Validation and Uncertainty Quantification in CASL

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What Is CASL?

- Consortium for Advanced Simulation of LWRs
  - An Energy Innovation Hub
- Objective: predictive simulation of light water reactors
  - Reduce capital and operating costs
    - Power uprates
    - Lifetime extension
  - Reduce nuclear waste
    - Higher fuel burnup
  - Enhance operational safety
    - Improved prediction of component failure
- End product: simulation tools for a virtual reactor

Find out more at www.casl.gov

Challenge Problems

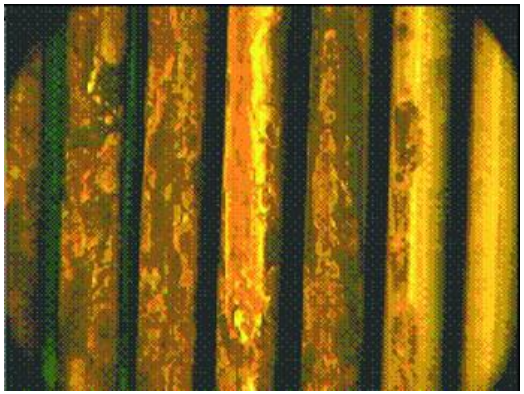
Industry partners ensure focus on relevant problems and identify important performance-limiting phenomena

Operational

- CRUD-induced power shift (CIPS)
- CRUD-induced localized corrosion (CILC)
- Grid-to-rod fretting (GTRF)
- Pellet-cladding interaction (PCI)
- Fuel assembly distortion (FAD)

Safety

- Departure from nucleate boiling (DNB)
- Cladding integrity under loss-of-coolant accident (LOCA)
- Cladding integrity under reactivity insertion accidents (RIA)
- Reactor vessel/internals integrity



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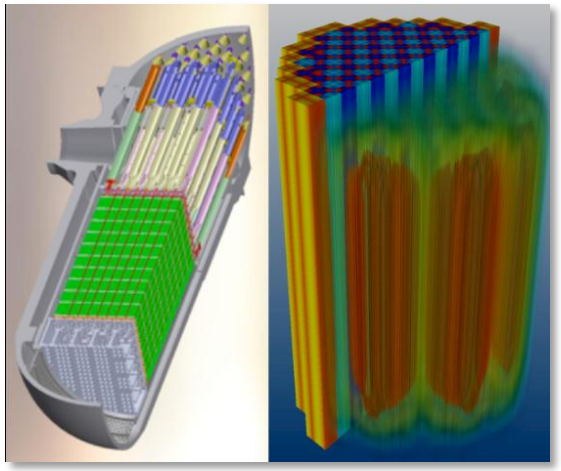
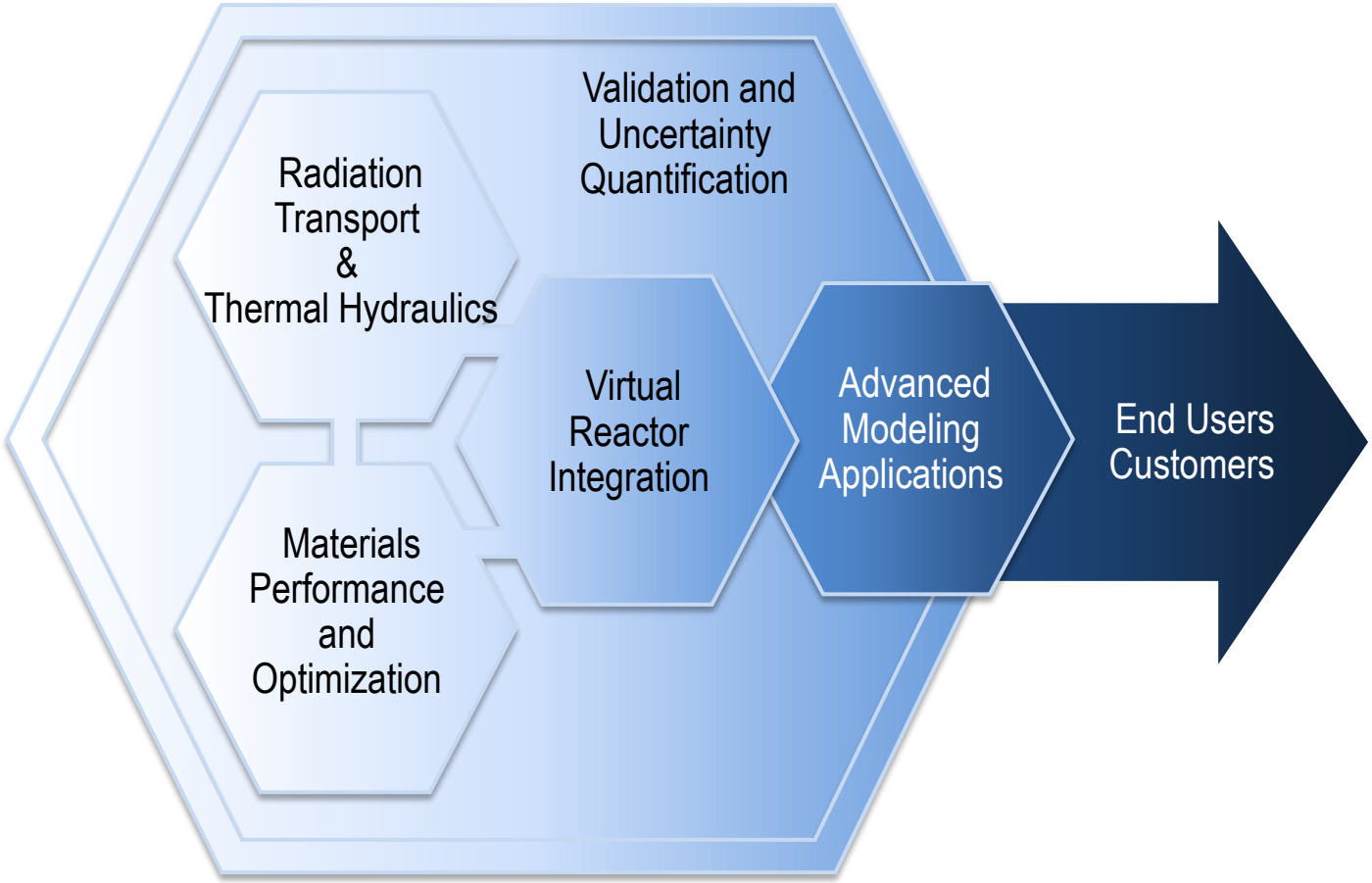
CASL Organization

- Organized into technical focus areas
  - Thermal-hydraulics
    - Multiphase fluid flow
    - Thermal transport in solids
    - Heat transfer at interfaces
  - Radiation transport
    - Pin-resolved neutron transport
  - Materials performance and optimization
    - First-principles performance prediction of fuel and cladding
    - Corrosion mechanisms
  - Virtual reactor integration
    - Flexible framework for multi-physics/multi-scale coupling
    - Verified physics components
    - Integral UQ
  - Validation and uncertainty quantification



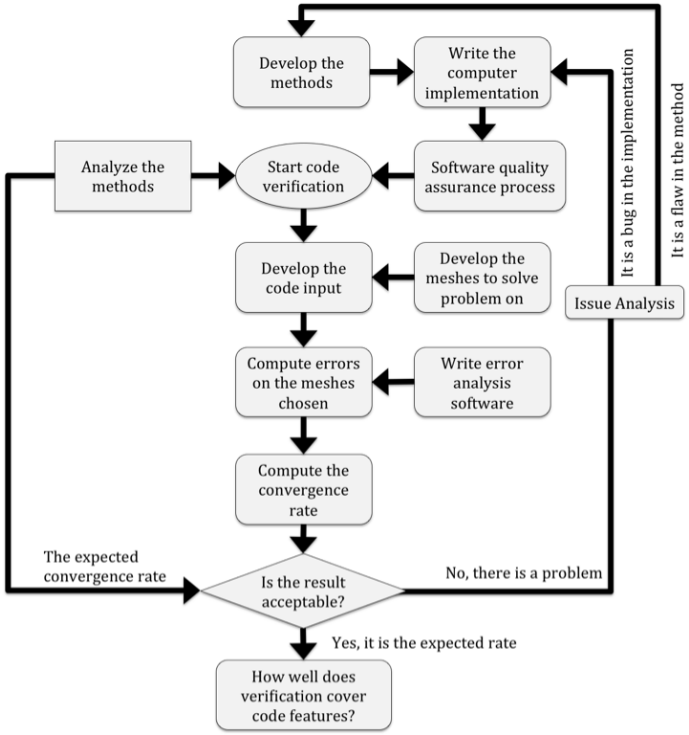
CASL VUQ Encompasses All Focus Areas



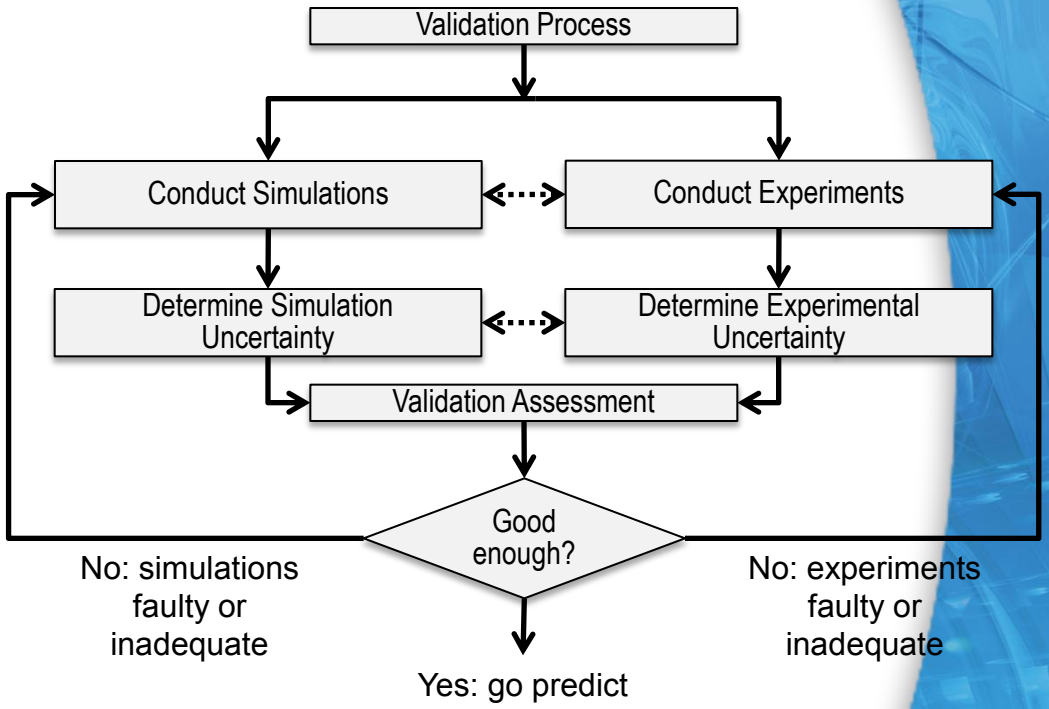
CASL/VUQ Goals, Outcomes and Impacts

- Continuous evolution towards *transformational, predictive computational simulation*
  - Best-estimate predictive capabilities with reduced uncertainties and quantified predictive maturity assessments
- Capability to quantify and reduce uncertainties for the CASL challenge problems
- New ways for experiments and simulations to work together, leading to predictions *with quantified confidence* of scenarios for which experimental data is not directly available
  - SA/UQ-driven process for guiding research & development investments

Verification, Validation, and UQ Workflows



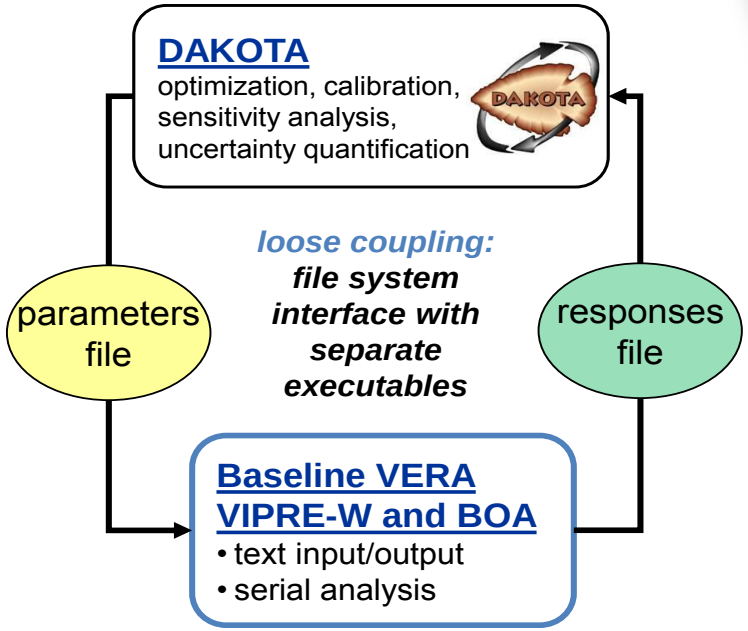
Code Verification Workflow



Validation Workflow

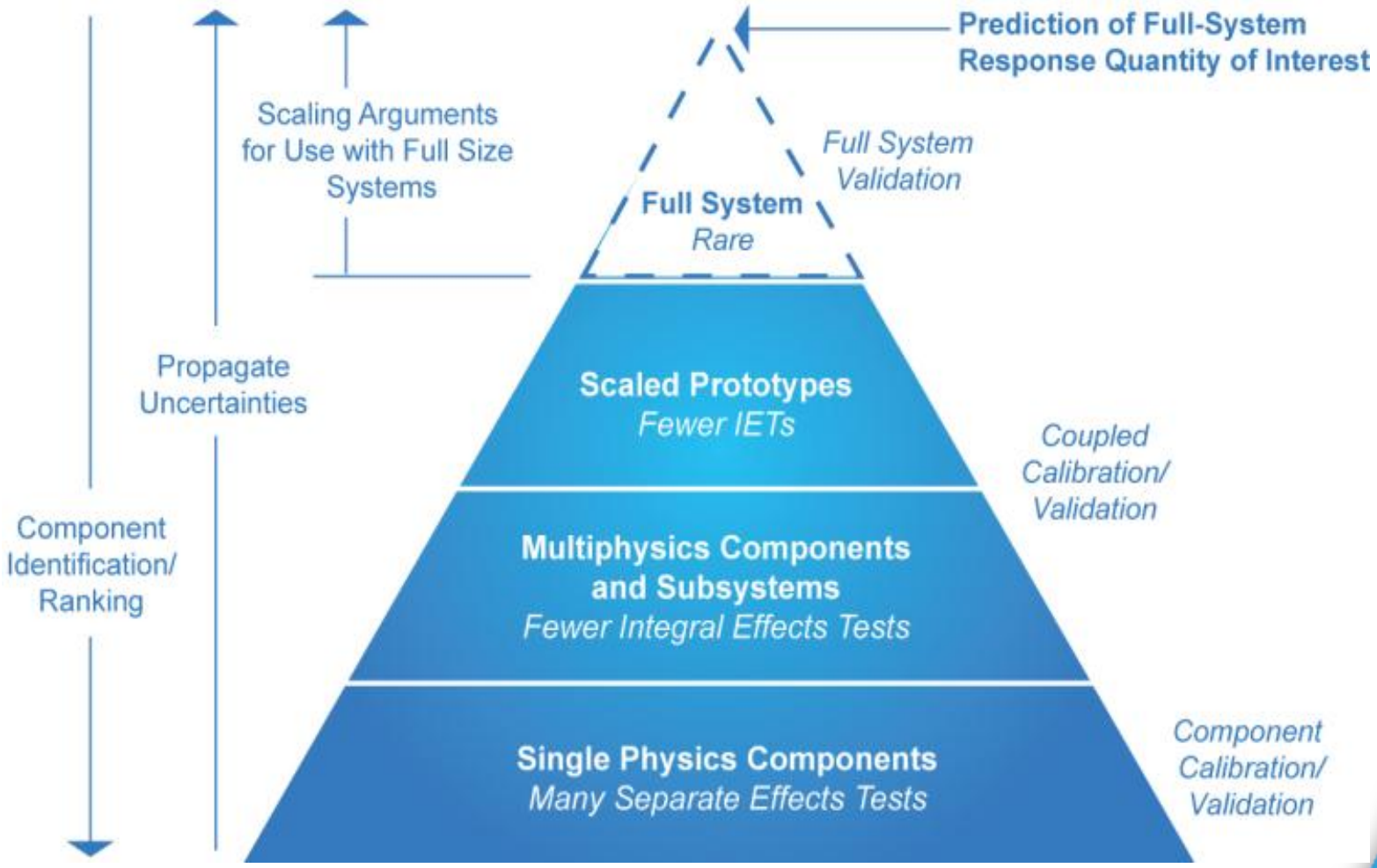
VUQ Methods and Capabilities

- Sensitivity analysis
- Uncertainty propagation
- Model form uncertainty
- Predictive capability assessments
- Data assimilation
- Verification tools

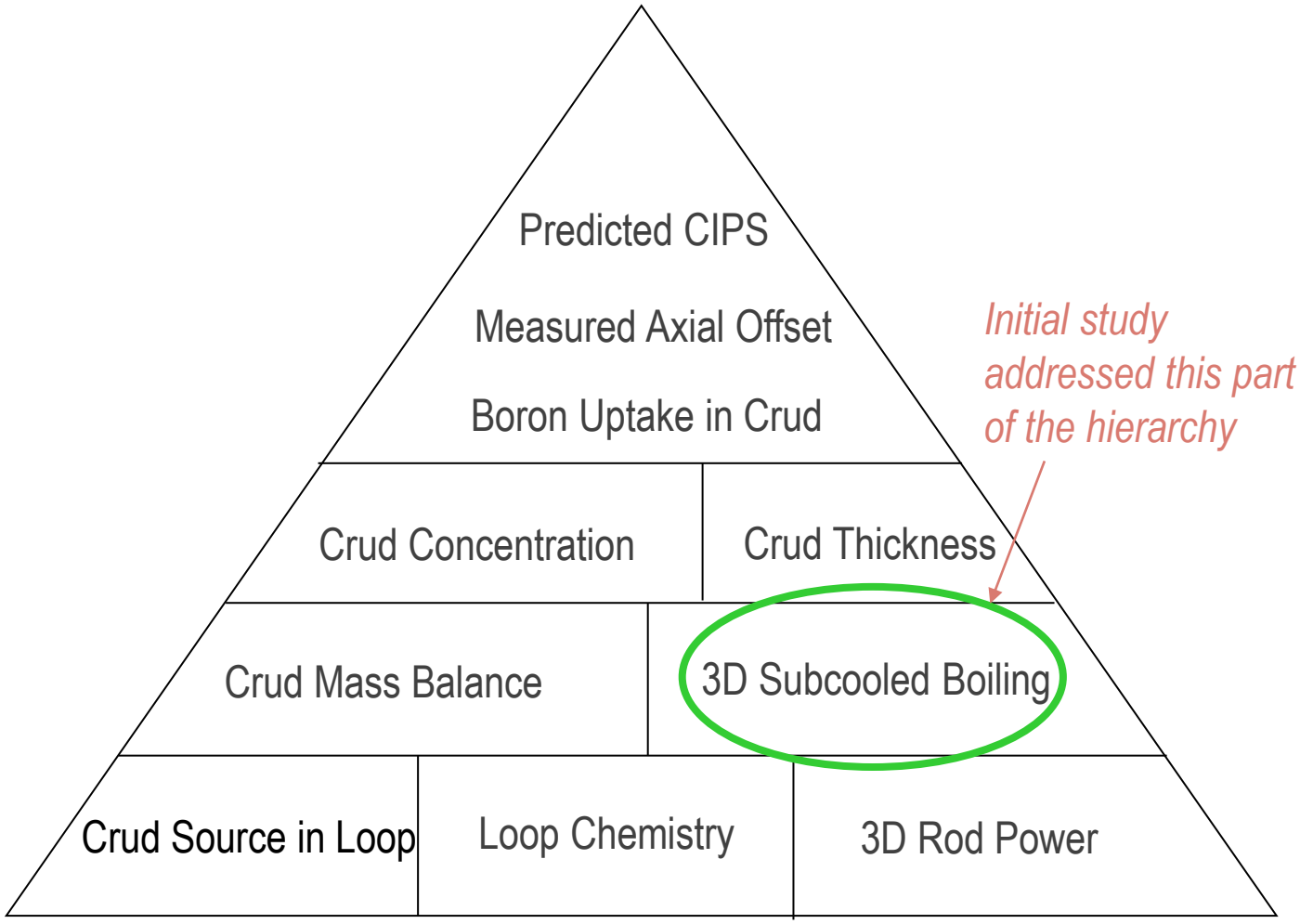


Uncertainty analysis has already led to new insights

Validation Hierarchy



Validation Hierarchy for CIPS

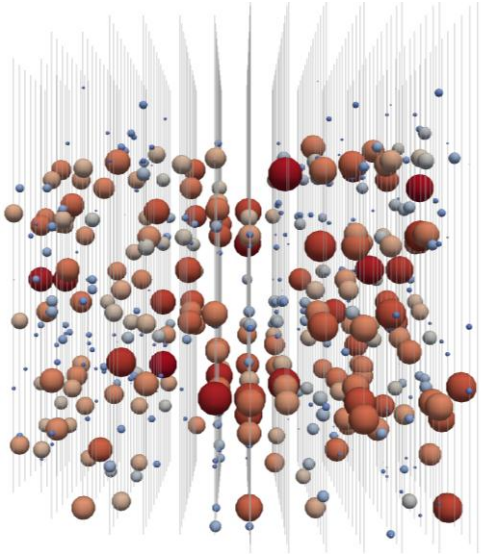


SA/UQ Demonstration for CIPS

work by B. Adams and W. Witkowski (SNL); J. Secker and Y. Sung (WEC)

- **Strategy:** Integrate SNL's *DAKOTA* UQ Toolkit with Westinghouse's VIPRE-W subchannel Thermal-Hydraulics simulator
- **Demonstration for Crud/CIPS problem (quarter-core geometry):** Assess influence of core operating parameters on mass evaporation rate
- **SA Methods:** Latin Hypercube Sampling, Morris One-At-a-Time, polynomial chaos with analytic Sobol' indices
- **UQ Methods**: Latin Hypercube Sampling, polynomial chaos
- **Results:** Affirmed well-known sensitivity (of mass evap. rate) to temperature and exposed sensitivity to pressure. Boiling model uncertainty is a key contributor.

Vertical lines are individual flow channels

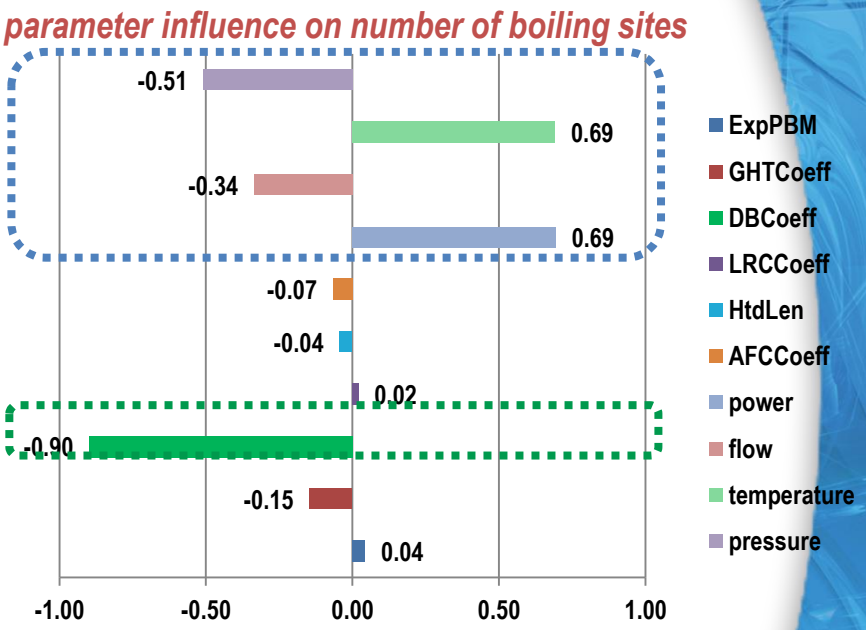


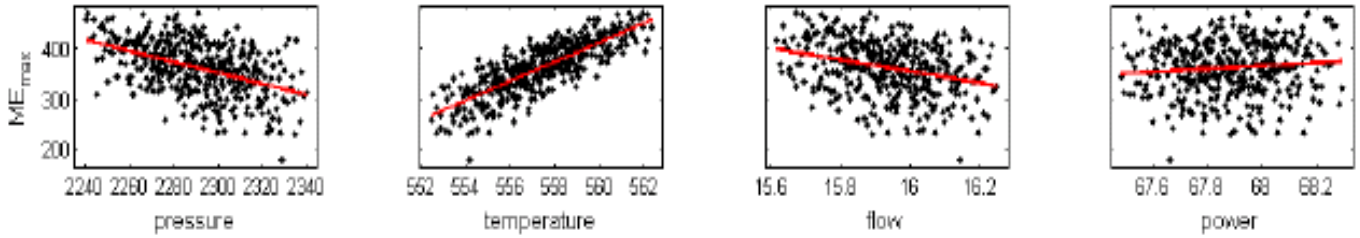
Spheres indicate where boiling occurs

- Size correlates to uncertainty
- Color correlates to mean boiling rate

Sensitivity analysis helps assess the influence of parameters on boiling rates

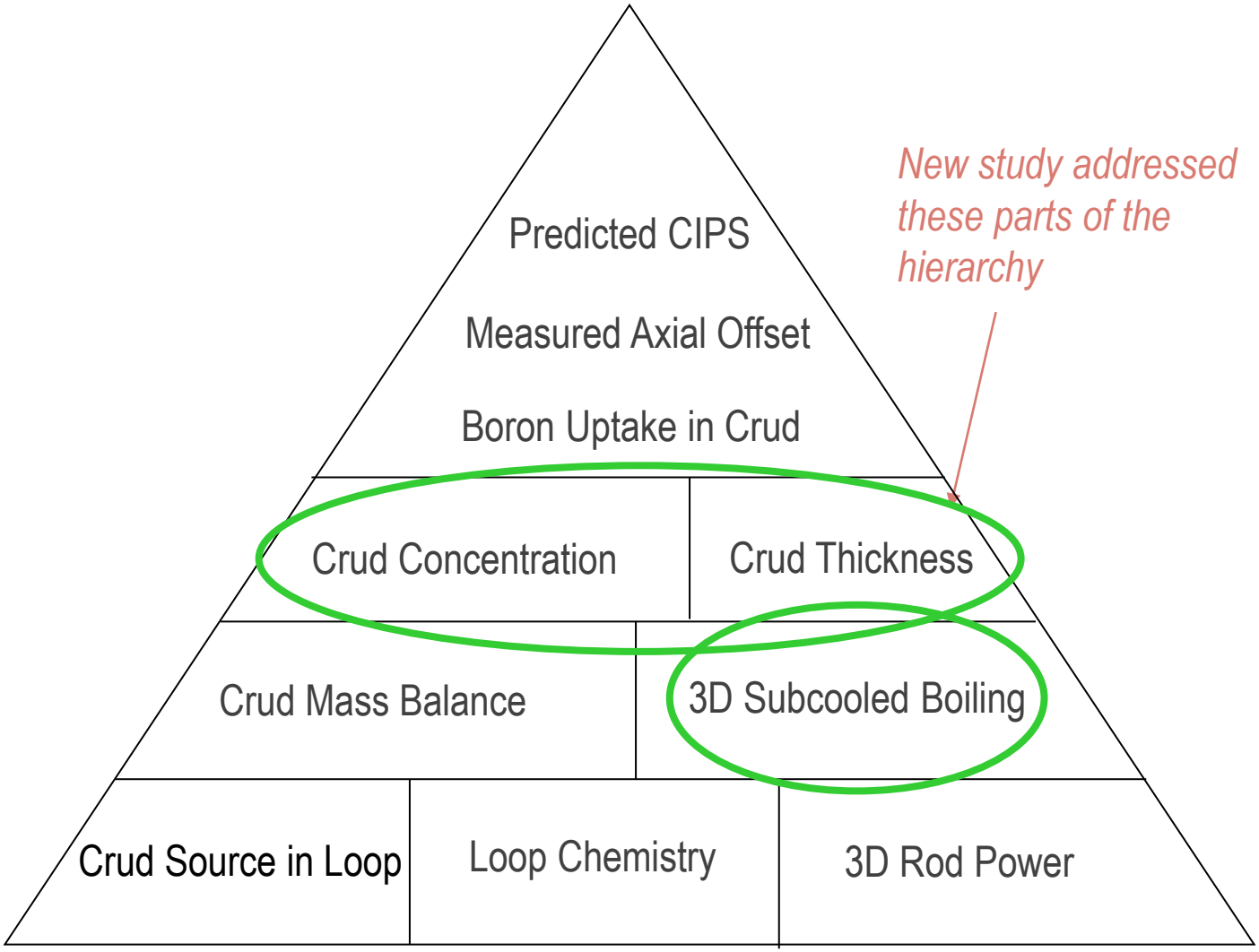
- DAKOTA correlation coefficients: strong influence of core operating parameters (pressure more important than previously thought)
- Dittus-Bolter correlation model may dominate the sensitivities
- Scatter plots help visualize trend in input/output relationships



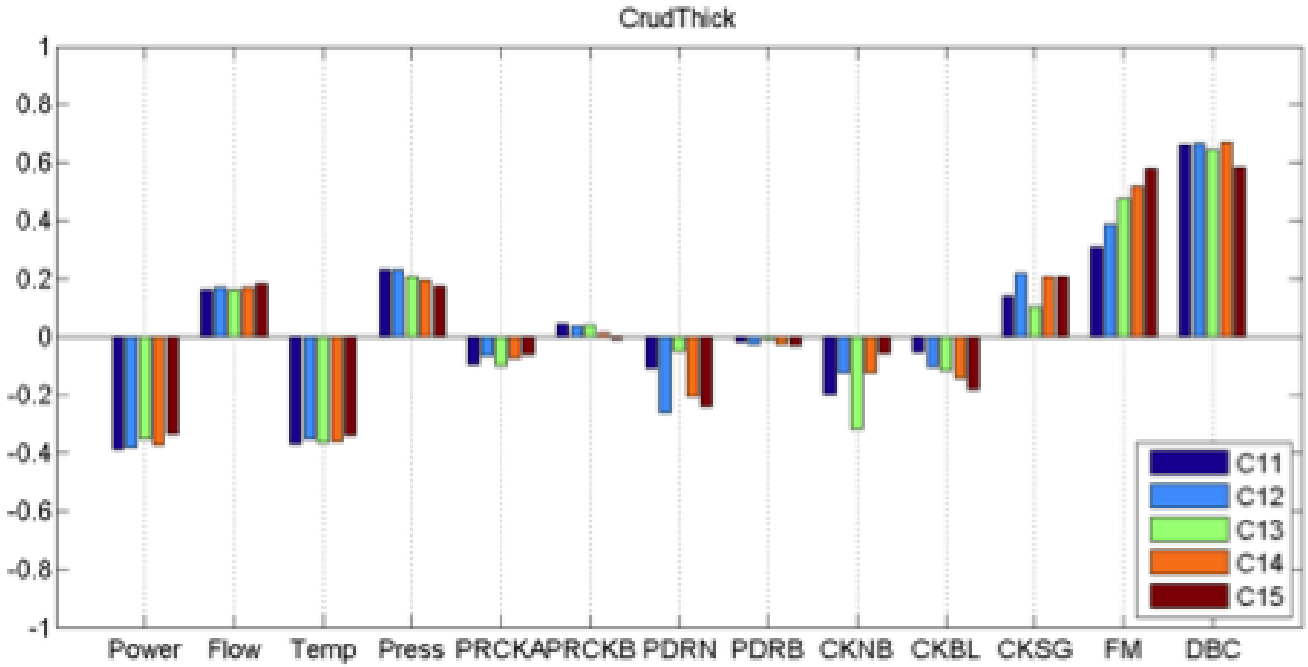


sensitivity of mass evaporation rate (max) to operating parameters

Continuing assessment: addition of CRUD model



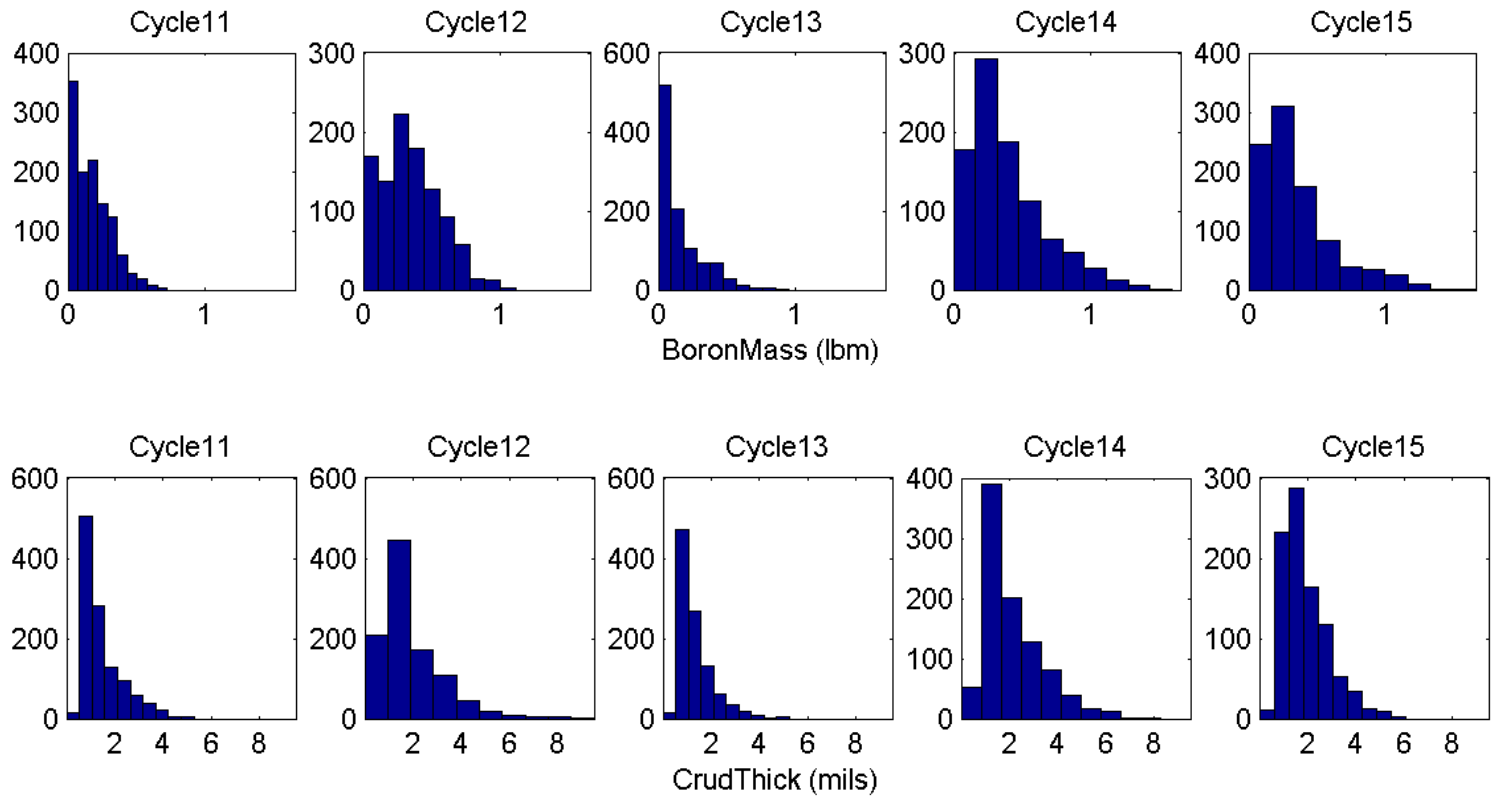
Global Sensitivity of CRUD predictors



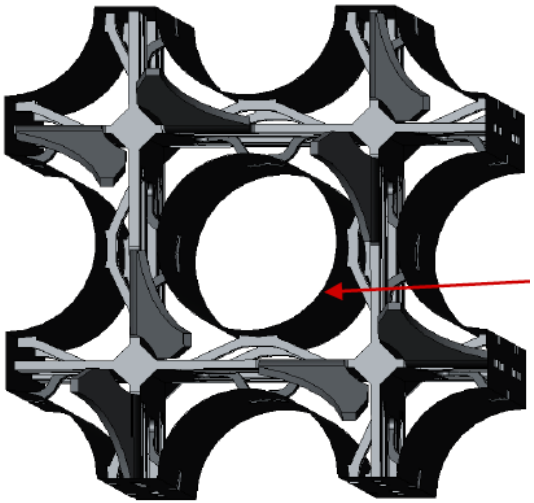
- Boron mass
- CRUD thickness
- Nickel/Iron Ratio

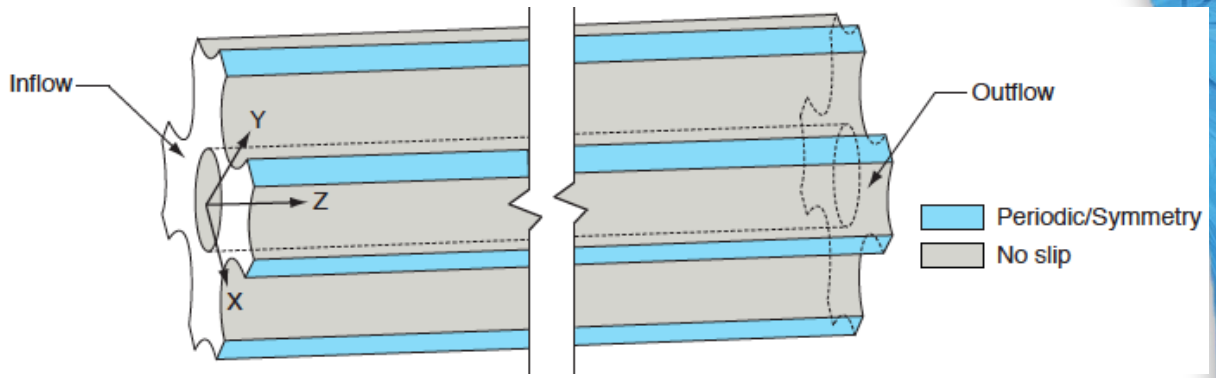
- Nickel Mass
- Median Nickel over 5 cycles
- Median Iron over 5 cycles

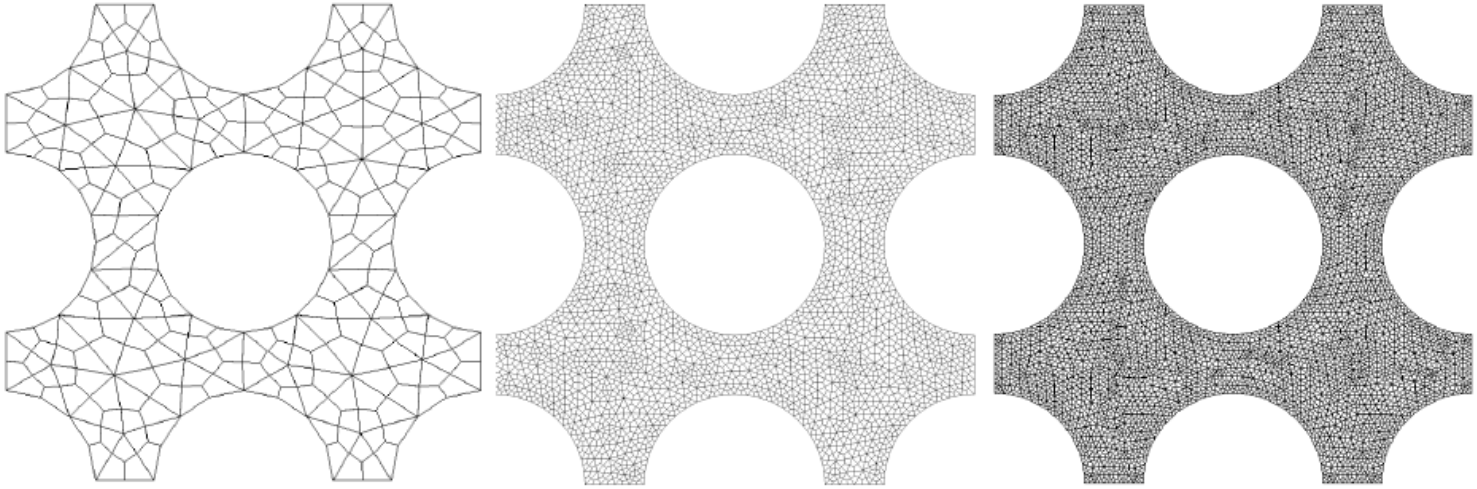
Output Distributions of CRUD Predictors



Next: Grid-to-rod fretting







VUQ Risks and Challenges

- Insufficient and/or poor-quality validation data
  - Will impact quality of predictions
- Verification
  - Sufficient mesh sequences
  - Identifying suitable manufactured solutions
  - Capacity HPC resources
- Scalable UQ
  - Curses: Nonlinearity, dimensionality, multi-physics/multi-scale
  - Coupling to verification
  - Constructing reliable uncertainty analysis for multi-physics simulations built from single physics components
    - Estimating errors incurred from loose coupling
    - Propagating uncertainty across coupling
- Social: perception that VUQ is adversarial
  - Decision-makers require a different level of evidence of correctness than scientific peers