U.S. DEPARTMENT OF ENERGY | Nuclear Energy

An Overview of NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Fiscal Year 2016 Annual Planning Webinar

Advanced Modeling & Simulation Office (NE-41)
Office of Science and Technology Innovation (NE-4)
U.S. Department of Energy

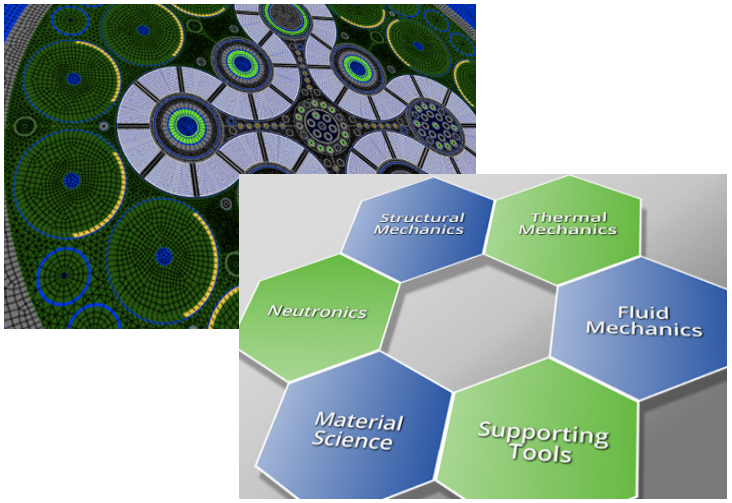
August 2015

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

Why pursue advanced modeling and simulation capabilities?

- **Modeling & simulation is a critical part of R&D** – *when integrated with theory and experiment, it enhances opportunities for new insights and more effective research*



- **Although modeling & simulation must be (and is being) integrated with theory and experiment in research programs, a concerted program is needed to develop advanced capabilities, demonstrate their utility, and help deploy them for use in R&D programs in government, academia and industry research** – *that's where NEAMS fits in*

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

What does NEAMS do, and what is its VALUE PROPOSITION?

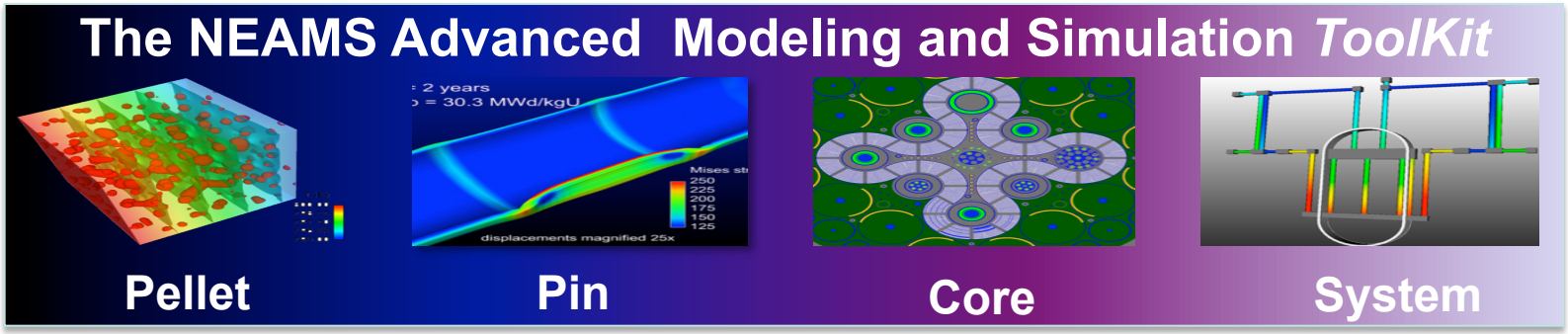
- Develops and deploys state-of-the-art predictive modeling and simulation tools (*the NEAMS ToolKit*) to the nuclear energy community; centered on enabling transitions:
  - *Descriptive to predictive models; single CPU to many CPU; single physics to multiphysics; single length/time scale to multiscale*
- Uses these tools in collaboration with field experts to solve important customer-driven high-impact problems (a key part of tool validation)
- Provides a foundational toolkit that supports the development of new advanced models and simulations (within R&D programs) to address the broad range of problems that are important to the nuclear energy community
- Empowers researchers/designers to transform nuclear technologies, and gain fundamental insights that are unattainable through experiment alone

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

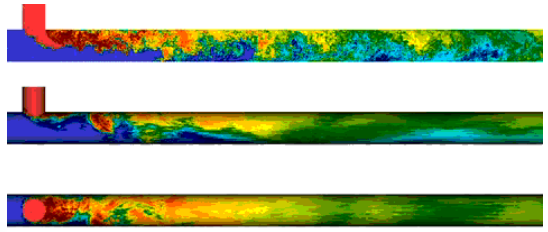
In other words NEAMS is guided by this Vision and Objective –

- **Vision:** *These advancements can be deployed as user-friendly simulation toolsets to both the R&D community as well as to industry – will impact existing, near-term and future reactors*
- **Objective:** *Develop and deploy advanced computational tools with extended capabilities to*
  - *Help achieve mission-critical goals for NE's R&D programs and industry partners -- some examples: critical down-selection of Accident Tolerant Fuels (ATF) concepts within the NE Advanced Fuels Campaign; planning for ATF experiments in the Transient Reactor Test Facility (TREAT); enhanced operation and research use of TREAT; and high-impact advances in innovative reactor designs such as SMRs*
  - *Help empower new R&D in universities*
  - *Help expand international and industry cooperation*

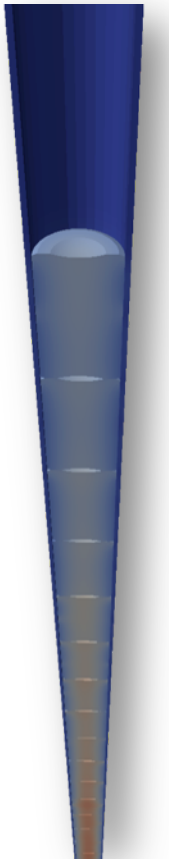


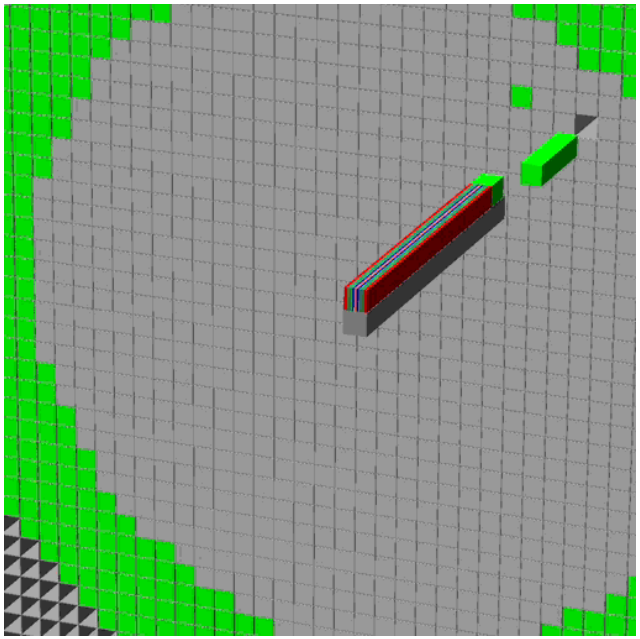
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS Focus on Problem Solving:
Initial Motivation and Drivers



- **Initial problems naturally focused on understanding limitations of conventional approaches to modeling and simulation**
  - Why does a directional bias appear in SFR fuel assembly temperature distribution measurements?
  - Can we predict thermal striping in a T-junction?
  - How is 3-D thermal prediction of deformation in a fuel pin using a model that explicitly considers the contact interactions between the pellets different from conventional 2-D models?
  - How accurately can we predict local neutron reaction rates?

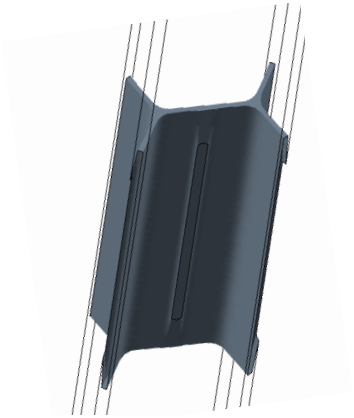


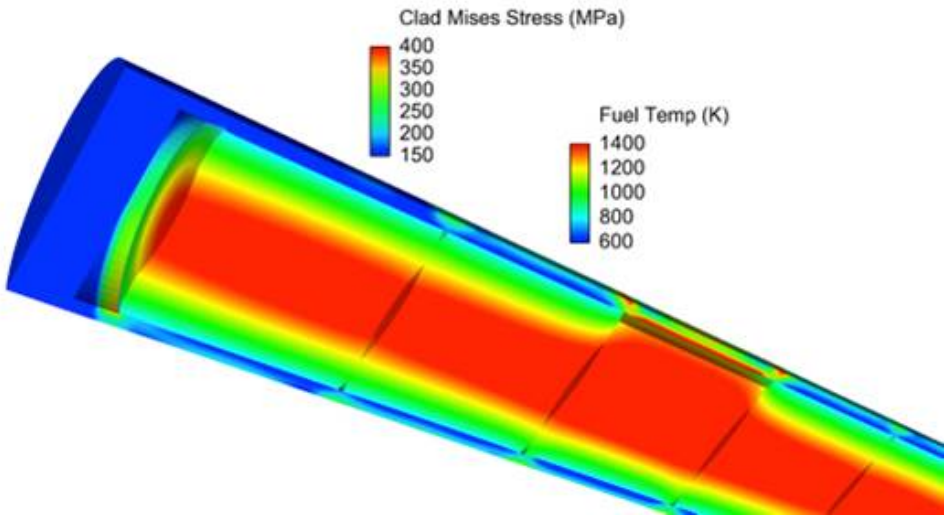


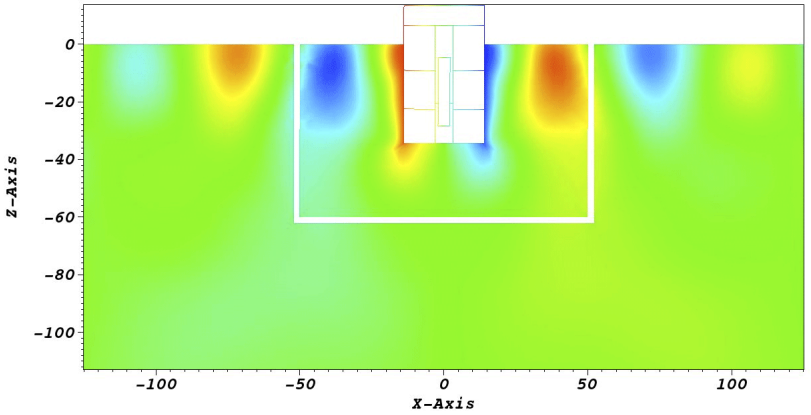
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS Focus on Problem Solving:
Capability Development

- **As we gained confidence through success in developing new capabilities, focus shifted to questions of design and design tolerances**
  - Should we use spacer grids or wire-wrapped spacers in tight-lattice bundles?
  - What is the impact of a missing pellet face on cladding performance?
  - How does soil structure interaction uncertainty impact seismic response predictions?



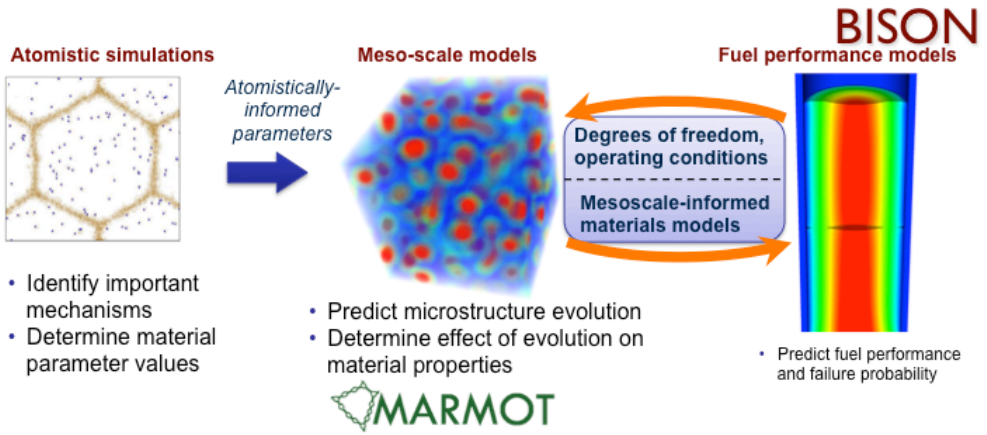




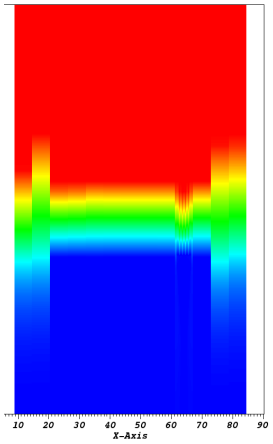
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS Focus on Problem Solving:
Capability Development & Challenge Problems

- **Both tool development and challenge problems have helped to drive multi-physics and multi-scale integration *AND* provide focus for initial validation**
  - Mulit-scale prediction of fuel performance in a conventional LWR
  - Multi-scale prediction of structural feedback contribution to passive shutdown in SFR ULOF transient



PROTEUS
+
Nek5000
+
Diablo



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Moving Forward with Solving High-Impact Problems (HIPs)

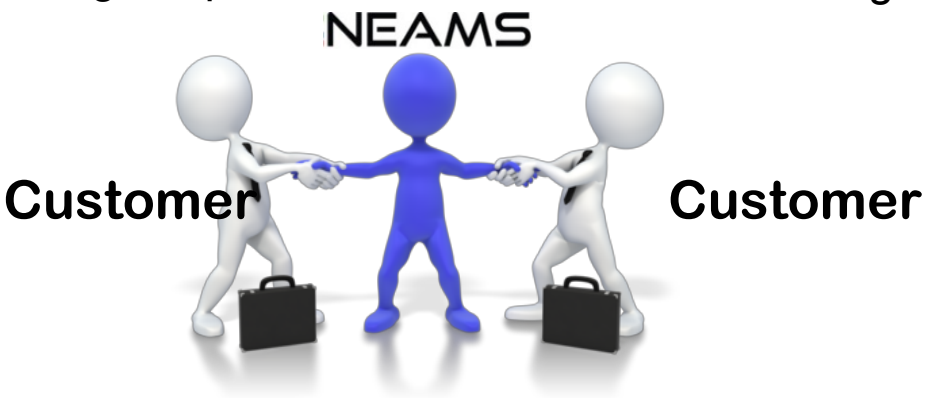
High-Impact Problem: a problem that has a solution which significantly improves, in a short period of time, an application of exceptional importance for the customer. Collaborative efforts to solve such problems will help demonstrate efficacy of NEAMS tools, and support their validation in well-defined applications, which is critical to their deployment (especially to industry), utility, and long-term value.

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

- Defines the problem
- Leads the scientific and engineering approach
- Demonstrates the high-impact

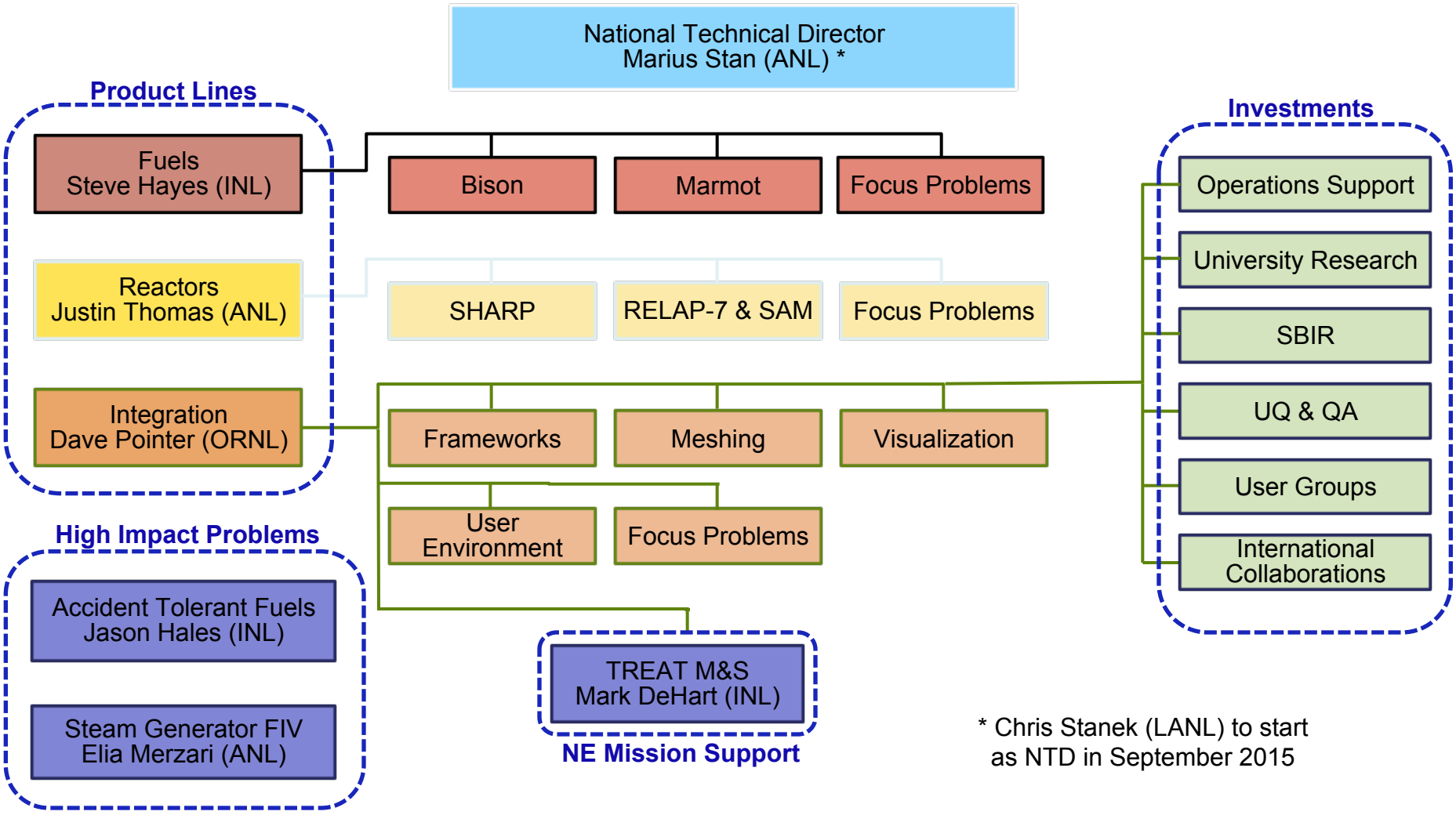
The Customer

- States the high-impact level
- Provides technical support, validation data, experiments, etc.
- Certifies the high-impact



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

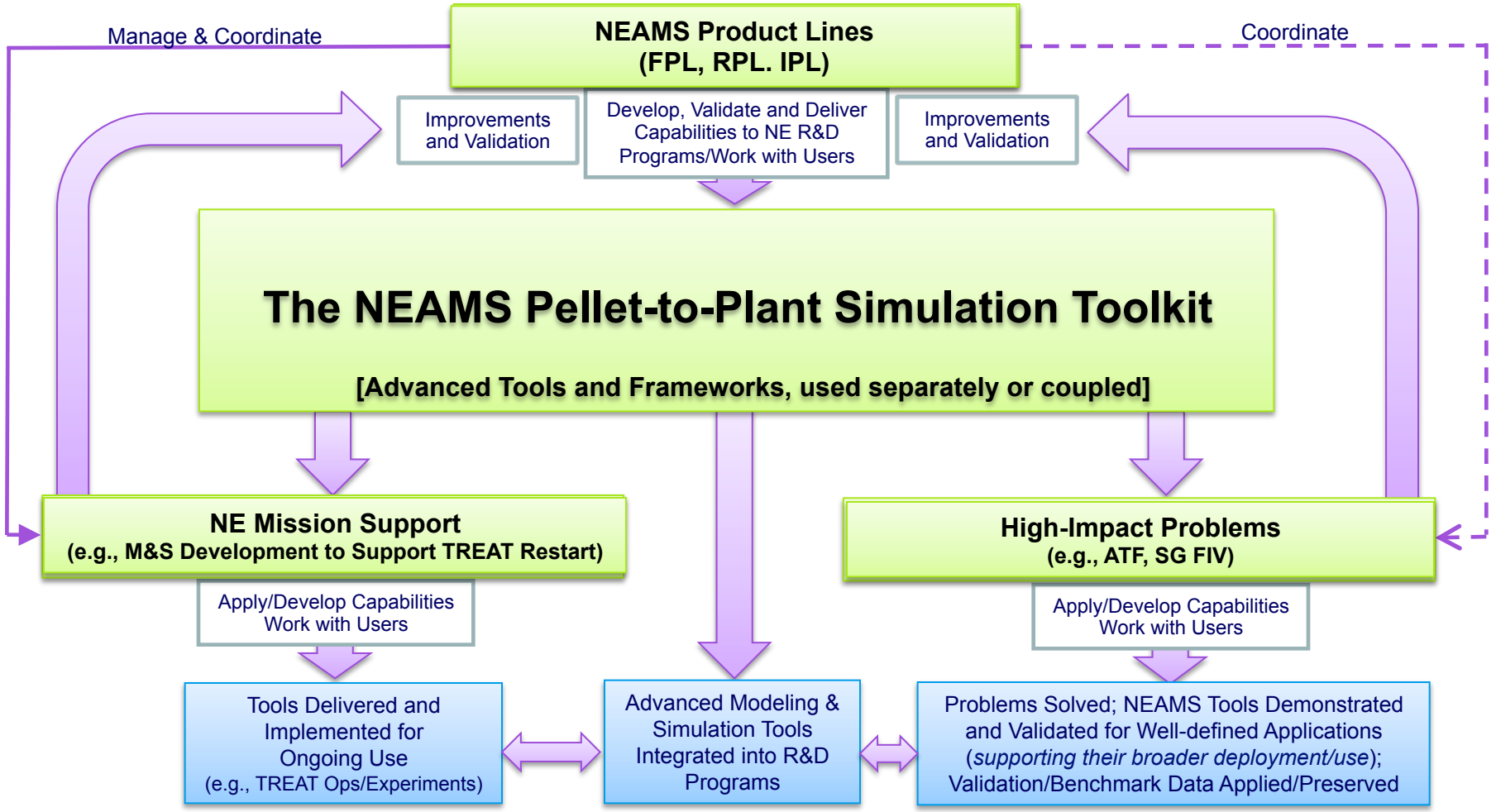
Nuclear Energy Advanced Modeling and Simulation (NEAMS)



* Chris Stanek (LANL) to start as NTD in September 2015

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

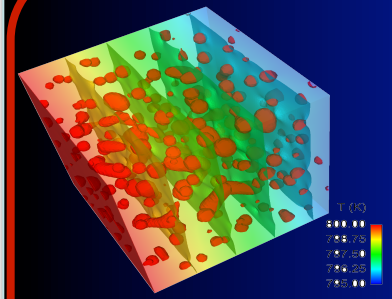


U.S. DEPARTMENT OF ENERGY
Nuclear Energy

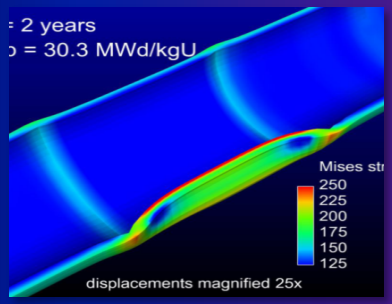
NEAMS – *Fuels Product Line*

- **The FPL spans "pellet to pin" fuel simulation**

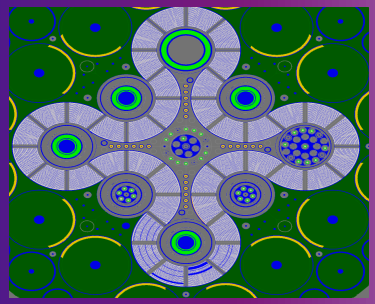
The NEAMS Pellet-to-Plant Simulation Toolkit**



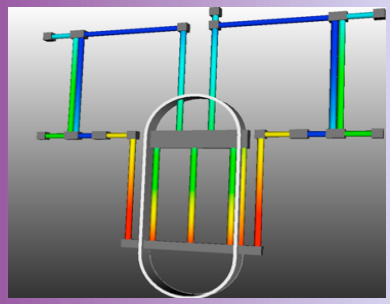
MARMOT (Pellet)



BISON (Pin)



SHARP (Core)



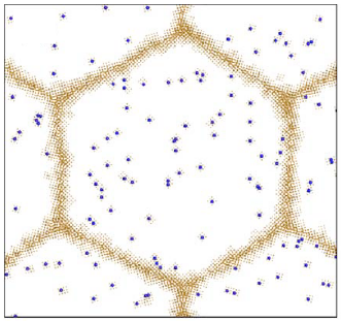
System Models (Plant)

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Fuels Product Line*

- **Central driver is to understand and be able to model the physics of microstructure changes in the fuel that are important to predicting fuel performance under operating and accident conditions over core life**
  - Empirical models can accurately interpolate between data but cannot accurately extrapolate outside of test bounds
  - Thus our goal is to develop improved, *mechanistic materials models* for fuel performance using hierarchical multiscale modeling

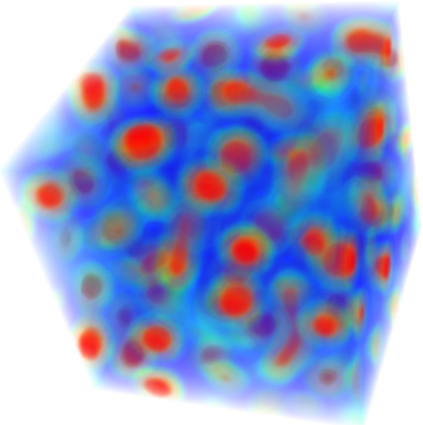
Atomistic simulations



- Identify important mechanisms
- Determine material parameter values

Atomistically-informed parameters

Meso-scale models

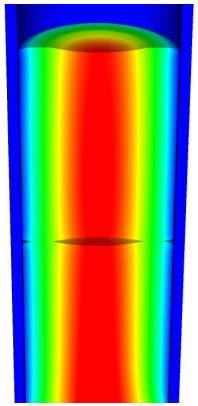


- Predict microstructure evolution
- Determine effect of evolution on material properties

Degrees of freedom, operating conditions

Meso-scale informed materials models

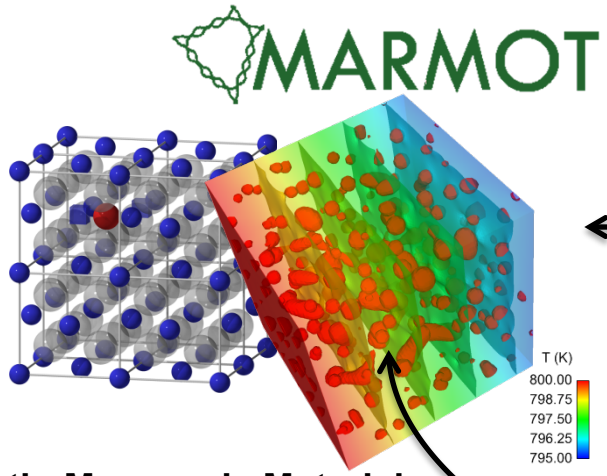
Fuel performance models

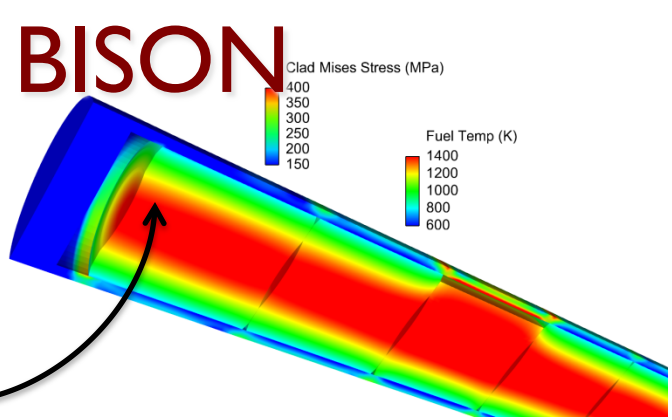


- Predict fuel performance and failure probability

NEAMS – *Fuels Product Line*

- **FPL Toolset: MOOSE-BISON-MARMOT (advanced, multiscale fuel performance capability)**





Atomistic-Mesoscale Material Model Development Tool

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

Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations
- **BISON Theory, Users, & Assessment Manuals (plus other good info) can be found at: http://www.inl.gov/BISON**

MOOSE

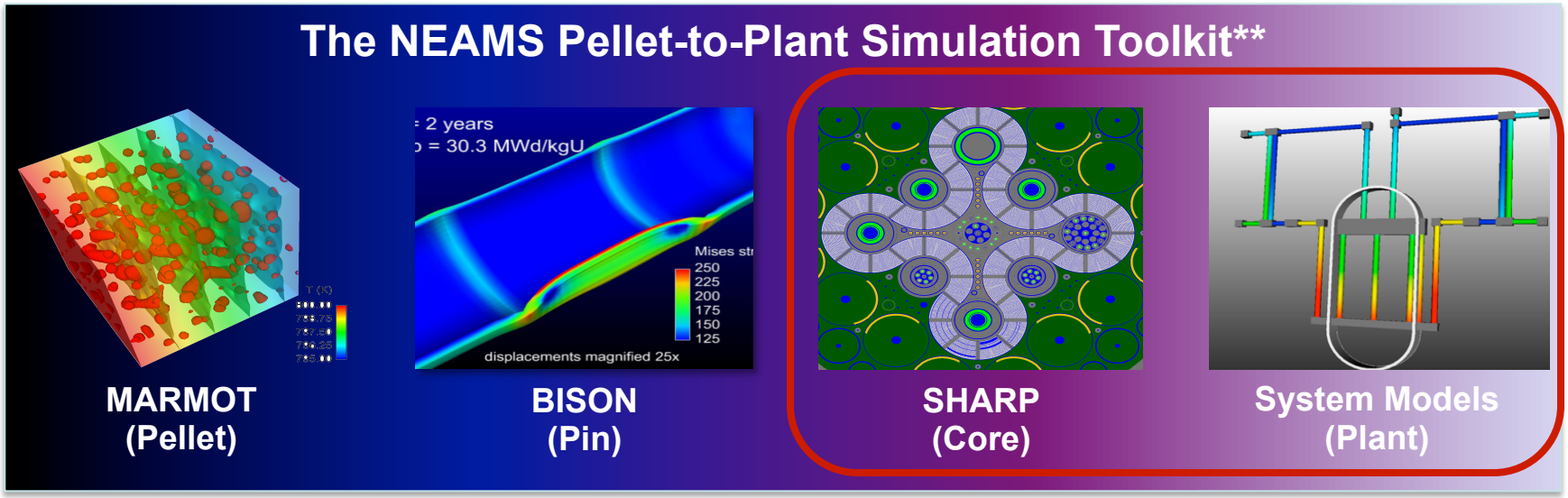
Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactors Product Line*

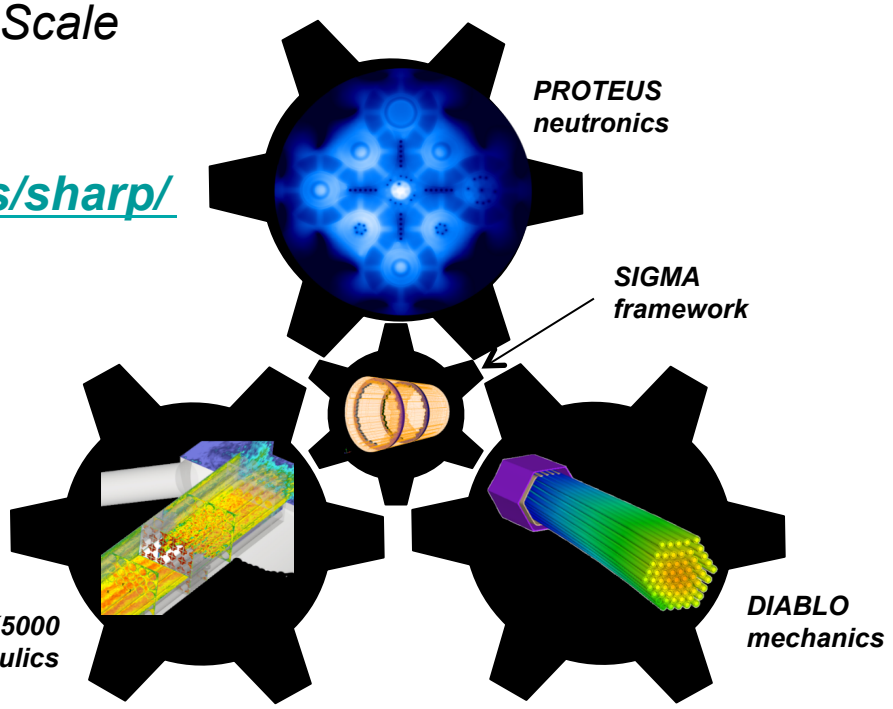
- The RPL spans the reactor "core to the full plant"



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line*

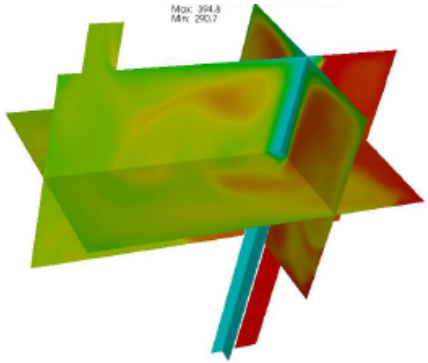
- **Central driver is to be able to achieve multi-scale and multi-physics simulations of core dynamics, core mechanics, and core thermal-hydraulics over time scales from picoseconds to seconds to days, and be able to achieve coupling and interoperability as needed**
- **SHARP/SIGMA – central to the "interoperability" approach**
  - *Intrinsically Multi-Physics and Multi-Scale*
  - *Coupling when necessary*
  - *Stand-alone when sufficient*
  - ***http://www.ne.anl.gov/capabilities/sharp/***
  - ***http://press3.mcs.anl.gov/sigma***

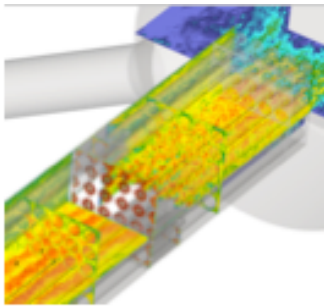


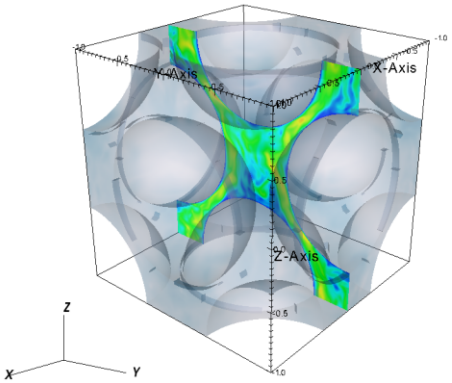
NEAMS – *Reactor Product Line*

Nek5000 –Thermal-Hydraulics Module

- **Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics**
  - Computational Fluid Dynamics (CFD) toolset using the Spectral Element Method (SEM)
  - Supports conjugate heat transfer analysis
  - Includes Stability Analysis toolkit with adjoint and Proper Orthogonal Decomposition capabilities
- **Open Source – available for download at nek5000.mcs.anl.gov**
- **Validation in progress for many nuclear energy applications**
  - T-junctions, spacer grids, wire-wrapped fuel assemblies, jet/plenum mixing
  - More needed
- **Demonstrated for up to 1,000,000 cpu processes and several billion geometric grid points.**
  - Also runs on desktop workstations

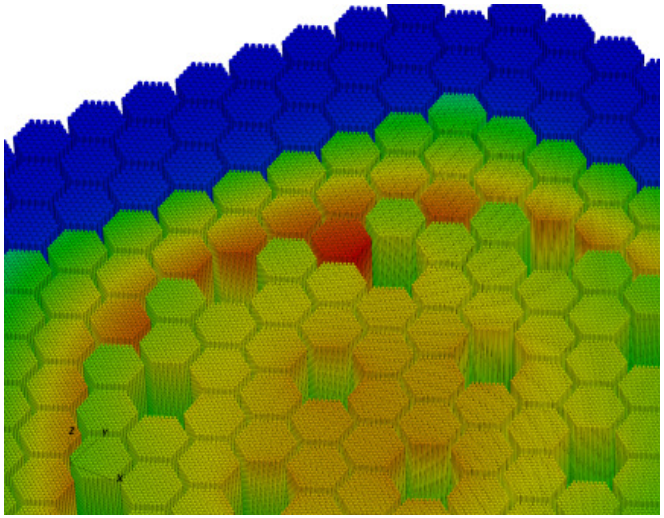


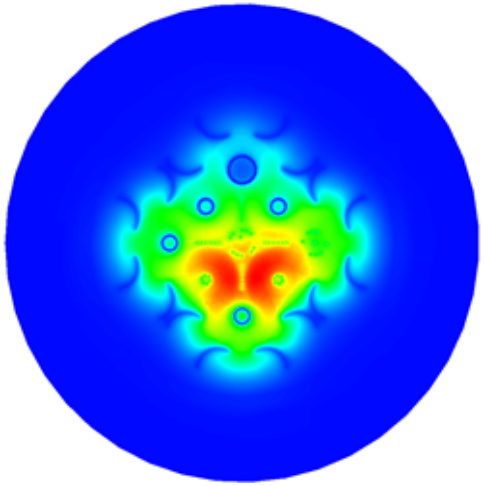




U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line*

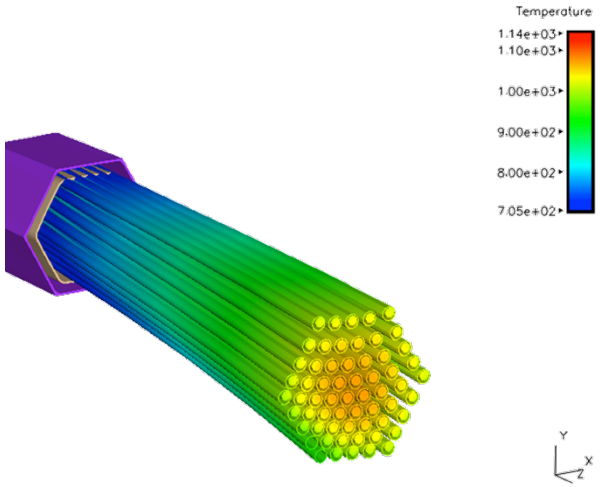


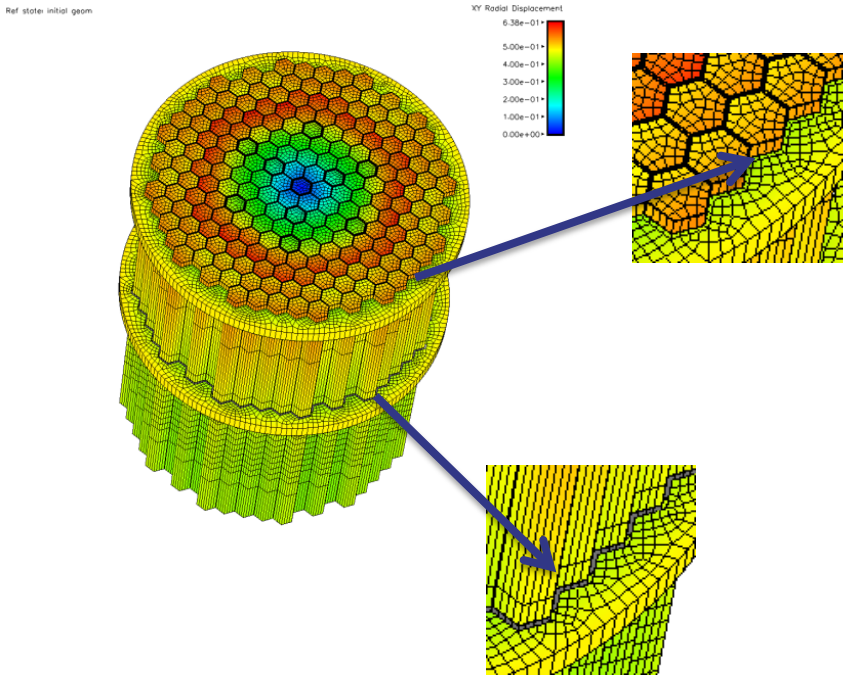


- **PROTEUS – the neutronics module**
  - Can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling
  - Additional information: http://www.ne.anl.gov/pdfs/PROTEUSbrochure_v6.pdf
- **Early user releases available, with user guides, methodology manuals, etc. in development**
- **Successfully used on real problems- ATR, ZPR, MONJU, PHENIX, EBRII…**
- **Validated against ZPR experiment foil reaction rates and k-effective**
  - More needed!
- **Demonstrated scalability to more than 200,000 CPU cores and billions of degrees of freedom.**
  - Also runs on desktop workstations

NEAMS – *Reactor Product Line*

- **The SHARP Structural Mechanics module, DIABLO**
  - 3-D thermal-structural and thermal mechanics analysis using a time explicit Finite Element Method (FEM)
  - prediction of deformation and stresses under structural and thermal loads
  - Includes a variety of contact modeling options
  - Includes connectivity to selected soil-structure interaction models for seismic analysis





- **Early user releases available, with updated user guides, methodology manuals, etc. in development**
- **Validated for a variety of standard structural mechanics benchmark**
  - Additional specific nuclear energy application validation needed
- **Demonstrated scalability to petascale computing platforms and large problems**
  - Also runs on desktop workstations

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **Program Support in Science & Technology Innovation – NEAMS-1; we are seeking proposals that contribute to improving the mechanistic models, computational methods, and validation of NEAMS tools in the toolkit, in four 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 and Structural Mechanics

- **Proposals should clearly define quantitative metrics of success for the proposed work that illustrate the return on investment (*e.g.*, the implemented model will reduce error in predictions of peak temperature in the selected benchmark problem by X%)**

- **Proposed model development and validation can span the entire hierarchy from single-scale and single-effects experiments designed to address individual phenomena to integrated models or experiments that address strong coupling of multiple phenomena**

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **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**
- **Collaboration with members of the NEAMS development team residing at DOE laboratories is strongly encouraged**
- **Please focus your application, if possible, on one of the four scope areas**
- **POCs**
  - Federal – Dan Funk (dan.funk@hq.doe.gov; 301-903-3845)
  - Technical – Dave Pointer (pointerwd@ornl.gov; 865-241-4472)

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **NEAMS 1.1 – Atomistic and Mesoscale Modeling and Simulation of Nuclear Fuels, Cladding, and Reactor Structural Materials**
  - Improve predictive capabilities for phenomena of interest such as corrosion, creep, chemical interaction, dislocation, and phase separation in multi-phase, multi-component systems in nuclear materials impacting their in-reactor performance
  - Extend the capabilities of MARMOT to a broader range of fuel and cladding materials, and improve the validation basis of the code. Validation should involve closely correlated experiments and modeling using MARMOT, as well as uncertainty quantification
  - Proposals on atomistic to mesoscale and physics coupling using MARMOT are also encouraged

- **NEAMS 1.2 – Macroscale Fuel Performance**
  - Aid in the development of theory-based models of advanced materials' properties
  - Offer more robust and efficient numerical algorithms
  - Extend capabilities of BISON to fuel forms that are currently under supported
  - Tackle fuel failure mechanisms in BISON
  - Improve the validation basis of BISON, particularly for 3-D problems
  - Proposals that employ coupling of BISON and MARMOT simulations using sequential, concurrent, or hybrid methods are encouraged

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **NEAMS 1.3 – Core Neutronics**
  - Improve predictive capabilities for complex transients
  - Provide capabilities for multi-resolution simulations with mixed homogenized-heterogeneous regions
  - Expand and demonstrate simulation capabilities of PROTEUS to other reactor types
  - Extend capabilities of PROTEUS for fuel cycle analysis with a wide range of reactor core configurations
  - Demonstrate improved accuracy for fuel performance simulations, and improve validation basis for NEAMS neutronics/depletion codes
  - Proposals that consider the integration of the NEAMS macroscale fuels and neutronics capabilities are also encouraged
- **NEAMS 1.4 – Thermal Hydraulics and Structural Mechanics**
  - Expand the turbulence modeling options available in Nek5000, demonstrate its applicability to a wider range of reactor types and conditions, and improve validation basis for the code
  - Develop new sets of measured data for validation of the two-phase boiling capability, including boiling water experiments (preferably at higher pressures) and/or experiments with detailed measurements in relevant fuel assembly geometries
  - Add models to Diablo or expand the validation of Diablo to enhance its ability to predict the behavior of reactor structures (possibly leveraging existing mesoscale and continuum material simulation capabilities such as MARMOT and BISON)
  - Proposals to integrate NEAMS tools for thermal-structural or fluid-structural applications are also encouraged