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NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Argonne NATIONAL LABORATORY

# NEAMS Update

Quarterly report for April – June 2012

Published July 2012

## Quarterly Highlights

- The interface of AMP was changed to prepare it for integration with Sharp (p. 2).
- Bison was enhanced with improved models for cladding and coolant channels (p. 2).
- FRAPCON and OECD-NEA databases are being used to evaluate Bison (pp. 2, 6, and 8).
- The validation of Bison is being implemented with the recently developed discovery, accumulation, and assessment process (p. 7).
- A study of microstructure and fission gas bubbles in $UO_2$ fuels showed how these characteristics affect fuel thermal conductivity (pp. 2 and 9).
- The thermal conductivity studies were informed by additional work on the kinetics of gas bubble evolution and cladding alloy properties, providing methods to express subcontinuum properties in continuum models (pp. 5 and 9).
- The new insights into the evolution of thermal conductivity in $UO_2$ fuels were used to drive mesoscale simulations with atomic-scale properties (pp. 2 and 9).
- The rapid development of Relap-7 continued, and initial modeling of a pressurized water reactor was successfully completed (p. 3).
- Extension of Relap-7 to novel reactor concepts provided opportunities to refine the code (p. 3).
- Risk grading of Relap-7 was completed (p. 8).
- Simulations of the Advanced Test Reactor show that Proteus is ready to use (p. 4).
- Simulations of an important pipe flow benchmark show that Nek5000 is also ready to use (p. 4).
- Mesh generation for Sharp has advanced to unprecedented complexity, with the capability to create a mesh with up to 1,500,000 elements in an intricate configuration (p. 4).
- A model for hydride reorientation in used fuel was demonstrated and implemented (p. 4).
- Work continued on the use of molecular dynamics to simulate the crystalline properties of structural materials (p. 5).
- Work continued on NiCE, the NEAMS user interface (p. 8).

## *Spotlight on Personal Achievements*

**Presidential Early Career Award.** On July 23, President Barack Obama named INL scientist Derek Gaston as one of 96 recipients of the Presidential Early Career Awards for Scientists and Engineers, the highest honor bestowed by the United States government on science and engineering professionals in the early stages of their independent research careers. As leader of the Computational Frameworks Group in INL's Fuels Modeling and Simulation Department, Gaston works in the field of multiphysics and has developed software tools being used by laboratories and research institutions around the world to create cutting-edge simulation codes.

More simply, he has developed an easier way for computers to solve systems of equations and create simulations of complex phenomena. Gaston developed MOOSE (multiphysics object-oriented simulation environment), which is being used in the NEAMS program for development of Relap-7.

**Landis Award.** ANL nuclear engineer Dave Pointer received the 2012 Landis Young Member Engineering Achievement Award from the American Nuclear Society (ANS). This annual award recognizes outstanding achievement in which engineering knowledge has been effectively applied to yield an engineering concept, design, safety improvement, method of analysis, or product utilized in nuclear power research and development or commercial application. The award was presented at the ANS annual meeting in June.

Pointer is a world-recognized authority on the CFD analysis of nuclear reactor thermal hydraulics, and serves as a DOE program manager and technical integrator for the Reactors Product Line Team. Among his responsibilities, Pointer leads the development of the Sharp code. To date, his contributions have led to a significantly greater understanding of the performance of wire-wrapped tight-lattice fuel assembly designs for advanced reactors, and the prediction of thermal mixing in reactor-relevant geometries such as t-junctions and large plena.

# Accomplishments

## Fuels IPSC

### *Assembly-scale code development*

The AMP assembly-scale code was modified to use a general interface instead of a libMesh native mesh format; this conversion is a prerequisite for integration with Sharp. Integration of AMP with the NiCE user interface to facilitate the Early User Program was initiated. [ORNL]*

### *Pin-scale code development*

Development of Bison for the engineering-scale simulation of nuclear fuel performance continued. Enhancements during this quarter include implementation of a nonlinear material model for Zircaloy cladding that simultaneously combines the phenomena of plasticity, thermal creep, and irradiation creep; implementation of a complete set of material properties and a creep model for stainless steel cladding; and modification of the coolant sub-channel model to better support simulations of loss-of-coolant-accidents.

Bison simulations are being compared to relevant empirical fuel pin data from the FRAPCON light water reactor (LWR) fuels database, with assistance from members of the Early Users Program. More than a dozen FRAPCON cases are being assessed using Bison. Although Bison development for use in predicting LWR fuel performance is still on-going, assessments continue to show Bison capable of generally good agreement with experimental data for many of the major fuel performance parameters, such as peak fuel temperature, fission gas release, and cladding deformation. The first Bison training workshop was held for code developers and early users at INL on May 30-31. [ANL, INL, LANL]

### *Lower-length-scale model development*

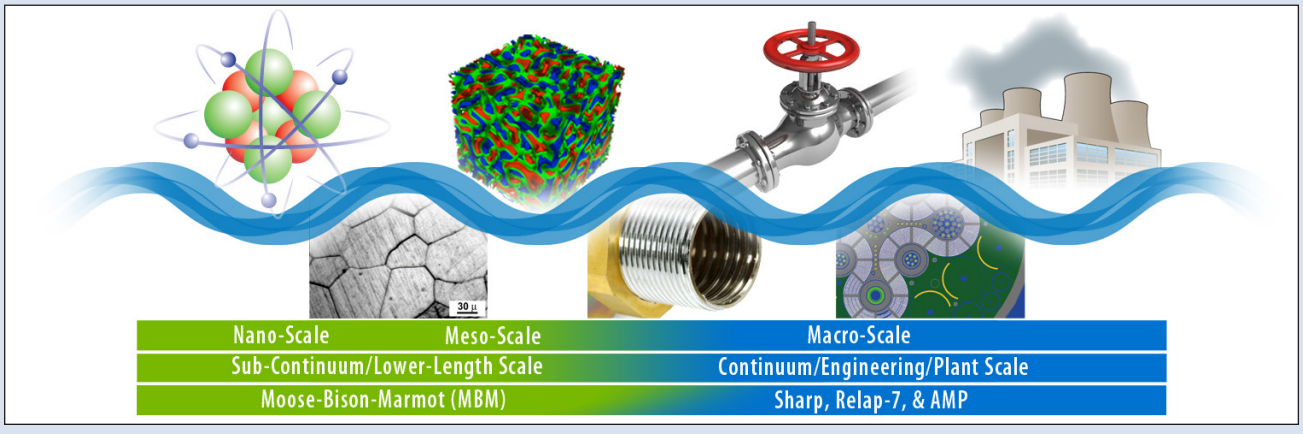
A comprehensive investigation of the impact of grain boundaries and fission gases on $UO_2$ thermal conductivity was brought to a conclusion. In all cases explored, the presence of Xe as a fission gas lowers the fuel thermal conductivity, which was not unexpected; however, it was discovered that the detailed configuration of Xe in the crystal is important factor in the magnitude of that degradation. Randomly distributed Xe atoms lead to a larger decrease in thermal conductivity than do Xe atoms precipitated into fission gas bubbles. Xe bubbles close to grain boundaries decrease the thermal conductivity more than the sum of the individual contributions. Thus, the interaction of Xe atoms with grain boundaries appears to be an important factor controlling the heat transfer in nuclear fuels. [LANL]

Simulations at the atomic scale were used to inform mesoscale simulations of microstructure evolution using Marmot and were then up-scaled to Bison. For details, see Technical Spotlight on page 9. [INL]

Work continued on development of a method to account for fuel cracking in engineering-scale analyses by calibrating the cohesive zone model for the fracture of $UO_2$ with results from molecular dynamics (MD) simulations to formulate a displacement-traction law. This should aid in developing a better oxide fuel restructuring model for Bison. [INL, LANL]

*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).

### Physical scale of NEAMS simulations



## Reactors IPSC

### *Relap-7 code development*

Relap-7 is a MOOSE-based nuclear reactor system safety analysis code. Development started in October 2011, and during the past quarter the initial capabilities of Relap-7 were demonstrated by simulating a steady-state single-phase pressurized water reactor (PWR) with two parallel loops and multiple reactor core flow channels (Fig. 1). The PWR configuration matched that of the Three Mile Island 1 LWR, which is a benchmark problem from the Organisation for Economic Co-operation and Development (OECD) / Nuclear Energy Agency (NEA). Although the simulation used a simplified system model, the resolution was consistent with the level of detail in current system safety analyses. [INL]

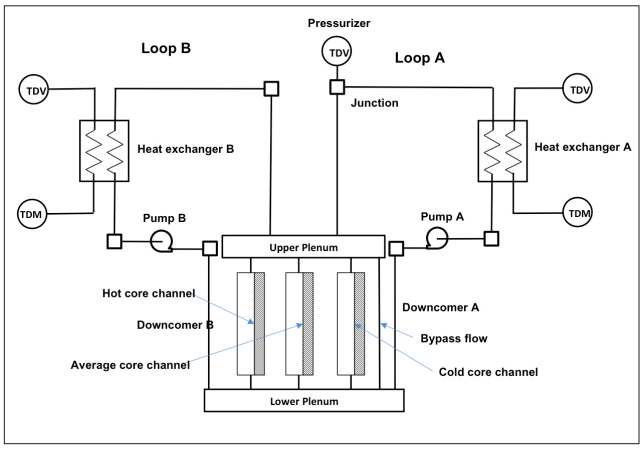



*Fig. 1. Schematic of the OECD PWR benchmark used in the initial Relap-7 demonstration.*

The simulation begins as a transient problem and progresses toward a converged steady state problem. The simulation results match the benchmark data very closely, within about 0.1 K of the benchmark reactor inlet and outlet temperatures. [INL]

Parallel to Relap-7 development for LWR analyses, component models are being developed for advanced sodium-cooled fast reactor (SFR) concepts. Several test SFR models have been developed based on the Advanced Burner Test Reactor (ABTR) conceptual design. Models for a five-channel core, primary loop, intermediate loop, and entire plant have been built. Steady-state parameters for the test problems agree well with expected ABTR operating conditions. [ANL]

During the development of the ABTR test problems, some issues in the Relap-7 component models were identified due to the very different operating conditions of an SFR and LWR. Most notably, when a sinusoidal power distribution was applied the predictions of the core channel inlet temperatures were not consistent with the upstream temperatures of other components, and the flow area for the secondary side of the heat exchanger component was incorrect. These issues are being corrected. [ANL, INL]

### *Sharp code development*

#### *Sharp neutronics module*

Copyright registration was initiated for code modules such as DIF3D, REBUS-3, VARI3D, and PERSENT; these are so-called “conventional modules,” relying upon previously developed methods. These tools form the backbone of the lower-fidelity methods in Proteus. The PERSENT code has been added to the NEAMS Toolkit to better support verification and validation. It allows three-dimensional (3D) transport-based sensitivity capabilities that do not exist in the neutronics field today. [ANL]

Work has continued on the development of a generalized sub-group method for cross-section generation. A Monte Carlo neutron-photon-based processing tool was created to demonstrate sub-group cross section generation. The initial application program interface for the sub-group was created. [ANL, ORNL]

The issues limiting the performance of the interface between the Sharp framework and the Proteus neutronics modules have been resolved and the integrated components are now ready for application. Figure 2 shows simulations of fast and thermal neutron fluxes in the Advanced Test Reactor (ATR), which were generated using the 2nd discrete ordinates method solver of Proteus. [ANL]

### Selected NEAMS Abbreviations

| | |
|---|---|
| ATR | Advanced Test Reactor (INL) |
| DAA | discovery, accumulation, and assessment |
| DD | dislocation dynamics |
| GB | grain boundary |
| IPSC | Integrated Performance and Safety Code |
| MD | molecular dynamics |
| NEAMS | Nuclear Energy Advanced Modeling and Simulation |
| NiCE | NEAMS integrated Computational Environment |
| PMI | predictive maturity index |
| PWR | pressurized water reactor |
| SQA | software quality assurance |
| UFD | used fuel disposition |

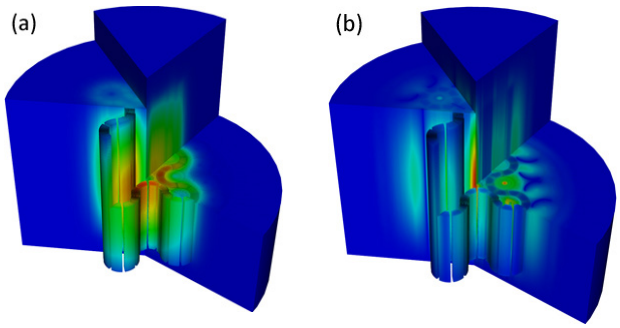



*Fig. 2. 3D ATR neutron flux plots: (a) fast neutrons and (b) thermal neutrons.*

### *Sharp thermal fluids module*

As part of the on-going Nek5000 validation efforts, a series of large eddy simulations (LES) have been performed for thermal stratification in a pipe. Results were in good agreement with the experiment and the simulation data has provided insight into the physics of the flow. An additional series of simulations of the OECD-NEA MATiS-H benchmark has also been completed using intermediate-fidelity modeling approaches, such as k-epsilon, k-omega shear stress transport, and ID detached eddy simulation, as well as one high-fidelity approach (LES). The data has been submitted to OECD-NEA (Fig. 3). [ANL]

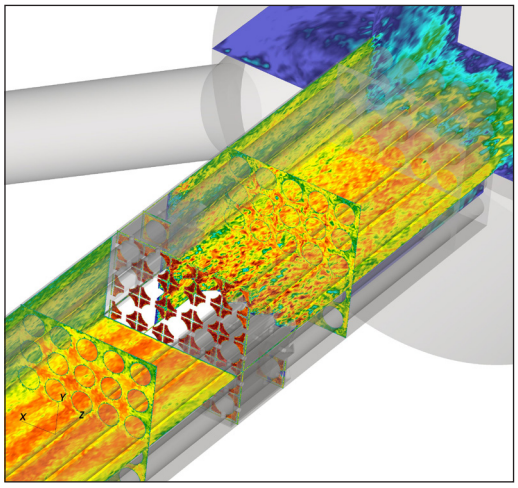


*Fig. 3 Velocity magnitude in MATiS-H spacer grid with swirl-type vanes.*

### *Sharp supporting elements*

During this quarter, the framework team was involved in two primary efforts, mesh generation and implementation of a MOAB-based coupled multi-physics simulation. For mesh generation, finishing touches were put on three major, high-complexity hexahedral meshes, and support was provided for their use in various simulations:

- MATiS-H, an OECD-NEA experiment for single-phase flow over a rod bundle and grid. [ANL]
- Nuscale, a hexahedral mesh of the core internals of the Multi-Application Small Light Water Reactor, a 1/3-scale mockup of the Nuscale reactor. [ANL]
- XX09, a high-fidelity model of the XX09 test fuel assembly used in the EBR-II Shutdown Heat Removal Test experiments. [ANL]

These meshes each had 500,000-1,500,000 elements and geometric complexity that exceeds that of any other reactor simulations done recently under NEAMS. In the area of coupled multi-physics analysis, a coupled Nek5000-Proteus simulation tool was implemented, based on MOAB's solution transfer and a new Coupé coupled multi-physics driver. The tool was used to demonstrate parallel, coupled analysis of a simple seven-pin reactor assembly, and it is currently being applied to the XX09 model described above. [ANL]

## Waste IPSC

Substantial progress was made on both the one-dimensional (1D) waste transport code deployed last quarter for Used Fuel Disposition (UFD) Program use and a new 3D version for higher-fidelity studies. Both codes use the same equations and solution algorithms. A shared graphical user interface is now being developed for input processing, material property database utilization, and initialization and display of simulation results. An equilibrium precipitate model was implemented and tested in the 1D code, and the first version of the 3D code was successfully tested on eight CPUs. Software developed under other federal programs for UFD-relevant phenomena is being evaluated for potential integration with NEAMS-developed software. [SNL]

After several meetings and discussions with experts on the various details of the Electric Power Research Institute (EPRI) hydride reorientation model and the results that it generates, the waste team completed implementation of a hydride mechanical model based on the EPRI model. A demonstration prototype of the new J2Fiber Damage Model, consisting of a mock ring compression test, was used to exercise the model for the behavior of hydrided material, with encouraging results. The model was delivered to the fuels team at the end of June for implementation in AMP. [SNL]

## Fundamental Methods and Models

### *Modeling of gas bubble evolution in polycrystalline fuels*

A generic phase-field model was used to simulate the growth kinetics of intra-granular gas bubbles in a single crystal and inter-granular gas bubbles in a bicrystal in two dimensions during post-irradiation thermal annealing. The model is based on the disparate thermodynamic and kinetic properties of defects in grain boundaries and a single crystal, which were obtained from atomistic simulations and experiments. The model accounts for many mechanisms, including gas atom and vacancy diffusion, trapping and emission of vacancies at defects, absorption and resolution of gas atoms and vacancies at gas bubbles, internal pressure in gas bubbles, elastic interaction between defects and bubbles, and the inhomogeneous thermodynamic and kinetic properties of both the matrix and grain boundaries. [PNNL, INL]

Predicted intra-granular gas bubble growth kinetics in a single crystal agreed well with experimental results, as shown in Fig. 4. Preliminary results for a bi-crystal (Fig. 5) demonstrate that the model can reproduce the equilibrium thermodynamic properties and correct wetting angles of gas bubbles at the grain boundary for given interfacial energies. The model enables parametric study of the affects of defects on gas bubble evolution kinetics in polycrystalline fuels and simulates the heterogeneous gas bubble microstructures needed to predict the evolution of thermo-mechanical properties. [PNNL, INL]

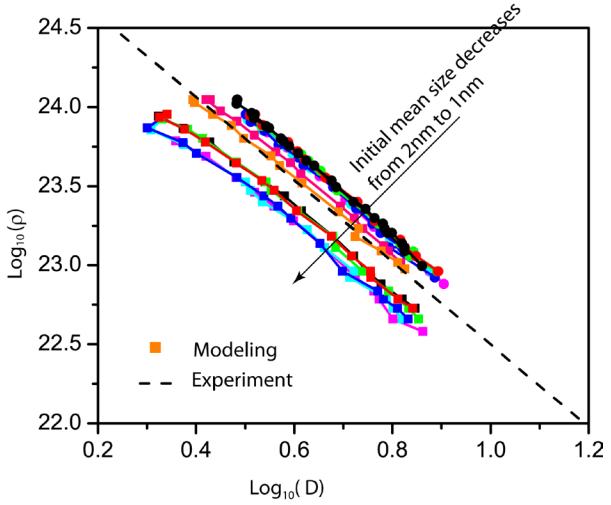



*Fig. 4. Simulated gas bubble evolution kinetics in a single crystal (ρ and D are the density and mean diameter of gas bubbles, respectively).*

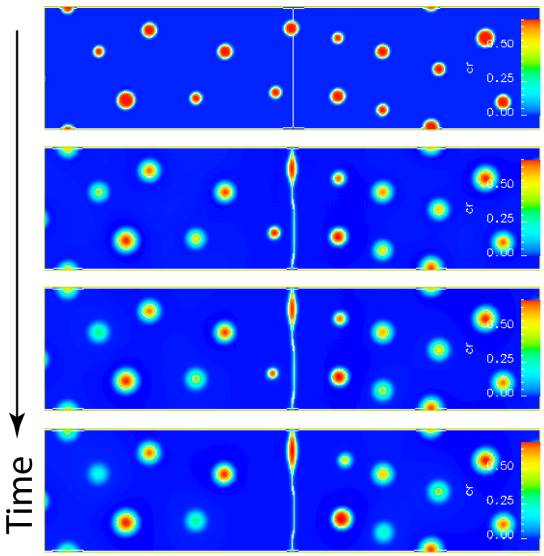



*Fig. 5. Simulated gas bubble evolution near grain boundaries; the color indicates the concentration of gas atoms, with red referring to the highest concentration (0.7).*

### *Thermodynamic and kinetic data for generic phase field*

The FMM team has completed the calculation of critical sizes and rates for the nucleation of α' precipitates in FeCr alloys. Low-chromium ferritic martensitic steels are promising candidates for structural materials in Gen-IV nuclear reactors. They offer good swelling resistance and mechanical properties under high temperatures and irradiation doses. Pure iron chromium (FeCr) alloys are studied as a model system for the complex steels. A generalized calculation of critical sizes and nucleation rates has further applications in the area of nuclear fuels, such as fission gas bubbles in $UO_2$, and as such is of broad importance for the NEAMS program.

FMM work combines the calculation of the FeCr free energy surface (Fig. 6) using MD simulations with recently published data for the interfacial free energies between the α and α' phases in FeCr to obtain thermodynamic and kinetic data on the nucleation in this system. The results are made available as a set of fitting functions and their parameters for integration into larger length scale models such as phase field, thereby bridging the gap between atomic and meso scales in a consistent way. [LANL]

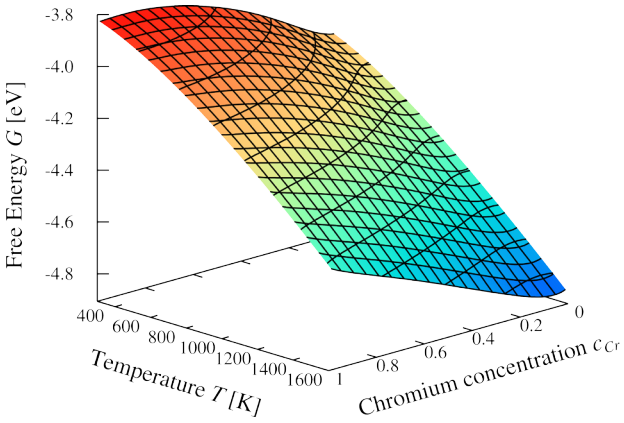



*Fig. 6. Free energy surface of the FeCr system calculated from classical MD simulations using CD-EAM.*

The free energy of the solid solution phase as a function of solute concentration and temperature was obtained using a switching Hamiltonian method in an MD simulation using an empirical concentration-dependent embedded atom model (CD-EAM). Critical nucleus sizes were calculated by applying classical nucleation theory. Nucleation rates (Fig. 7) furthermore contain experimentally determined Cr diffusivities in Fe. Work is in progress to construct a new FeCr potential for MD and kinetic Monte Carlo simulations that addresses the kinetic aspects through accurate defect formation and migration energies. [LANL]

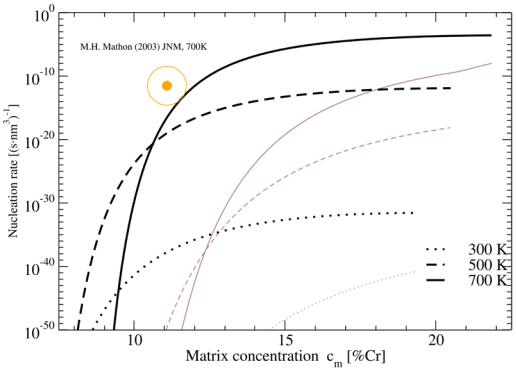


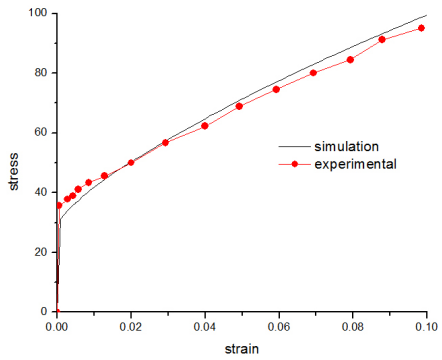

*Fig. 7. Nucleation rates derived from the free energy surface using classical nucleation theory (black lines) and assuming local solute concentration (gray lines) compared with an experimental data point.*

### *Large-scale DD simulation of crystal plasticity*

A multiscale simulation framework is needed to bridge MD, discrete dislocation dynamics (DD), and continuum DD models. To this end, the motion of an edge dislocation was simulated at various stress levels and temperatures. The MD results revealed that dislocation mobility depends on the temperature and concentration of the solute. A power law was formulated to fit the computational results and provide the basis for scalable universal laws of mobility that can be applied to discrete DD simulations at larger length and time scales. The dislocation evolution mechanisms generated by discrete DD can be used in continuum DD to accurately predict the strength and deformation behaviors of single-crystal α-Fe with the consideration of anisotropic Peierls stress and cross slip. [PNNL]

The predicted stress strain curve of single-crystal α-Fe with uniaxial tension loading along the crystal orientation <001> is in good agreement with experimental results, as illustrated in Fig. 8. The parameters used in the simulation are either experimentally measured or calculated from the discrete DD simulation. [PNNL]

*Fig. 8. Measured and predicted stress-strain curve of single crystal*




*α-Fe under uniaxial tension along the <001> direction.*

## Verification, Validation, and Uncertainty Quantification (VU)

### *Uncertainty quantification*

This quarter, the VU team worked with the Fuels team to perform sensitivity analysis on Bison using the Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) software, a suite of optimization and uncertainty quantification methods. Preliminary sensitivity analyses were performed for the Halden IFA-432 case (OECD-NEA Data Bank). The analyses focused on the thermal conductivity of both the gas in the gap and the fuel. The

studies verified the importance of certain input-output relationships, such as a high correlation of thermocouple temperatures with respect to fuel thermal conductivity. The studies also showed that certain combinations of parameters lead to very high temperatures in the fuel and lack of convergence in the solutions. [SNL, LANL]

### *Predictive maturity*

Work continued on the previously developed discovery, accumulation, and assessment (DAA) process to plan, track, assess, and communicate VU activities and results. DAA was applied to the Bison sensitivity analysis described above, and the results were exported to Synopsis, the DAA management tool. [SNL, LANL, INL]

Building on previous sensitivity studies of the LIFE-IV nuclear fuels code, a recently completed VU study focused on a methodology by which experimental campaigns may be devised to improve code calibration. Specifically, a principal component analysis is performed on the input parameters of the experiments, and the experiments that offer the least residual error when reconstructed from the principal components are proposed as those that should be conducted first. In this way, the experiments are ranked according to their ability to "cover" the input design space, or in this case, a low-dimensional representation of the input design space.

A comparison of two sequences examined in this study is provided in Fig. 9, which shows the predictive maturity index (PMI) approaching an asymptotic value more quickly with the early incorporation of experiments that offer more coverage of the input design space (vis-à-vis lower reconstruction errors) and also yield better-calibrated models (insofar as stability of the model predictions is concerned). [LANL]

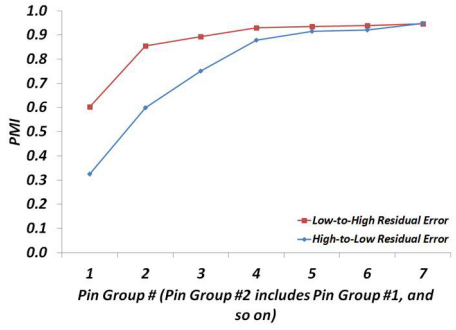



*Fig. 9. Comparison of PMI produced by two sequential calibration studies.*

Figure 10 shows the Bison DAA hierarchy with color-coding to provide a snapshot of the completeness of the Bison validation effort. The placeholders used to determine completeness are specific questions or items that must be identified, such as the physical quantities measured in the experiment. For Bison, about 230 placeholders need to be filled to complete the description of the validation effort. One can see that the initial steps in validation have been taken (e.g. acquiring a description of the experiment and data), and that more planning, verification, simulation, and validation comparison work remains to be done. If this data is collected periodically, one can plot project progress over time with Synopsis.

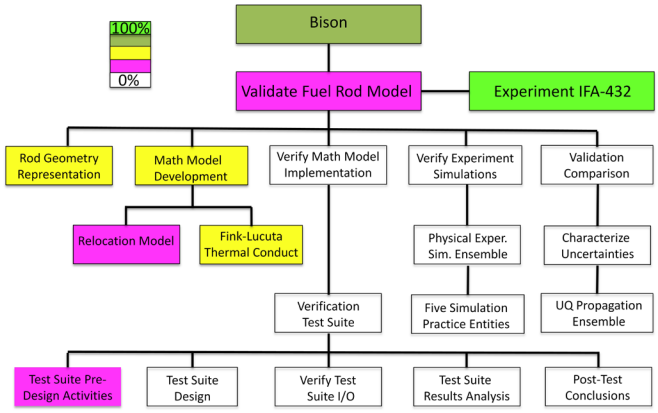
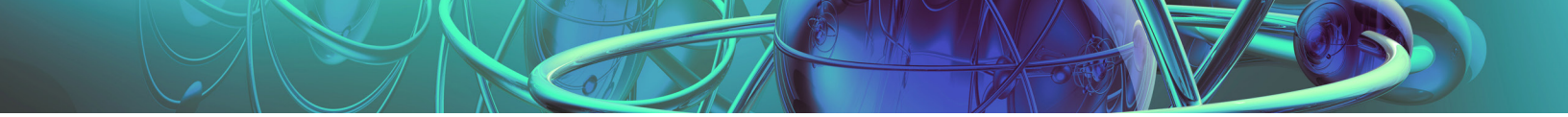



*Fig. 10. Initial Bison fuel rod DAA structure with current status (% complete is defined as the number of filled placeholders / total number of placeholders).*

### *NE-KAMS*

The objective of the NE-KAMS (Nuclear Energy - Knowledge base for Advanced Modeling and Simulation) project is to establish a comprehensive knowledge base for verification and validation of nuclear reactor analysis codes. The security requirements for the NE-KAMS demonstration were determined, and the network design using the existing *Gen IV Materials Handbook* infrastructure was completed. [INL, ORNL]

In the third quarter, the VU team started collecting experimental data sets to benchmark them against a set of verification and validation requirements and standards for such data. Several computational fluid dynamics (CFD) datasets from the MAX thermal hydraulics experiments at ANL were collected and their structure analyzed to develop guidelines for the NE-KAMS database structure design. Collection of additional MAX data is



planned. Other CFD and thermal-hydraulic data that can be used for the demonstration are being evaluated. [INL, Bettis Laboratory, SNL, ANL]

## Capability Transfer

Early User Program activity increased during the past quarter, with several groups evaluating the capability and usability of NEAMS software packages, including Nek5000, AMP, and Bison, in a variety of contexts. The Nek5000 evaluation focused on understanding and evaluating the core simulation capabilities of the package for turbulent flows, the effects of Reynolds number, driving forces, mesh refinement, points per cell, and averaging time on the solutions produced by the code for simple reactor modeling scenarios. [INL, TAMU]

Two different groups have been exercising the AMP fuels modeling code. After verifying the thermal solution for a single pellet and cladding benchmark problem (NEA/OECD Data Bank IFA-432 rod 6), the groups have been modeling a variety of simple pin configurations, including both solid and hollow pellets, with a focus on thermal performance and heat transfer from the pellet to the cladding. [ORNL]

Bison users have carried out simulations of a number of NEA/OECD benchmark cases (IFA-539.3 and Riso AN3 and AN4) and begun others (IFA-513 rod 1 and Oconee-1 rod 15309). Detailed simulations have been compared with experimental data, as well as results from the FRAPCON code. Evaluation results are being provided to the Bison development team. [ANL, INL, LANL, ORNL, Texas A&M University]

Work continues in the establishment of a working relationship with the Nuclear Regulatory Commission and the development of recommendations for program-wide policies for software licensing, release, and distribution. Preliminary reports on both of these topics, as well as discussion of issues relevant to planning for FY2013, were delivered at the end of June.

## Enabling Computational Technologies

An initial static analysis of AMP was completed. Key issues were triaged and discussed with the AMP team. Initial work used an older version of AMP, and Klocwork® revealed memory limitations and bugs. System memory was quadrupled, and Klocwork® developers were engaged to fix the bugs. The ECT team has now switched to the current development version of AMP. [LLNL]

The ECT team is preparing to support the static analysis of Bison.

Development and revision of content for the NEAMS web site is proceeding. In particular, content supporting several different aspects of the message of advanced modeling and simulation has been developed. Two reviews of current content organization as well as database back-end functionality to support its revision and extension have been completed, with several changes being made to, for example, the organization and back-end maintenance interface. [LLNL and subcontractors]

Risk grading of Relap-7 was completed and a NEAMS-specific software quality assurance (SQA) plan was started. The risk grading tool used to grade NEAMS codes was released for public use. An Advanced Simulation Capability for Environmental Management (ASCEM) collaborator was identified to help complete the ASCEM half of the NEAMS/ASCEM overarching SQA implementation plan. To make the NEAMS SQA plan applicable throughout the DOE complex, the ECT team started a revision of the NEAMS overall SQA plan to make it fully compliant with all DOE standards applicable to software. [LLNL]

Development of the NiCE Updater, a real-time monitoring library, was completed. Two new NiCE capabilities were started: NiCE MultiLaunch and NiCE Web Client. The multi-launch tool will support batch and chained launches of multiple jobs on the same or different machines. The web client will enable users to interact with NiCE from anywhere they can run a web browser. The ECT team also performed integrated tests of NiCE with AMP. Results were fed back to fix bugs and enhance usability. Improvements were demonstrated to selected NEAMS stakeholders. [ORNL]

The Cubit mesh generator was restructured to run with the TetGen mesher and OpenCascade modeler, two open-source alternatives to commercially licensed components. These changes support ECT's open-source strategy for Cubit. [SNL]

# Technical Spotlight: Multiscale Material Model Development for Fuel Performance Codes

### *Coupling the Atomistic, Meso, and Engineering Scales*

Fuel behavior is complex because it is governed by numerous coupled phenomena. Two key phenomena are (1) fission gas retention and release and (2) dimensional changes of the fuel pellet. Understanding both of these processes is critical for accurate prediction of the interaction between the fuel pellet and the cladding, which ultimately governs fuel performance. The most important variable governing these two phenomena is the temperature distribution within the fuel element, which is controlled by a combination of the heat generation due to fission and the fuel thermal conductivity. The latter property degrades during fuel irradiation due to increased concentration of point defects, formation of fission products and product precipitates, redistribution of fission gases and gas bubbles, and changes in the oxygen-to-metal ratio.

Current models of thermal conductivity typically rely on high degrees of empiricism and do not explicitly resolve changes in the microstructure induced by irradiation. Rather, they combine such effects into burnup-dependent factors. To develop models for a wider range of operating conditions and advanced fuel forms, a multiscale model is needed to couple the fuel microstructure and composition to thermal conductivity via internal state variables (ISVs) representing the fuel microstructure. Since, for example, the distribution of fission gas bubbles both depends on and affects fuel temperature, a more sophisticated simulation of thermal conductivity requires a fully multiscale approach.

As gaseous fission products build up within the fuel, they migrate to grain boundaries (GBs) and form a network of bubbles. These GB bubbles interconnect and grow until fission gas escapes from the fuel into the gap between the fuel and cladding. This fission gas release degrades fuel performance, as it reduces thermal conductivity within the gap between the fuel and cladding and increases the cladding pressure. Fission gas retained within the fuel inhibits heat transfer, decreasing thermal conductivity within the fuel, which can create a temperature gradient, further increase fuel temperature, and drive additional gas release. These changes reduce reaction efficiency, shorten fuel life, and increase the risk of cladding failure.

To model thermal conductivity in nuclear fuel, an ISV model was developed to evolve the fission gas within the grains and on the GBs.[1] MD simulations were used to calculate the thermal resistance of various $UO_2$ GBs at increasing temperatures (Fig. 11).

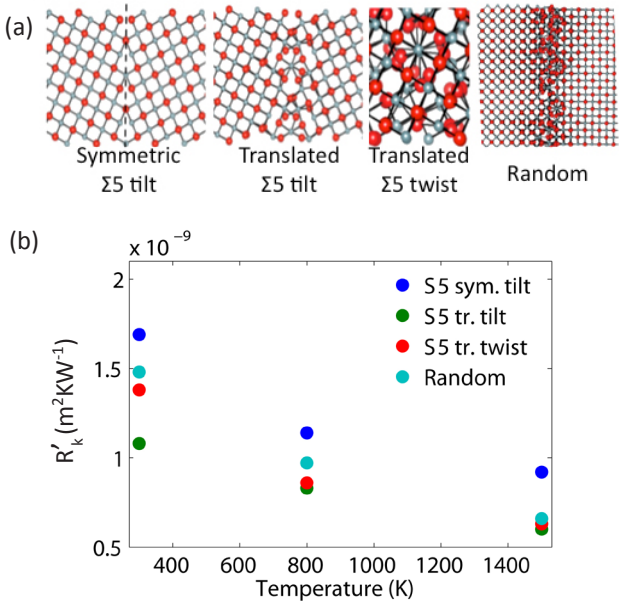



*Fig. 11. Atomistic calculation of the GB thermal resistance in $UO_2$ for four types of GBs: (a) GB structures[2] used in the MD calculations and (b) GB thermal resistance for each structure at three temperatures.*

The thermal resistance values were used in mesoscale heat conduction simulations with Marmot to determine the effective GB thermal resistance, including the effect of gas bubbles. In this way, the local thermal conductivity was coupled to the microstructure via state values calculated with MD. The mesoscale variables were grain size, temperature, GB type, and GB coverage (the percentage of GBs covered by fission gas). These simulations showed that the effective thermal conductivity is insensitive to grain size and GB type. Thus, a relationship was obtained for the effective thermal resistance ($R_k'$) as a function of GB coverage (Fig. 12).

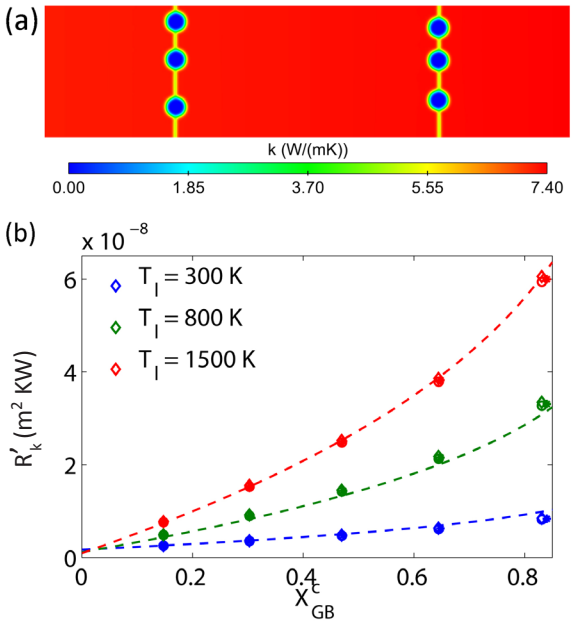



*Fig. 12. Mesoscale heat conduction calculation of effective GB thermal resistance: (a) the simulation domain with spatially varying thermal conductivity and (b) effective thermal resistance vs. GB coverage at various temperatures.*

The next step was to do some preliminary work to replace numerically generated microstructures with realistic microstructures reconstructed from optical scans of irradiated fuel (Fig. 13). This approach will add more accuracy to the mesoscale calculation and is the subject of future work.

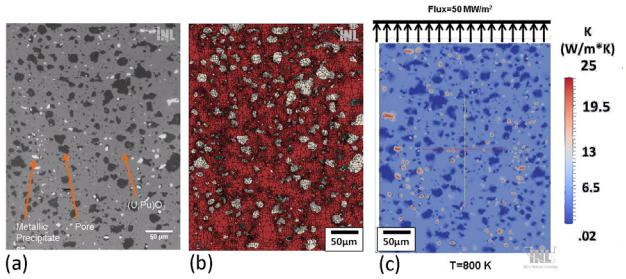



*Fig. 13. Mesoscale heat conduction simulation on a reconstructed fuel microstructure: (a) optical micrograph of high burn-up ACO-3 metal oxide fuel, (b) reconstructed simulation mesh, and (c) simulation setup, with initial values for thermal conductivity overlaid on the mesh.*

With thermal resistance defined as a function of GB coverage, the effect of GB bubbles on thermal conductivity can be incorporated into an engineering-scale fuel performance code, such as Bison. The existing fission gas release model in Bison already defines the evolution of the two state variables of interest (intragranular porosity and GB coverage). Thus, the ISV model was coupled to Bison using these values, which the ISV model used to provide thermal conductivity values to Bison. The coupling was demonstrated in a 2D axisymmetric simulation of a 10-pellet rodlet, modeled over three years under typical PWR conditions. Figure 14 shows results from this simulation, which yielded different values for fuel thermal conductivity in comparison to simulations performed without the ISV model.

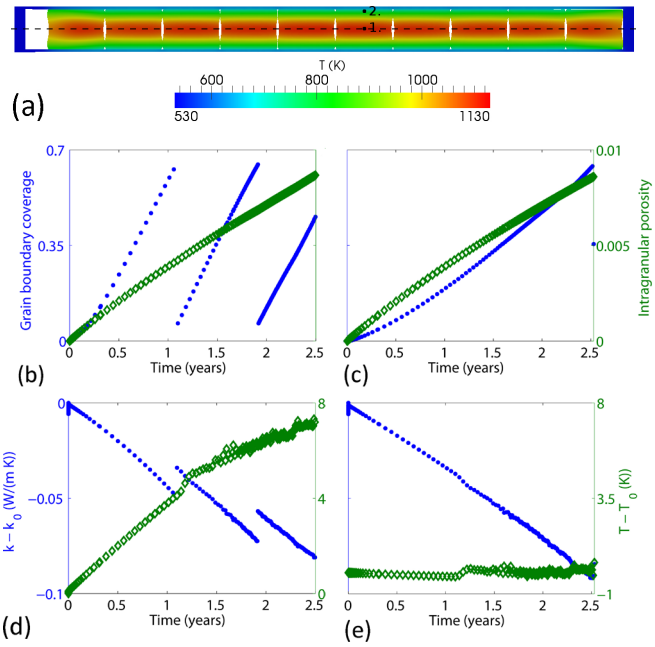
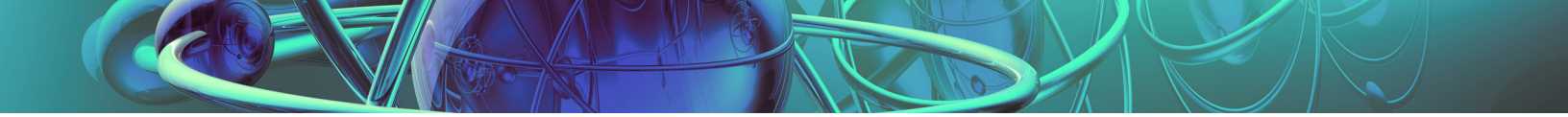



*Fig.14. Simulation results using Bison and the ISV model of thermal conductivity: (a) the simulation domain, a 10-pellet rodlet (note points 1 and 2), (b and c) GB coverage and intragranular porosity at points 1 and 2, respectively, and (d and e) change in the thermal conductivity and temperature at points 1 and 2 with respect to a reference simulation not using the ISV model.*

In summary, the empirical materials models currently used in fuels performance codes cannot be extrapolated to accident conditions or new fuel types. Therefore, multiscale modeling, encompassing all scales from atomistic to engineering, was used to develop new, a more mechanistic ISV model. Ongoing efforts will develop many more multiscale models, including an improved model of the fission gas release. This work has the potential to revolutionize fuel performance modeling.




### *References*

1. K. Forsberg, A.R. Massih, J. Nucl. Materials 135 (1985) 140–148.
2. P.V. Nerikar, et al., J. American Ceramics Soc. 94 (2011) 1893–1900.



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# FYI: NEAMS Computer Codes

Bison provides an engineering-scale simulation of 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.

MOOSE is a modular, adaptive architecture that greatly simplifies the addition of new physics "kernels" and coupling them together. This modularity, as well as the consistent way that MOOSE handles nonlinear material properties and boundary conditions, enable rapid prototyping and fast development of production-ready massively parallel code.

Relap-7 evaluates the performance and safety of a complete nuclear power plant system under a variety of operational and accident conditions. Relap-7 relies on one- and zero-dimensional engineering models of fluid flow, heat transfer, core power, and structural response to pressure and heat. The models in Relap-7 are calibrated by and validated against experimental data. Relap-7 was developed using MOOSE.

Sharp evaluates the performance and safety of nuclear reactor cores or other large components using higher-fidelity, physics-based methods that greatly reduce the dependence on calibrated engineering models. The Sharp toolset predicts neutronics, fluid flow, heat transfer, and structural mechanics. Sharp can be used by itself or in tandem with Relap-7, to improve Relap-7's accuracy, range of applicability, or both.

# Recent and Upcoming Level 1 and 2 Milestones

| Completed during this Quarter | | | |
|---|---|---|---|
| **Milestone ID** | **Description** | **Due Date** | **Finish Date** |
| M2MS-12PN0606017 | Benchmark gas bubble nucleation and growth in irradiated $UO_2$ in concert with other mesoscale models | 4/11/2012 | 4/11/2012 |
| M2MS-12IN0603336 | Simulate steady-state single-phase PWR (normal operations) with Relap-7 | 5/15/2012 | 4/27/2012 |
| M2MS-12AN0603278 | Complete multi-physics simulations of a sodium fast reactor fuel assembly using the Proteus, Nek5000, and AMP | 4/30/2012 | 4/30/2012 |
| M2MS-12IN0603337 | Complete Relap-7 SQA plan | 5/31/2012 | 5/29/2012 |
| M2MS-12IN0602061 | Demonstrate implementation of atomistic results into a combined MBM simulation | 5/31/2012 | 5/30/2012 |
| M2MS-12IN0603339 | Complete Relap-7 development plan | 6/30/2012 | 6/27/2012 |
| M2MS-12SN0605074 | Develop and demonstrate final hydride reorientation model for UNF-VLTS | 6/30/2012 | 6/30/2012 |
| M2MS-12AN0603018 | Expand collaboration plan for Sharp modeling and simulation area | 6/30/2012 | 7/9/2012 |

See back page for upcoming milestones.


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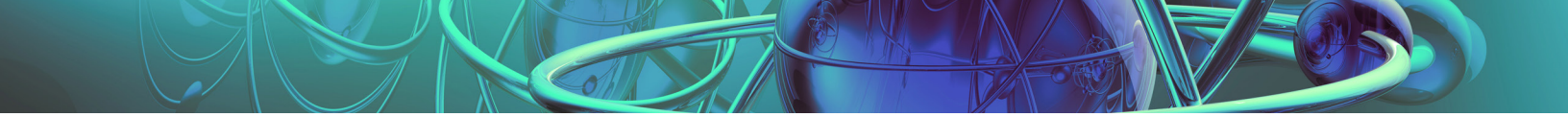

## Milestones Coming Due during the Next Quarter (July–September 2012)

| Milestone ID | Description | Due Date | Status |
|---|---|---|---|
| M2MS-12LL06031213 | Report final results of seismic gap analysis workshop | 7/27/2012 | Delayed (new due date) |
| M2MS-12PN0606016 | Complete strength model for Fe-Ni-Cr system with grain boundary segregation and irradiation effects | 7/30/2012 | On schedule |
| M2MS-12AN0601123 | Develop NEAMS project schedule for FY13 and beyond | 7/31/2012 | Accelerated (new due date) |
| M2MS-12IN0603338 | Plan for Relap-7 support of Mark 1 BWR major power level increase application | 7/31/2012 | On schedule |
| M2MS-12LL06090613 | Perform static QA analysis of three NEAMS codes, including Bison | 8/30/2012 | On schedule |
| M2MS-12LA0602071 | Demonstrate implementation of atomistic results into MBM simulation | 8/31/2012 | On schedule |
| M2MS-12OR0604041 | Complete separations plant-level model, including voloxidizer, dissolver, solvent extraction, and analysis | 8/31/2012 | Delayed (new due date) |
| M2MS-12OR0608117 | Report recommendations for NEAMS engagement with the NRC | 9/1/2012 | On schedule |
| M2MS-12AN0601061 | Complete extensible code for integrating separations system models | 9/28/2012 | On schedule |
| M2MS-12AN0603081 | Demonstrate Sharp framework support for a coupled physics problem | 9/28/2012 | On schedule |
| M2MS-12AN0603092 | Implement Nek5000-based uRANS module | 9/28/2012 | On schedule |
| M2MS-12AN0603118 | Complete initial development of the Proteus-2D1D module | 9/28/2012 | On schedule |
| M2MS-12IN0602111 | Report on progress in phase field methods development | 9/28/2012 | On schedule |
| M2MS-12LA0602131 | Report progress in up-scaling atomistic data for use in mesoscale models in Marmot or continuum-scale models in Bison | 9/28/2012 | On schedule |
| M2MS-12LA0604021 | Issue report on integrated separations plant model | 9/28/2012 | On schedule |
| M2MS-12OR0602032 | Deliver AMP 2.0 to RSICC for release | 9/28/2012 | On schedule |
| M2MS-12PN0602121 | Issue joint Fuels/FMM report on development of phase field methods | 9/28/2012 | On schedule |
| M2MS-12SN0605061 | Demonstrate simulations collaboratively defined with UFD Program | 9/29/2012 | On schedule |
| M2MS-12AN0603279 | Complete integrated multi-physics simulations of a BWR fuel assembly with Proteus, Nek5000, and AMP | 9/30/2012 | On schedule |
| M2MS-12IN0602041 | Release Bison to users for nominal simulation of $UO_2$ in an LWR | 9/30/2012 | On schedule |
| M2MS-12IN0602183 | Demonstrate application of Bison to an accident-tolerant fuel design | 9/30/2012 | On schedule |
| M2MS-12IN0603108 | Demonstrate Sharp/Pronghorn interoperability by modeling a prismatic core with the MOOSE platform | 9/30/2012 | On schedule |
| M2MS-12IN06033310 | Release Relap-7 1.0 | 9/30/2012 | On schedule |
| M2MS-12OR0609091 | Release NiCE 2.0 | 9/30/2012 | On schedule |

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