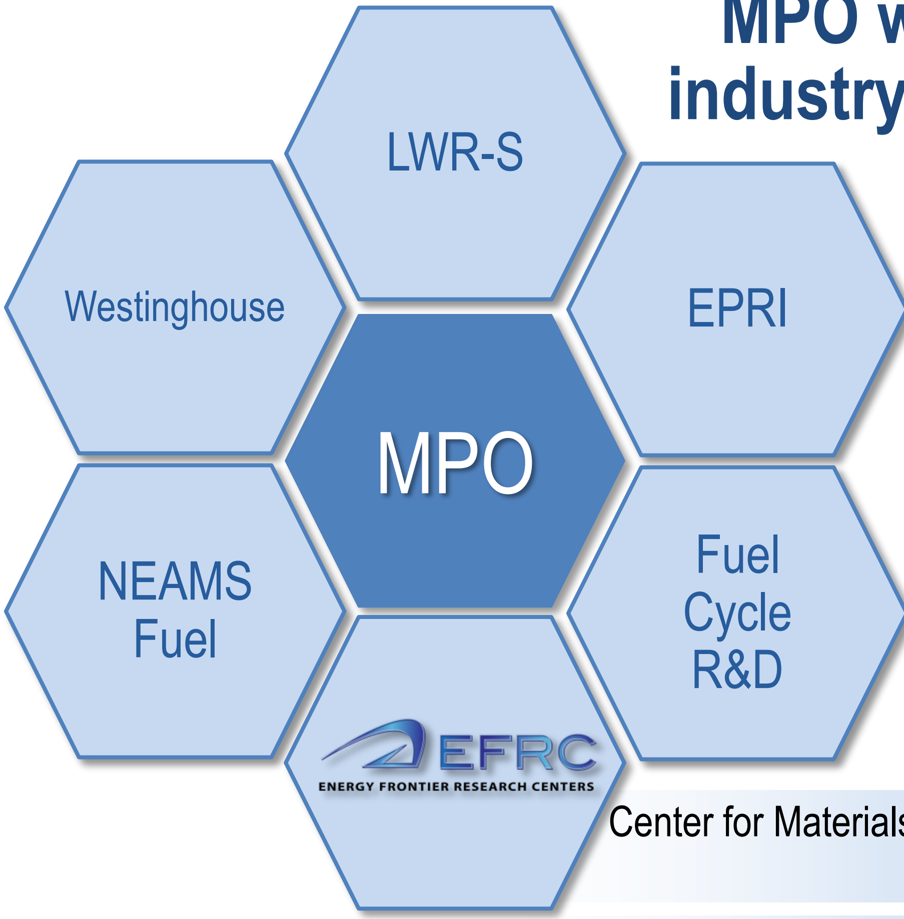
MPO science innovation is micro-meso coupling in both complexity of physical phenomena and modeling and simulation capability



Project	
1	CMPM
2	Microstructure evolution: Fuel
3	Microstructure evolution: Clad
4	Corrosion of clad/internals
5	CRUD deposition
6	Failure modes

Interactions: *External*

MPO will leverage existing DOE, industry, and university programs



Aggressive strategy requires cooperation with Office of Science, Office of Nuclear Energy, etc., programs for the development improved fundamental physics, mechanics and chemistry models

Center for Materials Science of Nuclear Fuel
INL/NCSU/UF/FSU

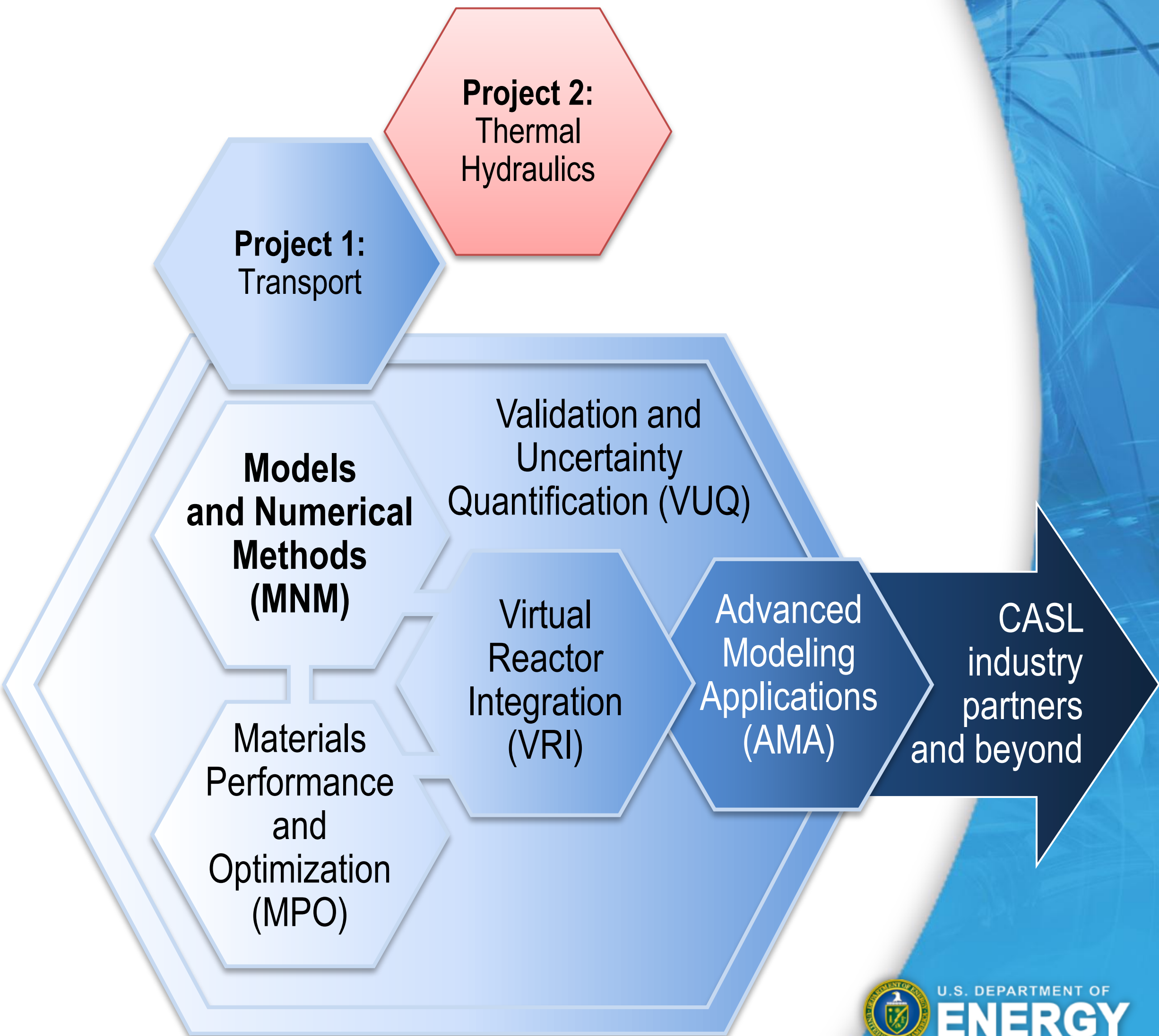
Extreme Environmental Tolerant Materials via Atomic Scale Control of Interfaces
LANL/MIT

Center for Defect Physics of Structural Materials
ORNL

MNM will deliver state-of-the-art transport and T-H simulation tools to the Virtual Reactor

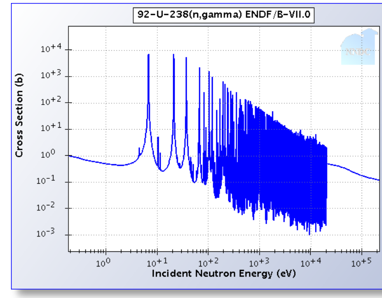
MNM Goals:

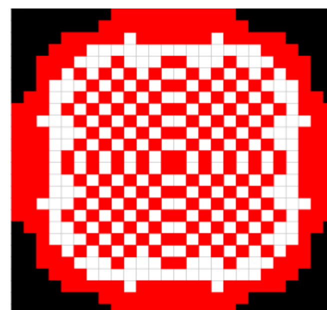
- Deliver next-generation, non-proprietary, scalable transport and T-H simulation tools to VRI, interfaced with the latest VUQ technologies
- Accommodate tight coupling of physics: neutronics, T-H, conjugate heat transfer, structural mechanics (GTRF), fuel performance

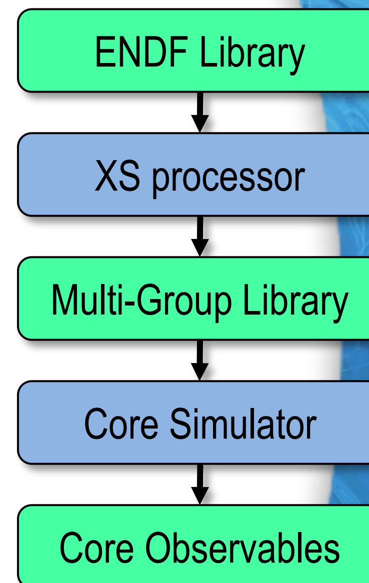


Specific goals for MNM Transport and T-H

Radiation transport	• Fully resolved capability to determine heat deposition rates, neutron fluence for isotopic evolution and radiation damage for generalized geometries and multiphysics feedback using deterministic and stochastic methods
Thermal-hydraulics	• Fully resolved CFD based multiphase flow and conjugate heat transfer capability for complex flow geometries and heat transfer surfaces with reduced dependence on empirical models and closure relationships
Numerical methods	• Methodologies in support of model implementation and multiphysics integration on parallel architectures







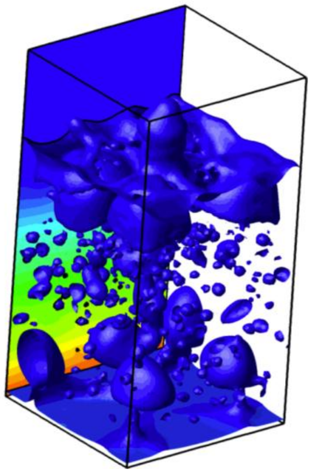
Improved predictive capability to foster improved product performance

MNM transport has 5 primary sub-projects

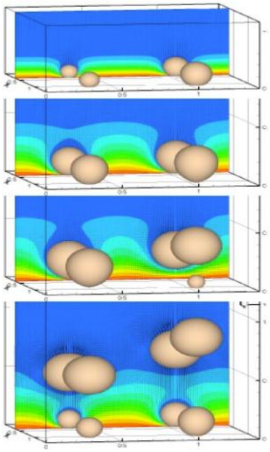
1. **Sn transport:** Development of non-proprietary, scalable, verified and validated 3D Sn transport code for steady-state and transient full core analysis *(Primary development path for deterministic transport)*
2. **MOC transport:** Development of non-proprietary, scalable, verified and validated 3D (or 2D/1D) MOC transport code for steady-state and transient full core analysis *(Alternation development path for deterministic transport)*
3. **Monte Carlo transport:** Continued development and enhancement of existing non-proprietary Monte Carlo codes for realistic full-core analysis
4. **General transport:** Development of generic transport methods including new energy condensation methods and transient methods
5. **Coupled transport:** Development of low-order/high-order coupling techniques for tight coupling of multiphysics to neutronics

MNM T-H has two primary sub-projects

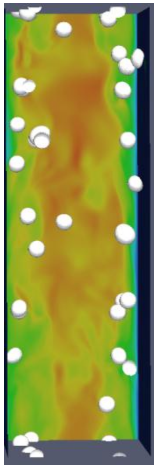
1. **Computational Fluid Dynamics (CFD)**: Development of non-proprietary, scalable, verified and validated *macroscale* CFD tools, that complement capability in existing commercial codes
2. **Interface Treatment Methods (ITM)**: Generate *microscale* simulation results and experimental data for CFD closure models and validation



Simulation of film boiling from a flat surface (D. Lakehal)



DNS simulation of bubbles growing and detaching from four prescribed nucleation sites (G. Tryygvason)



Wall-peaked low quality bubbly flow (M. Podowski)

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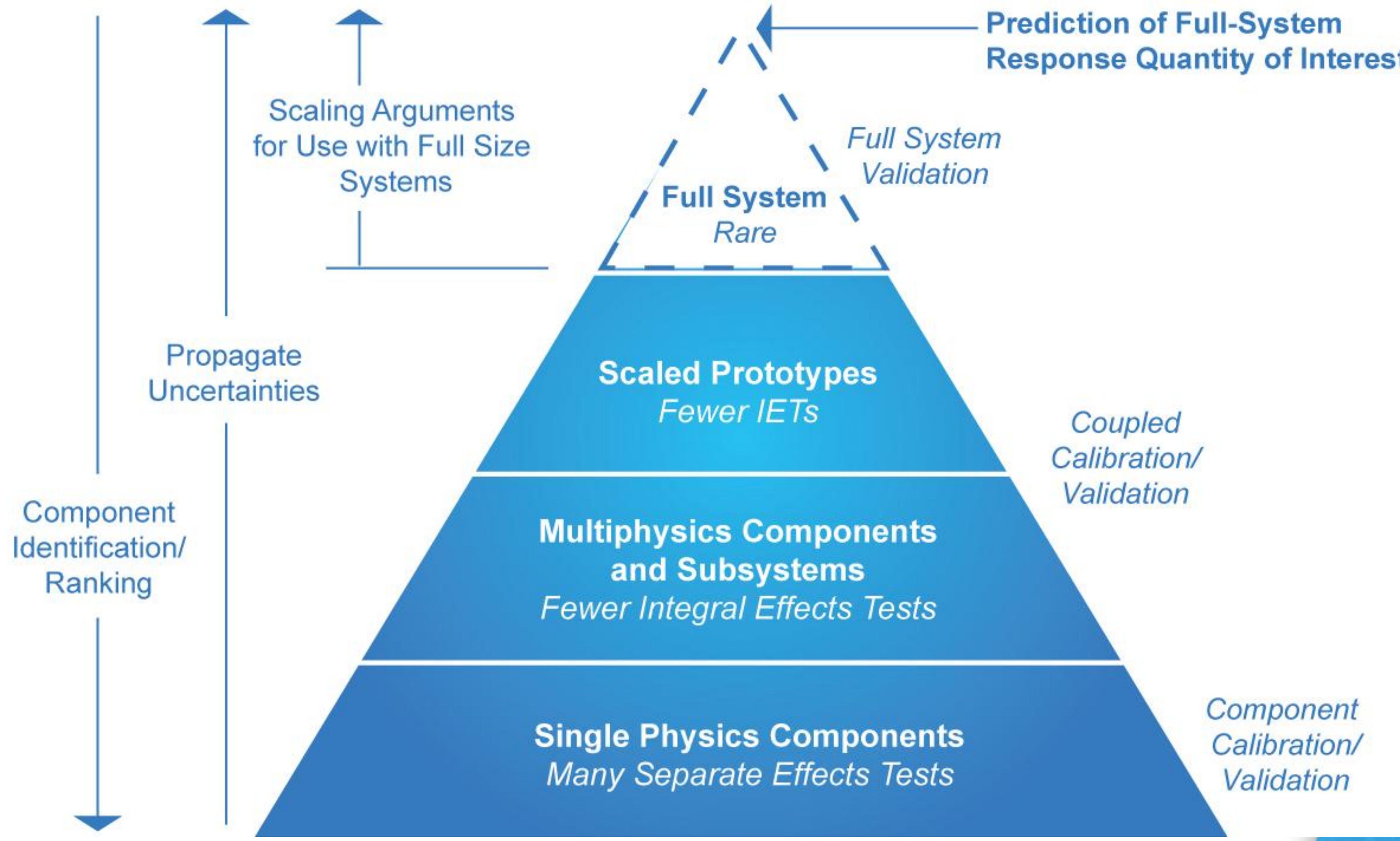
Validation and Uncertainty Quantification (VUQ)
Achieving credible, science-based predictive M&S capabilities



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Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive M&S capabilities

Consortium for Advanced Simulation of LWRs

- VUQ is dedicated to developing overall V&V UQ approach
- We will develop and deliver **new methods** for the VUQ *capability areas*
  - ✓**Project 1**: Verification, Validation, and Calibration through Data Assimilation
  - ✓**Project 2**: Sensitivity Analysis and Uncertainty Quantification
- VUQ has an **experienced team** across each of these areas
  - ✓**Mathematical foundations** (supported by publications)
  - ✓**Software** (SNL's DAKOTA, Trilinos, and Encore toolkits)
  - ✓**Complementary programs** (e.g., NEAMS, LWRS, ASC V&V)

Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive M&S capabilities

Requirements Drivers

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

Outcomes and Impact

- **Continuous evolution** towards transformational, predictive M&S.
- Capability to **quantify** and reduce **uncertainties** for the CASL challenge problems.
- Ability **to predict *with defined confidence*** scenarios for which experimental data is not (directly) available.

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 virtual reactor (VERA) against challenge problems

Validation data support plan

CASL
Consortium for Advanced Simulation of LWRs

Data sources

- Plant and in-core diagnostics
- PIE of used fuels
- In- and out-of-pile testing of prototypic fuels
- Separate-effect tests
- Integral effect tests

Knowledge/data base

Acquire and use [TVA] plant and PIE measured data to support VR-based data assimilation

Near term (1–3 years)

Review, collect, qualify, and use selected past experimental data for validation of VR-critical models and methods

Identify and rank needs, develop recommendations and support design of experiments to support VR validation (in coordination with other programs, e.g., LWR-S, NEUP, EPRI)

Years 4–7:
VR validation and UR-guided experiments operational, including tests conducted under auspices of CASL in phase II

- Operational conditions
- Fuel performance (crud, corrosion, fretting, failures)
- Fuel behavior and capacity limits
- “Elementary” physics (T/H, S/M, M/S)
- Multi-physics and system dynamics

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

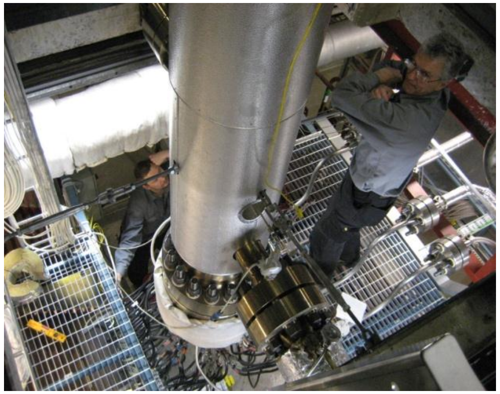
Westinghouse Test Facilities will Support Validation

But more data is always needed

VISTA Loop 5x5 testing
pressure drop & vibration

FACTS Loop Single Assembly
Pressure drop and vibration

VIPER Loop Dual Assemblies
Rod Vibration and Wear



Oden Loop 5x5 and 6x6
DNB and Mixing tests

WALT Loop single rod
CRUD and thermal testing

Mechanical Assembly Test
Forced Vibration & Seismic/LOCA

Overall CASL Cadence

- CASL is executing per 6-month *Plan of Record (PoR)* tasks, deliverables, and milestones
  - Imposes more agility and flexibility in our plan and actions
- We plan to release our virtual reactor (VERA) regularly and follow an evolutionary delivery life cycle
  - Place our M&S products into hands of users early and often
  - Follow quarterly "treadmills": science delivery, release, assessment, solution
- We encourage & need collaborations and partnerships to succeed
  - This is too hard of a problem; our partnerships (formal and informal) will likely change as we encounter new problems and solve old ones

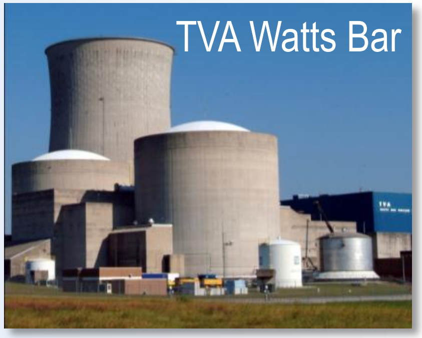
CASL will need industry interaction and collaboration and the leveraging of other DOE Programs to succeed

CASL is applying a remarkable set of assets

- A U.S. team focused on U.S. leadership in nuclear energy
  - Carefully picked to leverage and pair partner strengths
  - A distinguished record of LWR regulatory and design accomplishments
- Industry partners are embedded to assure relevance and focus
  - Representing the entire U.S. nuclear industry landscape: Vendors, owner-operators, R&D for nuclear utilities
- Implements a new paradigm: University-industry-lab leadership balance
- Unparalleled collective institutional knowledge and nuclear science and engineering talent
  - The lead DOE laboratories in science, nuclear energy, and national security
  - Preeminent university nuclear engineering programs (Core + contributing partners: 7 of top 10 nuclear engineering programs)
  - Intimately connecting key science challenges to the nuclear energy enterprise: Unmatched expertise in materials science, chemistry, nuclear engineering, and multi-scale/multi-physics computational science
- Leaders in HPC (top 3 systems) and computational science (production code)

Executing a clear, milestone-driven technical strategy for real-world NPP solutions

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

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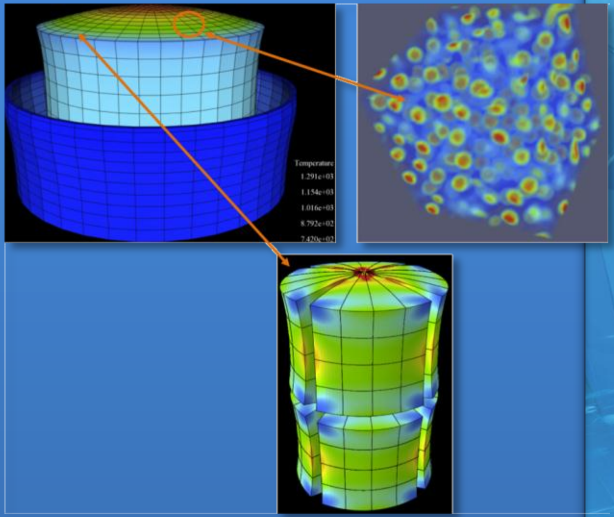
CASL legacy:
A preeminent computational science institute for nuclear energy

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

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