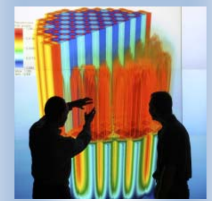
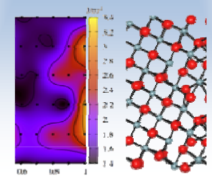




# CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

Douglas B. Kothe (ORNL)

CASL
Consortium for Advanced Simulation of LWRs

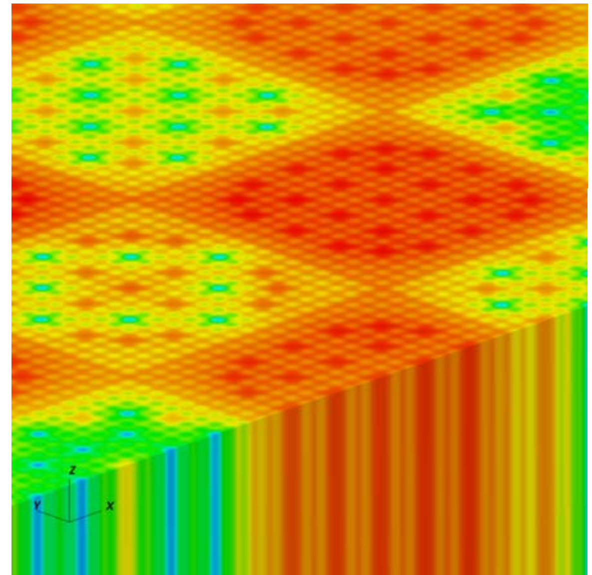
U.S. DEPARTMENT OF ENERGY | Nuclear Energy

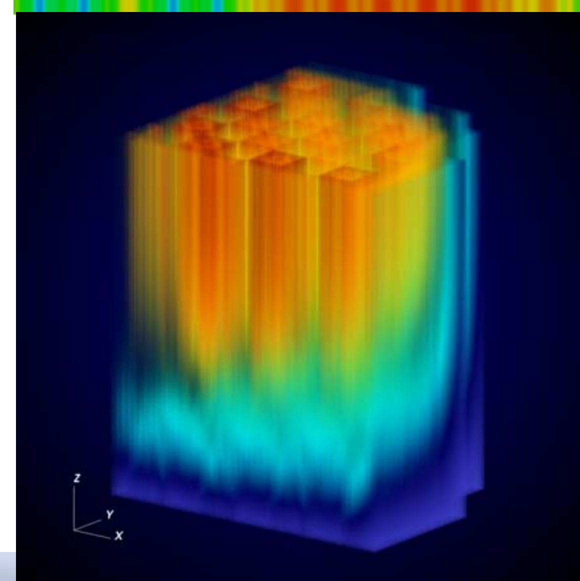
2nd DOE/NRC/NEI Workshop on U.S. Nuclear Power Plant Life Extension R&D, Feb 22-24, 2011

# 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 (govt, 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)

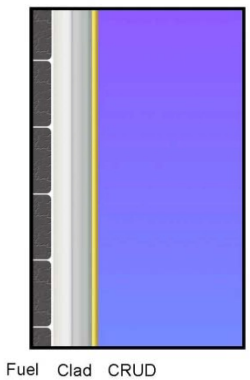
# Key Challenge Problems Limiting Reactor Performance

| | 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 | × | | × |

# CRUD Nucleation and Growth Affects Localized Fuel and Overall Reactor Performance*

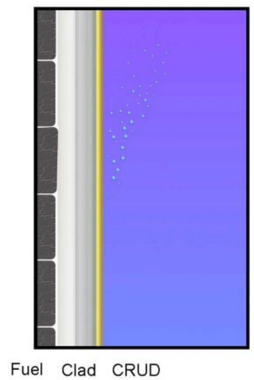
## A complicated, localized phenomenon that has global whole-core effects

### Step 0 – Normal Operation



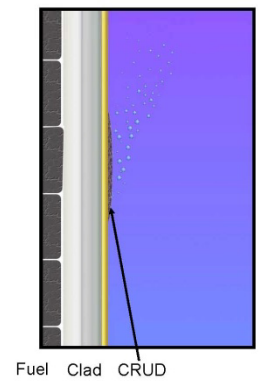

- Minimal sub-nucleate boiling
- Normal clad temperature
  - No serious fuel/clad contact yet

### Step 1 - Nucleation




- Initiating event causes local clad temperature to rise
  - Could be PCI, etc.
- Induces more sub-nucleate boiling
  - This causes local supersaturations of Ni,Fe ions
  - If they can't diffuse away fast enough, they can precipitate out on the clad

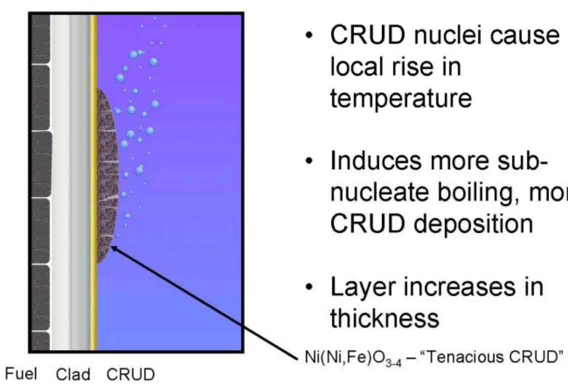
### Step 1 - Nucleation




- Sub-nucleate boiling nucleates CRUD
  - Supersaturates ions at boiling surface[1]
  - These ions (mostly Fe, Ni) crystallize out, forming CRUD[1]
- Little boron accumulation
- Slight temperature rise in clad

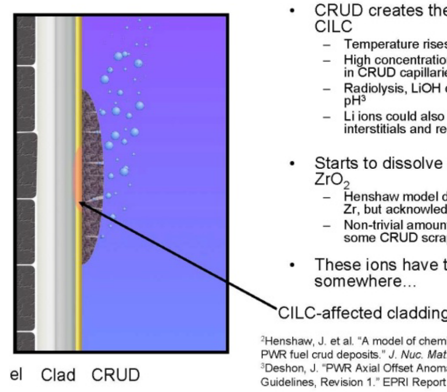
[1]Secker, J. R. "BOA Theory and Methods." Presentation to MPO, 9/2010.

### Step 2 - Growth




- CRUD nuclei cause local rise in temperature
- Induces more sub-nucleate boiling, more CRUD deposition
- Layer increases in thickness

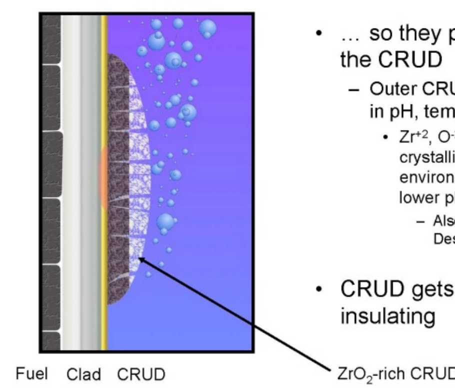
### Step 3 - CILC




- CRUD creates the environment for CILC
  - Temperature rises beneath CRUD
  - High concentrations of ions are trapped in CRUD capillaries
  - Radiolysis, LiOH cause localized high pH[3]
  - Li ions could also migrate into $ZrO_2$ as interstitials and release $Zr^{+2}$ ions
- Starts to dissolve $Zr^{+2}$ ions from $ZrO_2$
  - Henshaw model does not account for Zr, but acknowledges it[2]
  - Non-trivial amount of $ZrO_2$ observed in some CRUD scrapes[3]
- These ions have to go somewhere…

[2]Henshaw, J. et al. "A model of chemistry and thermal hydraulics in PWR fuel crud deposits." *J. Nuc. Mat.* 353 (2006), pp. 1-11
[3]Deshon, J. "PWR Axial Offset Anomaly (AOA) Guidelines, Revision 1." EPRI Report 1008102, 6/2004

### Step 3 - CILC

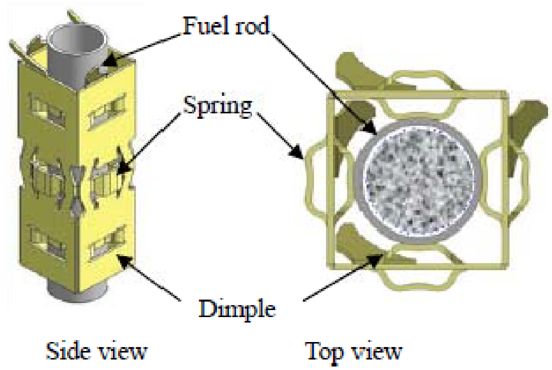


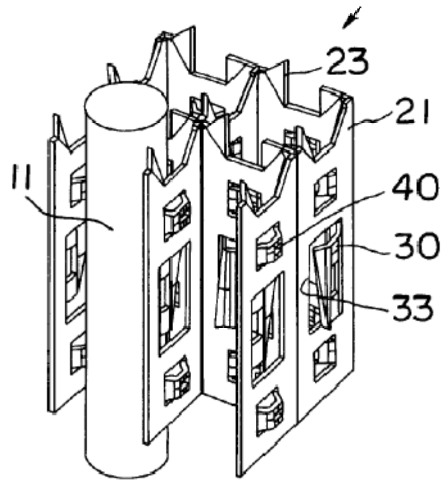

- … so they plate out on the CRUD
  - Outer CRUD layer is lower in pH, temperature
    - $Zr^{+2}$, $O^{-2}$ ions restabilize & crystallize in less harsh environment, lower temp., lower pH
      - Also hypothesized by Deshon[3]
- CRUD gets thicker, more insulating

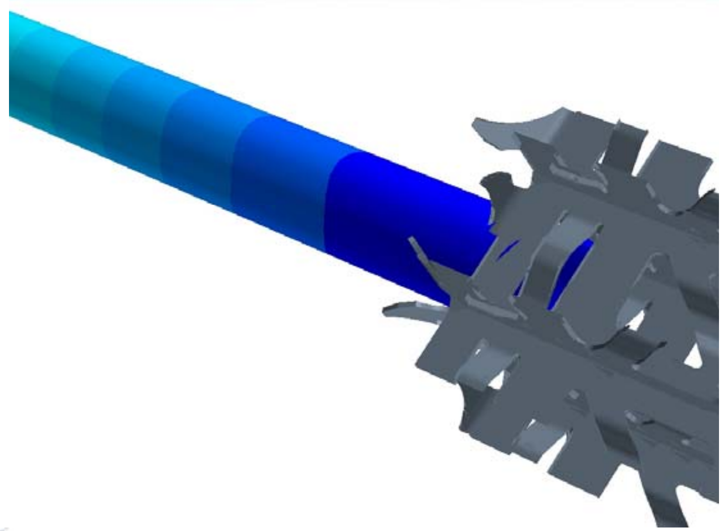
*figures courtesy of Mike Short (MIT)

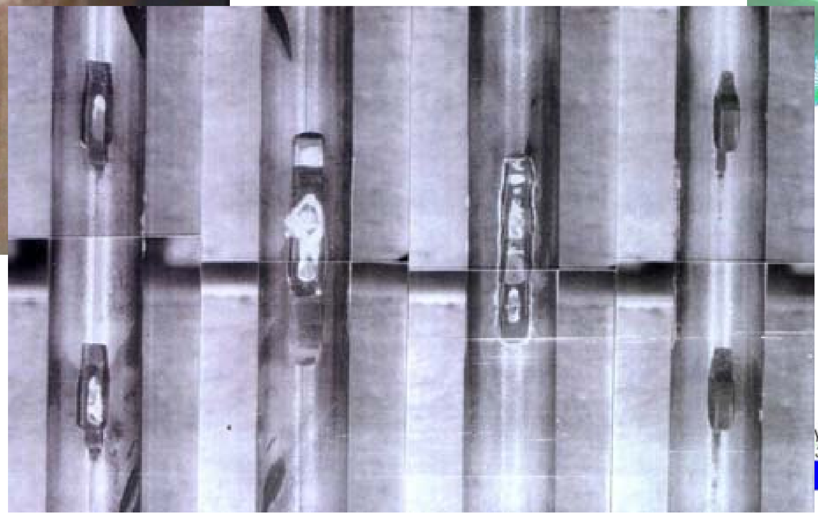
# Grid-to-Rod-Fretting (GTRF)

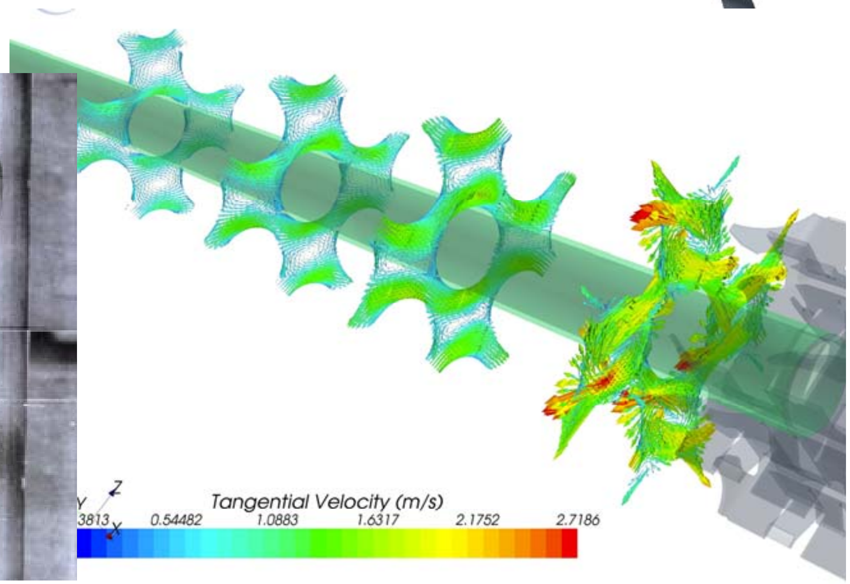
## Spacer Grid with Springs/Dimples







# 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 (RELAP/RETRAN)
  - 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 are Executing the Plan

## MPO
**Materials Performance and Optimization**

Chris Stanek, Lead
Sid Yip, Deputy
Brian Wirth, Deputy

- VERA Integration
- Fuel microstructure
- Clad/internals microstructure
- Corrosion
- CRUD deposition
- GFRF

## 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
- Challenge Problem Integration

## 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 CASL Organization

**Board of Directors**
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**U.S. Department of Energy**

**Director**
Doug Kothe

**Deputy Director**
Ronaldo Szilard

**Chief Scientist**
Paul Turinsky

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**Operations Manager**
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Victoria Shope
**Administrative Support**
Linda Weltman (executive)
Marsha Henley
**Contracting Authority**
Jo Ann Fitzpatrick
**Quality Manager**
Matt Sieger
**Facilities Project Manager**
John Shaw Jr.
**Web & Database Design**
Lara James
**IT Project Manager**
Danny Honeycutt
**Export Control**
Sam Howard
**Cyber Security**
Vickie Kurtz

**Technical Focus Areas**

**MPO**
**Materials Performance & Optimization**
Chris Stanek
Sid Yip
Brian Wirth

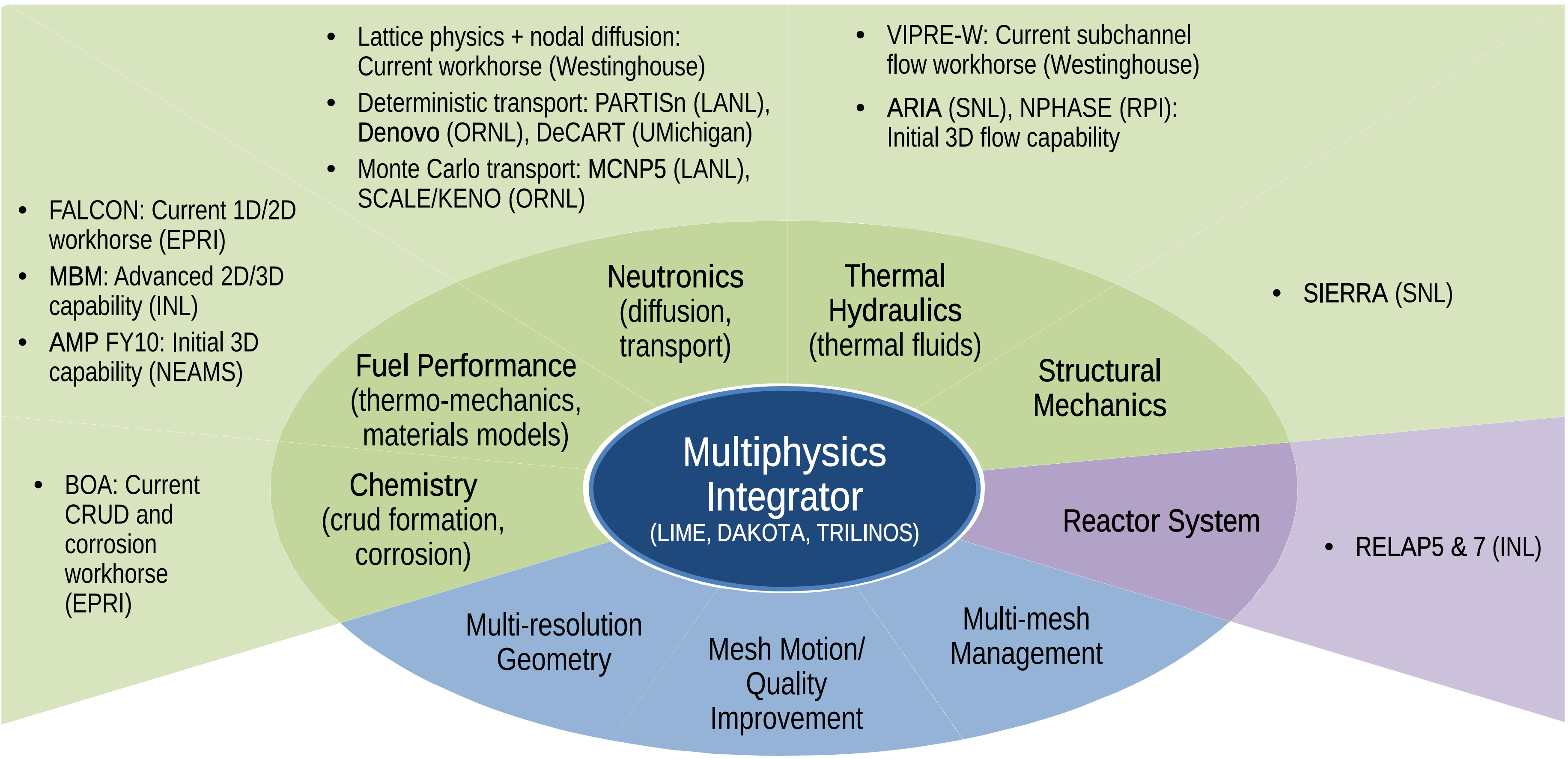
**VRI**
**Virtual Reactor Integration**
John Turner
Randy Summers
Rich Martineau

**AMA**
**Advanced Modeling Applications**
Jess Gehin
Zeses Karoutas
Stephen Hess

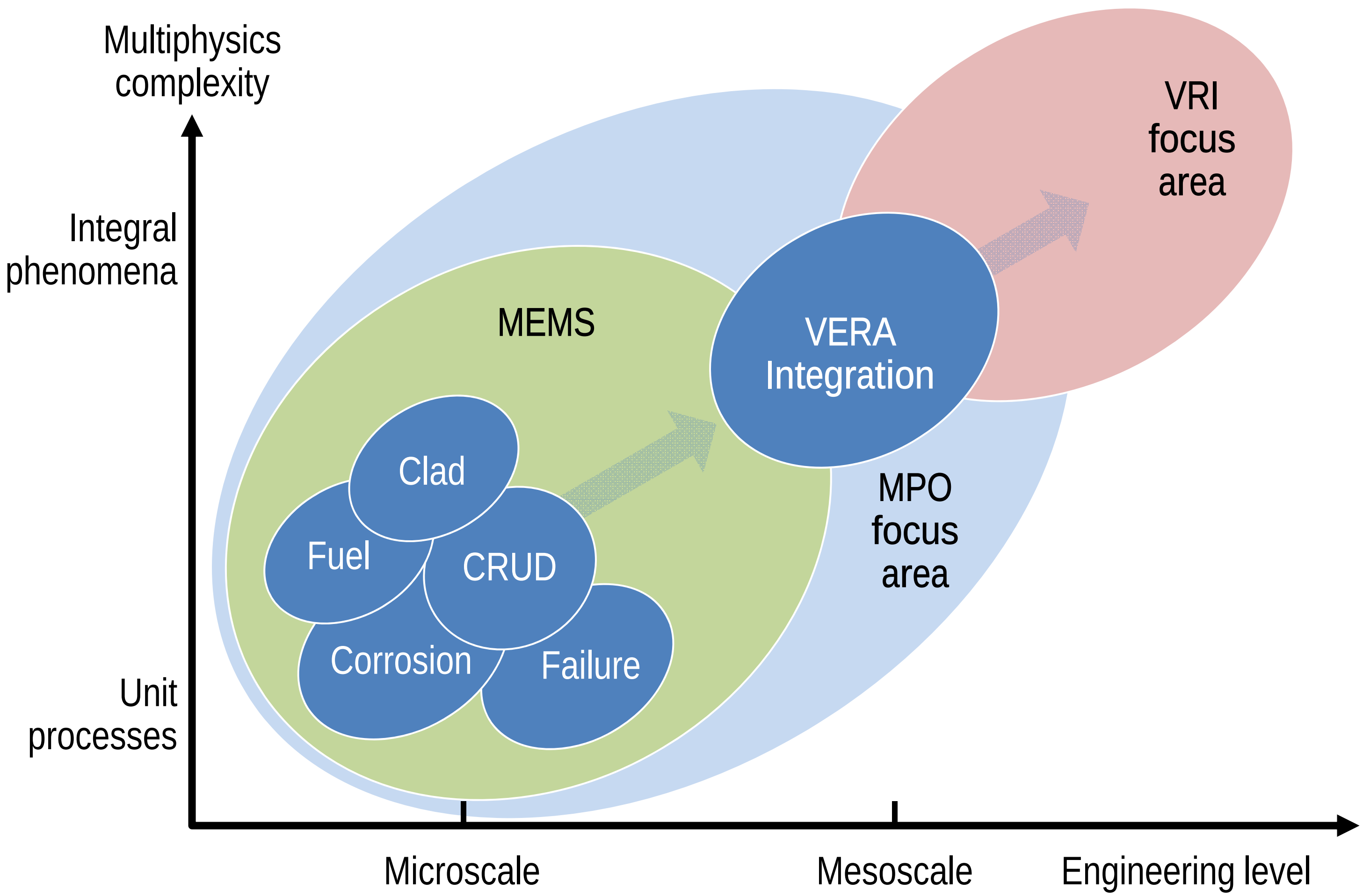
**MNM**
**Models and Numerical Methods**
Bill Martin
Rob Lowrie

**VUQ**
**Validation & Uncertainty Quantification**
Jim Stewart
Dan Cacuci

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

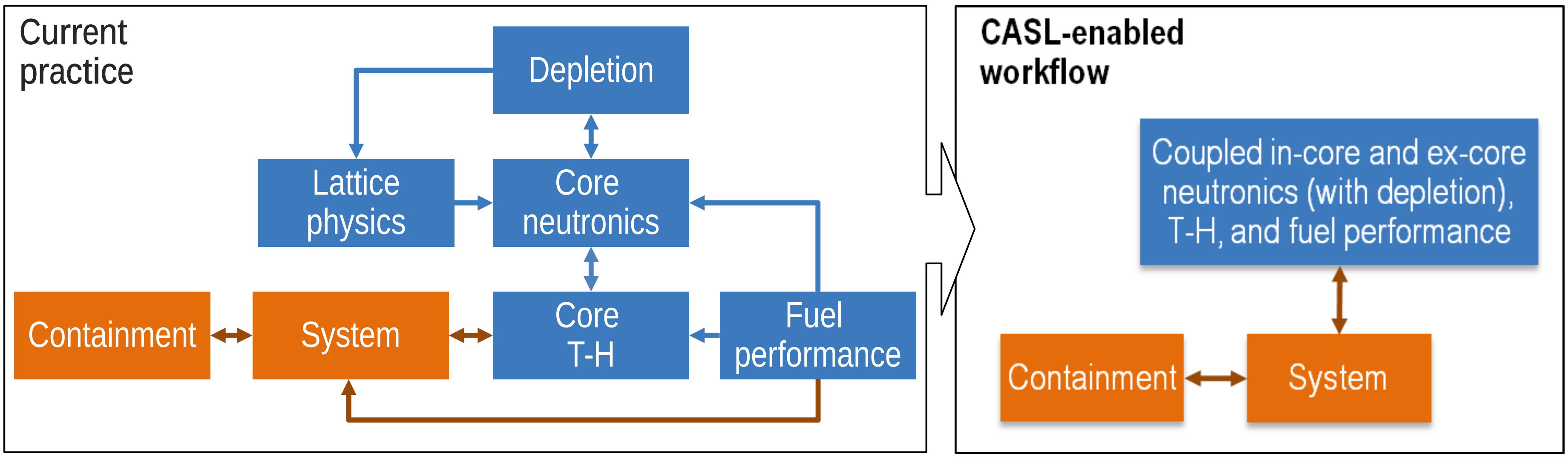


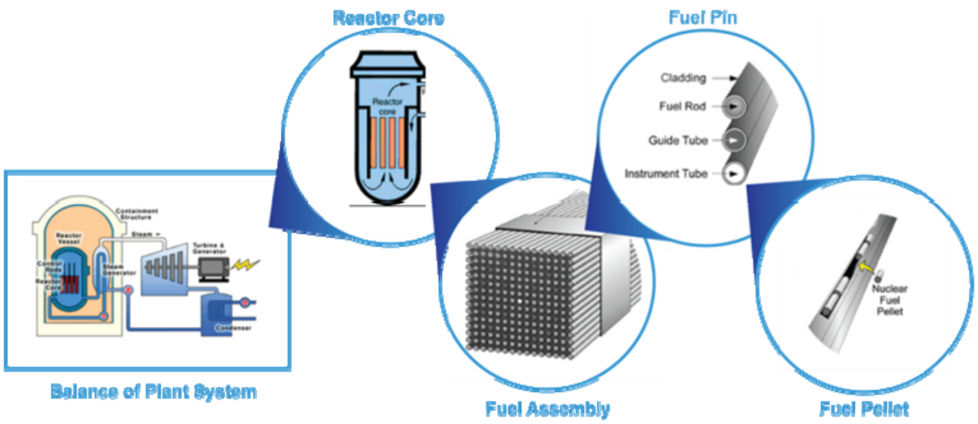
# MPO science innovation is micro-meso coupling in both complexity of physical phenomena and modeling and simulation capability




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

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

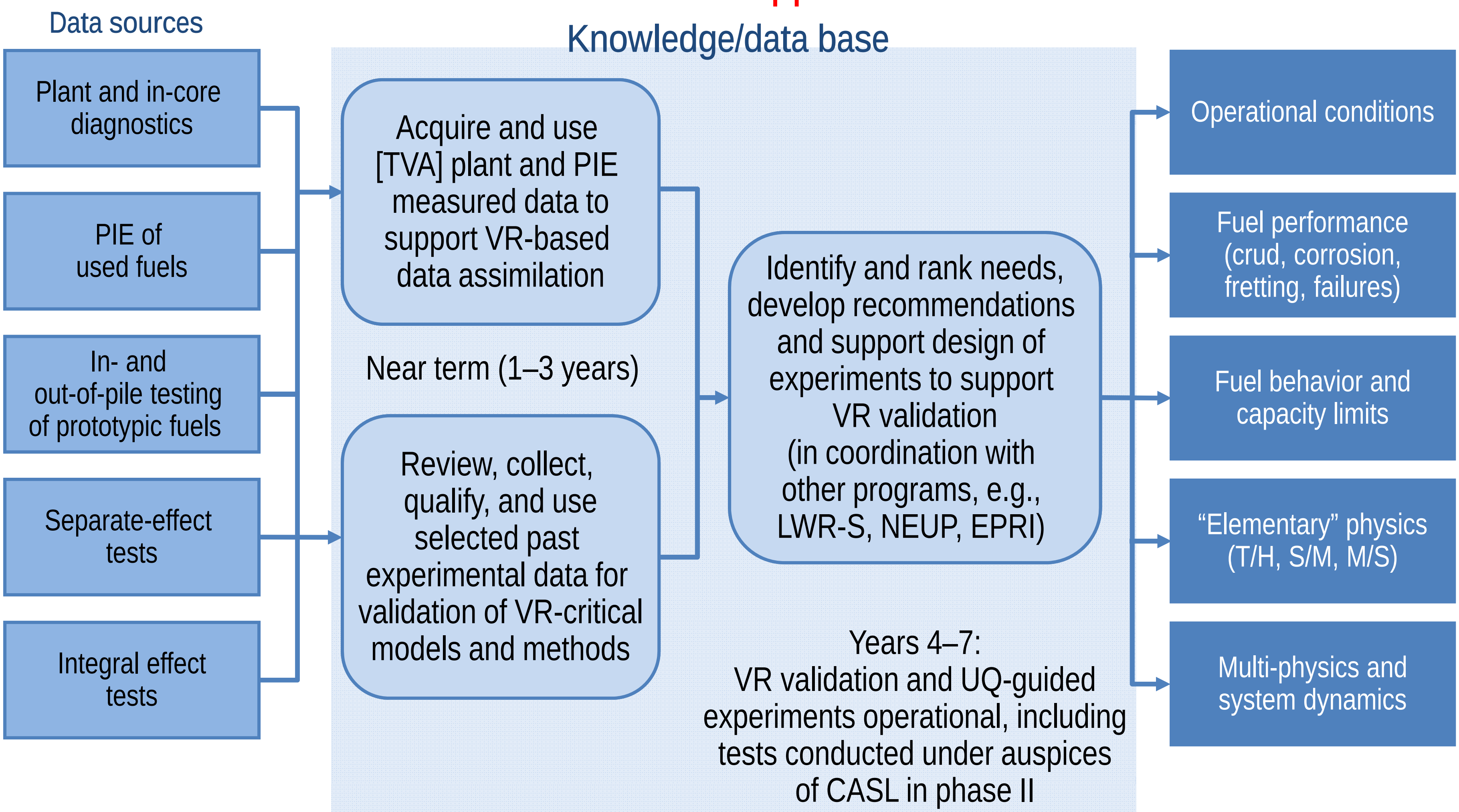



Suite of advanced yet usable M&S tools and methods, integrated within a common software infrastructure for predictive simulation of LWRs

# Validation data support plan

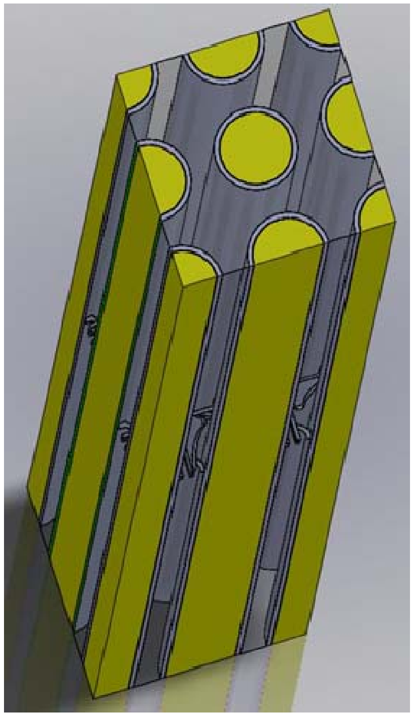
Validation data for fuels & materials, T-H & radiation transport would benefit from a coordinated approach

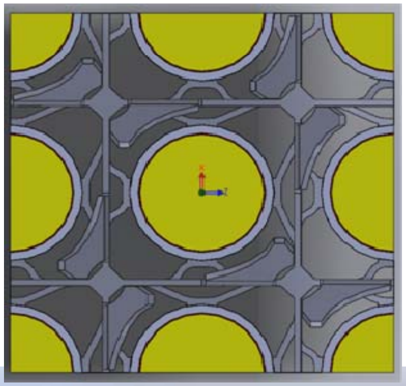


# We Plan to Develop Advanced Tools as Guided by a Systematic Scale Up

## 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**

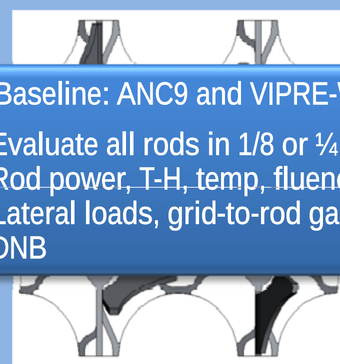
- Evaluate fuel temp, RIP, Corrosion Stress, Strain, Hydrogen, Growth, PCI
- Hot Cell, PIE, Halden, Stiudsvik data

### 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

### 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

**Baseline: link RETRAN, then RELAP5**

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

### 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

# TVA Plant Model Development is Underway

# Summary

- Advanced modeling & simulation will help us address key Challenge Problems for power uprates, high burnup and life extension
- Coupling existing capabilities will guide us in developing advanced ones
- CASL has important synergies and dependencies on relevant life extension programs (DOE/LWRS, NRC/LB60, EPRI/LTO)
  - Users and co-developers of our tools, providers of key validation data

www.casl.gov or info@casl.gov