An Overview of U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation program

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Abstract: Under the U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, advanced simulation tools are being developed using modern computational techniques and innovative methods to support design of advanced nuclear reactor concepts. The NEAMS program is organized along three modular production lines: fuels, reactors, and integration production lines. The fuels production line is focused on developing predictive computational tools for fuel performance design and analysis. The reactors production line is developing multi-physics, multi-scale tools that can support a broad spectrum of modeling and simulation needs of advanced reactor concepts. The focus of the integral production line is to integrate these fuels and reactors simulation tools in an easy-to-use common analysis environment that enables the end users to apply these high-fidelity simulations to inform the conventional lower-order models for the design, analysis, and licensing of advanced nuclear systems. This lecture note presents an overview of the NEAMS program and tools, focused on the RPL tools.
Keyword: nuclear energy; modeling and simulation; NEAMS; SHARP

1 Introduction

Reactor design and operation require a wide range of modeling and simulation (M&S) tools that can accurately predict the key system performance and safety characteristics. Advanced M&S capabilities based on first principles as closely as possible would allow for radical improvements in (1) reducing reliance on multiple costly integral experiments, (2) removing unnecessarily conservative design margins, (3) acquiring new knowledge to direct the innovative design features and approaches, and (4) global optimization of the future reactor system designs.

To support the current and future nuclear reactor analysis needs, the Office of Nuclear Energy of the U.S. Department of Energy (DOE) is running two nuclear energy modeling and simulation programs: Nuclear Energy Advanced Modeling and Simulation (NEAMS)[1] and Consortium for the Advanced Simulation of Light water reactors (CASL)[2]. The NEAMS program was established in 2009 to develop a high-fidelity simulation toolkit using modern computational techniques and innovative methods and solvers to support design and deployment of advanced nuclear reactor concepts. The CASL was established in 2010 as the first DOE Energy Innovation Hub with the mission to provide leading-edge M&S capabilities to improve the performance of currently operating and future Light Water Reactors (LWR's).

The NEAMS mission is to provide leading-edge computational tools for accelerating development of advanced reactor concepts and promoting innovative solutions to important nuclear industry problems.[3] These advanced M&S capabilities are expected to (1) help transformative scientific discovery and insights, (2) solve problems identified as significant by industry, (3) enhance opportunity for industry to commercialize advanced concepts, and (4) allow industry to implement innovations that improve the economics of both existing and future nuclear power plants.

The NEAMS program is organized along three modular product lines: Fuels Product Line (FPL), Reactors Product Line (RPL), and Integration Product Line (IPL). The FPL is focused on developing mechanistic predictive computational tools for nuclear fuel performance analysis and design. Under the RPL, high-fidelity neutronics, thermo-fluid, and structural mechanics analysis codes are being developed for reactor design and analysis. The IPL focus is to integrate these computational tools being developed in

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the FPL and RPL in an easy-to-use common analysis environment.

This lecture note presents an overview of the NEAMS program and tools, focused on the RPL tools. In Section 2, the overall structure of NEAMS is briefly described with its frameworks. The reactor analysis codes being developed in RPL are discussed in more detail in Section 3. Section 4 provides a summary.

2 NEAMS structure and frameworks

Currently, the NEAMS program consists of three modular production lines, two high impact problems, and a project to support Office of Nuclear Energy's mission. As mentioned in the introduction, the three production lines are FPL, RPL, and IPL. Table 1 presents the main M&S tools being developed in the FPL and RPL, including the framework discussed below and developing institute.

Table 1 Main M&S tools of NEAMS

Code	Purpose	Framework	Institute
MARMOT	Solid fuel microstructure modeling	MOOSE	INL
BISON	Solid fuel macroscopic modeling	MOOSE	INL
MC^2-3	Multi-group cross section generation	SHARP	ANL
PROTEUS	Neutron transport	SHARP	ANL
Nek5000	Computational fluid dynamics	SHARP	ANL
SAM	System analysis module	MOOSE	ANL
Pronghorn	Pebble-bed thermo-fluid analysis	MOOSE	INL
Diablo	Computational structural mechanics	SHARP	LLNL

The high impact problems were introduced to direct the NEAMS tools to address the problems of applied relevance. At present, two high impact problems are defined. One is the Accident Tolerant Fuel (ATF) High Impact Problem (HIP) defined for the multi-scale, predictive tools of FPL. As part of this effort, the multi-scale modeling was performed for iron-chromium-aluminum (Fe-Cr-Al) cladding alloys[4]. The other is the steam generator Flow Induced Vibration (FIV) problem to be analyzed with the RPL thermos-fluid and structural analysis tools[5]. NEAMS also supports the development of the reactor physics analysis tool MAMMOTH [6] to support the transient tests of the TREAT facility[7] at Idaho National Laboratory (INL).

The NEAMS tools are being developed mainly based on two frameworks: the Multi-physics Object Oriented Simulation Environment (MOOSE)[8] developed at INL and the Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP)[9] developed at Argonne National Laboratory (ANL). MOOSE is a finite-element, multi-physics framework that simplifies the development of advanced numerical applications. It provides a high-level interface to sophisticated nonlinear solvers and massively parallel computational capability. MOOSE is open source and freely available at http://mooseframework.org/. SHARP is a suite of physics simulation software modules and computational framework components that enables the user to evaluate the impact of design decisions on performance and safety of nuclear reactors or their components. SHARP allows users to attach the new simulation modules to the older legacy codes, thereby avoiding costly rewriting of codes.

2.1 Fuels production line

The goal of FPL is to develop improved, mechanistic (rather than empirical), and predictive models for performance analysis of existing, advanced, and used fuels. For this, hierarchical, multi-scale modeling approaches are used from atomistic simulations to engineering scale fuel performance analysis. The MARMOT[10] and BISON[11] fuel performance tools are the FPL components being developed at INL based on the MOOSE framework.

MARMOT is a meso-scale fuel performance code to predict the co-evolution of microstructure and physical properties of nuclear fuels and claddings due to applied stress, temperature, and radiation damage. It utilizes the material parameter values determined from atomistic simulations and supplies the calculated microstructure and physical properties to the engineering scale fuel performance code BISON. MARMOT solves the phase field equations coupled to solid mechanics and heat conduction using the finite element method (FEM). The current physical models include:

- UO_2 fuel: grain growth, fission gas release, and fracture.

- U-Zr fuel: species transport, phase change, and swelling.
- U-Si fuel: fission gas transport and swelling.
- Zircaloy cladding: hydride formation.
- FeCr cladding: microstructure evolution.

BISON is a finite element based nuclear fuel performance code applicable to a variety of fuel forms, including LWR fuel rods, TRi-structural-ISOtropic (TRISO) particle fuel, and metallic rod and plate fuel. It solves the fully-coupled equations of thermo-mechanics and species diffusion in one-dimensional (1D) spherical, 1D layered, two-dimensional (2D) axisymmetric, 2D plane strain, or three-dimensional (3D) geometries. The current fuel models include temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. The cladding material models include plasticity, irradiation growth, and thermal and irradiation creep.

2.2 Reactors production line

The RPL has adopted a multi-physics, multi-scale approach to ensure that its tools can support a broad spectrum of modeling and simulation needs of advanced reactor concepts. Multi-physics integration connects separate phenomena, while multi-scale approach can cover different time- and length-scales of each phenomenon. This hierarchal structure allows the coarse 1D plant-level system models to be informed by high-fidelity, 3D neutronics, fluid dynamics, and structural mechanics simulations. The RPL develops the following high-fidelity, coupled-physics simulation capabilities for advanced reactors:

- MC^2-3[12]/PROTEUS[13]: neutronics suite of codes.
- Nek5000[14]: computational fluid dynamics (CFD).
- SAM[15]: system analysis module.
- Diablo[16]: computational structural mechanics (CSM).

The system analysis code SAM is based on MOOSE, while the other codes are based on the SHARP framework. The neutronics and thermo-fluid codes are being developed at ANL, and the CSM code Diablo is being developed at Lawrence Livermore National Laboratory (LLNL). Under the RPL, a medium-resolution thermo-fluid and neutronics analysis code Pronghorn[17] is also developed for simulation of Very High Temperature Reactor (VHTR) and Fluoride-salt-cooled High temperature Reactor (FHR) concepts. It approximates the interrelated phenomena via neutron diffusion solutions coupled to porous medium representation of coolant flow in pebble bed reactors.

2.3 Integration production line

The advanced tools of FPL and RPL often require large computational resources, can be difficult to install, and require expert knowledge to operate. This causes many analysts to continue to use traditional tools instead of exploring high-fidelity simulations. The objective of IPL is to address the needs of design and analysis communities by integrating the NEAMS high-fidelity capabilities and current production tools in an easy-to-use common analysis environment. This enables end users to apply high-fidelity simulations to inform lower order models for the design, analysis, and licensing of advanced nuclear systems[18,19].

The NEAMS Workbench is a new initiative to facilitate the transition from conventional tools to high-fidelity tools by providing a common user interface for model creation, review, execution, output review, and visualization for integrated codes[20]. The NEAMS Workbench will enable analysts to select the fidelity of each type of physics to be used in the simulation. Figure 1 shows a conceptual design of tools that can be integrated for advanced reactor analysis. Current production tools with advanced components supported by the NEAMS program such as those from the Argonne Reactor Codes (ARC)[21] and the SCALE code system[22] are shown in light gray, other production tools are shown in dark gray, core tools from the NEAMS Toolkit are shown in maroon, and tools from CASL are shown in black.

3 SHARP reactors analysis toolkit

3.1 MC^2-3/PROTEUS neutronics module

The neutronics module PROTEUS is a set of advanced neutronics modeling and simulation tools developed at ANL, including cross section generation codes, transport solvers, and mesh generation tools[13]. The PROTEUS toolset has been used to study various reactor types ranging from small thermal test reactors to large sodium cooled fast reactors, and numerous verification and validation tests have been performed.

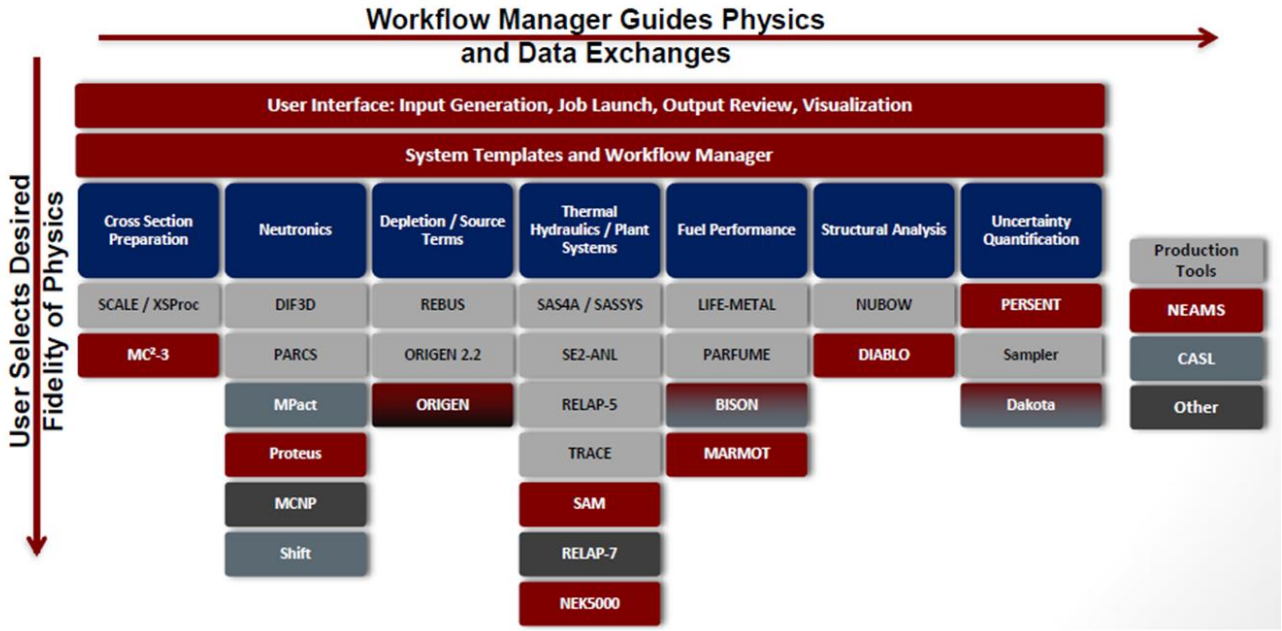

Fig.1 NEAMS Workbench for advanced reactor analysis[19].

Three different methods are available for multigroup cross section generation: MC^2-3, Cross Section API (CSAPI), and GenISOTXS. The MC^2-3 code[12] generates region-dependent multigroup neutron and gamma cross sections for fast reactor applications. It has been validated against various numerous fast reactor experiments and widely used for multigroup cross section generation for fast reactor design and analysis. MC^2-3 generates multigroup neutron cross sections by solving the neutron transport equation for a homogeneous medium or a slab or cylindrical unit cell problem in an ultrafine (~2,000) or hyperfine (~400,000) group level with detailed modeling of resolved resonances, unresolved resonances, and anisotropic scatterings. Gamma interaction cross sections are generated by performing gamma transport calculations in a 94-group structure[23]. Region-dependent cross sections are generated by accounting for region-to-region spectral transition with 2D whole-core transport calculation in cylindrical-z geometry in ultrafine group for neutron transport and 94-group for gamma transport. Recently, capabilities have been extended to provide thermal cross sections and 3D MOC calculations[24].

The CSAPI is a standalone functional module for generating thermal and fast reactor multigroup cross sections using the subgroup or resonance table method. The CSAPI module can be adapted to any transport code with a fixed source solver capability. The CSAPI allows transport solvers to generate self-shielded multi-group cross sections on-the-fly, accounting for the effects of heterogeneous geometry as well as temperature and composition. The cross section library is generated using MC^2-3 and NJOY[25] for the reactor spectrum type of interest. One-group fixed source transport calculations are performed to determine the background cross sections for each isotope. The CSAPI is implemented directly into the transport solvers of PROTEUS. The GenISOTXS code prepares multigroup cross sections in the ISOTXS format from Monte Carlo (MC) simulations with Serpent[26] and OpenMC[27]. Macroscopic cross sections are generated with Serpent whereas microscopic cross sections are generated with OpenMC. It is noted that in both MC codes, higher-order scattering moments are generated with scalar flux weighting.

The PROTEUS code was initially named UNIC and focused on developing three solvers based on unstructured finite element meshes[28]: PN2ND, SN2ND, and MOCFE. PN2ND is based upon the second-order even-parity transport equation and implements spherical harmonics for the angular approximation. SN2ND is also based upon the second-order even-parity transport equation but a discrete ordinates approximation is applied for the angular

approximation. These solvers are designed for massively parallel computation with reduced homogenization approximations (*e.g.*, pin cell level). MOCFE is a 3D method of characteristics (MOC) solver for the first-order transport equation, and its targeted application is for explicit geometry, fine-group problems with the short-term purpose of cross section generation and the long-term purpose of fine-level transport calculations without homogenization.

Currently, the development of PROTEUS is focused on the following three transport solvers: PROTEUS-SN, PROTEUS-MOC, and PROTEUS-NODAL. The PROTEUS-SN[29] code is the SN2ND solver above. It is a massively parallel neutron transport code solving the discrete ordinates formulation of the even-parity transport equation. The spatial discretization is based on a fully unstructured conformal finite element mesh and can handle more than 10^{12} degrees of freedom (DOFs) via parallelization in space and angle domains. PROTEUS-SN includes steady state and adiabatic quasi-static kinetics formulations, a fixed source solver, and forward and adjoint calculations. PROTEUS-SN has been used to model nuclear reactor cores ranging from the Advanced Test Reactor (ATR)[30], Zero Power Reactors (ZPRs), and various sodium cooled fast reactor designs. As an example, Table 2 compares the PROTEUS-SN k-effective values with the MCNP6[31] MC solutions for the two control rod configurations of the Advanced Burner Test Reactor (ABTR) design[32].

Table 2 Comparison of k-effective values of ABTR

Control rod configuration	MCNP6	PROTEUS-SN (Δk from MCNP)
Out	1.23388±0.00010	-152 pcm
In	1.04374±0.00011	26 pcm

PROTEUS-MOC[33] combines the 2D MOC method (with unstructured finite element mesh) with the discontinuous Galerkin finite element method in the axial direction to efficiently solve 3D axially-extruded geometries. PROTEUS-MOC is a promising tool to solve axially complex geometry problems without the limitations of the 2D/1D approach (*e.g.*, DeCART[34] and MPACT[35]). The PROTEUS-MOC has been used to model nuclear reactor cores including TREAT, Rensselaer Polytechnic Institute (RPI) reactor, VHTR, and C5G7 benchmark[36], demonstrating excellent accuracy even for core problems with significant neutron streaming. As an example, the PROTEUS-MOC results are compared with Serpent MC solutions for the two experimental core configurations of the TREAT reactor: the minimum critical core (MinCC) and the half-slotted M8CAL core. Table 3 shows the k-effective values, and Table 4 presents the maximum and Root-Mean-Square (RMS) differences of PROTEUS-MOC fuel element powers from the reference Serpent solutions. Currently transient analysis capabilities are being developed at the University of Michigan [37].

Table 3 Comparison of k-effective values of TREAT

Core configuration	Serpent	PROTEUS-MOC (Δk from MCNP)
MinCC	1.00490±0.00018	-1 pcm
M8CAL	1.00497±0.00018	66 pcm

Table 4 Comparison of fuel element powers of TREAT

Core configuration	Deviation from Serpent solution	
	Maximum	RMS
MinCC	0.44%	0.22%
M8CAL	1.25%	0.50%

The PROTEUS-NODAL is a nodal transport solver based on homogenized assemblies to provide a conventional fidelity solver in a consistent framework with the high-fidelity SN and MOC solvers. Two solution methodologies have been implemented: P_N and Simplified P_N (SP_N) approaches. The P_N approach is a modernized form of DIF3D-VARIANT[38] although the current version only handles diffusion theory on Cartesian, hexagonal, and triangular-z grids. For the SP_N approach, a transverse integrated nodal methodology is built on the hexagonal grid model utilizing up to a SP_3 approximation. PROTEUS-NODAL solves steady-state and transient problems.

PROTEUS includes an extensive set of mesh processing tools to assist users with the creation of unstructured finite element meshes without the need for licensed external software. Both hexagonal and Cartesian geometries are supported. Explicit pins, cladding, and ducts can easily be modeled with varying mesh fidelity. An EXODUS II[39] finite element mesh convertor utility is also available to

convert externally generated EXODUS II meshes (*e.g.* generated with CUBIT[40]) into the PROTEUS native mesh format. As an example, Fig. 2 shows part of the PROTEUS mesh used to analyze the ATR.

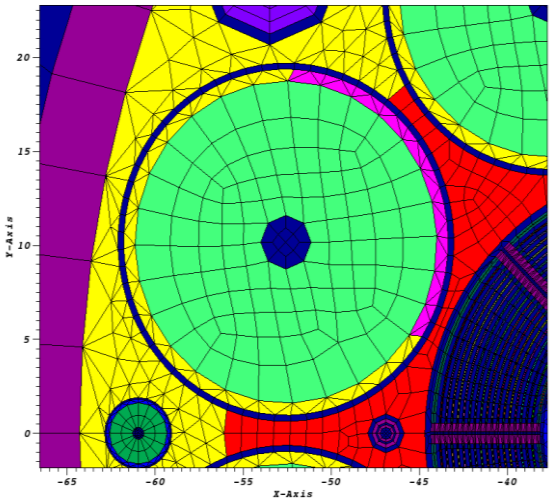

Fig.2 Part of PROTEUS mesh used to analyze ATR.

3.2 Nek5000 and SAM thermo-fluid codes

The SHARP thermo-fluid analysis capabilities include the CFD code Nek5000[14] and a new system analysis code SAM[15]. Nek5000 is an open source software for multi-dimensional heat transfer and fluid dynamics. It uses the spectral element method to achieve rapid spatial convergence and is highly scalable (up to 10^6 cores). Nek5000 has several advanced capabilities, including moving meshes, adaptive mesh refinement, overlapping multi-domain simulations, and ensemble averaging. The Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Unsteady Reynolds Averaged Navier Stokes (URANS) modeling options for turbulence can produce high quality reference solutions on high-performance computers. As an example, the axial flow distribution in a 217-pin wire-wrapped assembly of Sodium-cooled Fast Reactor (SFR) obtained with LES simulation is shown in Fig. 3. Nek5000 also includes porous media and momentum-source approaches to reduce the level of computational complexity to allow reliance on much smaller computing systems.

The SAM is a modern system analysis tool for advanced non-LWR safety analysis. It aims to provide fast-running, whole-plant transient analyses capability with improved fidelity for SFR, Lead-cooled Fast Reactor (LFR), Molten Salt Reactor (MSR), and FHR.

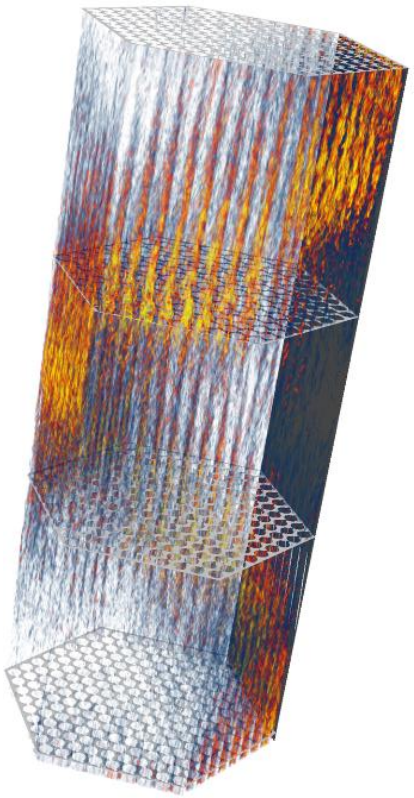

Fig.3 Axial flow distribution in 217-pin SFR assembly.

SAM is a MOOSE-based transient analysis capability with a robust and high-order FEM model of single-phase fluid flow and heat transfer[41]. SAM provides various flexible modeling capabilities:

- Flexible core modeling using single- or multi-channel representation of fuel assemblies with automatically generated core lattice and assembly structures. As an example, Fig. 4 compares average radial wall temperature distributions between SAM and CFD in a 7-assembly demonstration problem, where the periphery region of each assembly (Region 1 in Fig. 4) is represented by six channels to account for inter-assembly heat transfer.
- Flexible coupling between fluid and solid components enables a wide range of engineering applications.
- Enhanced built-in closure models and flexible modeling of fluid properties, friction, and convective heat transfer.
- Flexible coupling interfaces to allow for convenient integration with other advanced or conventional simulation tools for multi-scale and multi-physics modeling capabilities. Figure 5 shows an example for the coupled SAM and CFD

imulations of a Protective Loss-Of-Flow (PLOF) transient of ABTR.

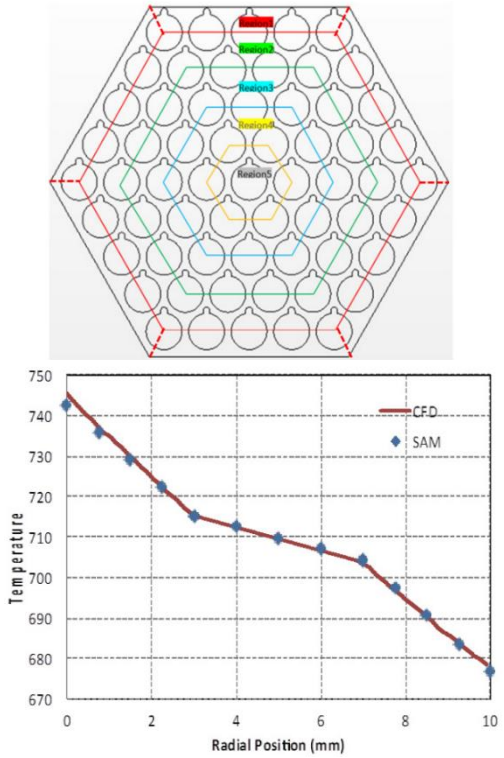

Fig.4 Comparison of average radial wall temperature distributions between SAM and CFD[15].

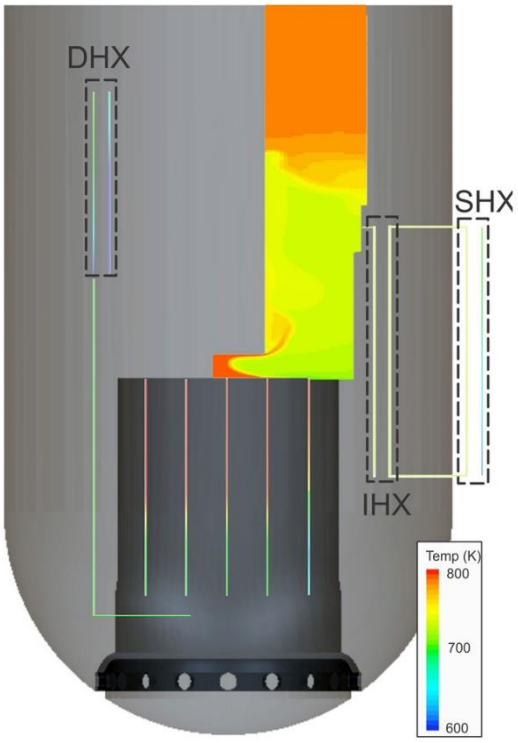

Fig.5 Snapshot of temperature distribution in the coupled SAM-CFD simulations of ABTR PLOF transient.

3.3 Structural analysis code Diablo

Diablo is a 3-D Lagrangian nonlinear structural-thermal-mechanics analysis code based on a time-implicit FEM[42]. A primary focus is nonlinear structural mechanics and heat transfer. It employs low-order spatial discretization (such as eight-node hexahedra for continua and four-node quadrilaterals for shells) and features a state-of-the-art contact (*i.e.*, the interaction between un-bonded material interfaces) modeling. Appropriate formulations are employed to accommodate nearly incompressible material models, such as for metal plasticity and rubber elasticity. Global algorithms include second-order and quasi-steady time integration and a number of approaches for nonlinear iteration: full Newton, modified-Newton, multiple quasi-Newton updates, and line search. Linear solvers are utilized from multiple libraries.

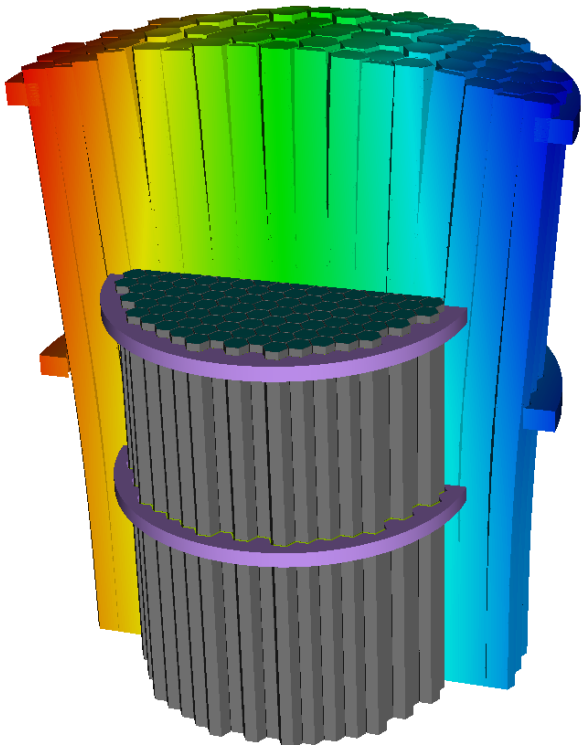

Fig.6 Predicted deformation of ABTR fuel assemblies.

Diablo is integrated into the SHARP multi-physics toolkit to support coupled neutronics and thermo-fluid-structural calculations, and coupled to Nek5000 for a novel high-fidelity FIV analysis capability (applied to prediction of FIV in helical steam generators for small modular reactors). As an example, Fig. 6 show the deformation of ABTR fuel assemblies predicted by a coupled simulation of PROTEUS, Nek5000, and Diablo. In the PROTEUS model, the

internal fuel pin, cladding, and coolant within each assembly were homogenized, but the duct walls were represented explicitly. Similarly, Nek5000 employed a porous media representation of the flow within each fuel assembly, while it predicts the temperature along the duct wall. Using this information, Diablo predicts the multi-dimensional thermal strain associated with these thermal gradients. The neutronics simulations were repeated on the deformed geometry provided by Diablo. For this steady-state exercise at the hot core condition, these SHARP iterations were repeated several times to achieve a converged k-effective value.

4 Summary

Advanced M&S capabilities are being developed under the NEAMS program of U.S. DOE, including the fuel performance analysis codes MARMOT and BISON, the neutronics codes MC^2-3 and PROTEUS, the thermo-fluid analysis codes Nek5000 and SAM, and the computational structural mechanics code Diablo. These codes are being integrated under the NEAMS Workbench in an easy-to-use common analysis environment that enables the end users to apply high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems

Relative maturity of NEAMS advanced M&S tools is coinciding with the current surge in advanced reactor startups. The DOE's Gateway for Accelerated Innovation in Nuclear (GAIN) initiative is catalyzing the necessary interactions between NEAMS (and other DOE-NE programs) and advanced reactor industry community that will enable productive use of advanced M&S tools.

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