U.S. DEPARTMENT OF ENERGY | Office of Nuclear Energy

An Overview of NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

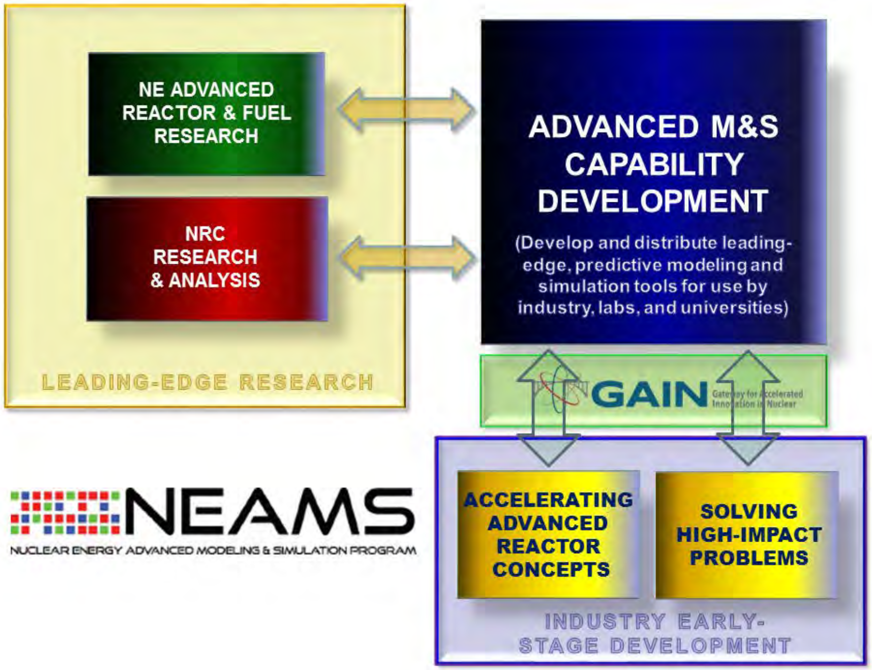
Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Fiscal Year 2017 Annual Planning Webinar

Office of Advanced Innovation in Nuclear Energy (NE-51)
Office of Nuclear Energy Innovation and Application (NE-5)
U.S. Department of Energy

August 2017

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

The NEAMS Mission: provide leading-edge computational tools, currently not available to industry, for accelerating early-stage development of advanced reactor concepts and promoting innovative solutions to important nuclear industry problems; these advanced M&S capabilities will –



NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

- Enable transformative scientific discovery and insights otherwise not attainable or affordable
- Solve problems identified as significant by industry, and consequently expand validation, application, and long-term utility of these advanced tools
- Enhance opportunity for industry to commercialize advanced concepts
- Allow industry to implement innovations that improve the economics of both existing and future nuclear power plants

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NEAMS Organizational Structure

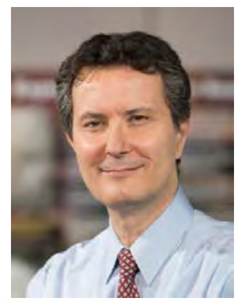
National Technical Director
Chris Stanek
(LANL)

Leadership Council

ATF HIP
Jason Hales
(INL)

Fuels Product Line
Steve Hayes
(INL)

Integration Product Line
Brad Rearden
(ORNL)



Reactors Product Line
Tanju Sofu
(ANL)

SGFIV HIP
Elia Merzari
(ANL)

Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

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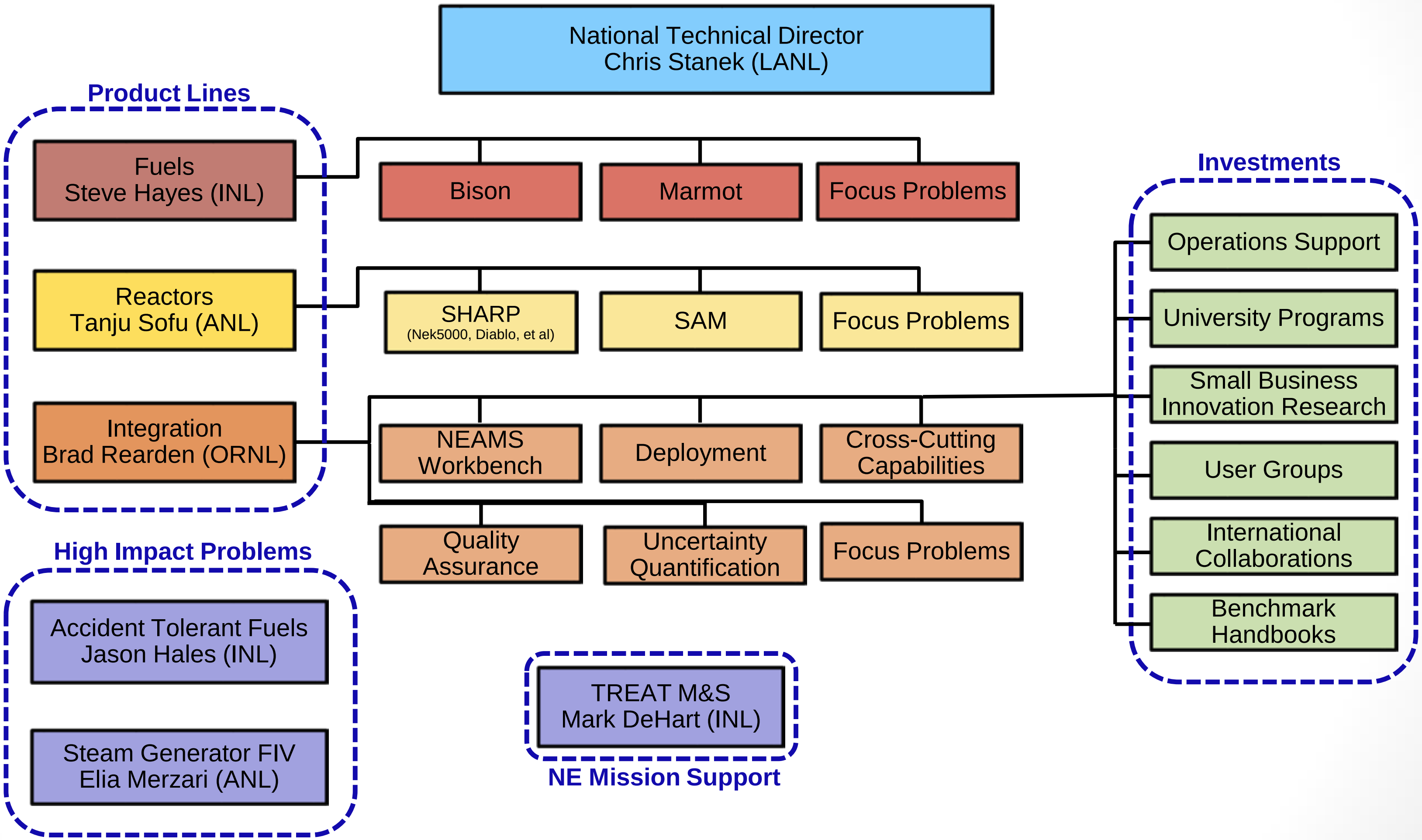
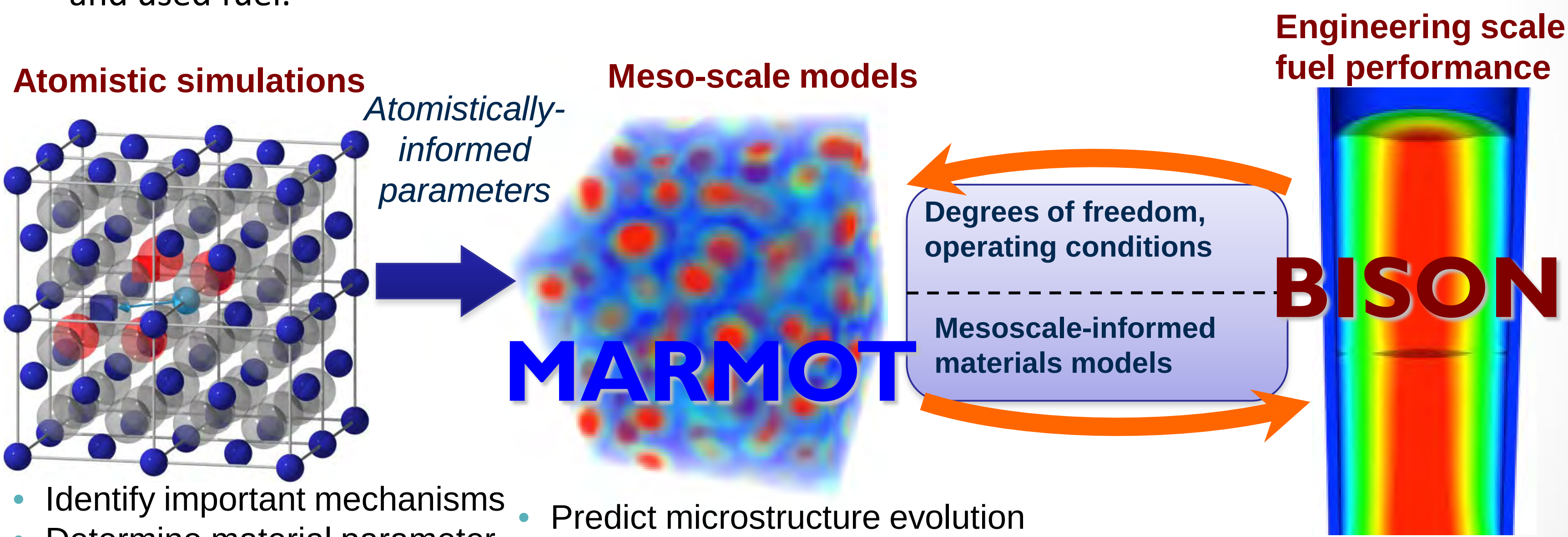
NEAMS Mission Areas



FPL

NEAMS - Fuels Product Line (FPL)

- Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds
- Goal: Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling - applied to existing, advanced (including accident tolerant) and used fuel.



- Identify important mechanisms
- Determine material parameter values

- Predict microstructure evolution
- Determine effect of evolution on material properties

- Predict fuel performance and failure probability

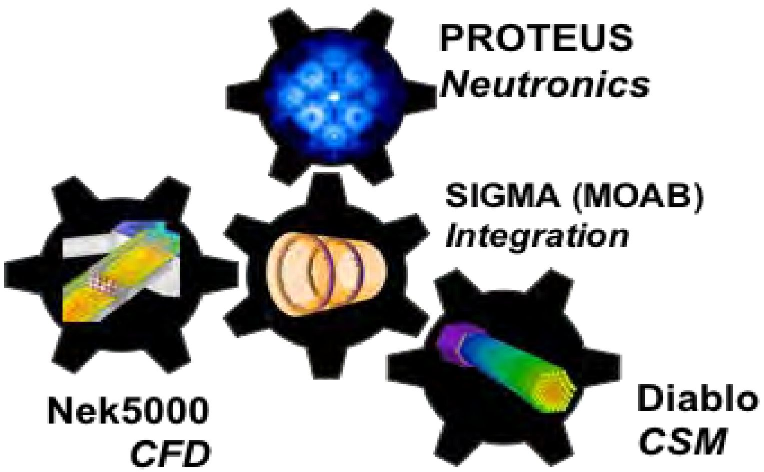
MOOSE

Multiphysics Object-Oriented Simulation Environment

NEAMS - Reactors Product Line (RPL)

RPL Focus:

- **System Analysis Module (SAM)**
- **Simulation-based High-fidelity Advanced Reactor Prototyping (SHARP)**
  - Pin-by-pin neutronics, T/H, CFD and CSM modules
  - Capabilities to integrate these modules for multi-physics simulations
  - Primarily targets leadership class computing platforms
  - A range of reduced-order models/methods are also being pursued for more common computing platforms



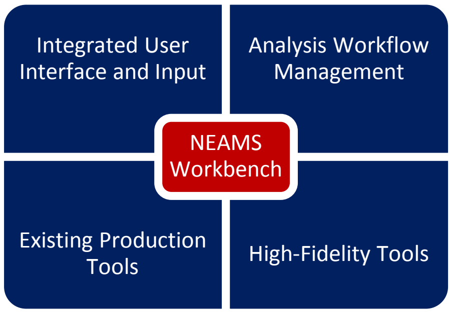
SHARP is comprised of several physical modeling tools and capability to integrate these tools for multi-physics analyses

- PROTEUS/MC^2-3/PERSENT for neutronics
- Nek5000 for CFD and T/H
- Diablo for structural mechanics
- SIGMA interface for multi-physics coupling

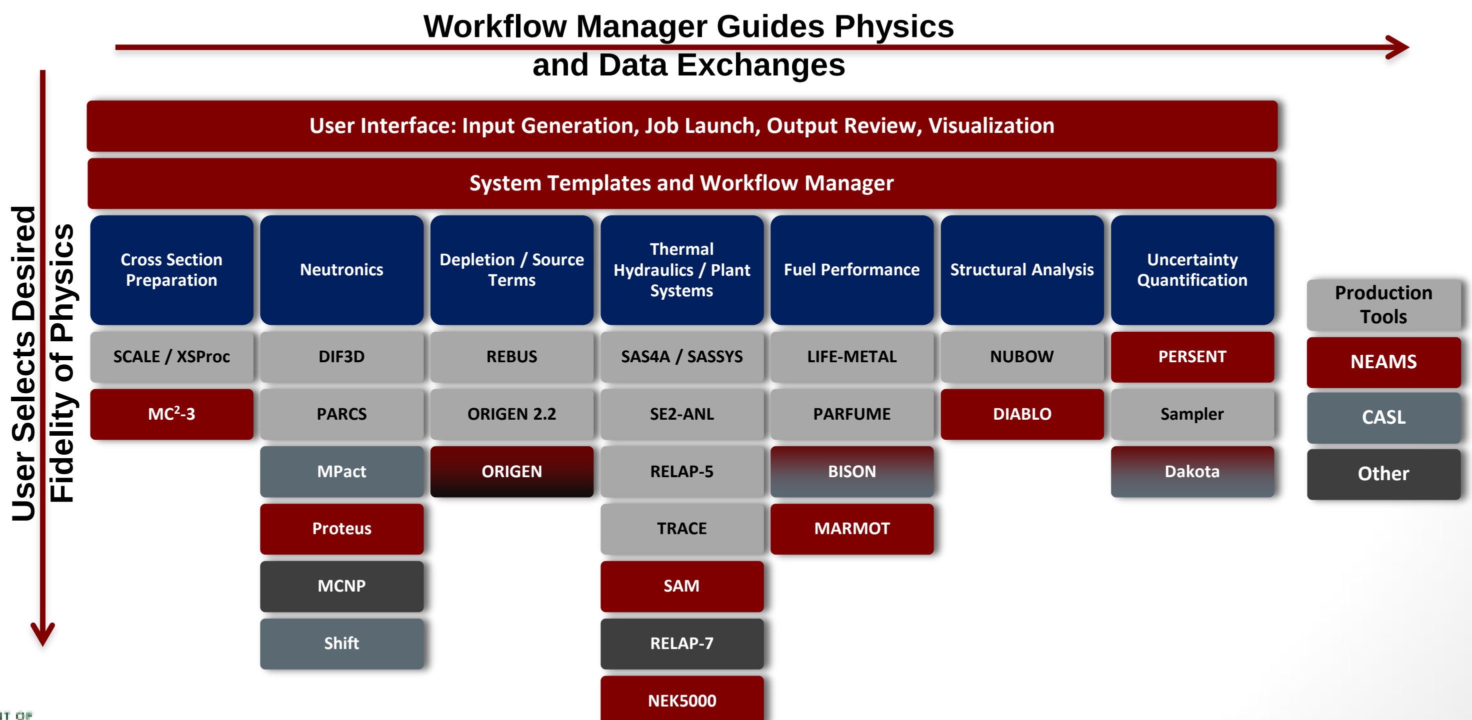
NEAMS – Integration Product Line (IPL)

IPL

The NEAMS Workbench



- Integrate current production tools with advanced tools under an integrated user interface and workflow manager
- Leverage modern user interface from SCALE, which is co-sponsored by NRC
- Leverage templating/input expansion engine from UNF-ST&DARDS and SCALE so that engineering parameters can be expanded to specific input for analysis with varying levels of fidelity in several codes
- Desire to integrate many tools for many types of systems and demonstrate use of high-fidelity simulations to inform lower order models



NEAMS – NEUP/CINR

Work-scope Description

- Program Support in Science & Technology Innovation – NEAMS-1 & 2; we are seeking proposals that contribute to improving the mechanistic models, computational methods, validation basis, and code integration and deployment for the NEAMS tools and their components in following topical areas:
  - NEAMS 1.1 – Atomistic and Mesoscale Modeling and Simulation of Nuclear Fuels, Cladding, and Reactor Structural Materials
  - NEAMS 1.2 – Macroscale Fuel Performance
  - NEAMS 1.3 – Core Neutronics
  - NEAMS 1.4 – Thermal Hydraulics
  - NEAMS 1.5 – Integration and Demonstration
  - NEAMS 1.6 – Two-Phase Flow for LWRs
  - NEAMS 2 -- Separate Effects Irradiation Testing for Validation of Microstructural Models in Marmot

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NEAMS – NEUP/CINR
Work-scope Description

- NEAMS 1.1 – Atomistic and Mesoscale Modeling and Simulation of Nuclear Fuels, Cladding, and Reactor Structural Materials (TPOC – Steve Hayes, steven.hayes@inl.gov)
  - Improve MARMOT predictive capabilities for additional phenomena of interest in nuclear fuels and materials impacting their in-reactor performance
    - Additional fuels and cladding materials include metallic fuels and stainless steel claddings for fast reactors
    - Additional phenomena of interest include mechanistic models for corrosion, creep, chemical interaction, swelling, and phase separation in multi-phase, multi-component systems in reactor materials including current and future reactors
  - Improve/extend the validation basis of MARMOT
    - Should involve closely correlated experiments and modeling using MARMOT, as well as uncertainty quantification
  - Atomistic simulations to enable/inform development of mechanistic models for MARMOT are also encouraged.
  - Reference: http://bison.inl.gov
- NEAMS 1.2 – Macroscale Fuel Performance (TPOC – Steve Hayes, steven.hayes@inl.gov)
  - Aid in the development/implementation of mechanistic models for material properties and irradiation behaviors at the engineering scale
    - Offer more robust and efficient numerical algorithms
    - Extend capabilities of BISON to fuel forms that are currently under supported or not supported (*e.g.*, metallic fuels and stainless steel claddings for fast reactors)
  - Improve the validation basis of BISON, particularly for 3-D problems (*e.g.*, enhancing 3-D multi-physics validation using a method of manufactured solutions approach would be encouraged)
  - Coupling of BISON and MARMOT simulations using hierarchical, concurrent, or hybrid approaches are encouraged.
  - Reference: http://moose.inl.gov/marmot

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NEAMS – NEUP/CINR

Work-scope Description

- NEAMS 1.3 – Core Neutronics (TPOC – Tanju Sofu, tsofu@anl.gov)
  - Needs associated with the new MC^2-3 modeling capability for 3D MOC-based neutron transport calculations to account for the heterogeneity effect of complex geometry problems more accurately
    - Performance improvements (computation time and efficiency and solution stability)
    - V&V of the new capabilities and uncertainty evaluations
  - Proposals are sought to improve solution accuracy, computational performance and efficiency, and V&V of MC2-3 for various fast and thermal reactor applications
    - Introducing Monte Carlo approaches
    - Coherent coupling with PROTEUS
    - Efficient parallelization and numerical algorithms
    - Advanced uncertainty evaluation techniques
- NEAMS 1.4 – Thermal Hydraulics (TPOC – Elia Merzari, emerzari@anl.gov)
  - To support development of System Analysis Module (SAM) and Nek5000 for modeling the mixing and thermal-stratification in large volumes (e.g., upper plena in LMRs), contributions sought for development of Reduced-Order Modeling (ROM) approaches
    - Based on techniques that may involve proper orthogonal decomposition (POD) or other structure recognition methods and machine learning.
    - Simulations performed with Nek5000 to obtain the necessary high-fidelity data to mine
    - ROM to be implemented in SAM to support conceptual design studies and license applications
    - Experimental contributions will not be considered, but coordination with existing experimental efforts funded under the ART NEUP component is encouraged

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NEAMS – NEUP/CINR
Work-scope Description

- NEAMS 1.5 – Integration and Demonstration (TPOC – Brad Rearden, reardenb@ornl.gov)
  - Proposals are sought to integrate high-fidelity as well as conventional tools into the Workbench;
  - Automate analysis workflows used in design studies
  - Provide convenient access to uncertainty quantification; and
  - Develop and demonstrate templates of complex system models, provide automated meshing, and demonstrate the use of the Workbench for practical studies
  - Proposals that demonstrate the value of the high-fidelity NEAMS tools as applied to collaborative benchmarks, validation, and industrial systems as well as the use of NEAMS tools to inform the improved use of conventional tools within the Workbench are strongly encouraged.

NEAMS – NEUP/CINR
Work-scope Description

- NEAMS 1.6 – Advanced Two-Phase Flow Simulation for LWRs (TPOC – Elia Merzari, emerzari@anl.gov)
  - Proposals are sought for developing a native three-dimensional sub-channel capability in RELAP-7 based upon the seven-equation two-phase flow model; these capabilities must:
    - be tightly coupled to the BISON nuclear fuels performance code
    - account for continuous heat flux across the fluid structure interface and the effect of fuel pin cladding displacement on the sub-channel geometry over the life of the fuel
  - Specific experiments are also sought to validate RELAP-7's seven-equation flow model, specifically regarding its advanced features that distinguish it from traditional two-phase models; validation data must:
    - account for the seven-equation model assumption that there are distinct phasic pressures for steam and water; and,
    - for validation of pressure relaxation coefficients of the seven-equation model, include measurement of the distinct phasic pressures and their rate of relaxation toward a common pressure under transient flow conditions

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NEAMS – NEUP/CINR
Work-scope Description

- NEAMS 2 – Separate Effects Irradiation Testing for Validation of Microstructural Models in Marmot (TPOC – Steve Hayes, steven.hayes@inl.gov)
  - Proposals are sought for innovative, separate effects irradiation tests of nuclear fuels and/or materials that would provide data important to informing and validating mechanistic, microstructure-based models of fuel behavior under development using MARMOT, the NEAMS tool for simulating microstructure evolution under irradiation
    - MARMOT models under active development are summarized under NEAMS 1.1 and in the MARMOT Assessment Report
    - Fuel systems of interest for which separate effects experiments are desired are:
      - The LWR fuel system (i.e., both the historic UO2 fuel and Zirconium-based cladding, as well as emerging Accident Tolerant Fuel concepts)
      - The SFR fuel system (*i.e.*, U-Zr and U-Pu-Zr metallic fuel and steel-based cladding)

NEAMS – NEUP/CINR
Work-scope Description

- Collaboration with members of the NEAMS development team residing at DOE laboratories as well as end users in industry or regulatory authorities is strongly encouraged.

- Running simulations or conducting experiments at DOE laboratories or and Nuclear Science User Facilities (http://atrnsuf.inl.gov/) in support of the NEAMS Toolkit are encouraged, although computation or experimentation at university laboratories is equally acceptable.

- Please focus your application, if possible, on one of the five scope areas

- Federal POC – Dan Funk (dan.funk@hq.doe.gov; 301-903-3845)

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NEAMS – NEUP/CINR

Back-Up Slides

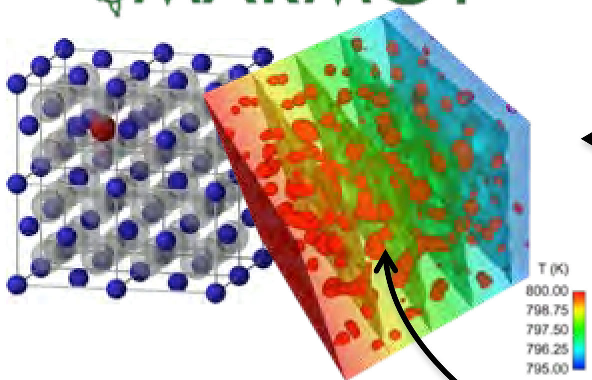
NEAMS - Fuels Product Line (FPL)

FPL

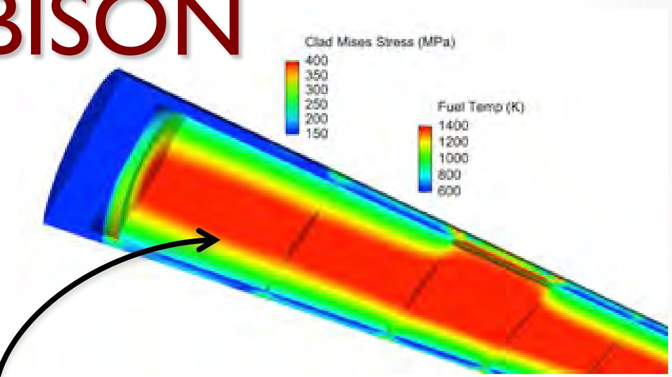
MOOSE-BISON-MARMOT

MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability

MARMOT



BISON



Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

R&D 100 2014 Winner

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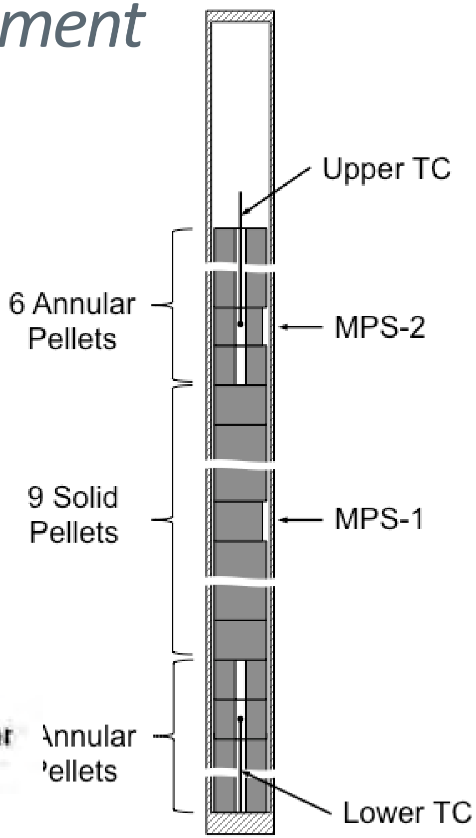
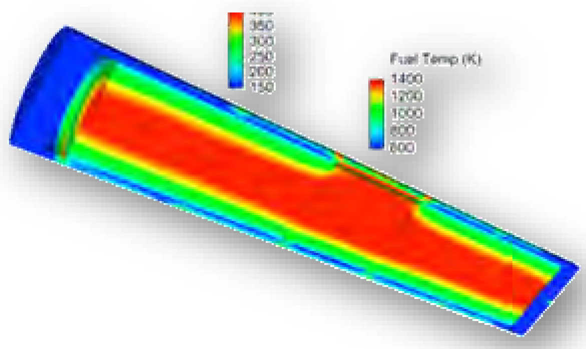
NEAMS – BISON Advanced Validation

Halden Missing Pellet Surface Experiment

FPL

- Manufacturing flaws ("missing pellet surface" defects) in fuel pellets have been root cause of fuel failures. Pellet-cladding interaction (PCI) is a CASL challenge problem.
- Validation experiment to begin in the Halden reactor this year.
- Example of a 3D fuel performance code addressing a 3D applied problem – which requires specific validation





The OECD Halden Reactor Project

Once validated, further analysis using BISON to define an MPS geometry threshold could used to inform fuel manufacturing tolerances.

FPL

NEAMS – MARMOT

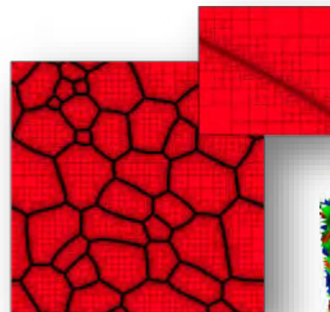
- MARMOT predicts coevolution of microstructure and physical properties in fuel and cladding materials due to applied load, temperature, and radiation damage

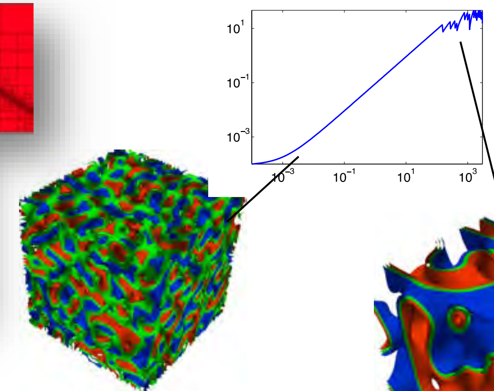
All models implemented in MARMOT are:

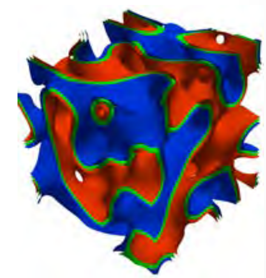
•1D, 2D or 3D

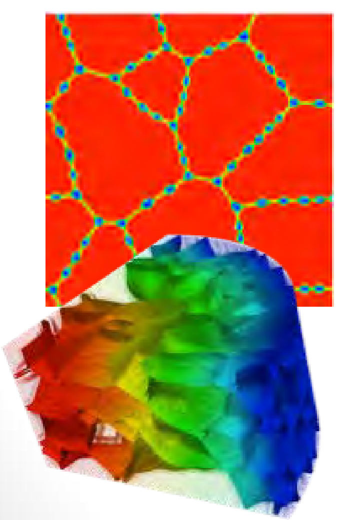
•Massively parallel, from 1 to 1000's of processors

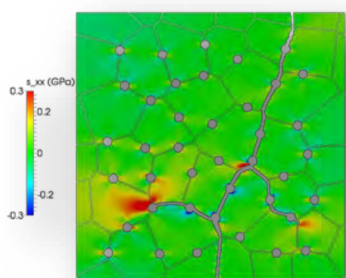
•Able to employ mesh and time step adaptivity

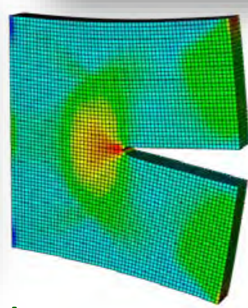


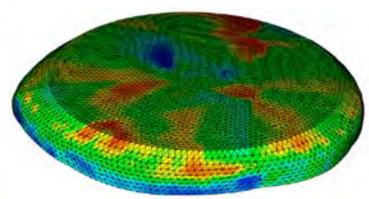












Physical models include:

- UO_2 (grain growth, fission gas release, fracture)
- U-Zr (species transport, phase change, swelling)
- U-Si (fission gas transport and swelling)
- Zircaloy cladding (hydride formation)
- FeCr (microstructure evolution)

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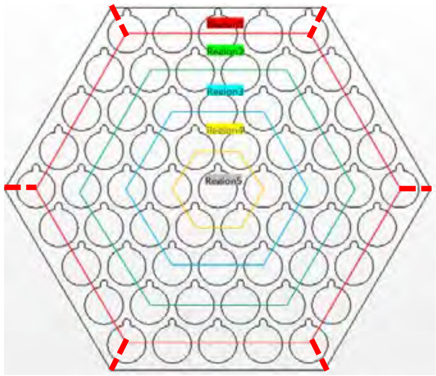
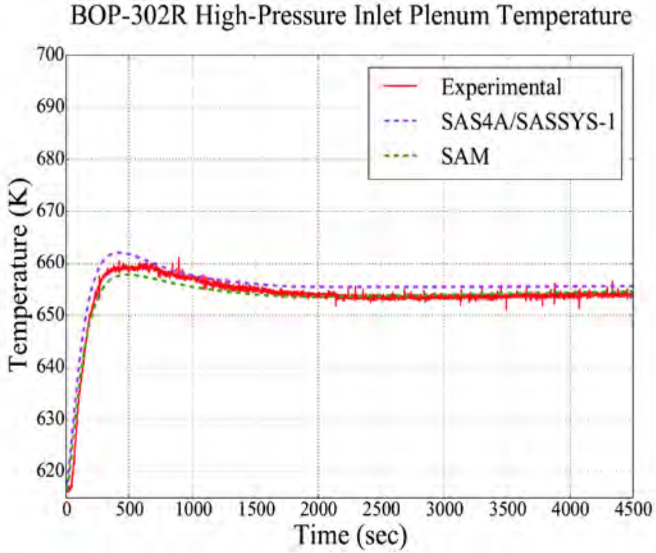
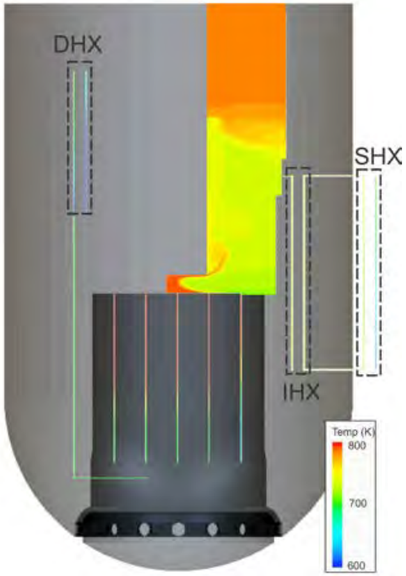
System Analysis Module: SAM

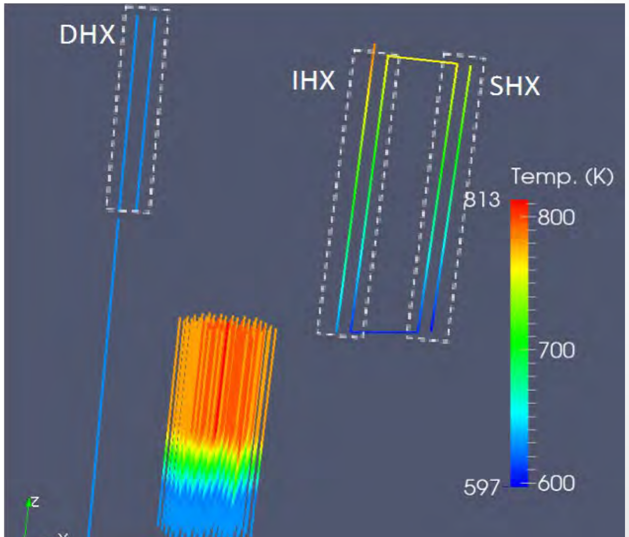


- A practical plant-level system analysis tool for advanced reactors (SFR, LFR, MSR/FHR)
- Advances in software environments and design, numerical methods, and physical models
- Built-on MOOSE framework and other modern scientific software libraries
- Flexible multi-scale multi-physics integration with other high-fidelity tools

EBR-II Loss-of-Heat-Sink Test



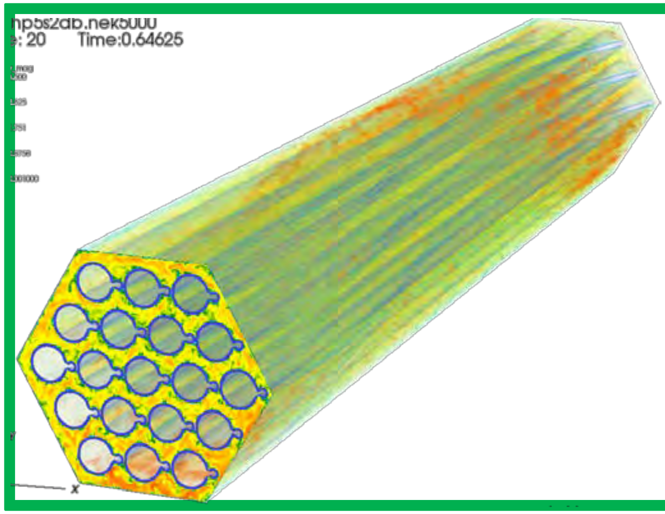




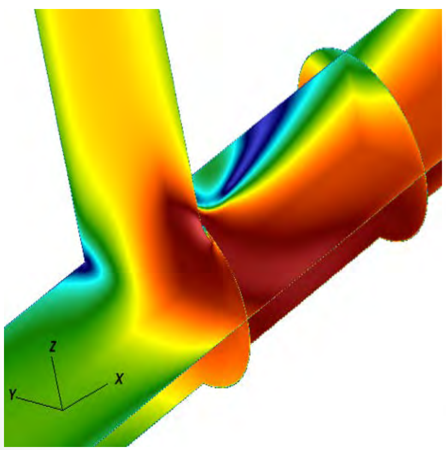
Simulation of ABTR PLOF

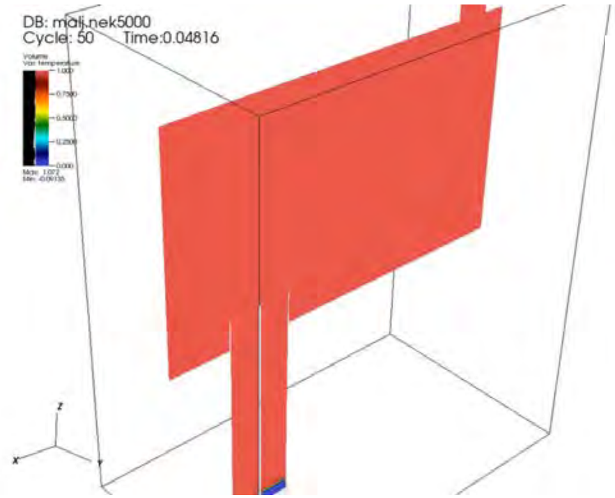
RPL

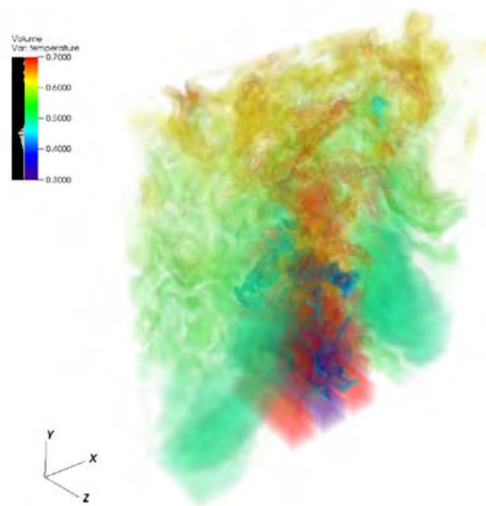
SHARP Thermal-Hydraulics: CFD Module: Nek5000



- CFD with high-order spectral elements on an unstructured (but conformal) hexahedral grid
- Incompressible and weakly-compressible flow
  - Eulerian two-phase boiling ht option
- DNS, LES, and RANS formulations for turbulence
- Excellent parallel scaling (1M+ ranks)
  - Gordon Bell and R&D-100 awards







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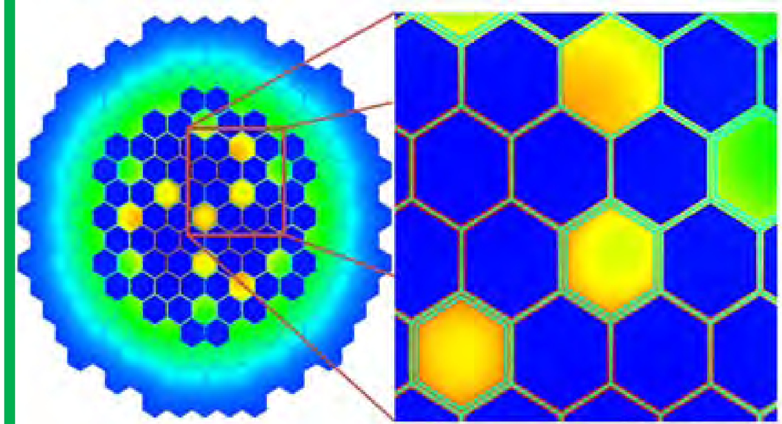
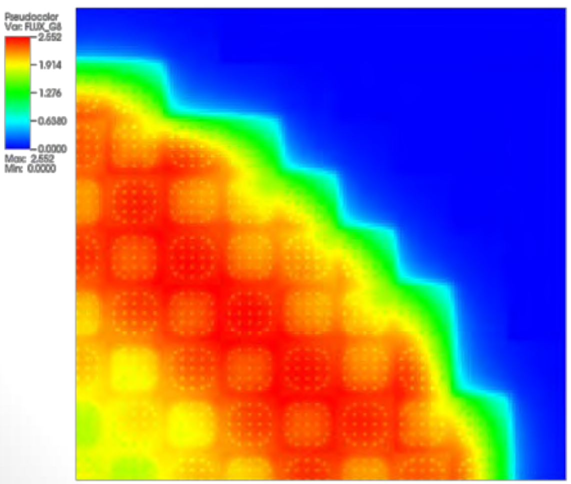
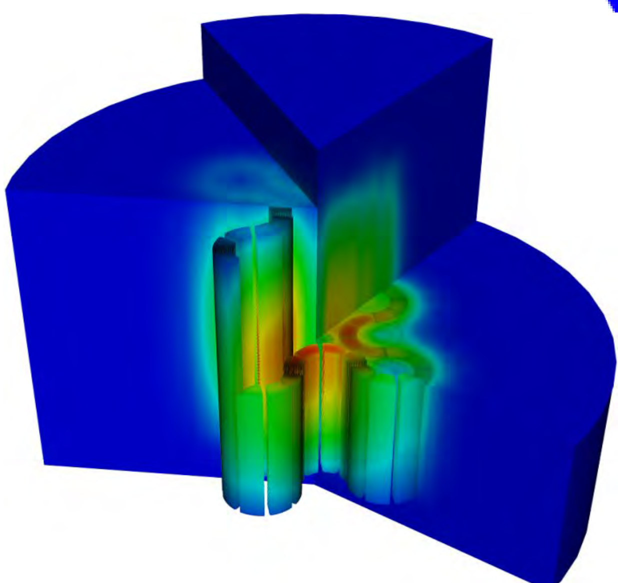
RPL

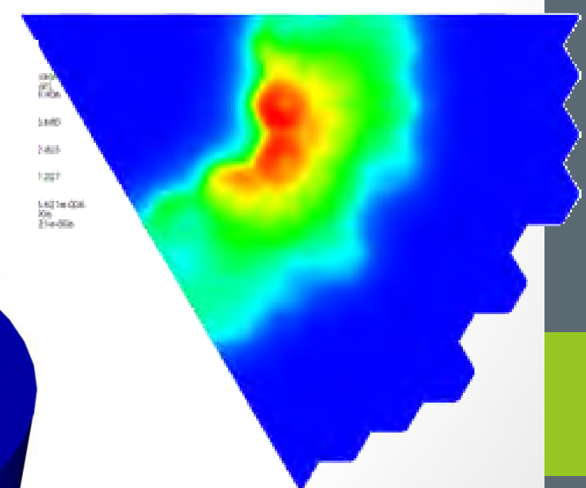
SHARP Neutronics: PROTEUS/MC^2-3/PERSENT



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







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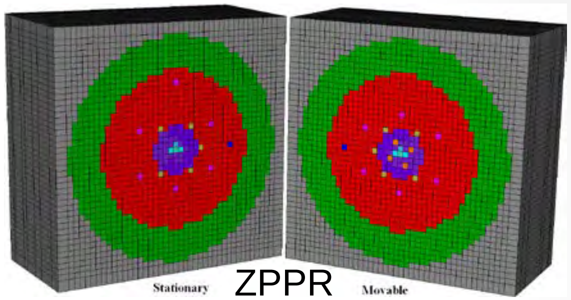
RPL

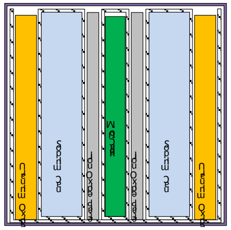
SHARP - MC²-3

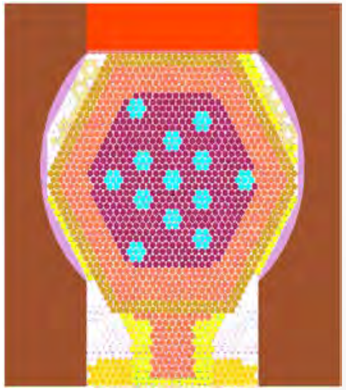
Multi-group Cross Section Generation Code

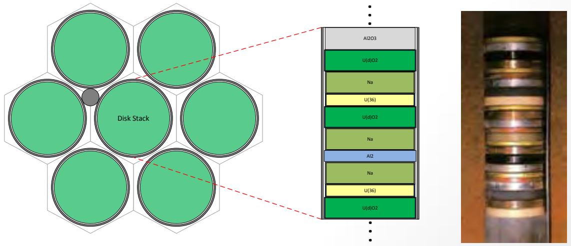
- Generate thermal and fast spectrum multigroup cross sections for diffusion and transport solvers
  - Improved resonance self-shielding using pointwise cross section integration (including analytic Doppler broadening)
  - Improved modeling of the local heterogeneity effect based on 1D geometry
  - Accurate multigroup cross section accounting for the whole-core spectrum effect by coupling with TWODANT
- V&V using numerous fast reactor benchmark problems and experiments
- Recent Progress
  - 3D MOC-based neutron transport capability to account for the heterogeneity effect of complex geometry problems more accurately
  - Thermal cross section capability which allows the code to be used for thermal reactor applications
  - Generation of ENDF/B-VII.1 cross section library



ZPPR


ZPPR Fuel


BFS



BFS Fuel

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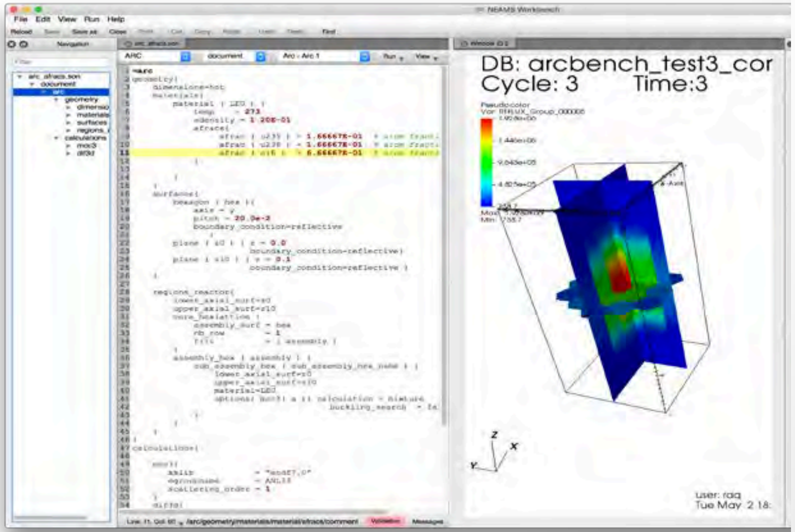
IPL

NEAMS - Integration Product Line (IPL)

- NEAMS FPL and RPL provide many advanced tools, but they often require large computational resources, can be difficult to install, and require expert knowledge to operate.
- Goal: Respond to needs of design and analysis communities by integrating robust multi-physics capabilities and current production tools in easy-to-use versioned deployments that enable end users to apply high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems.

Desired attributes:

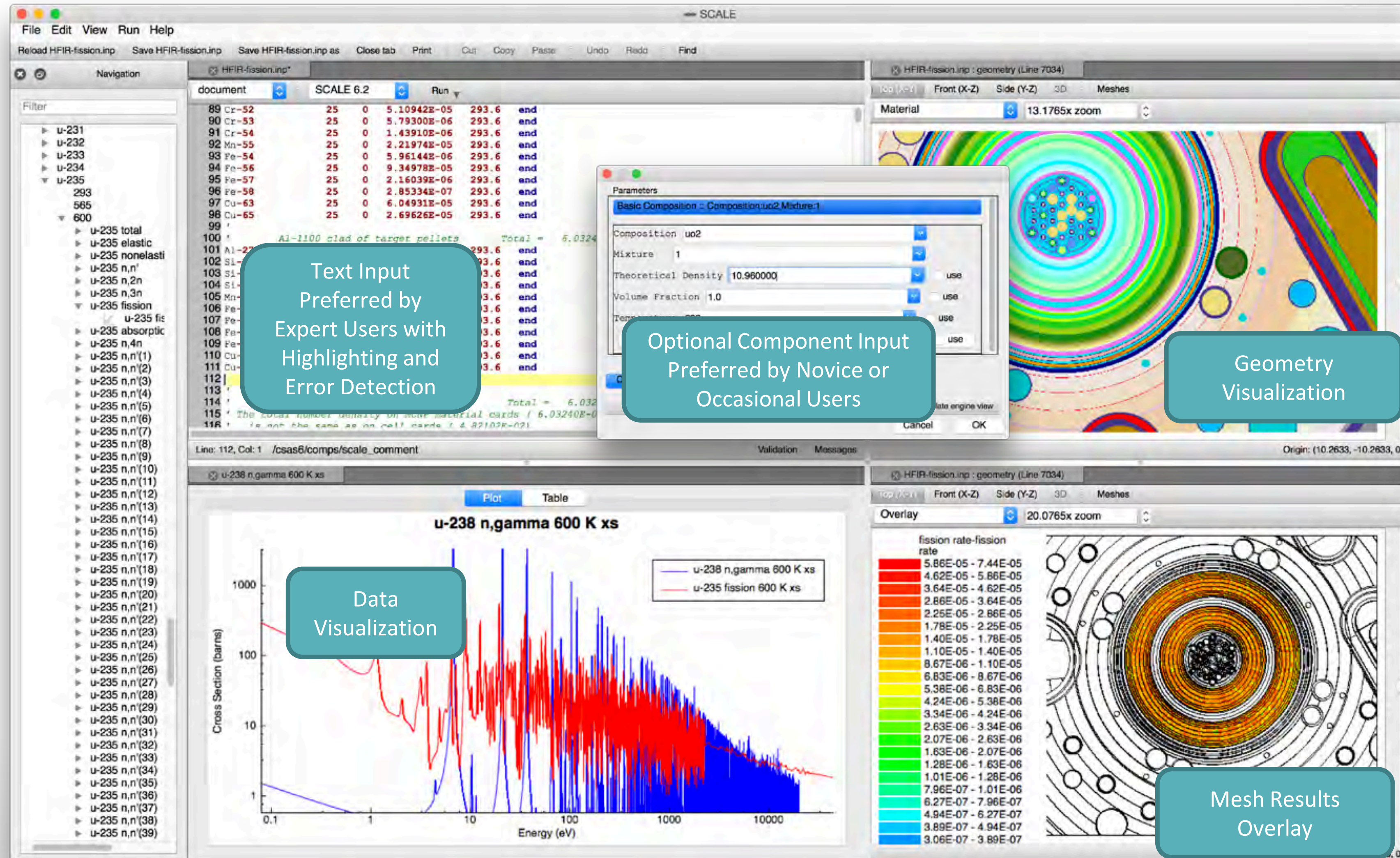
- Convenient access to high-fidelity simulations to inform lower-order models
- Common user interface
- Simplified common input to many codes
- Visualization
- Uncertainty quantification
- Quality assurance
- Verification and validation
- Application to design systems and recognized benchmarks



IPL

NEAMS – Workbench User Interface

Snapshot of Fulcrum (from SCALE)



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IPL

Templated Common Input – Use with Many Codes

Similar to CASL VERA-IN concept; Leverages Template Engine used for UNF-ST&DARDS and SCALE

Engineering-style problem specific input
(type of system, materials, dimensions, timesteps, etc)

Database of supported system configurations

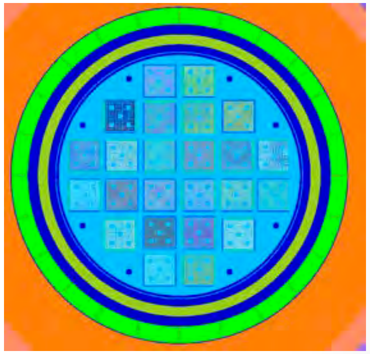
- Known systems and customizable features
- Input requirements and options for each code
- Code and problem specific information (mesh geometry, etc.)

Template Engine Expansion

Input for Code A

Input for Code B

Input for Code C



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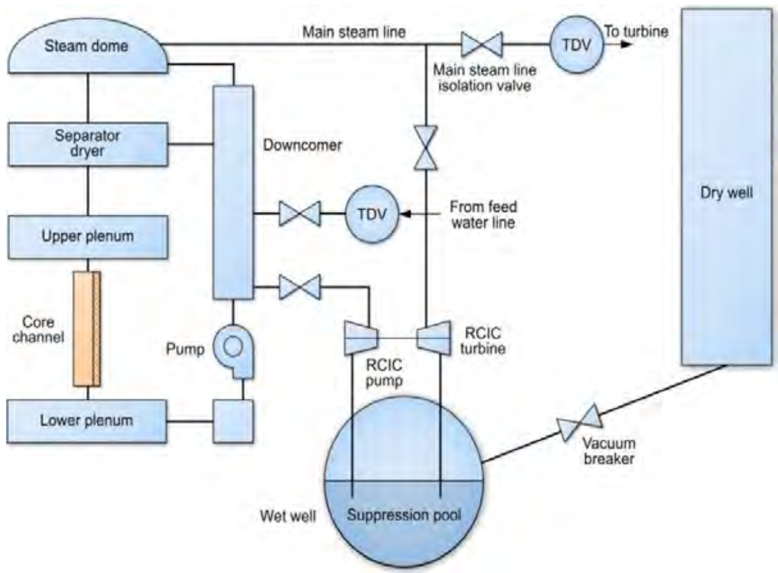
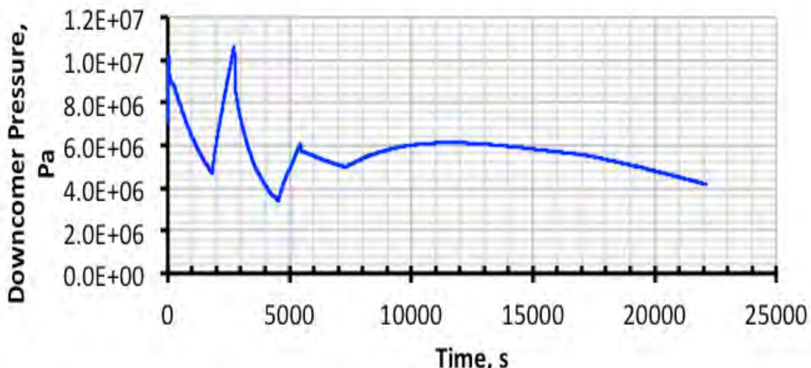
RELAP-7

(*Reactor Excursion and Leak Analysis Program*)





- RELAP-7 is the current nuclear systems safety analysis application being developed at INL.
- RELAP-7 development began in FY-2012 to support the Risk Informed Safety Margins Characterization (RISMC) Pathway of the Light Water Reactor Sustainability (LWRS) program.
- Funding Source: LWRS (NEAMS in 2012)
- 50% initial development goals completed.
- The overall design goal of RELAP-7 development is to leverage 30 years of advancements in software design, numerical integration methods, and physical models.

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RELAP-7 Design Concept

- **Modern Software Design:** *What MOOSE brings to the table.*
  - Object-oriented C++ construction (www.mooseframework.org)
  - Designed to be easily extended (modular physics) and maintained
  - Strict adherence to SQA (meeting NQA-1 requirements)
- **Advanced Numerical Integration Methods:**
  - Multi-scale time integration, both 2^{nd}-order accurate implicit and semi-implicit
  - 2nd-order accurate spatial discretization (continuous and discontinuous Galerkin)
- **State-of-the-Art Physical Models:**
  - All-speed, all-fluid (vapor-liquid, gas, liquid metal) flow – agnostic of reactor concept (PWR, BWR, SMR, SFR, MSR, FHR, HTGR, etc.).
  - 7-equation two-phase flow model incorporating IAPWS-95 equation of state.
  - New two-dimensional core heat transfer model based upon fuel, gap, clad.
  - Closure relations from the TRACE V5.0 code.
  - Designed for multiphysics analysis (BISON and MAMBA) or to couple to multi-D core simulators (CASL's VERA or NEAMS Pronghorn and TREAT simulators) with MOOSE MultiApp and Transfers.