ANL/NEAMS-14/4

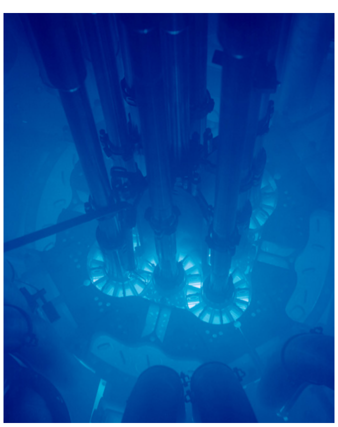
# NEAMS Update

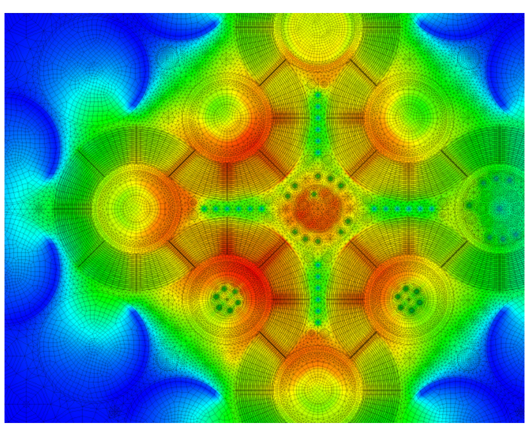
**Quarterly report for July - September 2014**

**Published February 2015**

## Overview

- BISON version 1.1 was released in September, and the BISON Assessment Report was updated.
- BISON was given a better capability for modelling hydrogen behavior in Zircaloy cladding.
- A sensitivity analysis of the gap heat transfer model for $UO_2$ fuel at high burnup was completed.
- The microstructure-based $UO_2$ fracture model was improved by using the fission gas bubble density at grain boundaries to inform the fracture criteria.
- Molecular dynamics simulations of oxide fuel thermal conductivities were performed and compared to experimental data.
- MARMOT continues to be used to investigate the impact of high-burnup microstructures on thermal conductivity.
- The development of new fission gas diffusion models from lower-length-scale simulations continued.
- PROTEUS was verified using various benchmarks.
- Cross section libraries applicable to various reactor types have been tested for nine benchmark sets.
- Japanese sodium experiments were simulated to evaluate temperature fluctuation characteristics and thermal fatigue.
- A coupling interface between the SHARP nuclear reactor multiphysics framework and the thermal hydraulics code Nek5000 is being developed.
- The NiCE team continued to improve its support of MOOSE-based applications.
- The SIGMA toolkit – comprising CGM (geometry), MOAB (mesh), and MeshKit (mesh generation) components – had a consolidated initial release in July.
- The MeshKit team has been developing a graphical user interface that includes several tests and examples for optimally handling large-scale reactor geometries.
- Numerous fixes were introduced to the lattice creation method in the Reactor Geometry Generator for nonsymmetrical rectangular reactor assemblies.
- The RAVEN group delivered a new sampling strategy that represents an evolution of the well-known dynamic-event-tree (DET) methodology.





Far left: The Advanced Test Reactor (ATR) at Idaho National Laboratory. The ATR is a light-water reactor (LWR) with a novel configuration that provides locations with different flux rates to test reactor materials.

Left: The ATR has been the subject of numerous NEAMS simulations.

# Fuels Product Line (FPL) Accomplishments

**Engineering Scale (BISON)**

The updated fuel performance tool BISON 1.1 was released in September, along with revised user and theory manuals. The major new or improved capabilities in BISON 1.1 included models for:

1. enhanced coolant channels, allowing the simulation of the full boiling curve;
2. high-temperature Zircaloy creep, needed for use in loss-of-coolant accident (LOCA) simulations;
3. Zircaloy microstructure phase changes at high temperature;
4. improved hydrogen diffusion/precipitation in Zircaloy;
5. transient fission gas release;
6. multiple nonlinear materials, an important and broadly applicable capability);
7. mechanical and thermal contact; and
8. mechanistic smeared cracking in three dimensions.

Many of the enhancements implemented in BISON during this past year have been with a view to providing a robust capability to simulate light water reactor (LWR) fuel performance during transient, off-normal events, specifically LOCAs and reactivity-initiated accidents (RIAs).

The BISON Assessment Report was also updated and released. In addition to all the previous validation cases being reassessed using BISON 1.1, 18 new cases from the FUMEX-II and III projects were added to the validation database. In general, BISON performance when assessed against international benchmark and validation databases for steady-state and ramp behavior has consistently met or exceeded the performance of other modern codes currently in use around the world. In addition to work on BISON validation, considerable advances were made the area of code verification, with special attention paid to needs specific to fuel performance software. The BISON team published a favorable comparison of BISON to other fuel performance codes (Annals of Nuclear Energy, Sept. 2014, vol. 71, pp. 81-90). [INL]

Significant improvements have been made in BISON's capability to model hydrogen behavior in Zircaloy cladding. Specifically, previous constraints that often necessitated small time steps have been entirely removed. This upgrade enables large, multi-dimensional simulations to be executed efficiently while still capturing hydrogen pickup, diffusion, precipitation, and dissolution in the cladding (***Fig. 1)***.

Work on validating the hydride model has also progressed. In a recent comparison of BISON calculations to results from a classic 1960 experiment involving hydrogen transport, precipitation, and dissolution in Zircaloy-2 under a temperature gradient, BISON successfully predicted all the major features from the experiment (see ***Fig. 2)***. [INL, Penn State University]

*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).

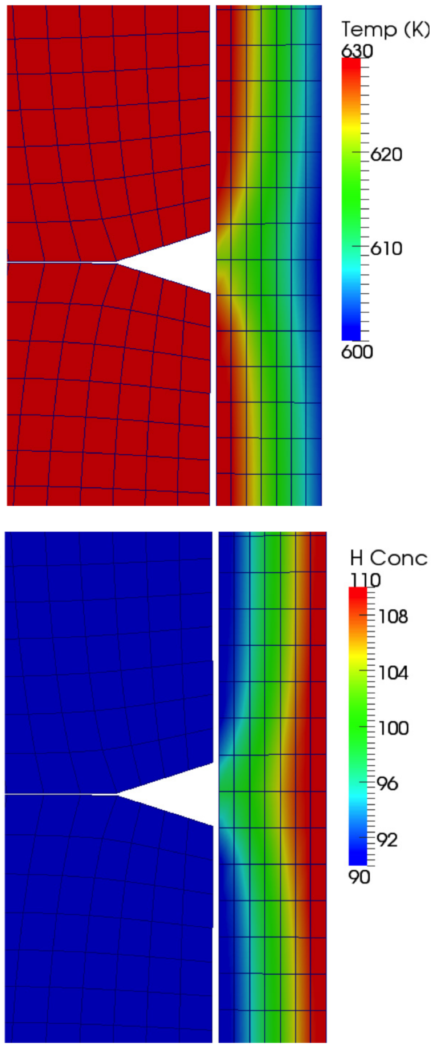



*Fig. 1. Example of temperature (top) and hydrogen (bottom) concentrations in cladding near a pellet-pellet interface using BISON hydride model.*

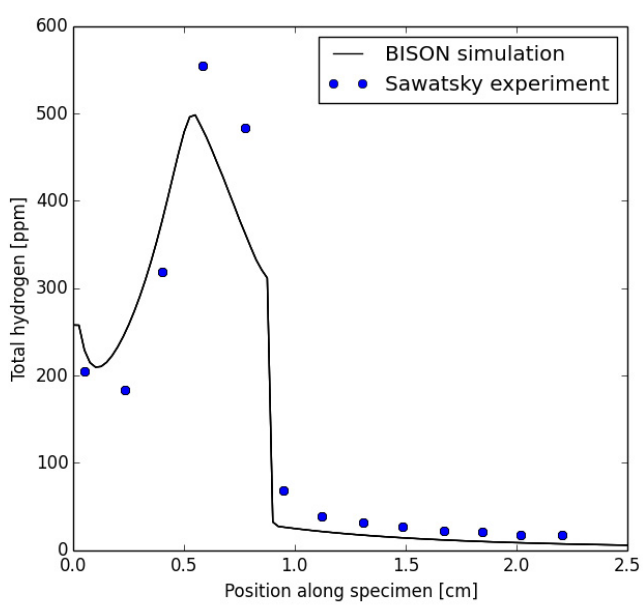



*Fig. 2. Comparison of BISON hydride model predictions to classic hydride redistribution experiment.*

In a small activity initiated this year, full coupling of BISON to the microscale depletion/isotope production capability under development in MAMMOTH was completed. As a test of coupled performance, a high-resolution microscale depletion calculation over 350 effective full power days (EFPDs) for a pressurized water reactor (PWR) fuel rod having 20 radial rings was performed using MAMMOTH. The power density results provided to BISON by the concurrent MAMMOTH simulation were comparable with those of the internal, static, Lassmann-style model that resides in BISON. The depletion capability in MAMMOTH, however, will be more generally valid for diverse simulation scenarios, whereas the current BISON model is restricted to normal PWR conditions. [INL]

A sensitivity analysis of the gap heat transfer model for $UO_2$ fuel at high burnup was completed. The insight obtained from this analysis will be used to guide improvements to the BISON gap conductance model in the future. [SNL]

Finally, a BISON training workshop was held on July 29-30 at the DOE Germantown facility. Federal staff from the Fuel Cycle Research & Development (FCRD) and LWR Sustainability programs participated. [INL]

## Subcontinuum Scale (MARMOT and Atomistic Simulations)

A significant step was made in the development of a microstructure-based fracture model for $UO_2$ in which the grain boundary fission gas bubble density informs the fracture criteria. The model has been developed using both molecular dynamics (MD) and MARMOT fracture simulations. Intergranular brittle fracture in $UO_2$ was simulated using a phase-field based formulation in MARMOT. Sensitivity studies were performed to ensure that the length scale and viscosity parameters used in the phase-field model are appropriate and were chosen to independently derive growth of sharp cracks (***Fig. 3***).

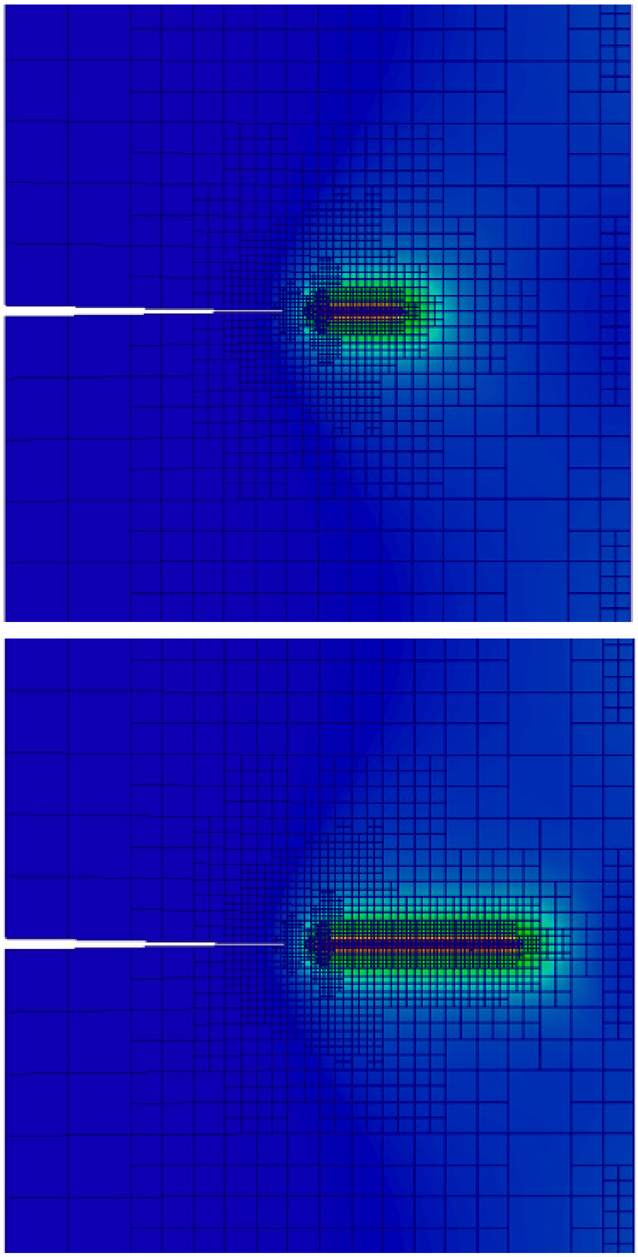


*Fig. 3. Crack growth simulations in MARMOT at two stress levels. Note the use of adaptive mesh refinement with crack propagation.*

The energy release-rate type parameter used in the phase-field model was calibrated from MD simulations. Subsequently, a numerical sensitivity study was performed whereby the effect of porosity and pore and grain size on the fracture behavior was explored. The response from the micromechanical simulations were then fit to a stress-based model usable at the engineering scale. Presently, predictions are made solely based on brittle intergranular fracture. However, transgranular and ductile fracture will also be incorporated following a similar methodology to obtain improved predictions.

The multiscale approach in BISON bridges three different scales and allows engineering-scale model development using a minimal number of experiments. In the future, BISON's macroscale model will be expanded to also account for pore radius. [INL]

In the area of thermal conductivity modeling and validation, MD simulations of the $UO_2$ and $UO_{2+x}$ thermal conductivities were performed and compared to experimental data collected in the low (<300 K) and high (>500 K) temperature ranges. The MD simulations were corrected for missing spin scattering, as established in previous studies. Above 800 K, the MD simulations overestimate the thermal conductivity, while it is underestimated below this temperature. The change in thermal conductivity with increasing oxygen content is correctly reproduced in each temperature range. At 800 K, $UO_{2+x}$ transitions from a two-phase $UO_2$+$U_4O_9$ mixture to a $UO_{2+x}$ solid solution, which explains why the model exaggerates conductivity estimates below and above this temperature as compared to experiments. Future work will assess the sensitivity of the absolute thermal conductivity values to the potential employed.

Surprisingly, the low-temperature measurements on $UO_{2.04}$ show increased thermal conductivity above the Néel temperature compared to stoichiometric $UO_2$. This may indicate a strong coupling between scattering by interstitial oxygen ions and spin-phonon scattering. Additional work is required to resolve this problem. [LANL]

INL continued to use MARMOT to investigate the impact of high-burnup microstructures on thermal conductivity. A comparison was made of the effective thermal conductivity of microstructures with large grains and small grain boundary bubbles (typical irradiated fuel structure) and small grains with large bubbles (***Fig. 4***). Current results predict lower thermal conductivity in high-burnup microstructures, probably due to the high density of grain boundaries. This will require the incorporation of additional effects (e.g., dispersed point defects) in future enhancements to the thermal conductivity model. [INL]

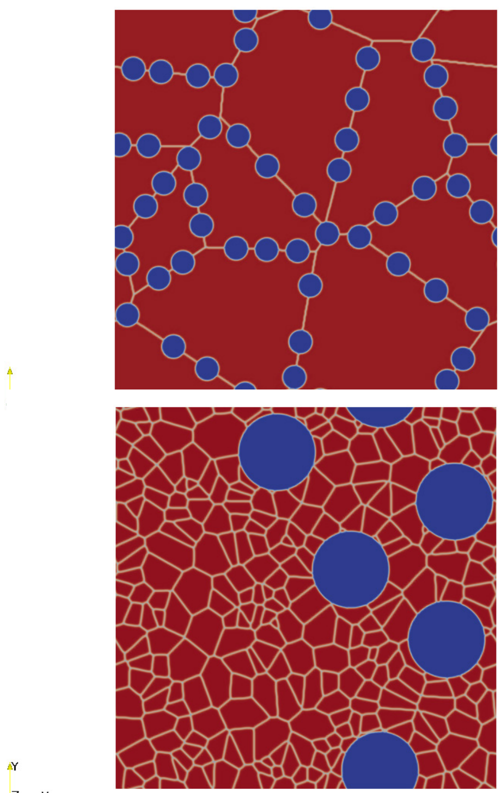


*Fig. 4. Microstructures used in MARMOT simulations of UO2 fuel thermal conductivity at (top) low burnup, and (bottom) high burnup, which is shown to have lower thermal conductivity.*

The development of new fission gas diffusion models from lower-length-scale simulations continued. And assessment of these models in terms of annealing experiments and fission gas release simulations using BISON was initiated. Based on the mechanisms established from density functional theory (DFT) and empirical potential calculations, continuum models for diffusion of Xe in $UO_2$ were derived for both intrinsic conditions and under irradiation. The model illuminated the importance of the large $XeU_3O$ cluster (Xe atom in uranium + oxygen vacancy trap site with two bound uranium vacancies), which is a consequence of its high mobility and stability. These models were implemented in MARMOT to calculate effective Xe diffusivities for various irradiation conditions and fission gas release for a number of test cases. [LANL, INL]

Finally, the first edition of the MARMOT Verification and Validation Report was issued. This report will be updated annually with additional validation cases. [INL]

# Reactors Product Line (RPL) Accomplishments

### Neutronics (PROTEUS)

As a verification effort for PROTEUS, the two-dimensional C5 PWR benchmark problem, which was modified from the OECD C5G7 benchmark, was simulated by PROTEUS and Monte Carlo N-particle (MCNP) methods using the identical 23-group multigroup cross sections. Using Legendre-Tchebyshev angular cubature order L3T15, PROTEUS and MCNP solutions agreed very well (within 125 pcm for eigenvalue – see ***Fig. 5)***. This work verifies that the PROTEUS solver accurately solves heterogeneous geometry problems when eliminating the cross section generation procedure as a source of error.

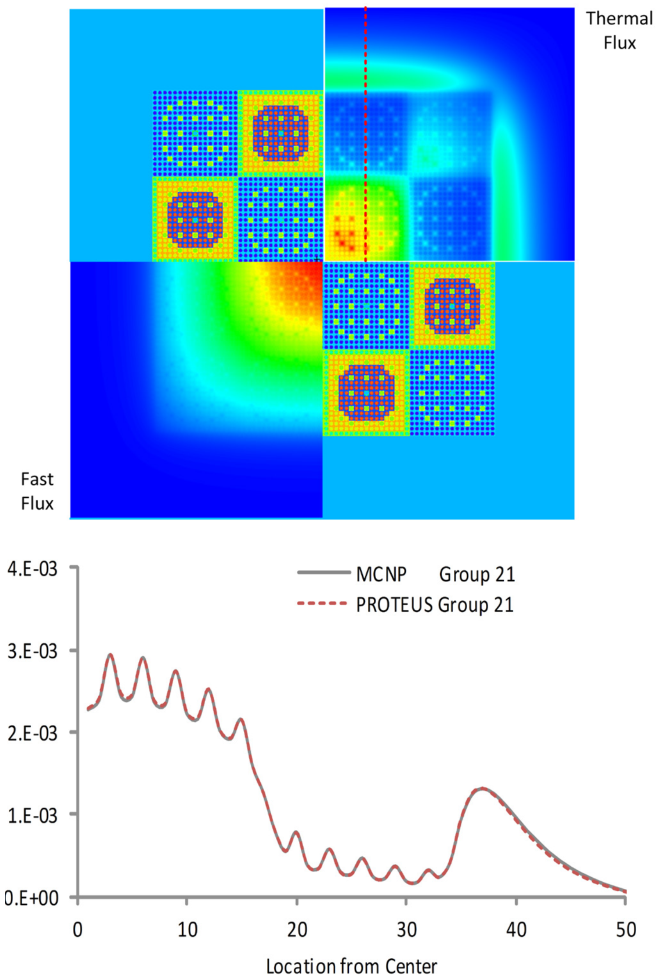



*Fig. 5. Flux distributions (top) and thermal flux distributions (bottom) along the red dotted line of the C5 PWR benchmark problem.*

The PROTEUS code has been verified against continuous energy MCNP for a variety of geometries derived from the Advanced Burner Test Reactor (ABTR) design. This work was conducted to support the multiphysics simulation of the ABTR with the SHARP toolkit. For the verification tests, the multigroup cross sections were generated with the fast-reactor multigroup cross section code $MC^2$-3. Initial verification results showed excellent agreement with reference MCNP solutions for homogeneous, partially homogeneous (explicit duct), and fully heterogeneous models of a fuel pin, fuel assembly, and small core. Work is ongoing to extend test models to the full core and to assess different strategies of heterogeneous multigroup cross section generation.

The cross section libraries applicable to various reactor types, based on the resonance table approach, have been tested for nine selected pin and assembly cases of the VERA PWR benchmark set. Test results using DeCART showed good agreement in eigenvalues with MCNP (continuous energy) within 140 pcm. Further tests are ongoing using the cross section application interface of PROTEUS, which includes the subgroup and resonance table options.

A utility code was developed to translate Exodus II formatted finite element meshes directly to PROTEUS mesh format. This code is available to external users and provides a path for generating PROTEUS meshes that have access to Cubit (Sandia National Laboratory version) or Trelis (commercial version) finite element software. A corresponding manual is also available.

### Thermal Hydraulics (Nek5000)

The particular phenomenon of thermal striping is encountered in liquid metal-cooled fast reactors (LMFR), in which temperature fluctuation due to convective mixing between hot and cold fluids can lead to a possibility of crack initiation and propagation in the structure due to high-cycle thermal fatigue. Using sodium experiments of parallel triple jets configuration performed by the Japan Atomic Energy Agency (JAEA) as a benchmark, numerical simulations were carried out to evaluate the temperature fluctuation characteristics in fluid and the transfer characteristics of temperature fluctuation from fluid to structure, which is important to assess the potential thermal fatigue damage. In this study, both steady (RANS) and unsteady (URANS, LES) calculations were applied to predict the temperature fluctuations of thermal striping by using commercial tool STAR-CCM+ and Argonne's advanced CFD tool Nek5000 (***Fig. 6***).

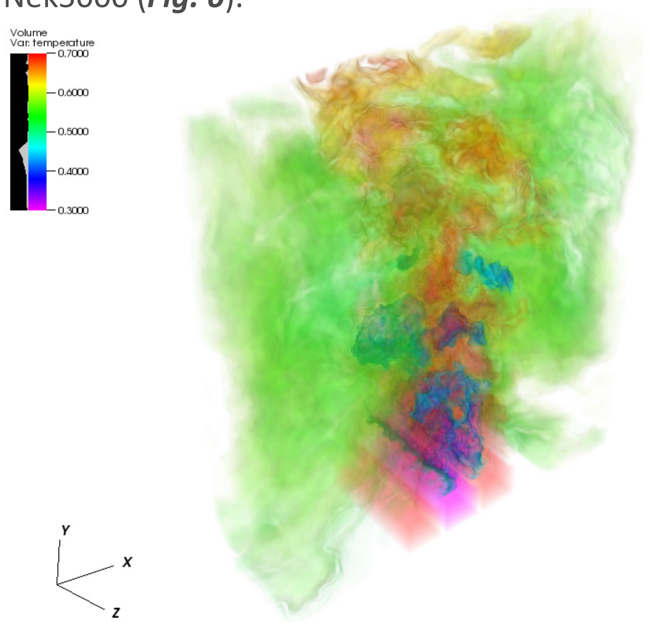



*Fig. 6. Volume rendering of temperature in Nek5000 unsteady LES simulations.*

# Integrated Product Line (IPL) Accomplishements

### Code Integration Activities

The code integration and packaging effort focused on the improvement of the coupling interface between the SHARP nuclear reactor multiphysics framework and the thermal hydraulics code Nek5000 (***Fig. 7***). Specifically, this work improves the solution accuracy of SHARP multiphysics calculations by improving the solution-transfer mechanism between PROTEUS neutronics calculations and Nek5000. Additionally, the SHARP build system was improved to allow for the easy integration of Diablo structural mechanics calculations. [ORNL]

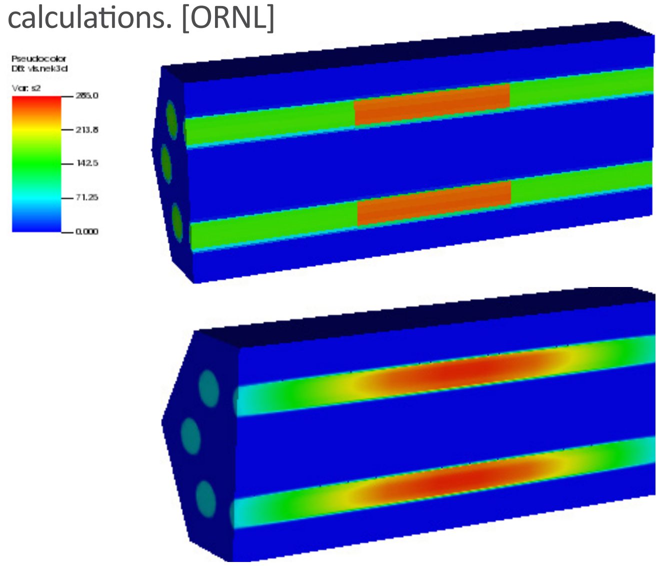



*Fig. 7. Simple (left) and improved (right) solution transfer between Nek5000 and PROTEUS.*

### NiCE User Environment

The NiCE team continued to improve its support of MOOSE-based applications (***Fig. 8***). These improvements include the ability to import existing MOOSE input files, view 3D reactor plant models, and import comma-separated value (CSV) data files for plotting. This new tool is capable of creating scatter plots, line and bar graphs, and contour plots. The NiCE team ended July with a successful trip to DOE headquarters in Germantown, MD, to demonstrate the latest NiCE support for BISON. [ORNL]

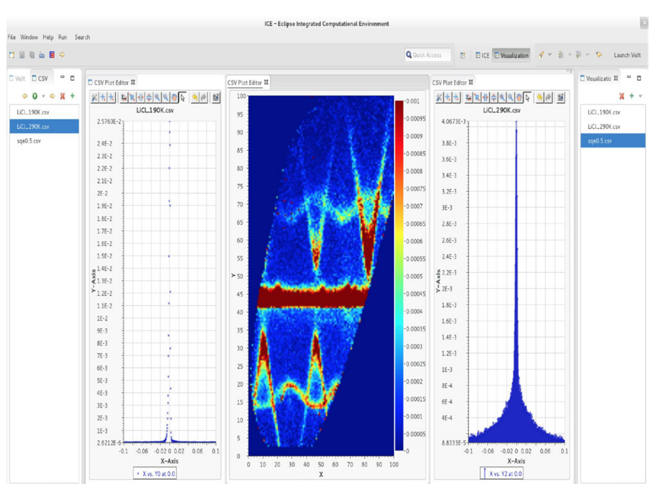


*Fig. 8. NiCE screen shot showing improved visualization and data analysis features for MOOSE-based applications, such as BISON.*

## Geometry Interfaces (SIGMA)

SIGMA (Scalable Interfaces for Geometry and Mesh-based Applications) provides several tools to access geometry data, create high-quality unstructured meshes along with unified data-structures to load, and manipulate parallel computational meshes for various physics applications to enable efficient solver implementations. The SIGMA toolkit – comprising CGM (geometry), MOAB (mesh), and MeshKit (mesh generation) components – had a consolidated initial release in July. Several key enhancements simplified the complex process of mesh generation and handling unstructured meshes.

Efforts to improve the parallel scalability of solution transfer between highly resolved physics meshes were also performed and demonstrated to have good computational efficiency on petascale systems at Argonne. Verification of the coupled physics methodology and improvements to the interfaces in the coupled physics solver (CouPE) were incorporated to utilize scalable solvers from PETSc to resolve the nonlinearity between physics components. These improvements enabled completion of several demonstration problems involving heterogeneous single-assembly geometry involving neutronics (PROTEUS) and thermal-hydraulics (Nek5000) that were utilized to ascertain the coupled solution consistency in SHARP.

Key improvements in CouPE were also introduced to enable interfacing to Diablo and solve spatially resolved fast reactor problems accurately. This work will be further refined to tackle full-reactor-core problems with full resolution and all three physics in the coming year. [ANL]

## MeshKit

In collaboration with Kitware, the MeshKit team has been developing a graphical user interface that includes several tests and examples for optimally handling large-scale reactor geometries. The interfaces in the Reactor Geometry Generator (RGG, implemented in MeshKit) were made consistent to enable seamless use of the serial versions of the tools. Some effort was also focused on improving the build system for the RGG interface and MeshKit. Several enhancements, bug fixes, and overall code maintenance were performed in the RGG interface after user tests involving the Kitware team. To showcase our recent efforts, Bob Obara (Kitware) presented a talk titled "RGG for Building Models & Meshes for Nuclear Reactor Design" at the SuperComputing conference (SC14) in the Kitware booth.

Description and creation of Neumann set boundary conditions in the RGG were also developed during this period. A parallel effort to improve the NetGen-based surface meshing has been progressing well, and currently it is being more tightly integrated with MeshKit to enable creation of hex meshes with OCC geometries.

Numerous fixes were introduced to the lattice creation method in RGG for nonsymmetrical rectangular reactor assemblies. A paper, titled "Generating Unstructured Nuclear Reactor Core Meshes in Parallel," presented the parallel scalability results of RGG at the International Meshing Roundtable 2014. At the roundtable, an industry representative showed interest in using RGG for other reactor designs. The RGG was used to create different meshes for heat exchanger simulations (pincell-like structure), and simulations were performed using the MOAB-Nek5000 plugin on the Argonne supercomputer Blues. The final results were validated against standard Nek5000 runs. Current work is focusing on modeling bigger, more realistic heat-transfer problems. [ANL]

### Scenario Simulation (RAVEN)

In September, the RAVEN group delivered a new sampling strategy that represents an evolution of the well-known dynamic-event-tree (DET) methodology, adaptive DET (ADET). The ADET technique brings several advantages with respect the conventional event-trees approach, among which is the fact that it employs system simulators to model the actual accident evolution.

As shown in ***Fig. 9***, starting from an initiating event, the ADET methodology allows the system code (i.e., RELAP5-3D, RELAP-7, etc.) to determine the pathway of an accident scenario. The likelihood of probabilistic events changes during the simulation, and the simulation branches when these probabilities reach thresholds defined by the user. The simulation spoons n different branches.  In each of them, the branching event determines a different consequence (including associated probabilities). Each sequence continues until another event occurs and a new set of branches is spooned.

As seen in ***Fig. 10***, when uncertain parameters directly influence the outcome of the goal function, the ADET method naturally tends to search for the "limit surface" (LS), which separates failure from success.

Among the several benefits that this methodology brings in the exploration of the uncertain domain, the following two are important:

- The initial training set, used to guess the initial location of the LS, is more accurate and evaluates events at lower computational cost.
- When, in the LS research process, the points in the input space that need to be explored are requested, the ADET approach can be used to avoid repeating the parts of the simulation that are in common with previously explored points

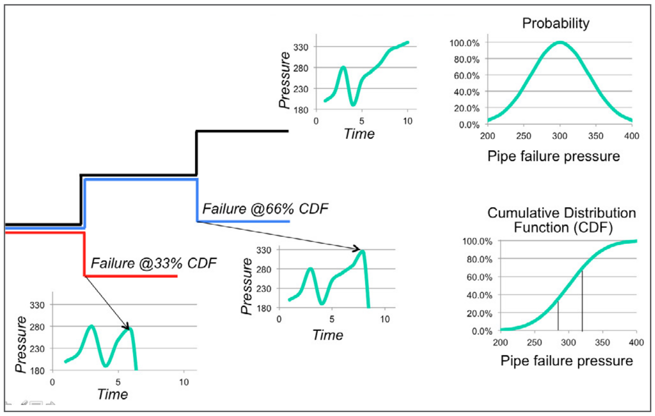



*Fig. 9. ADET logic flow.*

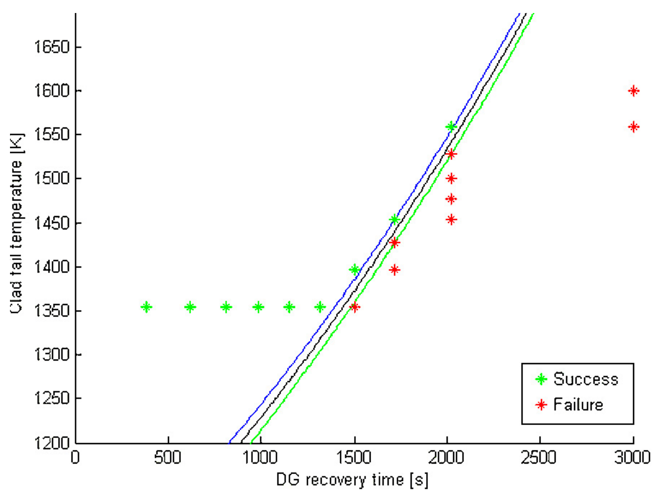



*Fig. 10.Example the set of point explored in the input space by the ADET vs. the location of the limit surface.*

Thus, the ADET methodology starts with a standard DET that performs the initial exploration of the input space, exploiting its capability to investigate the domain of uncertainty in a reasonably short time.  In fact, as shown in ***Fig. 10***, when success/failure is directly influenced by one (or more) uncertain parameter(s), ADET tends to increase the sampling density in proximity to the transition boundaries. This means that the initial guess of the LS location is more accurate and it improves the convergence speed of the method. After the initial DET, the adaptive scheme starts. Every time a new point in the input space is requested, a search in the DET database is performed to leverage already-existing common parts of the simulation. Every time a new branch ends, it is added to the database and can be used to reduce the length of subsequent runs.

***Fig. 11*** shows that the set of points explored at convergence (i.e., at the location of the LS) does not change, but adds more explored points in the input space. [INL]

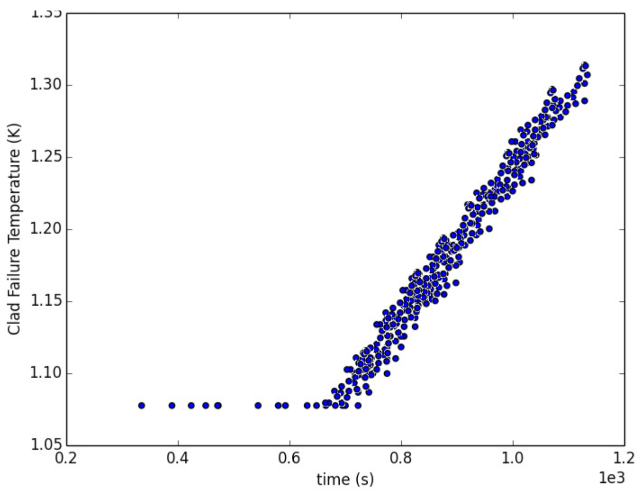


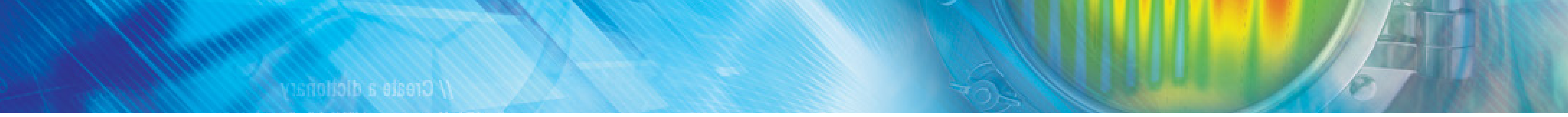

*Fig. 11. Adaptive DET density of sampled points*

### Dakota-BISON Analyses

A report was completed documenting the results of a set of sensitivity analysis studies involving Dakota and BISON. The report, Sensitivity Analysis of the Gap Heat Transfer Model in BISON (SAND2014-18550), examined the model used in the BISON code for heat transfer in the gap between the fuel rod and the cladding. The report includes three different case studies:

1. Development of a standalone model of the equations governing gap heat transfer.
2. Evaluation of the sensitivity of the model parameters at the beginning of life.
3. Evaluation of the sensitivity of the model parameters in highly irradiated fuel.

The results were similar for the three studies. In the highly irradiated fuel study, the variable with the most significant main effect on mid-plane centerline temperature was the fuel thermal conductivity multiplier. For the mid-plane gap conductance, both the roughness coefficient and the fuel thermal conductivity multiplier were significant. The Kennard temperature jump model coefficient and the contact model coefficient did not exhibit significant effects on either response (centerline temperature or gap conductance). [SNL, INL]



# Abbreviations

## Computer Codes

| | |
|---|---|
| CouPÉ | Coupled Physics Environment |
| Dakota | Design Analysis Kit for Optimization and Terascale Applications |
| MBM | MOOSE, BISON, AND MARMOT (integrated configuration) |
| MCNP | Monte Carlo N-particle |
| MOAB | Mesh-Oriented dAtaBase |
| MOOSE | Multiphysics Object-Oriented Simulation Environment |
| NiCE | NEAMS integrated Computing Environment |
| RELAP | Reactor Excursion and Leak Analysis Program |
| RGG | Reactor Geometry Generator |
| SHARP | Simulation-based High-efficiency Advanced Reactor Prototyping |
| SIGMA | Scalable Interfaces for Geometry and Mesh-based Applications |

## Other Abbreviations

| | |
|---|---|
| ABTR | Advanced Burner Test Reactor |
| API | Application programming interface |
| ATR | Advanced Test Reactor (INL) |
| BWR | Boiling water reactor |
| DET | Dynamic event tree |
| FPL | Fuels Product Line |
| HTGR | high-temperature gas reactor |
| IPL | Integrated Product Line |
| JAEA | Japan Atomic Energy Agency |
| LES | Large eddy simulation |
| LMFR | Liquid metal-cooled fast reactor |
| LOCA | Loss-of-coolant accident |
| LS | Limit surface |
| LWR | Light water reactor |
| MD | Molecular dynamics |
| OECD | Organisation for Economic Co-operation and Development |
| PWR | Pressurized water reactor |
| RIA | Reactivity-initiated accident |
| RPL | Reactors Product Line |
| SFR | Sodium fast reactor |
| UO | Uranium oxide |
| VHTR | Very high-temperature gas-cooled reactor |
| Xe | Xenon |

**Availability of This Report**
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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.

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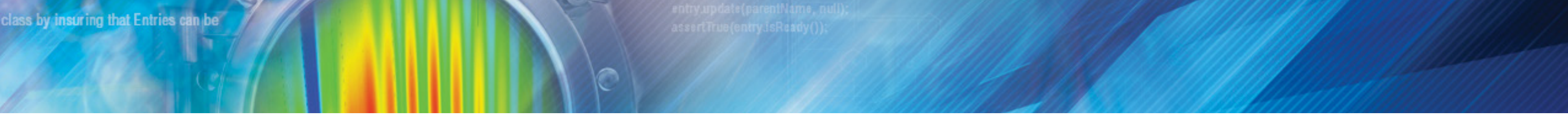


# Status of Level 2 Milestones

## Completed Milestone

| Milestone ID | Description | Due Date |
|---|---|---|
| M2MS-14AN06030210 | Simulate single assembly with online mesh deformation | 10/5/2014 |
| M2MS-14AN0603022 | Release version 1.0 of the CouPE coupler/driver | 10/1/2014 |
| M2MS-14AN0603024 | Release MeshKit version 2.0 | 9/30/2014 |
| M2MS-14AN0603038 | Update and demonstrate the SFR system simulation capability | 9/26/2014 |
| M2MS-14IN0602022 | Release BISON update for LWR fuel performance in quasi-steady-state and off-normal conditions | 9/29/2014 |
| M2MS-14IN0602023 | Update BISON validation and assessment report | 9/29/2014 |
| M2MS-14IN0602032 | Deliver an initial quantitative fracture model for BISON implementation | 9/26/2014 |
| M2MS-14LA0602042 | Deliver a new heirarchical diffusion model for BISON implementation | 9/30/2014 |
| M2MS-14LL0603072 | Update the NEAMS structural mechanics module to support FY14 demon-strations | 7/31/2014 |
| M2MS-14OR0602051 | Perform a benchmark problem with Thermochimica-MOOSE/BISON/MAR-MOT for oxygen potential in high-burnup LWR fuel | 9/30/2014 |
| M2MS-14OR0603062 | Demonstrate PROTEUS for selected reactor benchmarks and problems | 8/27/2014 |
| M2MS-14OR06030627 | Implement and demonstrate prototype ORIGEN API for integration with other codes | 9/30/2014 |
| M2MS-14OR06030647 | Complete initial review of SHARP integration interfaces and implement improvements | 9/30/2014 |

## Upcoming Milestone

| Milestone ID | Description | Due Date |
|---|---|---|
| M2MS-14AN0603039 | Provide update on testing and development of Nek5000 thermohydraulic capability | 11/30/2014 |

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