U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Benchmark Experiments to Validate Multiphysics Simulations for Nuclear Energy Systems

Bhupinder P. Singh
David Pointer
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IRP Goals

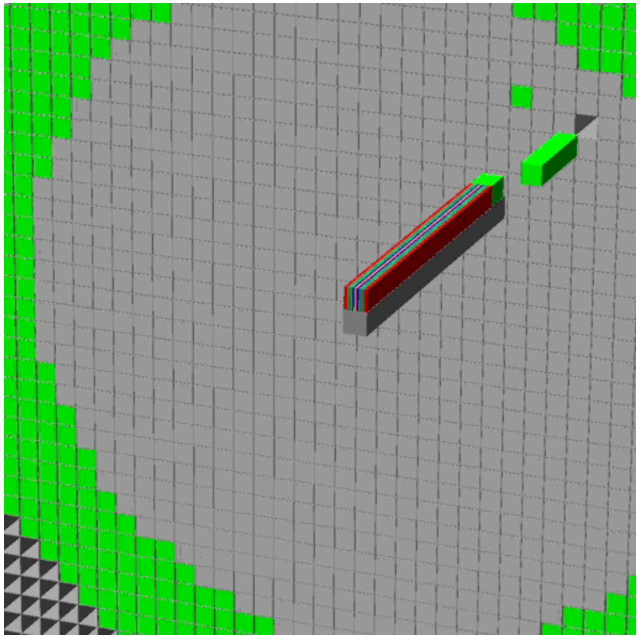
- **Make progress toward establishing benchmarks for validation of high-fidelity multiphysics codes for assessment of fuel and safety performance in an nuclear reactor core.**
  - Example — model the phenomena governing light water reactor accident tolerant fuel behavior in postulated accident conditions.
- **Establish new approaches to validation experiment development which recognize special requirements for validation of high-fidelity multiphysics codes**
  - Provide adequate data resolution in time and space, adequate measurement of boundary conditions, and adequate characterization of uncertainty
  - Develop methods to assess the impact of individual phenomenological impact on integral data for strongly-coupled multi-physics simulations

IRP Objectives

- **Develop a state-of-the art experimental multiphysics validation benchmark**
  - Modeling application of high importance
  - Demonstrating high-fidelity experimental methods for strongly-coupled phenomena while delineating phenomenological contributions
  - Enhancing validation and uncertainty quantification approaches
- **Support the use and adoption of high-fidelity multiphysics modeling and simulation tools developed by the Department of Energy's Nuclear Energy Programs (e.g., NEAMS, CASL, LWRS, FCR&D) by expanding their validated regimes**
- **Support the efforts of the DOE Nuclear Energy Knowledge and Validation Center (NEKVaC) to establish methods and guidelines for validation and uncertainty quantification of high-fidelity multiphysics simulations**
- **Support NE collaborations with the OECD/NEA on high-fidelity multiphysics validation and uncertainty quantification**

IRP Scope

- **Plan, design, and conduct an experiment that can serve as a benchmark for critically assessing the results predicted by a multiphysics simulation code for a nuclear energy system.**



- **Document the methods for designing the experiment including those for collection of data and quantification of uncertainties.**

- **Collect, store, reduce and present the data in a context which preserves all of the expert knowledge and rigor that went into the design and execution of the experiment.**

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Multiphysics Integration in DOE-NE Software Projects

			Major HPC Software Projects												
			MBM		SHARP				MAMMOTH			VERA-CS			
Physics Areas		Codes	Bison	Marmot	PROTEUS	Nek5000	Diablo	ORIGEN	RattleSnake	RELAP-7	MAMMOTH	MPACT	CTF	HYDRA-TH	Mamba
Physics Areas	Fuel Performance	Bison	–	X	X	O		X	X	X	X	X	X		
		Marmot	X	–											
	Neutron Transport	MPACT	X					X				–	X		X
		PROTEUS	X		–	X	X	X							
		RattleSnake	X						–	X	X				
	Isotopic Depletion	ORIGEN	/		X			–				X			
		MAMMOTH	X						X		–				
	Thermal Hydraulics	CTF	X									X	–		X
		HYDRA-TH												–	X
		Nek5000	O		X	X	X								
		RELAP-7	X						X	–	X				
	Coolant Chemistry	Mamba											X	X	–
	Structural Mechanics	Diablo			X	X	–								

Key: X – ongoing O – planned

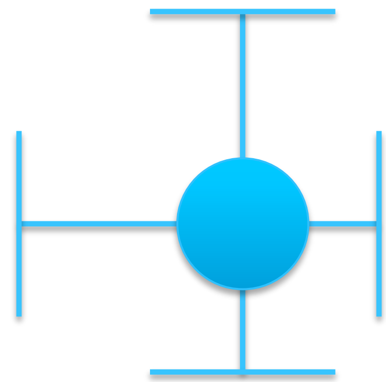
Six Key Characteristics of a Validation Experiment

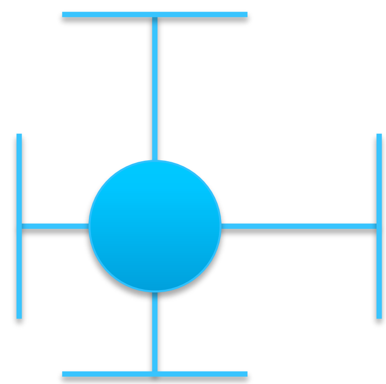
1. A validation experiment should be jointly designed and executed by experimentalists and computationalists.
2. A validation experiment should be designed to capture the relevant physics, all initial and boundary conditions, and auxiliary data.
3. A validation experiment should leverage the inherent synergisms attainable between experiment and computational approaches.
4. Independence between computational and experimental results should be maintained where possible.
5. A hierarchy of experimental measurements should be made which presents an increasing range of computational difficulty.
6. Carefully employ experimental uncertainty analysis procedures to delineate and quantify random and correlated bias errors.

Reference: W. L. **Oberkampf** and C. J. **Roy**, Verification and Validation in Scientific Computing, Cambridge University Press, Cambridge, 2010.

Experimental Uncertainty Quantification is Challenging

- **Reported instrumentation error**
- **Instrumentation bias**
- **Repeatability error**
  - Systematic data acquisition errors
  - Phenomenological time scale errors
  - Environmental biases
- **Experiment scaling bias**
- **Experimentalist bias**
- **Data user bias**
  - Comparison method bias





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Requirements for Successful Proposals

- **Validation is application specific**
  - Define a clear application of high importance
  - Select an appropriate modeling and simulation strategy
  - Propose a multiphysics validation benchmark based on a new experiment
  - Explain the gap in the available data that is filled by the proposed work
  - Explain why the identified gap is a high priority
- **Validation is only as good as the uncertainty quantification supporting it**
  - Define a clear approach to UQ for proposed experiment
  - Explain why the proposed UQ strategy is both necessary and sufficient
- **Validation benchmarks must be well-documented and quality assured**
  - Define a clear quality assurance plan for the benchmark to be generated
  - Identify standards which will be satisfied
  - Explain why the proposed QA strategy is both necessary and sufficient

Desired Outcomes

- **Demonstrate a successful approach for high-fidelity multiphysics code validation experiment and benchmark development**
- **Add value to DOE-NE multiphysics code development efforts through development of a validation benchmark for an application of high importance**
  - IRP teams may propose to exercise the specific selected code application and compare results from the code and the benchmark experiment.
- **Support establishment of practical methods and guidelines for uncertainty quantification in high-fidelity multiphysics benchmarks which supports NEKVaC and NE activities with OECD/NEA**
- **Support development of appropriate quality assurance and knowledge management strategies for high-fidelity multiphysics benchmarks by NEKVaC and OECD/NEA**
- **Incorporate knowledge learned in a college course to advance the state-of- the-art on VVUQ**