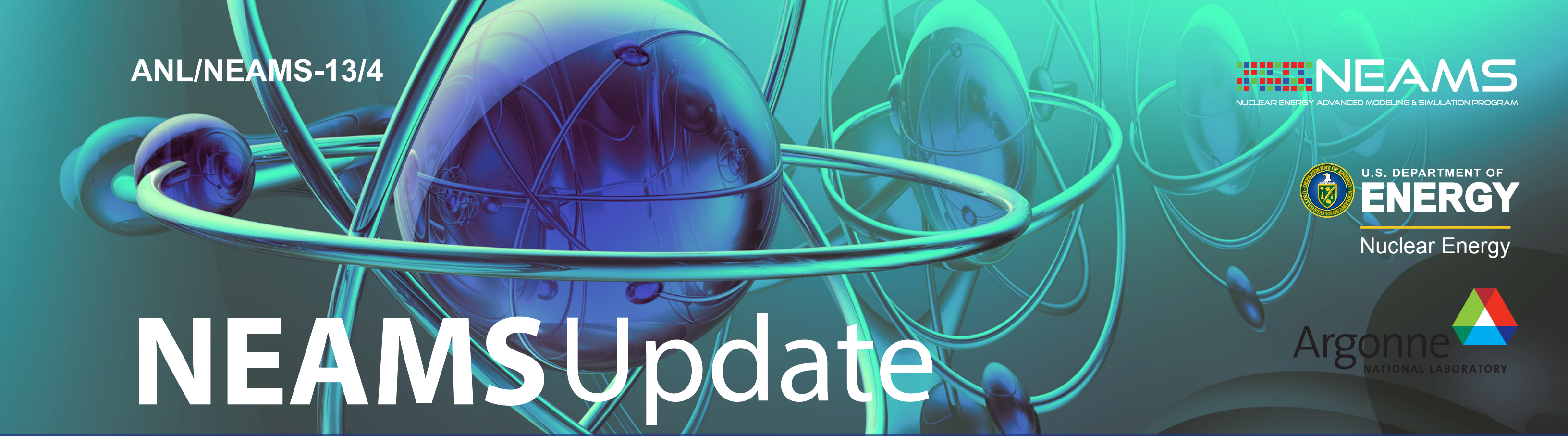
ANL/NEAMS-13/4



NEAMS Update

Quarterly report for July– September 2013

Published December 2013

Quarterly Highlights

- The FPL team released BISON 1.0 (see article below) and made it available to Westinghouse fuels engineers.
- For the first time, BISON simulated a loss-of-coolant accident using the full complement of components developed for the NEAMS ToolKit (page 2).
- MARMOT was enhanced to better simulate fission gas behavior, fuel cracking, and nucleation (page 3).
- SHARP performed a multiphysics simulation of the full EBR-II core for the first time (page 4).
- The thermal fluids team developed an intermediate-fidelity turbulence model and continued to work with I-NERI collaborators on code validation (pages 4 and 5).
- The neutronics team transferred PROTEUS-SN to the early user team and continued to develop tools for neutron cross-section libraries (page 5).
- The Reactor Analysis and Virtual Control Environment (RAVEN) was extended with a dynamic event tree capability for evaluating failure modes of nuclear power plant systems (page 7).
- The RPL team released MeshKit 1.0 (page 8).
- Work continued on other NEAMS components, such as CouPE, MOAB, and NiCE (page 8).
- Work started on a seismic soil-structure interaction model in the Diablo structural mechanics code (pages 8-9).

BISON 1.0 Released

After 4 years of development, BISON 1.0 was officially released during September 2013. BISON provides a comprehensive capability to simulate uranium oxide reactor fuels, including TRISO-coated particle fuels.

Before its release, BISON was vigorously tested with data collected from 21 fuelrod experiments. BISON successfully replicated results for (1) fuel rod temperatures at various life-cycle stages, (2) fission gas release, (3) cladding profilometry, and (4) cladding elongation. ***Fig.1*** illustrates a BISON simulation of TRISO fuel. See page 2 for the rest of the story.

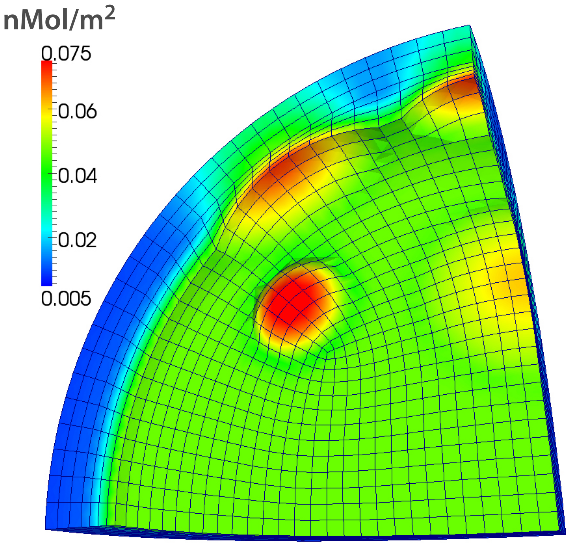
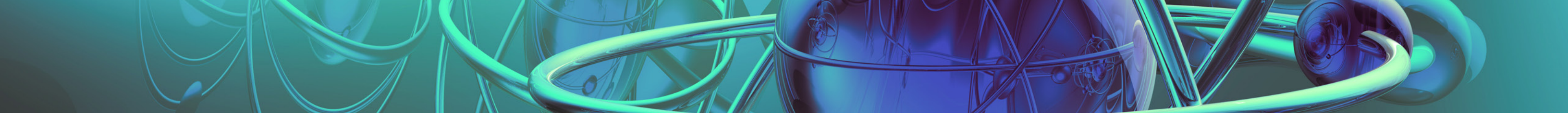


Fig. 1 BISON Simulation of cesium-137 accumulation at a TRISO cladding/fuel interface. (Source: Report INL/MIS-12-27485)



FPL Accomplishments

Engineering Scale (BISON)

During the final quarter of FY2013, the BISON development team reached three important Fuels Product Line (FPL) milestones for simulation capability, code completeness, and user testing.

First, enhancements to BISON that had been underway for several months finally made it possible to perform a first demonstration simulation of a loss of coolant accident (LOCA). The LOCA demonstration included decay heat and reduced coolant flow rate and pressure. Also key to performing the simulation were BISON's transient operators with adaptive time-stepping, arbitrary geometry with large deformation mechanics, implicit numerics with fully coupled physics, and coupled fission gas release and swelling models.

Although this first LOCA simulation was not a validation case and cannot be compared to experimental data, the temperature versus time response shown in ***Fig. 2*** appears very reasonable. In this simulation, the variable coolant conditions had to be supplied as time-varying boundary conditions that were independently estimated, which highlights a pressing need to directly couple fuel and thermal-fluid simulations. [INL]*

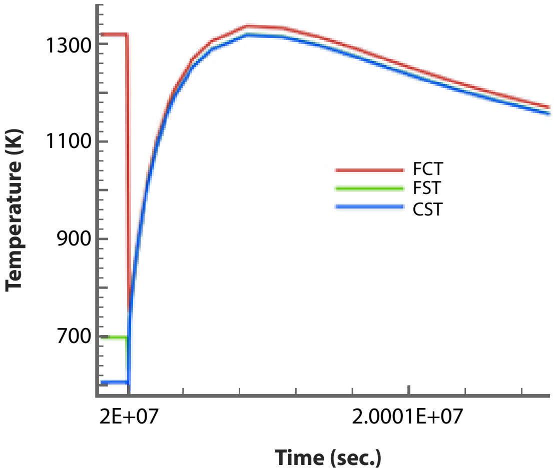


Fig. 2. Fuel centerline temperature (FCT), fuel surface temperature (FST), and cladding surface temperature (CST) as calculated by BISON for a simulated LOCA.

Second, BISON 1.0 was officially released. This version of BISON provides an enhanced, mature, and increasingly comprehensive capability to simulate oxide fuels for light water reactors (LWRs) under quasi-steady-state and off-normal conditions, as well as developing capabilities to model metallic and oxide fuels for sodium fast reactors (SFRs), TRISO-coated particle fuels, and even research reactor fuels. The release of BISON 1.0 was accompanied by the publication of a theory manual, user manual, and assessment report (INL/MIS-13-30307, INL/EXT-13-29930, and INL/MIS-12-27485, respectively).

Table 1 summarizes the BISON benchmark simulations of 21 integral LWR fuel rod experiments that were performed to complete version 1.0. See ***Figs. 1 and 3*** for example simulations from the assessment report. The report also provides benchmark results for TRISO-coated particle fuels, the current fuel of choice for high-temperature reactor technologies. In general, BISON predictions seem to be as good as or better than industry standard fuel performance codes for these validation cases. (See the discussion of fuel benchmarks in the May 2013 *NEAMS Update*.) [INL]

Table 1. Summary of Published BISON Assessment Results

Fuel	Benchmarks*	Behavior	State or Property
LWR	• IFA 431, 432, 515.10, and 597.3 • Risø AN3 and GE7 • OSIRIS • AREVA (idealized) • RUMIX-II (simplified) • REGATE	Thermal	• Beginning of life • Through life • Power ramp tests
		Fission gas	Release
		Mechanical (end of life)	• Cladding elongation • Cladding diameter • Cladding profile
TRISO	13 cases from the IAEA Coordinated Research Program for High-Temperature Gas Reactors	Thermo-mechanical (end of life)	• Internal gas pressure • Tangential stress at coating inner surface

*LWR rod designations omitted for brevity.
Source: Report INL/MIS-12-27485

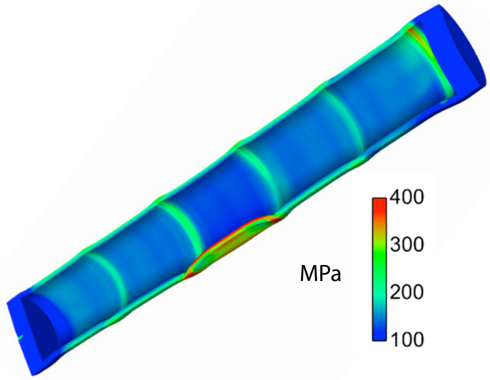
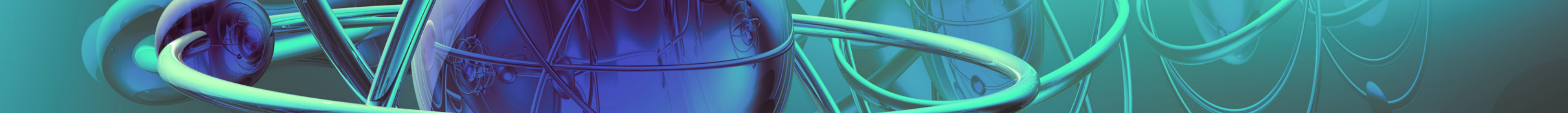


Fig. 3 BISON simulation of the nonelastic deformation of a fuel rod with a surface defect. (Source: Report INL/MIS-12-27485)

---

*The organizations that performed the work are listed in brackets at the end of each topic. The national laboratories performing NEAMS work are Argonne (ANL), Idaho (INL), Lawrence Livermore (LLNL), Los Alamos (LANL), Oak Ridge (ORNL), Pacific Northwest (PNNL), and Sandia (SNL).



Finally, the BISON user community grew significantly as BISON was installed on a new high-performance computing cluster at the Westinghouse International Headquarters in Cranberry Township, PA, and BISON developers gave Westinghouse fuels engineers a 2-day BISON training session on-site in late August. Westinghouse engineers will begin exercising BISON on several fuels problems of particular interest to Westinghouse in the coming months. [INL]

Subcontinuum Scale (MARMOT and Atomistic Simulations)

Fission gases

Understanding the behavior of fission gases in oxide fuels continues to be one of the highest priority efforts at the subcontinuum scale. Models for intrinsic and radiation-enhanced Xe diffusion have been implemented in MARMOT. The diffusion models account for Xe atoms, vacancies, interstitials, Xe-vacancy and vacancy-vacancy clusters, segregation to grain boundaries, and annihilation reactions between interstitials and vacancies. These models in MARMOT were tested by simulating Xe segregation to grain boundaries in both one and two dimensions. These enhancements to MARMOT will enable the simulation of different and competing mechanisms more accurately than the simplified rate theory approaches that have been used to date. [LANL]

Two major structural enhancements to MARMOT were completed. First, the team implemented a more intuitive user interface for the grain boundary model. Second, the capability to run MARMOT simulations using explicit (in addition to implicit) time integration was added. [INL]

Fuel cracking

The development of models to account for cracking in oxide fuels is an important effort due to the major influence cracking has on thermal and gas transport, fuel-cladding mechanical interaction, and accurate predictions of the pellet stress state – an important parameter in many fuel behavior models. A first-of-a-kind multiscale modeling approach to predict crack initiation and propagation yielded good results during 2013.

At the subcontinuum scale, molecular dynamics simulations have been used to investigate intergranular fractures for multiple grain boundary types. At the engineering scale, cracking of fuel pellets has been studied using statistical fracture mechanics. The objective of this work is to estimate the amount of fragmentation that occurs in real fuel pellets (within certain probability limits) for a given amount of initial damage (i.e., initial porosity, micro-crack density, etc.) during irradiation without having to explicitly model the underlying microstructure.

To generate a database of results for the statistical analysis, an eXtended Finite Element Method (XFEM) was used. The XFEM approach accurately accounts for the singular stress fields of cracks and efficiently simulates crack nucleation, merging, and branching. ***Fig. 4*** illustrates the results being obtained from the XFEM simulations, which start with randomly distributed microcracks. [INL]

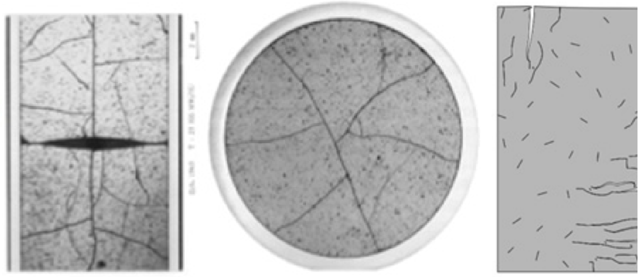


Fig. 4. Cracking patterns common in oxide fuels and results (far right) from an XFEM simulation of fragmentation behavior.

Nucleation

Another important effort has been to accurately model homogeneous precipitate nucleation within the phase field methodology used by MARMOT. Nucleation is a ubiquitous physical phenomenon in nuclear fuels undergoing irradiation. Homogeneous nucleation occurs spontaneously and randomly, but it requires significant thermodynamic imbalances, such as supersaturation, superheating, or supercooling of the medium. Computer simulations of homogeneous nucleation are extraordinary difficult, in part due to the stochastic nature of the process and the relatively short time scales over which it occurs.

Two phase-field modeling approaches have been adapted and implemented in MARMOT for the purpose of predicting a particular homogeneous nucleation phenomenon, namely precipitation kinetics. This enhancement to MARMOT will allow quantitative simulations of precipitate evolution, which can be compared with experimental results. [PNNL]

Finally, work was completed on the direct coupling of the Thermochimica tool with BISON in fuel performance simulations. This will give BISON developers and users an alternative to having to supply the thermochemical data needed in their fuels simulations. Thermochimica now gives BISON simulations run-time access to a large, growing, and self-consistent library of thermodynamic data. To demonstrate the coupling, BISON was used to successfully calculate the distribution of hydrides in zirconium cladding under postulated LWR conditions using thermodynamic data supplied by Thermochimica as needed during the simulation. [ORNL]

Supporting Tools

Work continued in the use of DAKOTA to support model development and implementation in BISON. Three areas of advance during the past quarter were: (1) calibration of the relocation model, which is a legacy empirical model still in use while mechanistic models for fuel cracking are under development; (2) sensitivity analyses of the new fission gas release model; and (3) sensitivity analyses and uncertainty quantification of simulations on beginning-of-life versus irradiated fuel. [SNL]

RPL Accomplishments

Multiphysics Simulations (SHARP)

In the last quarter, the SHARP team of the Reactors Product Line (RPL) has focused on simulating the full EBR-II core (excluding the blanket region). Part of the core (the XX09 assembly) has been treated heterogeneously, while the rest has been treated homogeneously (***Fig. 5***). Resolving the geometry pin-by-pin only in a small portion of the domain dramatically cuts the computational cost. The user can increase the local resolution to match the available resources and desired accuracy. A set of pseudo-transient and full-transient simulations has been carried out for a simplified loss-of-heat-sink transient. [ANL, LLNL]

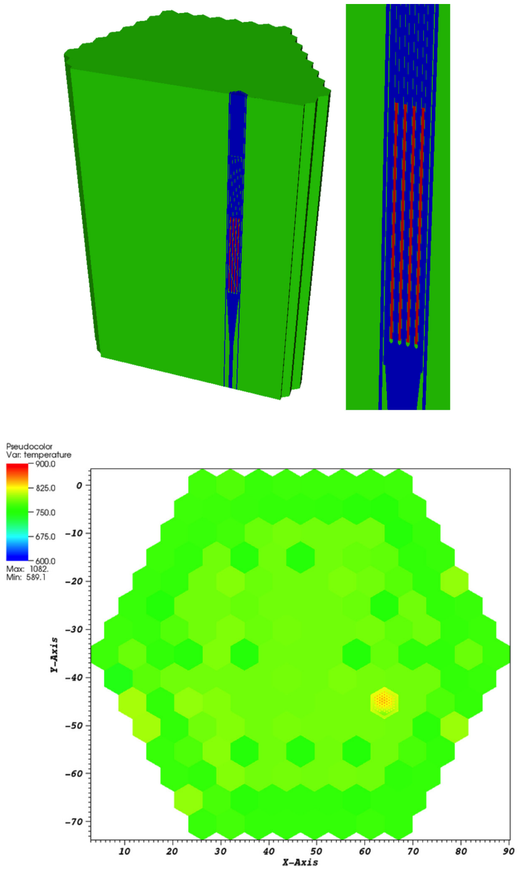
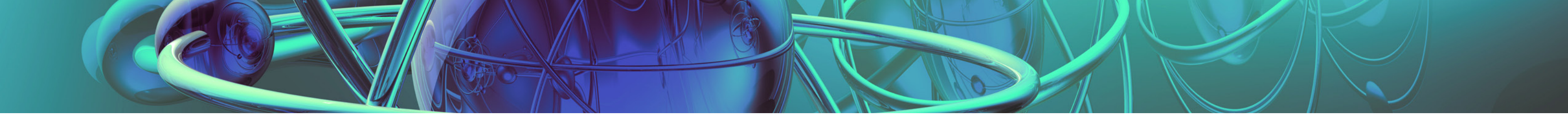


Fig. 5. View of the EBR-II core domain (top) and its temperature distribution in the multiphysics simulation (bottom).

Thermal Fluids (uRANS and Nek5000)

The NEAMS thermal fluids team has focused on four main projects: development of unsteady Reynolds-averaged Navier-Stokes (uRANS) capability, MAX experiment sensitivity study, Euratom collaborations under the International Nuclear Energy Research Initiative (I-NERI), and an update of the Nek5000 development plan. [ANL]

The main focus was the implementation, verification, and validation of a few variants of the k-ω uRANS model of turbulence, including a novel regularized approach to wall boundary conditions. These intermediate-fidelity tools enable fast-turnaround capability for complex geometries in Nek5000 that could also be used to improve the existing lower-fidelity tools and provide a better initial guess for intermediate-fidelity simulations. ***Fig. 6*** shows results of modeling a wire-wrapped fuel bundle with the Nek5000 uRANS regularized k-ω shear stress transport (SST) model. [ANL]



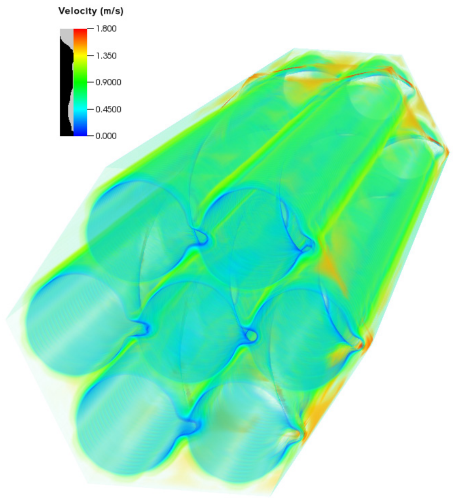


Fig. 6. Velocity field contours in a wire-wrapped 7-pin fuel bundle.

The unprecedented high-resolution data provided by the MAX experiment will be used for validating numerical simulation capabilities at various levels of fidelity through a future blind benchmark exercise. To this end, simulations have performed with various numerical methods, levels of fidelity, flow parameters, and boundary conditions to thoroughly study the modeling sensitivity of the MAX geometry. ***Fig. 7*** shows the destabilizing influence of relatively minor perturbations of inlet geometry on the vertical flow velocity. [ANL]

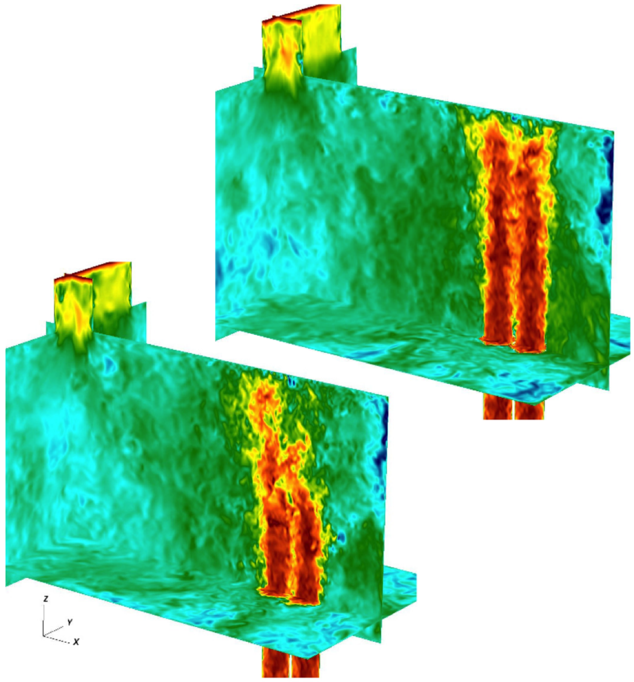


Fig. 7. Instantaneous vertical velocity field for two MAX experiment mixing chamber inlet configurations: (top) default setup with protruding inlets and (bottom) alternative case where the inlets are flush with the chamber floor.

As part of the I-NERI collaboration with Belgium (NRG) and the Netherlands (SCK-CEN), ANL issued report ANL/NE-13/20, which compares results of different models for the 7-pin bundle shown in Fig. 6. Ongoing collaborations on benchmarks like this are instrumental for verification and validation activities. The RPL team is also collaborating with Texas A&M University to perform direct numerical simulations of pebble bed reactors for several configurations and Reynolds numbers (***Fig. 8***), leading to a deeper insight into the flow physics of this geometry. [ANL]

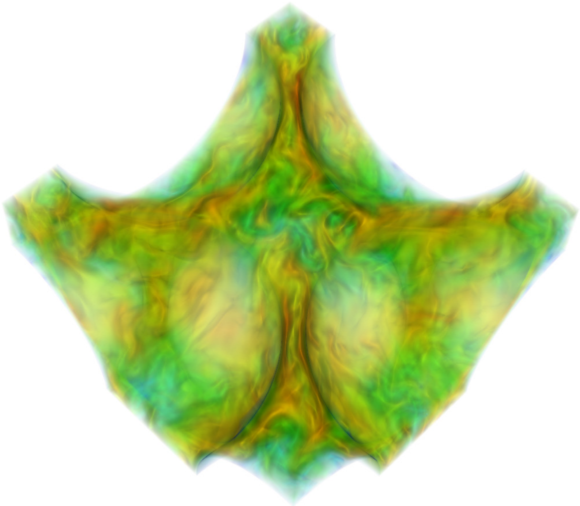
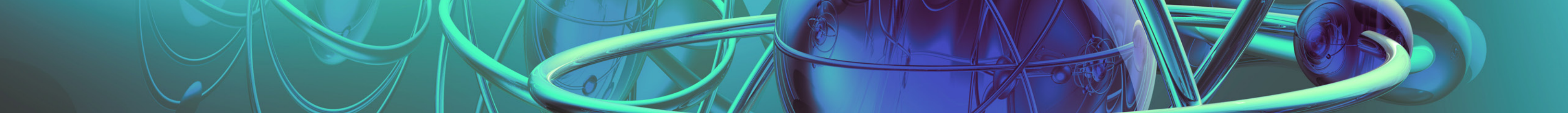


Fig. 8. Volume rendering of the flow field in the interstitial region between 6 fuel particles in a pebble bed reactor.

The NEAMS thermal hydraulics development plan outlines a 5-year improvement and implementation strategy for Nek5000. Implementation tasks include coupling Nek5000 to the NEAMS integrated computing environment (NiCE) and to DAKOTA, an uncertainty quantification package. [ANL]

Neutronics (PROTEUS and Cross-section Libraries)

During the last quarter of FY2013, the PROTEUS-SN code, including a user manual and benchmark cases, was transferred from the development team to the early user team. The user team installed PROTEUS on a local Linux cluster at ORNL, executed test problems, and reviewed available documentation. The review criteria include user accessibility and friendliness, geometry construction capability, numerical accuracy of the transport solver, and computational efficiency. [ANL, ORNL]



The neutronics team continues to develop appropriate cross-section libraries, which provide the neutron-nucleus reaction probabilities needed to calculate reaction rates during simulations. Verification tests for the generalized cross-section libraries have been performed using fuel compositions from various reactor types, including LWRs, SFRs, and high-temperature reactors. The base ultrafine library was produced by the GeneCS code using the cross-section data generated from MC^2-3 and NJOY. The base library was condensed to a broad group library using reactor-specific condensation optimization.

Initial verification results of the new libraries indicated that the eigenvalues were estimated within 200-300 pcm when compared to the Monte Carlo continuous-energy-group solutions (pcm is a measure of relative core reactivity used by reactor design engineers and in this case corresponds to predictions within 0.2-0.3% of the Monte Carlo solutions). [ANL, ORNL]

The cross-section application programming interface (API) implemented in PROTEUS-MOC (method of characteristics) was verified using homogeneous composition and single and 2×2 pin-cell cases based on the VERA pressurized water reactor benchmarks. Eigenvalue tests indicated that all subroutine and function components worked as designed. [ANL, ORNL]

An updated, embeddable version of the Oak Ridge Isotope Generator (ORIGEN) depletion and isotope decay code has been developed to support the varied needs of multiphysics analyses. A newly developed OrigenLibraryBuilder aggregates data defining decay and reaction transitions for over 2,200 nuclides, producing an ORIGEN library object for depletion/decay calculations (see ***Fig. 9***).

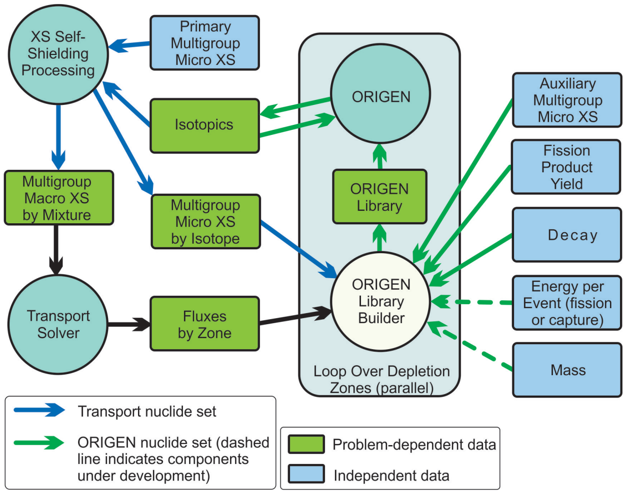


Fig. 9. Data flow in a depletion/decay calculation using the updated ORIGEN module (XS = cross-section).

The builder component also integrates AMPX microscopic cross-section library resources with the "main" cross-section library (self-shielded ENDF) and microscopic cross-sections in the "auxiliary" library (infinitely dilute JEFF-3.0/A). Contemporary data structures suitable for high-performance computing environments are now available for all major data components. Data structures for the minor components are currently being developed. [ANL, ORNL]

Preliminary testing of OrigenLibraryBuilder showed performance better than that of SCALE/Couple, the legacy module of SCALE (Standardized Computer Analyses for Licensing Evaluation) that performed the same task. OrigenLibraryBuilder includes additional generalization beyond what is available in Couple, such as allowing daughter products from any incident particle type (e.g., a proton) and handling multiple metastable daughter states (Couple could only handle one metastable daughter state). Fortran interfaces are currently being developed. [ANL, ORNL]

SFR Module (RELAP-7)

The SFR primary systems module was enhanced with new components for tracking the liquid level change in open 0D volumes and the heat transfer between 0D volumes through solid structures. These changes provide better modeling of the pool dynamics, which is important for transient evolution in an SFR. As discussed in the Sept. 2013 *NEAMS Update*, the SFR system simulation capabilities have been successfully demonstrated by modeling the Advanced Burner Test Reactor protected loss of flow transient. [INL, ANL]

Balance of Plant (RAVEN)

RAVEN is a MOOSE-based application that provides a user interface with RELAP-7 for performing risk-informed safety margin characterization (RISMC). (RISMC is a methodology for evaluating risk and supporting plant decisions to improve economics, reliability, and safety in nuclear power plants.) Two major RAVEN activities were completed during the last two quarters of FY2013: (1) work completed during first half of the year was tested in a probabilistic risk analysis (PRA) and (2) a dynamic event tree (DET) analysis capability was implemented in the code. [INL, ANL]

A station blackout, i.e., the loss of both normal and emergency power, was the scenario for the PRA demonstration, during which all of RAVEN's statistical functionalities were tested to sample the distributions for input parameters.

Fig. 10 compares histograms of the maximum temperature reached by the core fuel cladding (resulting from auxiliary systems recovering at different times) and of the failure temperature of the cladding (based on a triangular distribution of recognized safety limits). The figure illustrates a key conceptual advancement of the RISMC framework: both the load (maximum cladding temperature) and capacity (to withstand extreme temperatures) are defined in a probabilistic sense. The area of intersection between the two distributions defines the region where cladding failure is possible. This approach is more realistic than the classical approach, where cladding failure would be defined as all simulations that exceeded the mean cladding failure temperature (the histogram peak). [INL, ANL]

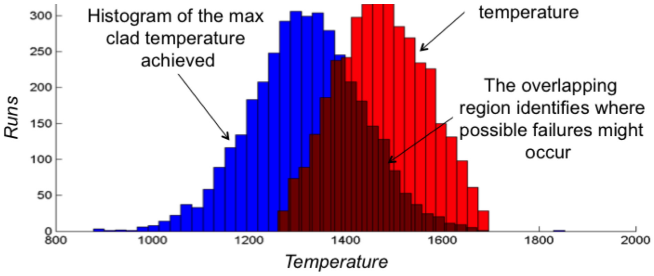


Fig. 10. The use of histograms to predict cladding failure.

The demonstration provided the opportunity to exercise the RAVEN graphical user interface and make it more user-friendly. The 3D visualization of the plant is shown in ***Fig. 11***. [INL, ANL]

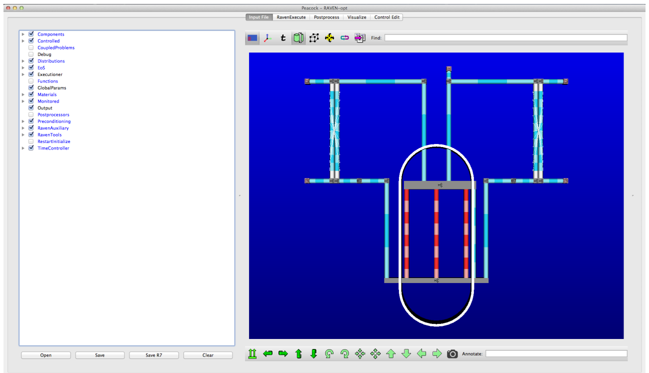


Fig. 11. 3D plant visualization in RAVEN.

RAVEN relies upon Monte-Carlo methods. While Monte Carlo is the most robust methodology to perform statistical analysis, it is also the most expensive. One of the most promising methodologies to decrease computational costs is DET analysis. This method provides a way to evaluate and manage the number of possible events and event sequences that the model will account for. However, it requires control logic flexibility that is not available in most of the existing safety codes. ***Fig. 12*** shows the output of a DET analysis. The plotted outcomes define a plane, usually referred to as a limit surface, that clearly separates success from failure. The next enhancement will incorporate adaptive sampling strategies based on artificial intelligence algorithms. [INL, ANL]

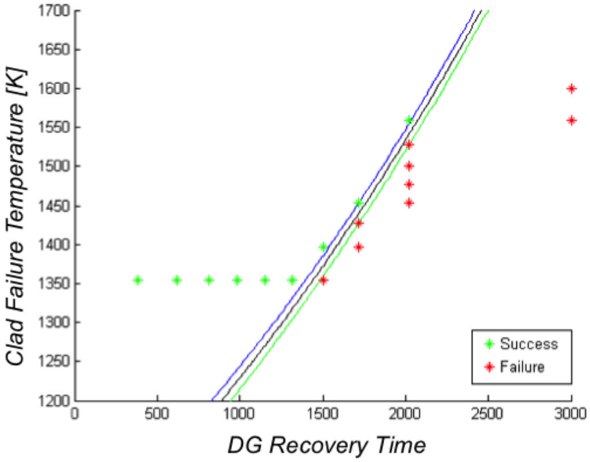


Fig. 12. Limit surface defined by DET outcomes.

MeshKit

MeshKit 1.0 was released as an open-source package on Sept. 30, 2013. Version 1.0 includes improved documentation; new boundary layer insertion, sweeping, and interval assignment algorithms; and algorithms for generation and manipulation of all-hexahedral and tetrahedral meshes. These features are critical when modeling the complex geometries of advanced nuclear reactor cores. [ANL]

Integrated Framework (CouPE and MOAB)

CouPE, which executes and controls the timing of data exchanges between different physics modules, has been updated to include support for quasistatic neutronics, the ability to enforce user-specified perturbations, and interfaces to libMesh and Deal.II libraries to support a variety of frameworks, including SHARP and MOOSE. These enhancements were used to perform coupled fluid dynamics/neutronics/structural mechanics simulations of 3D single- and multiple-assembly reactor cores. [ANL]

The solution transfer capability in MOAB, which enables data exchanges between physics modules, is being redesigned to enable different types of search trees, implement a more efficient parallel mesh searching algorithm, and allow the use of application-provided discretization evaluation functions. Initial evaluations indicate a 25-65% reduction in processing time for shape function evaluations. [ANL]

Computing Environment (NiCE)

The NiCE user environment provides tools to ensure a uniformly positive user experience when using the NEAMS ToolKit. Recent enhancements to NiCE include complete implementation of support for the BISON fuel mechanics code. Additional features have been added to the reactor analyzer to enable users of legacy codes to more easily transition to the higher-fidelity NEAMS tools, with an initial focus on LWR core geometries and fuel assemblies. The toolset is presently being extended to hexagonal lattice cores and fuel assemblies. The NiCE user environment can be seen in action on the jayjaybillings YouTube channel. (See the back page for links to the new features.) [ORNL]

Technical Spotlight: Modeling Structural Mechanics with Diablo

Diablo is a structural mechanics modeling tool that combines basic conservation laws with a variety of material and interface models. The code uses implicit, Lagrangian finite element methods to simulate nonlinear structural mechanics and heat transfer. Diablo supports parallel computation and leverages discretization techniques developed and user-tested in previous codes. Its architecture is based on Fortran 95 data objects and a message-passing programming model.

The Diablo code now incorporates an interface to SHARP via the MOAB backplane. The interface has been demonstrated by using temperature fields from coupled thermal-hydraulics (Nek5000) and neutronics (PROTEUS) simulations to model heat-induced structural deformations. This is important for evaluating passive safety features. SFRs, for example, can be designed to moderate the neutron flux and ramp down the power when the core is deformed by extreme heat.

A recent demonstration used a model of the EBR-II core with one pin-resolved assembly (XX09); the balance of the core was represented as a set of homogenized assemblies. ***Fig. 13*** shows the lateral pin displacements determined by Diablo from asymmetries in the power and temperature fields.

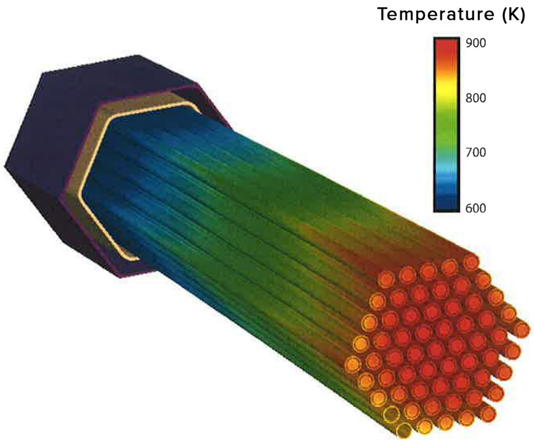


Fig. 13. Diablo simulation of thermal distortions in the XX09 assembly model (exaggerated 25x for display).

In addition to the effects of structural response within the reactor core, structural mechanics intersects with multiple systems in the balance of plant. Providing adequate margins of structural performance under earthquake loadings is a significant driver of overall plant capital costs. Tools that capture seismic response with greater fidelity can enable design choices that minimize excessive safety margins and cost.

A recent effort examined the technologies needed to incorporate soil-structure interaction (SSI) during seismic response into Diablo. This topic is especially relevant given the current design trend toward subsurface placement of reactors.

The standard methodology for SSI relies upon a frequency-domain representation. (There are generally two choices for representing waves: by time or frequency.) This simplifies modeling far-field effects (i.e., outside of the modeling mesh) in layered geologic media, but at the price of limiting the ability to incorporate and thus evaluate nonlinear material response. The latter is important because nonlinear response is the most common means for structures and nearby soil to dissipate energy under extreme load events like earthquakes.

The linear Bielak method for applying wave boundary conditions was extended to handle non-linear soil models. This modified Bielak method applies the seismic loading upon an intermediate region within the model of the nearby geology. As shown in ***Fig. 14***, strong seismic waves are applied on Γ^b and in Ω_{III} to load the structure and adjoining soil. The outer domain Ω_{II} only needs to represent waves reflecting from the structure and are treated with absorbing boundary conditions on the outside boundary Γ^e to mimic their continued propagation to the far field.

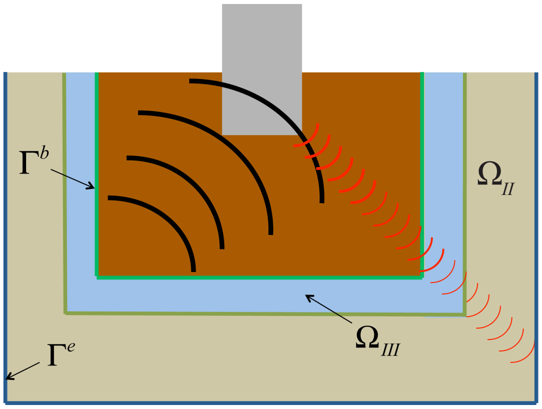


Fig. 14. SSI models must apply the seismic excitation while also allowing reflected waves (red) to escape to the far field.

The Diablo SSI study was intended to illustrate how advanced time-domain simulation approaches compare with and complement the standard frequency-domain approach for SSI. Simulations were performed on a buried small modular reactor configuration. The geologic conditions were derived from available data for the Savannah River Site. SSI experts exercised the standard frequency-domain tool on a comparable model. The study showed that the new time-domain approach provides comparable results for the excitation levels studied. This is a first step in establishing the method's credibility and can open the way to modeling more extreme structural response where nonlinear effects are dominant.

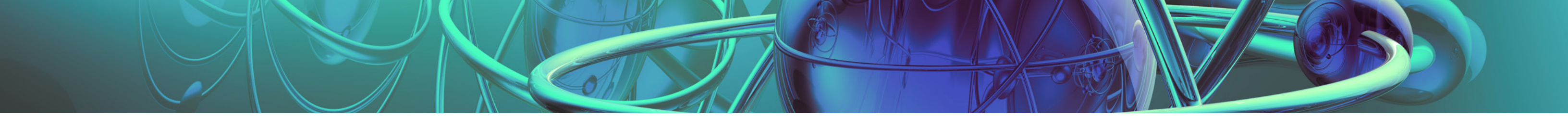
The Diablo team is Bob Ferencz, Jerome Solberg, Neil Hodge, and Russell Whitesides (all LLNL).

Synergy with Other Programs

NEAMS benefits from tools developed under other programs and also provides components used in other simulation toolkits. Some noteworthy instances are listed below:

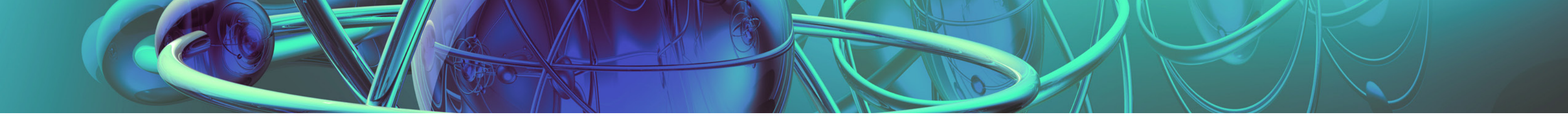
- Peregrine is a fuel performance code derived from BISON. The Consortium for Advanced Simulation of LWRs (CASL) created Peregrine for specific application to LWRs using proprietary models available only to CASL participants. The codes share a common framework and library for nonproprietary models, such that BISON development efforts benefit both programs.
- Development of RELAP-7 and RAVEN is co-funded by NEAMS and the Light Water Reactor Sustainability Program (LWRS Program).
- The CASL-developed Data TransferKit (DTK) generates parallel topology maps for transferring fields and other data between meshes. It relies upon MOAB for managing mesh data.

The mission of the CASL is to provide coupled, higher-fidelity, usable modeling and simulation capabilities needed to address pressurized water reactor operational and safety performance-defining phenomena. The LWRS Program is developing the scientific basis to extend existing nuclear power plant operating life beyond the current 60-year licensing period and ensure long-term reliability, productivity, safety, and security.

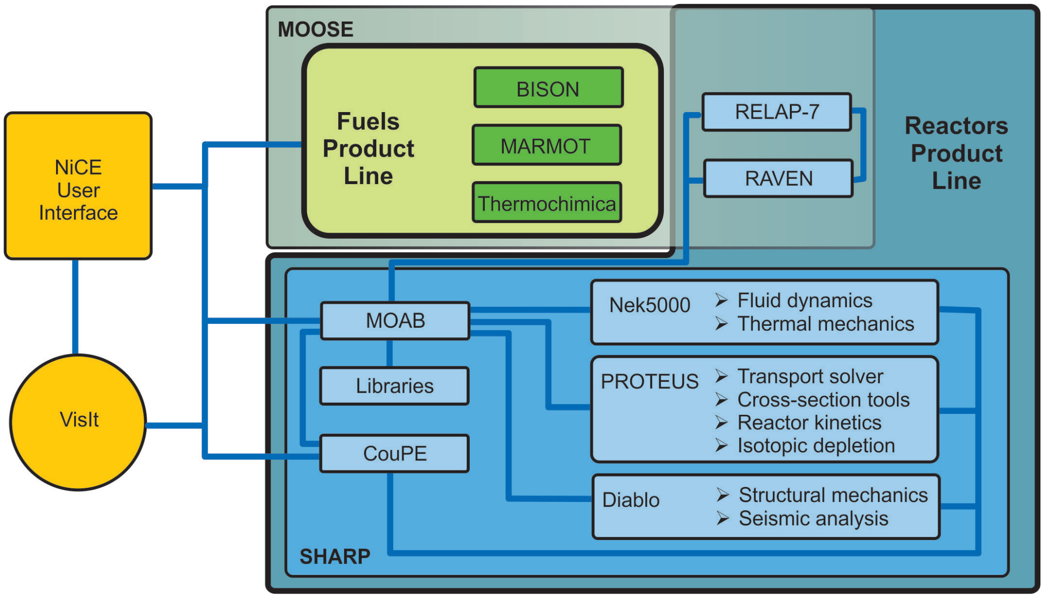


Computer Programs in the NEAMS ToolKit

Name	Purpose or Description
BISON	BISON is a MOOSE-based continuum-scale fuel performance code that simulates nuclear fuel physical characteristics for a wide range of operating and service conditions. BISON includes models for evolution and migration of fission products, fuel cracking, fuel cladding, coolant channels, thermal conductivity, and other reactor core components to predict the behavior of a complete fuel assembly.
CouPE	Coupled Physics Environment. CouPE is a multiphysics driver/coupler library that executes and controls the timing of data exchanges between different physics modules in SHARP.
DAKOTA	Design Analysis Kit for Optimization and Terascale Applications. DAKOTA provides a flexible, extensible interface between analysis codes and iterative systems analysis methods to facilitate sensitivity and uncertainty analyses for NEAMS components, as well as provide a bridge to some legacy codes.
Diablo	Diablo is a structural mechanics modeling tool that uses basic conservation laws and integration with a variety of material and interface models to simulate nonlinear structural mechanics and heat transfer. This is used within SHARP to evaluate structural stress, strain, and deformation and within RELAP-7 to evaluate seismic effects.
Mammoth	Mammoth is a MOOSE-based code used to couple RattleSnake and RELAP-7.
MARMOT	MARMOT is an object-oriented finite element framework for multiphysics phase-field (mesoscale) simulations. With BISON, it provides a single-pin fuel performance code for modeling microscopic response of nuclear fuel to irradiation.
MBM	Integration of MOOSE, BISON, and MARMOT that enables atomistically informed multiscale simulations of nuclear fuel microstructure.
MC^2-3	Version 3 of a fast reactor cross-section processing code for calculating fast neutron spectra and multigroup cross sections. MC^2-3 is one of the neutron cross-section library generators used in PROTEUS.
MOAB	Mesh-Oriented dAtaBase. MOAB is a highly scalable data management back-plane for mesh-based simulations. It transfers data and solutions between physics modules in SHARP.
MOOSE	Multiphysics Object-Oriented Simulation Environment. MOOSE is a parallel computational framework for coupled systems of nonlinear equations. It has a modular, adaptive architecture that greatly simplifies the addition of new physics "kernels." This modularity, as well as the consistent way that MOOSE handles nonlinear material properties and boundary conditions, enables rapid prototyping and fast development of production-ready massively parallel code.
Nek5000	Nek5000 is a multidimensional heat transfer andcomputational fluid dynamics code used in SHARP.
NiCE	NEAMS integrated Computing Environment. NiCE is the NEAMS user interface. It integrates MOOSE and SHARP applications and provides tools for model development, simulation and data set management, and data analysis and visualization.
ORIGEN	Oak Ridge Isotope Generator. A depletion and isotope decay code used to create neutron cross-section libraries in PROTEUS.
PETSc	Portable, Extensible Toolkit for Scientific Computation. PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It is used in MOOSE.
PROTEUS	PROTEUS is the neutron transport module in SHARP. PROTEUS models the fission reaction to determine temperature and power levels. Two versions are available: (1) PROTEUS-SN uses a second-order discrete ordinates method and (2) PROTEUS-MOC uses a method of characteristics solver.
RattleSnake	RattleSnake is a 3D kinetics code used with RELAP-7.
RAVEN	Reactor Analysis and Virtual Control Environment. RAVEN is a MOOSE-based application that provides a user interface with RELAP-7 for performing risk management evaluations.
RELAP-7	Reactor Excursion and Leak Analysis Program. RELAP-7 is a MOOSE-based single-zone (0D/1D) code for managing and coupling other simulation codes to model a complete nuclear power plant under a variety of operational and accident conditions.
SHARP	SHARP is a high-fidelity, 3D reactor core simulation framework for evaluating the impacts of design changes on reactor performance and safety. SHARP uses empirical physics-based methods that greatly reduce the dependence on calibrated engineering models.
Thermochimica	Thermochimica provides thermochemical property data for BISON and MARMOT.
VisIt	VisIt is an interactive parallel visualization and graphical analysis tool for viewing and animating scientific data in a variety of ways (scalar or vector, 2D or 3D, structured or unstructured meshes, etc.). VisIt is the primary visualization program in the NEAMS ToolKit.



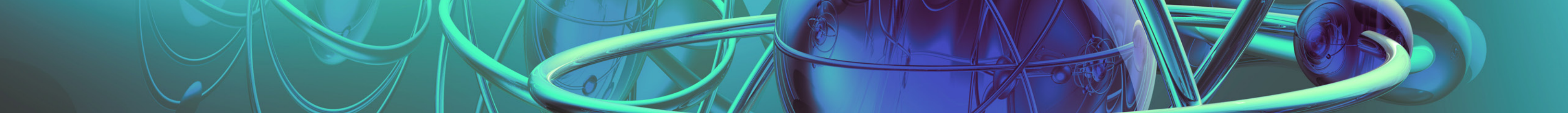
The NEAMS ToolKit



Recently Completed Level 1 and 2 Milestones

Milestone ID	Description	Due Date	Finish Date
M2MS-13AN06030213	Release initial version of thermal fluids (Nek5000-URANS) module to RPL team	7/31/2013	7/31/2013
M2MS-13IN0603032	Release initial version of integrated framework to RPL team	7/31/2013	7/31/2013
M2MS-13AN06030243	Complete validation comparisons with MAX data	8/30/2013	9/30/2013
M2MS-13LL0603074	Update development plan for the structural mechanics module	9/27/2013	10/31/2013
M2MS-13IN0602022	Release BISON update	9/30/2013	9/11/2013
M2MS-13OR0602061	Deliver the Thermochimica module for use by MBM team	9/30/2013	9/30/2013
M2MS-13OR06030520	Release initial graphical user interface for BISON	9/30/2013	9/30/2013
M2MS-13AN06030212	Update development plan for NEAMS thermal fluids module	9/30/2013	9/30/2013
M2MS-13AN06030215	Update development plan for NEAMS neutronics module	9/30/2013	9/30/2013
M2MS-13AN06030220	Complete integrated multiassembly multiphysics simulation	9/30/2013	9/30/2013
M2MS-13AN0603023	Release internal version of MeshKit to NEAMS Toolkit team	9/30/2013	9/30/2013
M2MS-13AN06030238	Complete 7-pin bundle simulation and exchange results with NRG/SCK-CEN/ Ugent as part of Euratom I-NERI	9/30/2013	9/30/2013
M2MS-13AN06030244	Complete validation pathways project summary	9/30/2013	9/27/2013
M2MS-13AN06030217	Report on ongoing subgroup software library development	9/30/2013	9/30/2013
M2MS-13AN06030218	Deliver initial SFR primary system simulation	9/30/2013	9/25/2013
M2MS-13PN0602054	Report on the Implementation of homogeneous nucleation scheme in MARMOT-based phase field simulations	9/30/2013	9/30/2013

Note: No milestones are due in the first quarter of FY2014.



NEAMS Vision

K. S. Bradley
NEAMS national technical director

The goal of the NEAMS program is to enhance DOE-NE's research and development portfolio through the development of advanced computational methods. The tools we are developing —the NEAMS ToolKit — will provide insights into the performance and safety of advanced reactor systems that we cannot obtain through experimentation alone. They will also complement experimental work by helping us design experiments that are more complex and informative and then helping us interpret the results of those experiments.

To achieve this, the NEAMS ToolKit will incorporate fundamental descriptions of the underlying physics that govern the critical behaviors we must understand and accommodate in new reactor designs. In other words, we strive to replace the empiricism and correlations typically employed in modeling and simulation tools with mechanistic descriptions that have been validated using experiments targeting each phenomenon in isolation as well as experiments conducted to address the interaction and competition between phenomena.

With this approach, the ToolKit will not only succeed at reproducing the results previously observed, but it will permit designers and analysts to predict performance in regimes beyond the test base, that is, where we have no direct experimental observations.

The NEAMS team hopes this quarterly report of our accomplishments will provide insight into our challenges and achievements.

The quality and utility of the NEAMS ToolKit will only be as good as the guidance we get from stakeholders. Please, reach out to the team if you have advice or ideas to share. Your input is essential to our success.

NiCE BISON plugin

NiCE reactor analyzer

NiCE SFR support

Acknowledgments
Argonne National Laboratory's work was supported by the U.S. Department of Energy, Assistant Secretary for Nuclear Energy, Office of Advanced Modeling and Simulation, under contract DE-AC02-06CH11357.

Availability of This Report
This report is available, at no cost, at http://www.osti.gov/bridge. It is also available on paper to the U.S. Department of Energy and its contractors, for a processing fee, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831-0062
phone (865) 576-8401 | fax (865) 576-5728
reports@adonis.osti.gov

About Argonne National Laboratory
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see www.anl.gov.

Editor Bryan Schmidt, ANL
Design Team Renee Carlson, ANL, & Larisa Blyudaya

CONTACT ▸ **Keith S. Bradley**
Argonne National Laboratory
630.252.4685
ksbradley@anl.gov

Argonne NATIONAL LABORATORY