U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Clean. Reliable. Nuclear.

Nuclear Energy
Advanced Modeling & Simulation

CINR Annual Planning Webinar - August 2018

Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Office of Nuclear Energy
U.S. Department of Energy

Office of Nuclear Energy Organization

Where in NE are programs for developing and deploying advanced modeling and simulation tools managed? Who manages them?

- NE-1 **Assistant Secretary for Nuclear Energy**
  - Nuclear Energy Advisory Committee
  - NE-20 Chief Operating Officer
  - NE-3 Deputy Assistant Secretary for Nuclear Infrastructure Programs
  - Deputy Assistant Secretary for Nuclear Technology Research and Development
  - NE-5 **Deputy Assistant Secretary for Nuclear Energy Innovation and Application**
    NE-4
    - **Office of Accelerated Innovation in Nuclear Energy**
    - **Office of Nuclear Energy Application**
  - NE-6 Deputy Assistant Secretary for International Nuclear Energy Policy and Cooperation
  - NE-7 Deputy Assistant Secretary for Idaho Site Operations and Contractor Assurance
  - NE-8 Deputy Assistant Secretary for Spent Fuel & Waste Disposition

NE Federal Manager for Advanced M&S

Dan Funk, dan.funk@hq.doe.gov (until August 31)

Dave Henderson, david.henderson@hq.doe.gov (after August 31)

Advanced Modeling & Simulation

NE currently executes two complementary advanced M&S programs, each tailored to focus on a particular reactor technology area using computational tools uniquely suited to the particular reactor moderator(s) and fuel(s).

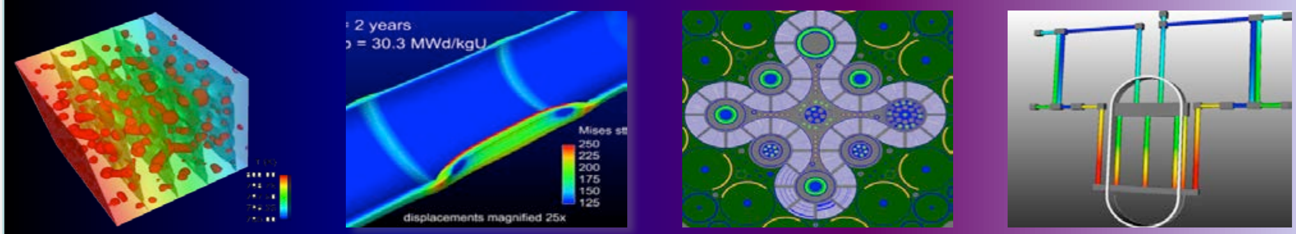
Energy Innovation Hub for Modeling and Simulation (Hub)

Objective: Develop and apply M&S tools focused on <u>LWR technologies</u> for an improved understanding of important operational and safety issues in existing reactors

Nuclear Energy Advanced Modeling & Simulation (NEAMS)

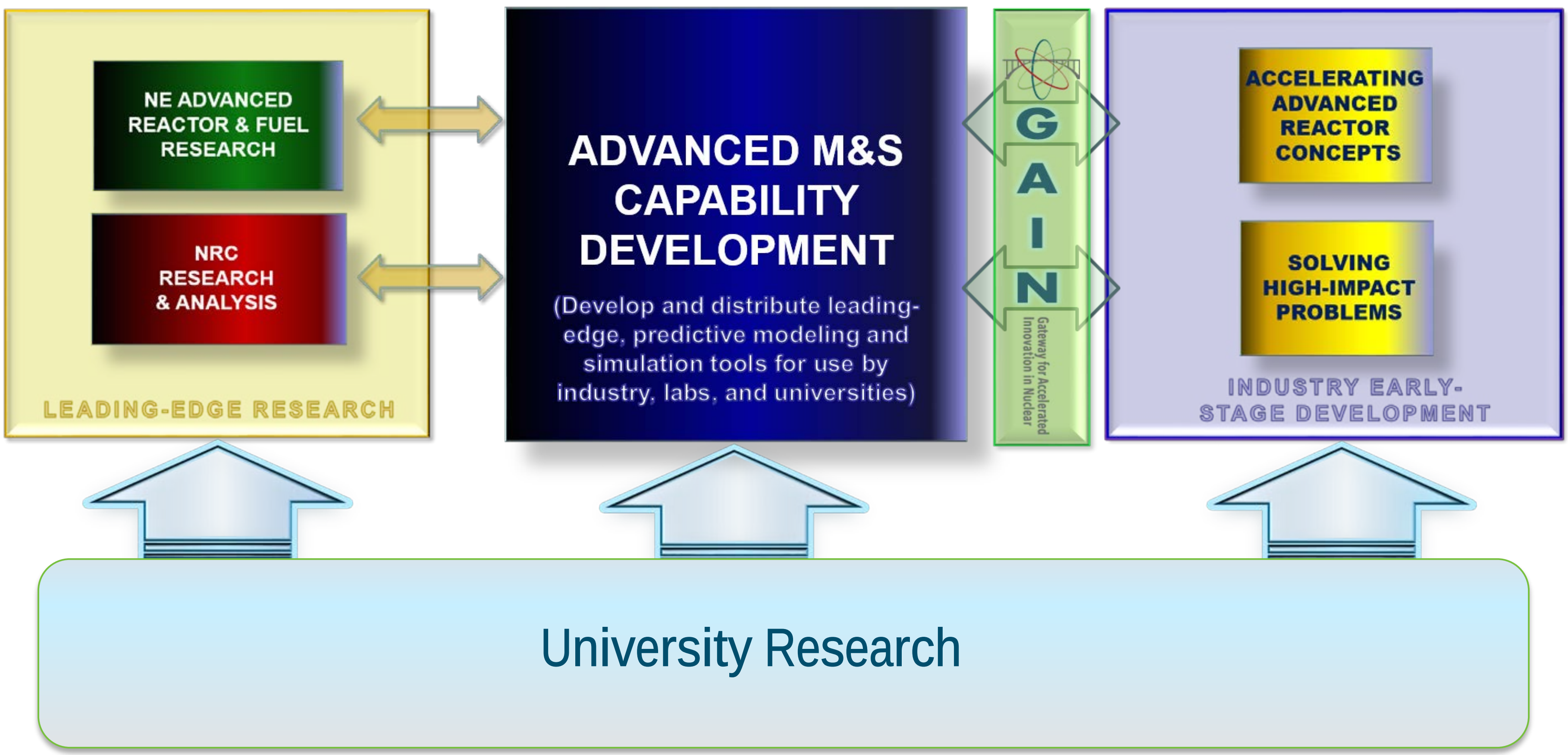
Objective: Develop and deploy predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems focused on <u>non-LWR technologies</u>

Advanced Modeling and Simulation Capabilities



Pellet | Pin | Core | System

Advanced Modeling & Simulation



Advanced Modeling & Simulation
Underpins NE's Mission Focus Areas

Existing Fleet

- **Address core performance issues that increase operational costs**
- **Assure the long-term availability and market competitiveness of nuclear energy**

Advanced Reactor Pipeline

- **Accelerate concept development and commercialization**
- **Meet otherwise cost-prohibitive data needs**
- **Support NRC confirmatory analyses**

Fuel Cycle Infrastructure

- **Confirm higher burn-up fuel strategies to slow production of used nuclear fuel (UNF) – VERA**
- **Support UNF R&D with high-fidelity analysis and prediction of fuel and cladding performance-NEAMS**

Advanced Modeling & Simulation
Supporting NE's Mission Focus Areas

Existing Fleet | Advanced Reactor Pipeline | Fuel Cycle Infrastructure

- **Critical role in accelerating design and deployment of advanced reactors**
  - Design optimization is required to fully realize the economic and technological advantages of advanced concepts
  - Advanced M&S tools will help the NRC expand capabilities as needed to perform confirmatory analysis on advanced reactor concepts
- **Only way for vendors to economically address data needs, which otherwise could require cost-prohibitive experimentation**
  - Reduce the amount of experimental testing needed
  - Identify, design, execute, and analyze more effective high-value experiments
- **The advanced reactor industry is already using our Advanced M&S tools to:**
  - Reduce cost and time for license applications to the NRC
  - Enhance potential for successful commercialization - accelerated development crucial to economic viability

Advanced Modeling & Simulation: *Tools to Solve Industry's Priority Problems*

- **Accelerating concept development for timely commercialization is absolutely critical to the future success of advanced reactors**
  - Without acceleration enabled by Advanced M&S, commercialization of promising advanced reactor concepts may not be possible, which could have a long-range adverse impact on the energy sector; certainly a major opportunity lost

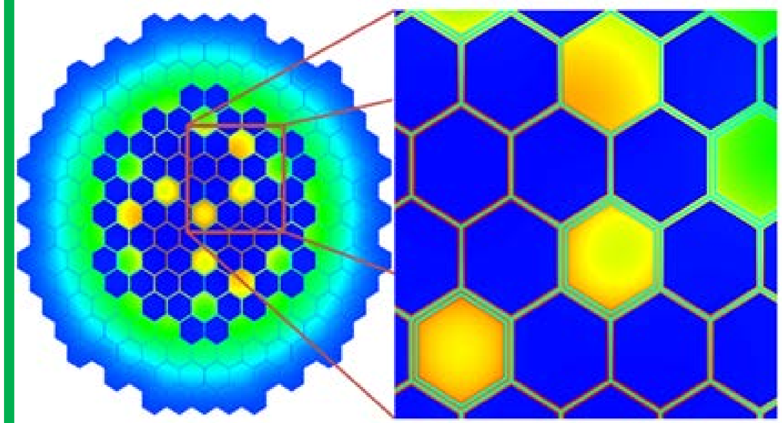
- **Similarly, application of Advanced M&S tools is critical to the optimized use of advanced test reactors that support advanced reactor and fuels development**
  - Establishing and executing a modern strategy to simulate experiments and analyze measurement data is central to maximizing the impact of any advanced test reactor experimental program
  - Deploying Advanced M&S tools as a tightly coupled research platform enables comprehensive understanding of the multi-scale and multi-physics performance of the advanced reactor experimental capabilities through intelligent feedback between simulations and experiments

Motivation for the
Advanced M&S CINR scope

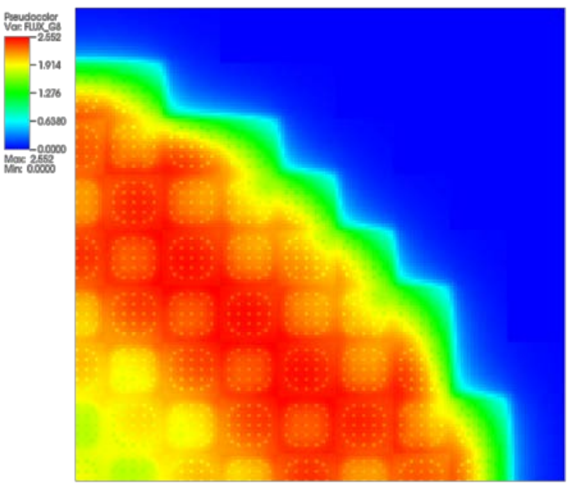
Advanced Modeling & Simulation:
Tools to Solve Industry's Priority Problems

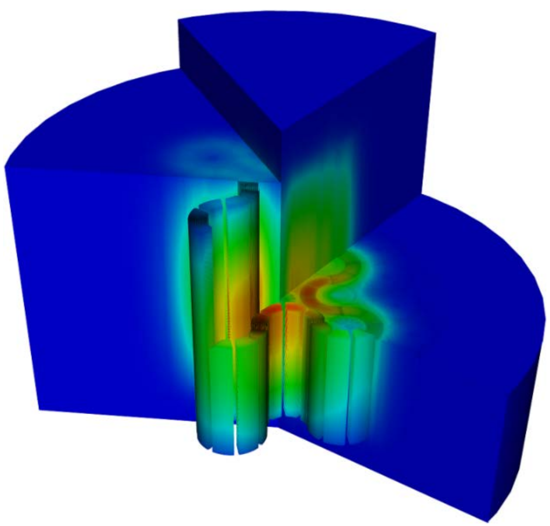
		LWRs (and water based SMRs)	Advanced Reactors
Integration		VERA	Workbench
System Analysis	Plant	RELAP-7	SAM
Core Analysis	Neutronics-Pin Resolved	MPACT	Proteus
	Neutronics-Monte Carlo	Shift/External Codes	External codes
	Neutronics-Kinetics/Depletion	MPACT	
	Neutronics-Cross Sections	AMPX/SCALE - MC2-3	MC2-3
	T-H Low Res	Cobra-TF (CTF)	SAM
	T-H Hi Res (CFD)	External codes/Nek5000	Nek5000
	Structural Mechanics	External codes	Diablo
Fuel Analysis	Continuum	BISON	BISON
	Microstructure	Marmot	Marmot
	Component Aging	Grizzly	Grizzly
	Chemistry	MAMBA	MAMBA

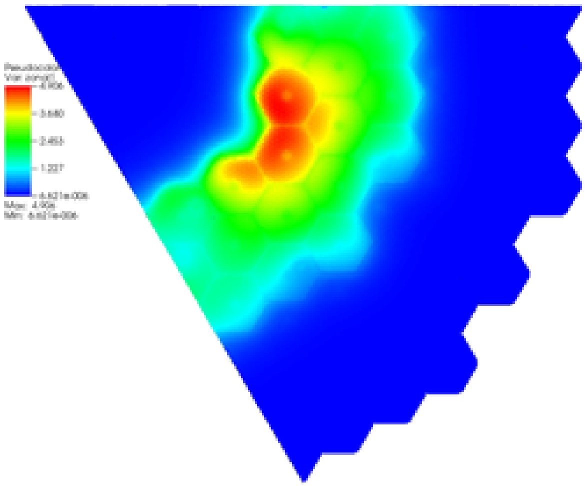
PROTEUS/MC^2-3
Pin Resolved Neutronics



- High-fidelity FEM neutron transport module and matching cross-section generation capabilities
- Unstructured grid for complex geometries
- On-line cross section generation
- Excellent scalability for parallel computing





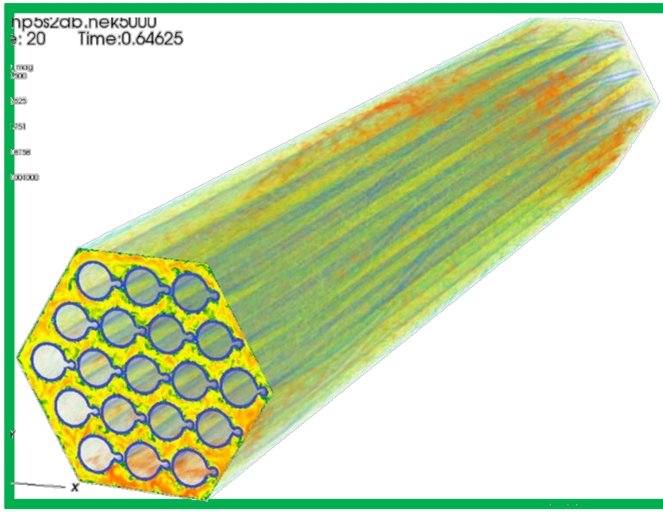


PROTEUS/MC^2-3
Papers

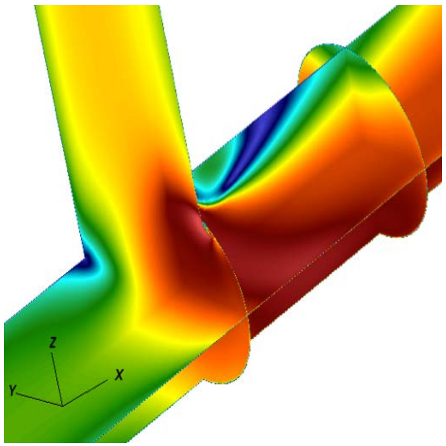
MC^2-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis (*Nuclear Science & Engineering*)	*Improved methods and performance of the MC2-3 code, which is a multigroup cross-section generation code for fast reactor analysis*
NEAMS Neutronics: Development and Validation Status (ICAPP)	*Status of advanced neutronics capabilities at Argonne National Laboratory (high-fidelity neutron transport code PROTEUS, and advanced multigroup cross section generation code MC^2-3); includes validation results and discussion*
High Fidelity Multiphysics Calculations Of Hot Channel Factors For Sodium-Cooled Fast Reactors	*Reduction or elimination of modeling uncertainties in the calculation of HCFs using high fidelity advanced modeling and simulation tools; high fidelity HCFs calculated with PROTEUS-MOCEX and Nek5000 are compared to legacy HCFs for similar reactor types (SFRs)*

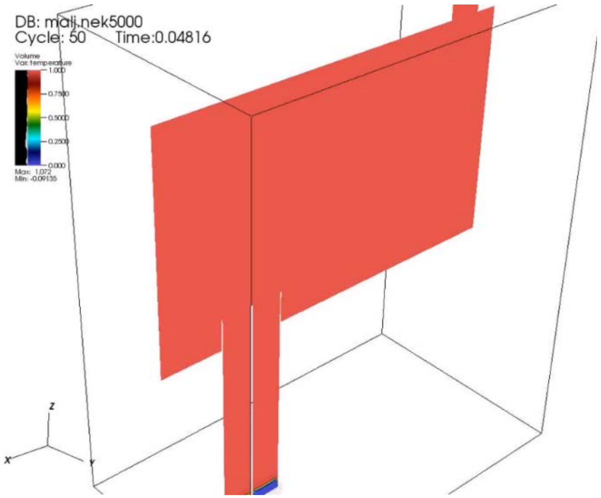
POC – Tanju Sofu (tsofu@anl.gov)

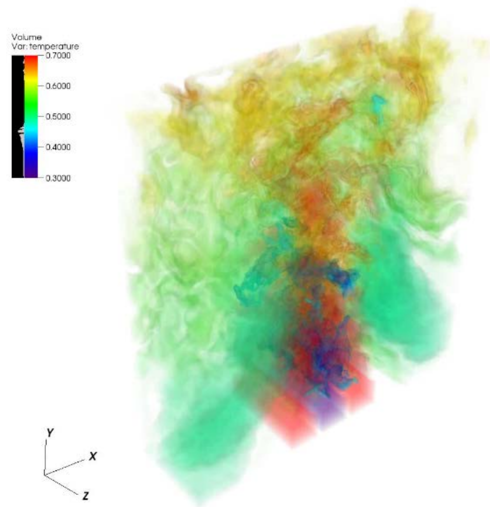
Nek5000
CFD/Thermal-Hydraulics



- CFD with high-order spectral elements on an unstructured (but conformal) hexahedral grid
- Incompressible and weakly-compressible flow
- DNS, LES, and RANS formulations for turbulence
- Excellent parallel scaling (1M+ ranks)







Nek5000
Papers

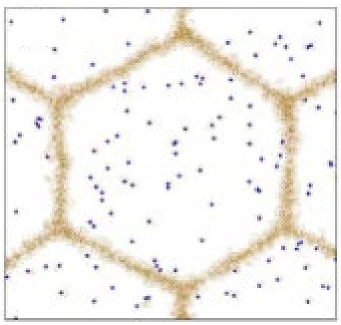
Comparison Of Experimental and Simulation Results On Interior Subchannel Of A 61-Pin Wire-Wrapped Hexagonal Fuel Bundle	*Joint project with AREVA, ANL, TAMU, and Terrapower. Comparisons are made between particle image velocimetry velocity field measurements to ANL's large-eddy simulation results at an interior subchannel for a Reynolds number of 19,000*

POC – Elia Merzari (emerzari@anl.gov)

BISON/MARMOT
Multiscale Mechanistic Modeling of Nuclear Fuels

- **<u>Objective</u>:** Use hierarchical, multiscale modeling for improved, mechanistic, and increasingly predictive models of fuel performance
- Mechanistic fuel behavior models: 1) minimize form errors, 2) provide insight were experimental data is sparse, and 3) may require less (or different) experimental data for validation

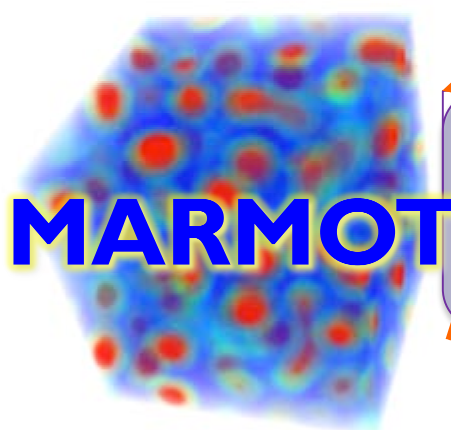
Atomistic simulations



Atomistically-informed parameters

- Identify important mechanisms
- Determine material parameter values

Meso-scale models

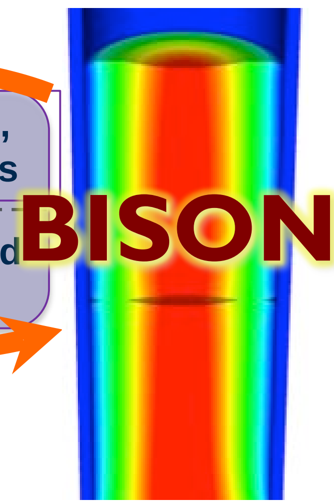


Degrees of freedom, operating conditions

Mesoscale-informed materials models

- Predict microstructure evolution
- Determine effect of evolution on material properties and fuel behaviors

Fuel performance models



- Predict fuel performance and failure probability

BISON/MARMOT
Papers & Manuals

Mechanistic materials modeling for nuclear fuel performance ***https://doi.org/10.1016/j.anucene.2017.03.005***	*Mechanistic materials modeling approach based on the current state of the evolving microstructure rather than on burn-up, with experimental data used to inform the development of these models.*
BISON Theory Manual: The Equations Behind Nuclear Fuel Analysis ***https://bison.inl.gov/SiteAssets/BISON_Theory_ver_1_3.pdf***	*Theoretical and numerical foundations of BISON for a range of fuel types and physical properties and behavior, with discussion of resulting models*
Assessment of BISON – A Nuclear Fuel Performance Analysis Code (Release 1.4) **https://bison.inl.gov/SiteAssets/BISON_assessment1.4.pdf**	*Perhaps the most important comprehensive report on Bison. Summary of assessments of Bison's predictive capability. Primary focus on LWR fuel, with secondary focus on TRISO fuel.*

POC – Rich Williamson (Richard.williamson@inl.gov)

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

- **Focus is extend the applicability and utility of the NEAMS tools to provide support for advanced fast reactors (*e.g*., micro-reactors) and for experimental use of fast test reactors**
  - Expected to support the experimental program (experiment design, analyses, et al) for the Variable Test Reactor project
  - Collaboration should include NEAMS and VTR project

- **IRP is comprised of two primary Tasks**
  - **Task 1** - Accelerate extension of NEAMS computational tools to simulation of relevant metallic fuel behavior and performance, including both high-fidelity and fast-running capabilities as needed.
  - **Task 2** - Accelerate coupled Neutronics and Thermal-Hydraulic Analysis capabilities to support experimental use of test reactors such as the VTR, and support related advanced fast reactor commercialization (*e.g*., micro-reactors)

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

- **Task 1 – Extension of BISON/MARMOT has two focus areas**
  - Mechanistic model and transient simulation developments that incorporate or enhance capabilities for key phenomena, including
    - Fuel and cladding temperature distribution (as calculated by the NEAMS neutronics and thermal-hydraulics analysis tools),
    - Fuel-to-cladding and cladding-to-coolant heat transfer,
    - Axial burnup distribution in the fuel,
    - Thermal conductivity of the fuel and cladding for fresh and as-irradiated fuel,
    - Thermal expansion of the fuel and cladding,
    - Fission gas production, transport, and release,
    - Production and transport of lanthanide fission products,
    - Solid and gaseous fission product swelling,
    - Fuel constituent redistribution,
    - Cladding strain due to internal fission gas pressure and fuel-cladding mechanical interactions, and
    - Thinning of the cladding due to fuel-cladding chemical interactions
  - Validation of new models by leveraging the available EBR-II and FFTF, and transient fuel testing data, to support both the VTR project as well as relevant industry end-users

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

- **Task 2 – Extend Coupled Neutronics and Thermal-Hydraulic Analysis Capabilities**

  - Review of the hot-pin/channel factors developed for the earlier SFRs (EBR-II, CRBR and FFTF)

  - Identification of a subset of these factors as potential candidates for reduction or elimination through high-fidelity simulations

  - Application of NEAMS multiphysics analysis capabilities to the calculation of hot-pin and hot-channel factors, where the overall mature capability is expected to subsequently support the test reactor experimental efforts and help meet certain advanced reactor concept commercialization needs

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

- **Program (IRP-NEAMS-1)**
- **Federal POC**
  - **Dave Henderson (david.Henderson@hq.doe.gov)**
- **TECHNICAL POCs**
  - **Chris Stanek (stanek@lanl.gov)**
  - **Tony Hill (hilltony@isu.edu)**
- **Up to 3 Years and $4,000,000**

Questions?

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