

Quarterly Highlights

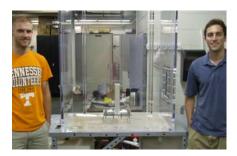
- The BISON team is refining and validating the new friction model for fuel-cladding interactions (pages 2 and 3).
- Gas bubble equilibrium configurations in UO₂ were simulated, an important step toward modeling fission gas movement in oxide fuels (page 2).
- Benchmark calculations for the thermal conductivity of UO₂ have been prepared as part of the effort to predict fuel degradation under irradiation (page 2).
- Work continued on models for fuel crack initiation, crack propagation, heat-induced grain boundary migration, and fuel relocation (page 2).
- The SHARP team has developed a targeted-resolution method that focuses computing power on specific locations within a model (page 5).

- The latest MeshKit release features new tools for boundary layers in multiple-volume domains (page 5).
- The cross-section library in PROTEUS was improved to more quickly generate reactor-specific neutron spectra (page 6).
- The thermal hydraulics team performed direct numerical simulations of pebble-bed reactor cores, which will lead to new computational fluid dynamics tools for very complex geometries (page 6).
- The NE-KAMS data warehouse is being extended to support an additional DOE-NE advanced simulation program (page 6).
- A plant systems analysis module is being developed for sodium-cooled fast reactors (page 6).

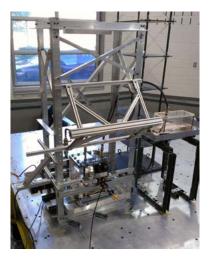
NEAMS Goes to College

NEAMS leverages current and prior investments in the Nuclear Energy University Program (NEUP) to meet empirical and validation objectives.

The University of Tennessee Twin Jet Facility shown below was originally developed in a NEUP project to explore flow mixing in large plena. The NEAMS validation pathways team will use the facility to measure fluid flows for comparison with computational fluid dynamics (CFD) results produced by the NEAMS ToolKit.



Cody Wiggins and Mark Crosskey show off the Twin Jet Facility they helped refurbish at the University of Tennessee.



The photo on the left shows a seismic testing facility under construction at George Washington University. This unique facility can shake a full-scale fuel assembly and measure subsequent changes in its form and structure. It very accurately mimics the motion of the earth during a wide range of earthquake scenarios.

FPL Accomplishments

Engineering Scale (BISON)

The Fuels Product Line (FPL) team continued development of a previous enhancement to BISON for simulating frictional slip between contacting independent bodies (e.g., pelletcladding contact and pellet-pellet contact). This was a major advancement in fuel performance modeling, and it has already accurately reproduced experimental observations that legacy fuel performance codes have been unable to address. (See the Technical Spotlight on page 3 for more detail on how mechanical contact is treated in BISON.) During the third quarter, the BISON team made tremendous progress toward developing a demonstration problem to simulate a pressurized water reactor (PWR) fuel pin under realistic lossof-coolant accident (LOCA) conditions. This demonstration, which depends on a high-fidelity treatment of fuel-cladding contact, will be completed during the fourth quarter. [INL]*

One of the challenges in assessing a tool like BISON against experimental data is that ongoing changes to BISON have the potential to make previous BISON assessment simulations unrepeatable. To guard against this, the BISON team is incorporating all assessment cases into a set of automated executions (along with unit and verification tests) that are automatically executed at regular intervals. Differences in results are monitored automatically and flagged for attention as necessary. [INL]

Subcontinuum Scale (MARMOT and Atomistic Simulations)

Understanding the movement of fission gases in oxide fuels continues to be one of the highest-priority efforts at the subcontinuum scale. Within this effort, complex Monte Carlo exchange moves of neutral units (UO_2 for one Xe and two vacancies) have been implemented to simulate gas bubble equilibrium configurations in UO_2 . The code is being systematically tested for accuracy to quantify the error contributions from approximations in the long-range coulomb energy calculation. Work has started on a complementary second vacancy detection algorithm that takes local crystallographic symmetry into account. [LANL]

A second high-priority subcontinuum effort is understanding fuel thermal conductivity and predicting its degradation under irradiation. Benchmark calculations for the thermal conductivity of UO₂ were performed using SNL's Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with nonequilibrium molecular dynamics. The results compared well with earlier results using LANL's Scalable Parallel Short-range Molecular dynamics (SPaSM) code. The effect of other fission products (such as Sr^{2+} , La^{3+} , Zr^{4+}) on the thermal conductivity of UO_2 will be explored using this method. [LANL]

The development of models to account for cracking in oxide fuels is also an important effort due to the major influence cracking has on thermal and gas transport, as well as fuelcladding mechanical interaction. Previously, progress was made in atomistic simulations to elucidate the role of metastable phase transformations at the onset of fracture. During the third quarter, a statistical analysis of the evolution of fragmentation as a function of initial pore density was completed. Work was also initiated on implementation of the extended finite element method (X-FEM), which allows for discrete cracking to occur in finite-element-based simulations (i.e., with MARMOT at the microstructure level and BISON at the continuum level). Thus, progress is being made on methodologies to predict the conditions necessary to initiate a crack, as well as to propagate a crack in finite element simulations. [INL]

Another phenomenon that strongly influences heat and gas transport in oxide fuels operated at higher temperatures (i.e., peak pins in light water reactors [LWRs] and nominal pins in sodium fast reactors [SFRs]) is restructuring, which leads to formation of a central hole. This tends to increase the thermal conductivity of the fuel in the restructured zone around the hole (due to reduction of porosity) and greatly increase fission gas release. The implementation of a model in MARMOT that allows simulation of restructuring by both void/pore and grain boundary migration under a thermal gradient was completed last quarter.

This quarter, grain boundary migration under a thermal gradient was studied in more detail. Results indicate that the temperature gradient has little influence on bulk grain growth behavior, although there is always significant movement of the grain boundary toward the hot end of every grain. [INL]

Implementation of a crystal plasticity model into MARMOT continued to be assessed against results from a continuum dislocation dynamics strain gradient model in the ABAQUS commercial finite-element code. [PNNL]

Supporting Tools

The DAKOTA and BISON teams are working to calibrate the oxide fuel relocation model, with the objective of determining the optimal value of the power activation threshold, and are initiating a sensitivity analysis on fresh fuel (beginning of life) vs. irradiated fuel. The parameters of interest in the sensitivity analysis will include power, fuel thermal conductivity, relocation, gap heat transfer, pellet-cladding geometry, and radial power distribution. [SNL]

^{*}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).

Technical Spotlight: The Challenge of Modeling Pellet/Cladding Contact

In legacy fuel performance analysis codes, it is common to model the fuel-cladding system as a 1.5D or 2D problem (1.5D indicates the presence of both 1D and 2D elements). In either case, the models consist of a "smeared" column of fuel rather than individual fuel pellets. An axial slice of fuel is paired with an axial slice of cladding. Heat transfer from the fuel to the cladding is accomplished by introducing 1D gap heat transfer elements that conduct heat across the gap. The mesh is severely constrained, in that the axial elements align one-to-one with elements in the cladding. In a physical system, this is analogous to the pellets and cladding being locked together as if glued.

Fig. 1(a) illustrates the legacy model. Since no other method is available within the model, these mesh constraints limit the types of problems the legacy codes are able to analyze. The legacy codes cannot model complicated fuel geometries, significant relative motion between the fuel and cladding, and other scenarios where fixed node pairing does not accurately represent the physics acting across the gap. **Fig. 1(b)** shows a system that the legacy model cannot simulate.

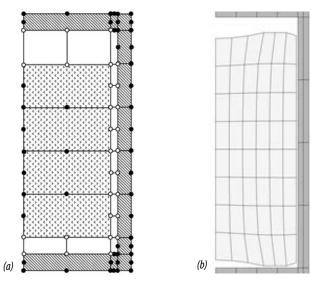


Fig. 1. (a) Axisymmetric legacy model of fuel and cladding with 8-node finite elements. Open circles are paired nodes connected with 1D elements. (b) Finite element model for which 1D node-to-node connections cannot be made.

The modeling of mechanical contact is similar. For 1D slices or simple 2D geometries, it is possible to introduce 1D node connections across the pellet/cladding gap. These connections become the locations for force transfer between pellets and cladding during the analysis. Again, this approach does not accommodate more complicated geometries or significant relative motion between the fuel and cladding. To overcome the limitations of legacy models, the BISON team is incorporating more general contact algorithms into BISON. These approaches allow for constraints between arbitrary finite element surfaces, rather than nodes, which enables analysis of individual fuel pellets as well as novel fuel designs.

One approach to model contact constraints is the node-on-face technique. In the node-on-face technique, nodes on one side of the interface are constrained (tied) in some way to a face on the other side of the interface. Search algorithms are required to establish the pairing of nodes and discrete face locations.

The penalty formulation is perhaps the most straightforward way to enforce node-on-face constraints. Taking mechanical contact as an example, we define the normal contact force as $t_N = \epsilon g$, where ϵ is a penalty parameter and g is the penetration distance of the node into the face. This formulation requires penetration in order to generate force opposing the penetration. With a sufficiently large penalty parameter, the gap becomes smaller and converged solutions will have a negligible penetration. Care must be taken not to choose such a high value for the penalty parameter that the condition number of the resulting stiffness matrix becomes large enough to affect accuracy and robustness.

The differences between a discrete and smeared-pellet analysis are illustrated in *Fig. 2*, which was calculated with a more complex node-on-face formulation. The inset shows radial displacement contours and the displaced shape of a pellet at the end of power-up. Displacements are exaggerated 100 times to show the pellet "hourglass" shape, which results from thermal expansion. Due to this shape, the ends of the pellet contact the cladding earlier than the middle, which makes contact about 2.5 MWd/kgU after the end makes contact. (*MWd/kgU* is a measure of fuel utilization, also referred to as "burnup.") As expected, the smeared-pellet model calculates a gap width that is an average of the end and middle locations given by the discrete-pellet model.

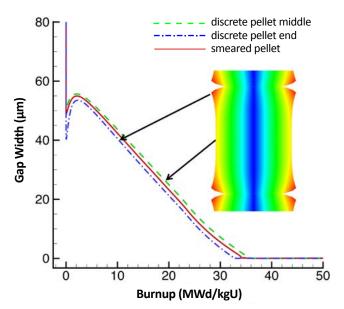


Fig. 2. Gap closure simulated by smeared and discrete pellet models. Inset coloring represents radial displacement.

Fig. 3 is a plot of the cladding radial displacement versus axial length at various times in fuel life. Results from both the discrete and smeared-pellet calculations are shown for comparison. Note that the discrete pellet simulation produces the commonly observed "bamboo" profile along the cladding axis. This profile develops well before any fuel/cladding contact because chamfering at the pellet ends reduces radial heat transfer. At first, high temperatures and coolant pressure push the cladding inward until gap closure and mechanical contact occur at about 35 MWd/kgU. At this point, the cladding creep reverses direction and fuel swelling begins to push the cladding outward. The discrete-pellet simulation shows how the profile formed by chamfering at pellet-pellet interfaces is then exaggerated by the hourglass shape of the pellets after contact.

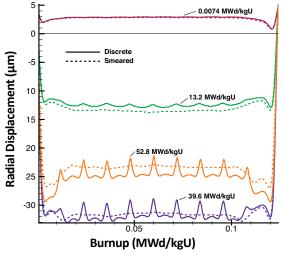


Fig. 3. Cladding radial displacement versus axial length over time.

As another example of contact constraints in BISON, *Fig. 4* shows the hoop stress in the cladding near a pellet surface defect. This figure highlights the need for more realistic friction modeling, as the calculated stresses are markedly different for the frictionless (no contact) and glued contact (no slip after initial contact) solutions. The correct solution lies somewhere between these two extremes.

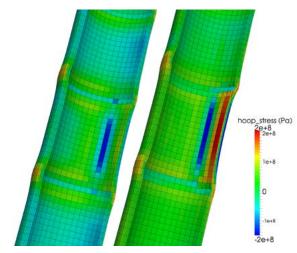


Fig. 4. Modeling of hoop stress in pellet with surface defect: (left) no contact and (right) qlued contact.

In addition to the node-on-face technique, other contact algorithms are under development in BISON. In particular, the mortar method, a face-on-face technique, promises to be an accurate approach for modeling mechanical and thermal processes, as well as interactions between separate numerical domains, such as heat transfer between the cladding and reactor coolant.

The BISON team is Rich Williamson, Jason Hales, Steve Novascone, Ben Spencer, Giovanni Pastore, and Danielle Perez (all from INL).

RPL Accomplishments

Multiphysics Simulations (SHARP)

During the third quarter, the coupled simulation team focused on implementing and testing a multiscale capability using the SHARP toolset. The team has developed a targeted-resolution method where the geometry can be resolved pin-by-pin in relatively small locations but represented more coarsely elsewhere in the core. This dramatically cuts the computational cost without sacrificing new high-fidelity capabilities. The analyst will have new flexibility to study in great detail a selected portion of the core with fewer computational resources. [ANL, LLNL]

The team is currently testing targeted resolution for application to a set of transients in a simplified reactor fuel assembly geometry **(Fig. 5)**, while working to extend it to the full EBR-II geometry. A significant effort is also underway to increase the usability of the code, as the demonstration simulations have moved from the development team to knowledgeable early users. [ANL, LLNL]

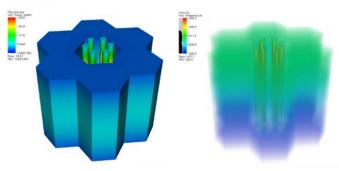


Fig. 5. Simplified six-assembly multiphysics simulation of both power (left) and temperature (right).

Framework (MOAB)

MOAB 4.6.0, the data backplane framework component of the Reactors Product Line (RPL), was released in early 2013. This release included improved MOAB examples and expanded user documentation. Also included were new conventions for handling spectral element meshes and various other mesh types of interest to current users. See the last page for a link to MOAB. [ANL]

MeshKit

The MeshKit module is now available for download as an open source toolset, see the last page. The last update included an improved post-meshing boundary layer tool, which improves handling of multiple volume (e.g., liquid/solid) models and provides more options for specifying the features of boundary layers in multiple-volume domains. Boundary layer meshing is critically important for high-quality CFD simulations and some structural mechanics simulations. [ANL]

New functionalities have been demonstrated in the development of a complex computational mesh describing the full core of the EBR-II reactor *(Fig. 6)*, with some regions homogenized and some regions included in full geometric detail. This model will be used by the applications and demonstrations team for upcoming multiphysics analyses of the EBR-II Shutdown Heat Removal Tests. [ANL]

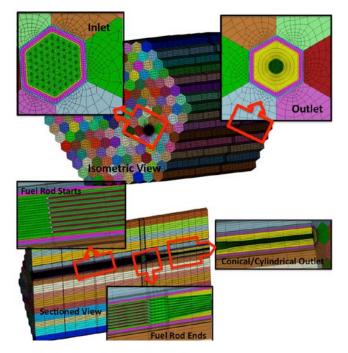


Fig. 6. EBR-II core model created with MeshKit. This version targets the XX09 test assembly for higher resolution.

Neutronics (PROTEUS)

For coupled multiphysics time-dependent simulation, a quasistatic kinetics methodology was derived and added to the PROTEUS-SN code using the second-order S_N solver. In the quasistate method, the point kinetics parameters are updated with the progression in time using a series of steady-state forward and adjoint spatial calculations. This method is sufficient to meet the needs of current NEAMS transient analysis capabilities while a fully spatial kinetics methodology is implemented with an efficient generalized minimal residual algorithm. Initial verification and benchmarking has been completed using standard benchmark problems to confirm the accuracy of the quasi-static kinetics implementation. [ANL] The new library improves upon the legacy cross-section codes by avoiding the development of many different library generation tools and providing for much broader applicability to current models. The approach may be useful within other transport codes. The new mothod has been tested for pin cell and lattice benchmark problems. [ANL]

Thermal Hydraulics (Nek5000)

As part of collaboration with researchers in Belgium and the Netherlands, benchmark results for a 7-pin wire-wrapped fuel bundle model from three institutions will be compared and reported next quarter. [ANL]

The thermal hydraulics team also performed a set of direct numerical simulations of pebble-bed reactor cores, which will be compared with data from the Nuclear Research Group in the Netherlands. At Texas A&M University (TAMU), a set of routines to calculate the turbulence kinetic energy budget has been implemented and tested successfully on turbulent channel flow. These routines will be applied to pebble bed simulations and will provide valuable benchmarking data for lower-fidelity CFD tools for very complex geometries. [ANL]

SFR Module (RELAP-7)

Development continues for advanced SFR primary system modeling capabilities in collaboration with the RELAP-7 team. A capability to more accurately model heat transfer in the reactor core has been developed by adding (1) a general liquid flow and solid structure interface model; (2) a new core channel component, including the solid fuel pin, coolant flow, and duct wall; (3) a bypass channel component; and (4) a reactor core component. The module can be coupled to the STAR-CCM+ CFD code, as described in the Program Spotlight on this page. [ANL, INL]

Validation Pathways

NEUP is both providing data for validation of RPL components and taking measurements to develop a better understanding of the sources of uncertainty in high-fidelity validation experiments. More details on the NEUP contributions pictured on page 1 are given below. [ANL, ORNL]

The NEAMS validation pathways team has upgraded the Twin Jet Facility with additional instrumentation and a revised external tank that will reduce distortion in optical measurements. The facility will support a campaign to better understand sources of environmental and user error in high-resolution measurements of flowing fluids after it is moved to TAMU this fall. Also, TAMU has leading-edge instrumentation that will generate very high-resolution data to support future uncertainty analyses. [Univ. of Tennessee, TAMU] The fuel assembly seismic response rig will be equipped with one-of-a-kind diagnostic instrumentation to collect multiphysics seismic response data for NEAMS ToolKit validation. The facility is 7 m tall and has a 3 × 3 m footprint. The rig is secured to a large shaker table that can very accurately mimic the motion of the earth during a wide range of earthquake scenarios. It can hold a full-scale fuel assembly, complete with spacer grids. [George Washington University]

NE-KAMS

The Nuclear Energy Knowledgebase for Advanced Modeling and Simulation (NE-KAMS) data warehouse is being developed in support of the collection, documentation, and archiving of NEAMS program experimental and computational data. To improve the efficiency of data archival and maximize the benefit to DOE-NE, the NE-KAMS data warehouse is being extended to support both NEAMS and the Consortium for Advanced Simulation of LWRs (CASL) programs. [Bettis, INL, ORNL, SNL]

To incorporate CASL data, the NE-KAMS team is developing a structured process for data collection, management, and archiving.. The intent is to establish an iterative and dynamic process that fosters open communication and collaboration among experimentalists and modeling and validation experts and boosts the system's credibility. A common process shared by NEAMS and CASL will broaden the availability of new simulation data from NEAMS and CASL users and new validation data from NEUP and other programs. [Bettis, INL, ORNL, SNL]

To date, four CASL datasets, three experimental and one computational, have been identified for collection, and the NE-KAMS team is working with cognizant CASL researchers to collect the CASL data. Collected data, associated metadata, and related information will be documented with some initial structuring and stored in the CASL Virtual Office Community and Computing Facility in preparation for integration with the NE-KAMS warehouse. [Bettis, INL, ORNL, SNL]

Program Spotlight: Developing an SFR Systems Analysis Tool

Because SFRs are the initial technology focus for reactors plant analysis, the NEAMS team is developing an SFR systems module for whole-plant safety analysis. This tool will solve equations for tightly coupled physical phenomena – including nuclear fission, heat transfer, fluid dynamics, and thermal-mechanical response – in SFR structures, systems, and components. It will work within the MOOSE framework which relies upon libMesh and PETSc for mesh generation, finite element analysis, and nonlinear solutions. The module will build upon RELAP-7 to define many of the objects that represent reactor components and systems. However, RELAP-7 is geared toward LWRs and sometimes cannot accurately represent components for advanced reactor concepts, such as SFRs, lead-cooled fast reactors, and fluoride-salt-cooled high-temperature reactors. Thus, the development of the SFR systems module is being coordinated with the development of RELAP-7 so that it can represent the typical features of advanced reactor systems.

Advanced systems are distinguished from light-water systems in their use of single-phase, low-pressure coolants with very low Prandtl numbers. This simple yet fundamental change has significant impacts on core and plant design, the types of materials used, component design and operation, fuel behavior, and the relative importance of specific fundamental physical processes during transients.

The SFR systems module will model and simulate SFR systems with high fidelity and will have well-defined and validated prediction capabilities. The module will:

- Provide fast-running, high-fidelity, whole-plant transient analysis capability, which is essential for design scoping and engineering analyses.
- Utilize the MOOSE framework to leverage currently available advanced software environments and numerical methods.
- Incorporate the latest advances in physical and empirical models for SFR systems.
- Provide multiscale multiphysics modeling capabilities through integration with other high-fidelity advanced simulation tools.
- Assist with RELAP-7 development by providing code verification and contributing general physics models and components applicable to all reactor types.

The SFR systems module is based on RELAP-7 and the MOOSE framework (see *Fig. 7*). The module leverages the common features between LWRs and SFRs (e.g., single-phase flow in a pipe and steam-system modeling for the balance of plant) and has direct access to the existing RELAP-7 physics models and component library. The SFR simulation effort is developing:

- A 1D finite element flow model using a pressure-based formulation with numerical stabilization schemes for use in incompressible sodium flows.
- A multiscale, single-phase flow coupling capability between the SFR systems module and the fluid dynamics code STAR-CCM+ to simulate the effects of multidimensional flow and thermal nonequilibrium.
- SFR-specific physics models and components based on both the density-based (RELAP-7) flow model and the pressurebased formulation.
- Advanced physics models and components compatible and available for use in RELAP-7.
- Demonstration problems for the newly added stand-alone system simulation capabilities and coupled multiscale or multiphysics simulation capabilities.

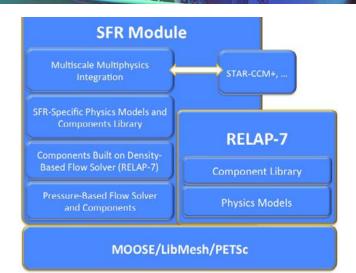


Fig. 7. Structure of the SFR systems analysis module.

The MOOSE and RELAP-7 based SFR system analysis module is currently under rapid development. Its capabilities have been demonstrated by the simulation of an SFR protected loss-of-flow accident. Major physics phenomena in the primary coolant system during the transient were captured. Multiscale coupling was demonstrated by modeling the same transient with the module coupled to STAR-CCM+. The importance of the targeted-resolution capability was confirmed by thermal stratification in the modeled outlet plenum and cold pool during the transient event (see **Fig. 8**).

Future enhancements include integration of the formulations, study of advanced preconditioning techniques, and alternative numerical integration schemes to accelerate the processing speed.

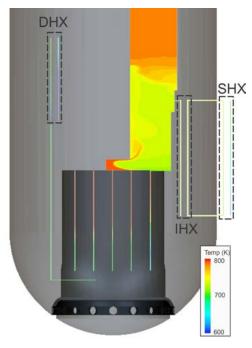


Fig. 8. Temperature distribution obtained in a coupled simulation of an SFR protected loss-of-flow transient.

The NEAMS Vision

The NEAMS program is developing advanced computational tools that will provide insights into the performance and safety of advanced reactor systems that cannot be obtained through experimentation alone.

To achieve this, the NEAMS ToolKit incorporates fundamental descriptions of the underlying physics that govern the key behaviors of nuclear reactors and power plants. In other words, the empiricism and correlations typically employed in current modeling and simulation tools will be replaced with mechanistic descriptions that have been validated using experiments targeting each phenomenon in isolation as well as during interactions 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 direct experimental observations are lacking.

The NEAMS team hopes this quarterly report of our accomplishments will provide insight into the program's challenges and achievements. Input from NEAMS stakeholders is essential for improving the quality and utility of the NEAMS ToolKit.

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

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Design Team Renee Carlson, ANL, & Larisa Blyudaya

Recent and Upcoming Level 1 and 2 Milestones

	Completed during this Quarter (April–June 2013)		
Milestone ID	Description	Due Date	Finish Date
M2MS-13LA06020410	Deliver atomistic data for fission gas diffusion and release in UO_2 fuel	4/3/2013	4/3/2013
M2MS-13IN0602032	Implement improved thermal conductivity model in BISON	4/30/2013	4/29/2013
M2MS-13IN0602033	Implement improved fission gas release model in Bison	5/31/2013	5/30/2013
M2MS-13IN0603038	Demonstrate probabilistic risk assessment on PWR reactor	6/30/2013	6/26/2013

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





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