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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 July – September 2012

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Quarterly Highlights

- AMP 2.0 was completed and distributed with an open license. (page 2)
- BISON was used to analyze a novel fuel design. (page 2)
- MARMOT simulations were performed to study grain growth and segregation in irradiated materials. (page 3)
- The Fuels and FMM teams completed multiscale modeling of the nucleation of Cr-rich phases in stainless steel. (page 8)
- The Reactors team executed the first true multiphysics reactor core simulations using only NEAMS SHARP components. (page 3)
- An initial integration of the Diablo structural mechanics code with SHARP was completed. (page 4)
- A coupled RELAP-7/PRONGHORN benchmark simulation was performed to show that the code can handle steep spatial gradients. (page 4)
- Dissolver and solvent extraction modules were integrated into the Safeguards and Separations Performance Model. (page 4)
- Analytical tools were developed for characterizing emission signatures during used fuel processing. (page 5)
- The Waste IPSC team completed groundwork for modeling long-term radioactive waste disposal. (page 5)
- The FMM team studied the tendency of grain boundaries to attract point defects. (page 5)
- A coupled Potts/phase-field simulation technique was use to model bubble evolution in nuclear fuel. (page 5)
- The aging behavior of Fe-Cr alloys was studied with phase-field modeling. (page 6)
- The VU team completed studies of importance sampling for uncertainty quantification. (page 7)
- The assessment of validation experiment datasets for NEKAMS was completed. (page 7)
- Early user program participants completed their evaluation activities for BISON/MOOSE, AMP, and Nek5000. (page 8)
- The NEAMS Common Software Stack (NEAMS-CSS) was developed and tested. (page 8)
- Static analysis was used to improve AMP, MOAB, HDF5, and VisIt. (page 8)
- The NEAMS web site was launched at neams.ne.anl.gov. (page 8)

Spotlight on Personal Achievements

Young Member Excellence Award. Elia Merzari (ANL) will be awarded the American Nuclear Society (ANS) Young Member Excellence Award at the ANS Winter Meeting in San Diego in November 2012. This award recognizes ANS Young Members who demonstrate overall excellence through involvement with the ANS national level, outstanding non-technical skills as well as technical or managerial ability, recognition by peers, and adherence to high quality and safety standards.

Dr. Merzari has demonstrated excellence as a nuclear engineer in the areas of reactor thermal hydraulics and computational fluid dynamics. He has made internationally recognized contributions to the understanding of turbulent fluid flows in the complex geometries of nuclear reactors. He organized a session focused on turbulent flow in tight lattice assemblies at the 2011 NURETH 14 topical meeting in Toronto, Ontario, Canada.

Dr. Merzari has published 14 articles on these topics in refereed journals and submitted scholarly articles to nearly 30 conferences. In 2010, he was awarded the ANS Thermal Hydraulic Division Best Paper Award.

ANS Fellow. The ANS has elected ORNL Distinguished Research Scientist Mark L. Williams to the grade of Fellow. The ANS recognized Dr. Williams for his contributions to nuclear science and engineering, including "extensive work in sensitivity/uncertainty methods, development of the 'contributon' transport theory and new techniques for lattice physics and resonance self-shielding computations, and reactor pressure vessel fluence analysis."

Dr. Williams is a member of the ORNL Reactor and Nuclear Systems Division, where he works on the internationally distributed SCALE nuclear analysis code system. SCALE is a comprehensive and unified set of codes and nuclear data libraries for reactor physics, radiation shielding, criticality safety, spent fuel characterization, and sensitivity/uncertainty analysis. His main focus areas within SCALE are currently reactor and lattice physics, nuclear data generation, and uncertainty quantification techniques. His contributions to NEAMS include developing efficient methods for computing self-shielded cross sections that can be integrated with highly parallel core physics calculations in SHARP.

Accomplishments

Fuels IPSC

Assembly-scale code development

In July, AMP 2.0 was submitted to the Radiation Safety Information Computational Center for distribution with an open license. This marked the completion of AMP development efforts under NEAMS. Future assembly-scale tool development is included in the Reactors IPSC (SHARP, for example). [ORNL]*

Pin-scale code development

Development of BISON for the engineering-scale simulation of nuclear fuel performance continued.
Major enhancements to BISON during this quarter included: (1) the capability to read volumetric power history information directly from neutronics code output, which greatly simplified input file generation; (2) implementation of thermal and mechanical material property models for mixed-oxide (MOX) fuel and stainless steel cladding, which was a major step toward enabling BISON to perform meaningful analyses of MOX fuels in sodium fast reactor (SFR) applications; (3) development and implementation of a heat transfer model that uses sodium in the fuel-cladding gap and plenum region, which allows for a much more accurate analysis of sodium-bonded metallic fuels; and (4) modification of the coolant sub-channel model to support loss-of-coolant-accident simulations.

An initial demonstration of the application of BISON to the analysis of a conceptual accident-tolerant fuel (ATF) design was performed and documented. The concept analyzed was one using annular oxide fuel with high-thermal-conductivity metallic inserts in the central annulus as well as between pellets. The BISON analysis showed that peak fuel temperatures could be reduced by a factor of two, offering potential performance improvement during off-normal events in which fuel temperatures escalate. Fig. 1 illustrates a temperature distribution calculated by BISON for the ATF concept. [INL]

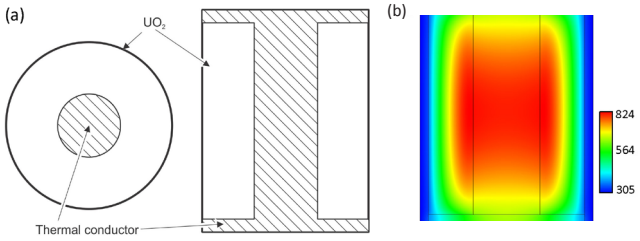
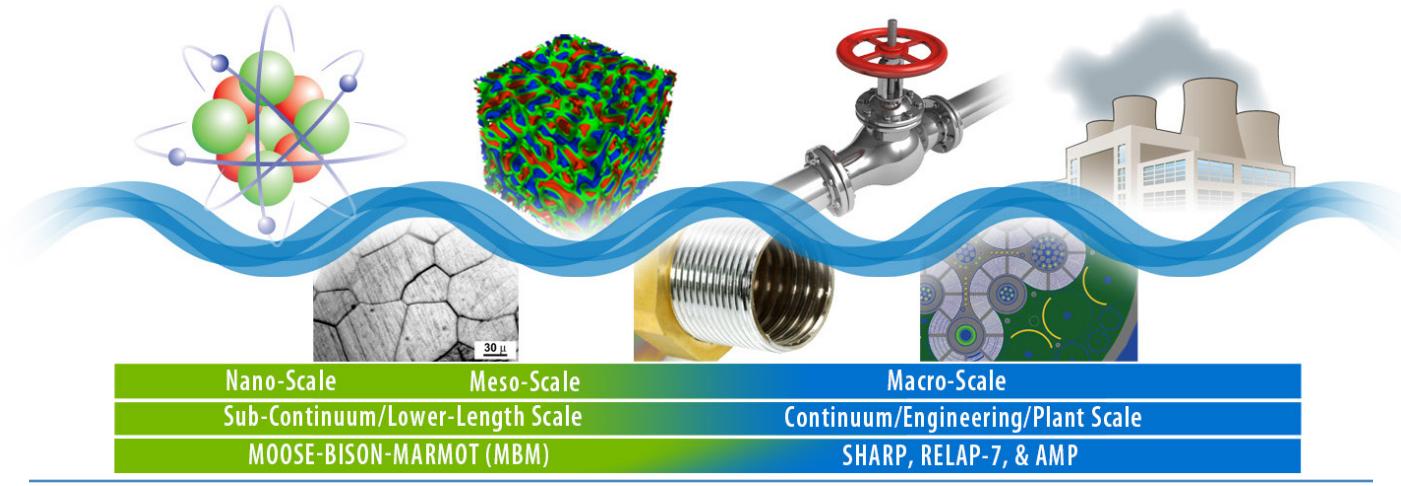


Fig. 1. ATF modeling in BISON: (a) Cross-sections of a conceptual ATF pellet and (b) calculated pellet temperatures (°C).

Finally, the release of BISON to a preliminary user community for the simulation of UO_2 under pressurized water reactor conditions was documented. Throughout FY2012, BISON was released to various institutions, including SNL, ANL, PNNL, LANL, ORNL, Penn State University, University of Michigan, University of Tennessee Knoxville, Anatech Corporation, National Nuclear Laboratory (United Kingdom), and Atomic Energy of Canada Limited. Each institution received training in the use of MOOSE and BISON, instructions for checking out the code from the INL repository, and help with installing and running the code. Each institution has used the code to varying degrees in analyzing oxide fuel performance under light-water reactor (LWR) conditions, and most of these users have provided important feedback on their experiences.

*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



Lower-length-scale model development

An improved climb-and-glide single-crystal deformation model was implemented in the Visco-Plastic Self-Consistent (VPSC) code, which models the inelastic behavior of solids under a load. Initial efforts to couple VPSC with MOOSE-BISON-MARMOT (MBM) at both the BISON and MARMOT scales were successful. The MBM-VPSC simulations of stress-strain response reproduced the stand-alone VPSC calculations. The VPSC improvement will enable, for example, visco-plastic deformation mechanisms to be included in the development of grain growth models for both fuels and cladding materials. [LANL, INL]

A series of MARMOT simulations were performed to elucidate the coevolution of grain growth and segregation behavior in materials under irradiation. Information gained from these simulations is providing valuable insight into the evolution behavior of fission products in polycrystalline UO_2 fuel, particularly the dragging of fission product gas atoms during grain growth, which is a potentially important mechanism in the process of fission gas release in restructured oxide fuels at elevated temperatures. [INL]

A major collaborative study on generic phase-field method development was completed and reported. For details, see the FMM section on p. 5 and the nucleation article on p. 8. [LANL, PNNL, INL]

Reactor IPSC

SHARP code development

SHARP integration

The final quarter of FY2012 saw the long-anticipated integration of many components. Most importantly, the Reactors team demonstrated the COUPÉ simulation driver module and successfully executed the first true multiphysics reactor core simulations using exclusively SHARP components developed by NEAMS. Simulations of steady-state conditions in the simple SAHEX SFR assembly (Fig. 2) utilized the MeshKit mesh generation module, the PROTEUS neutronics module, the Nek5000 thermal fluids module, the Mesh-Oriented dAtaBase (MOAB) mesh management module, and the COUPÉ driver module.

In addition, the broad applicability of MeshKit was successfully demonstrated in the generation of computational meshes describing a very high-temperature gas-cooled reactor (VHTR) core for use by the MOOSE-based PRONGHORN multi-dimensional reactor analysis code. Initial thermal-fluid/thermal-structural simulations were also carried out in SHARP using the MOAB data backplane component, which provides an interface between other simulation modules. [ANL]

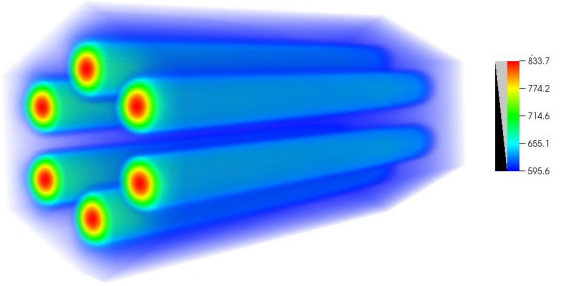


Fig. 2. Predicted temperature profiles in an integrated neutronics/thermal-fluid simulation of a simple SFR fuel assembly using the integrated SHARP toolset.

PROTEUS development

The SHARP neutronics module, PROTEUS, includes neutron and gamma transport solvers and cross-section processing tools as well as capability for depletion and fuel cycle analysis. [ANL, ORNL]

Efforts continued to complete and distribute the conventional code modules for fast reactor analysis, including DIF3D, REBUS-3, VARI3D, and PERSENT; these modules are based on proven methods that predate the NEAMS program. The development of the PERSENT code, built around the nodal 3-D transport solver in DIF3D, has been completed and demonstrated for a series of benchmark problems. PERSENT is a sensitivity analysis tool that enhances the verification and validation capabilities of the NEAMS toolkit.

A set of proof-of-principle simulations, based on the Takeda standard problem and a heterogeneous cylindrical heavy water system, were completed using the initial version of PROTEUS-2D1D (Fig. 3). The methodology of PROTEUS-2D1D is derived from the SHARP team's experience using and developing the 2-D/1-D capabilities of the DeCART code under the cooperative International Nuclear Energy Research Initiative agreement with the Republic of Korea. However, PROTEUS-2D1D is not a true 2-D/1-D method. Instead, it utilizes a simplified 3-D methodology in which the mesh used in the axial direction is a simple extrusion of the 2-D radial plane. This approach resolves the issues with axial discretization and axial discontinuities that plagued previous code modules using 2-D/1-D methods. [ANL]

SHARP thermal fluids module development

Validation continued for the computational fluid dynamics (CFD) capability provided by the spectral element thermal fluids module Nek5000. The Nek5000 team's submission to the Organisation for Economic Co-operation and Development's (OECD's) MATIS-H reactor fuel assembly spacer grid benchmark placed first among all submissions in the prediction of turbulent fluctuation magnitudes. The top

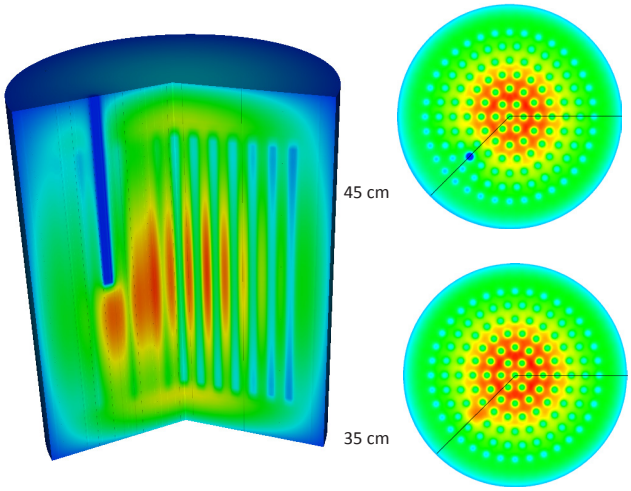


Fig. 3. PROTEUS-2D1D simulations of neutron flux in a cylindrical heavy water reactor. The images on the left and right are 3-D and 2-D representations, respectively.

six submissions, including Nek5000, gave nearly identical results for average velocities.

Additionally, an initial unsteady Reynolds-averaged Navier-Stokes (RANS) method was implemented in Nek5000 using a standard k-ω model. RANS methods use engineering correlations for the prediction of turbulent fluctuations rather than simulating those fluctuations directly, as in large eddy or direct numerical simulations. While this approach sacrifices accuracy in the predicted fluid mechanics behavior, the use of RANS models reduces the computational cost of typical reactor component simulations by a factor of 100 or more. [ANL]

SHARP structural mechanics model development

The initial integration of the structural mechanics module Diablo with the SHARP framework was completed. With the new connectivity provided by the MOAB library components, an integrated Diablo/Nek5000 simulation of conjugate heat transfer in a simple channel flow was completed. Diablo now has the ability to read more complex reactor geometry meshes and data stored on those meshes from the MOAB data backplane. This capability is currently being applied to a more typical thermal-fluid/thermal-structural reactor problem.

RELAP-7 code development

To develop a comprehensive nuclear reactor system safety analysis application, two existing models have been coupled: (1) RELAP-7, which models 1-D fluid flows through plant systems but lacks a nuclear reactor module, and (2) PRONGHORN, which was initially developed to model VHTRs and includes 3-D solvers for neutron diffusion, reactor core fluid flow, and conjugate heat transfer in a full reactor core. The coupling is "loose" in that each model functions independently with its own mesh and the join is accomplished via an exchange of data. Some modifications to RELAP-7 were necessary to align the fluid boundary terms.

Fig. 4 shows the coupled RELAP-7/PRONGHORN simulation of a simplified benchmark experiment from the OECD Nuclear Energy Agency (NEA). [INL]

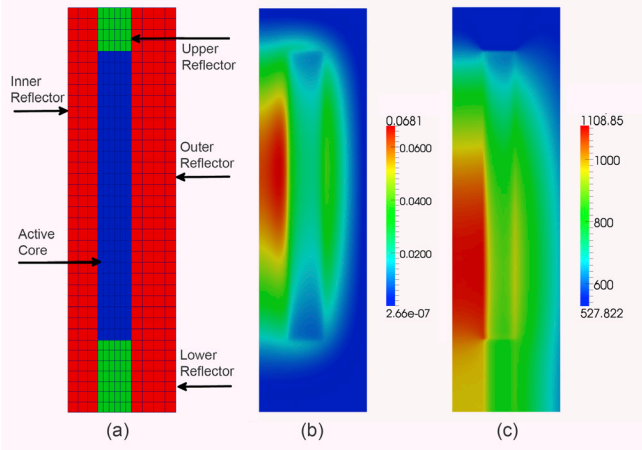


Fig. 4. Coupled RELAP-7/PRONGHORN simulations of the OECD/NEA MHTGR-350 Coupled Neutronics/Thermal-Fluids benchmark experiment: (a) Core geometry, (b) thermal flux, and (c) temperature of solid components.

Safeguards and Separations IPSC

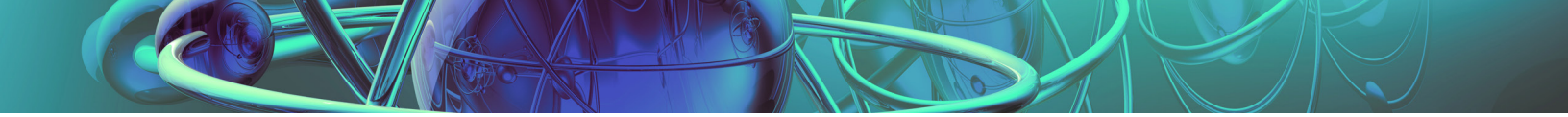
Plant-level model development

Previously developed concepts for processing commonality were used to create models for a voloxidizer, a dissolver, and solvent extraction. Visualization tools for the dissolver were developed. The voloxidizer model is based on volume holdup at each network stage, and the other models are based on chemical thermomechanical network transport. The results demonstrated the usefulness of the design approach for a wide range of processes. [LANL, ORNL]

In complementary efforts, the dissolver and solvent extraction modules were integrated into an end-to-end plant model, the Safeguards and Separations Performance Model. Initial demonstrations of the model have been completed, and additional topics for development identified. [ORNL, SNL]

Electrochemical modeling

A previously developed model for electrorefining was significantly improved by incorporating reaction kinetics (both electrochemical and chemical) at the electrode surface. Compared with previous models, most of which are based



on diffusion control and the assumption of reaction equilibrium, the new model can be applied to study nonequilibrium, mixed controlled (activation-diffusion controlled), and activation-controlled cases.

The model was validated by comparing it with experimental curves of UCl_3 and $PuCl_3$ cyclic voltammetry (CV), an electrochemical process similar to electrorefining of spent fuels in molten salts. The model can also capture some other features of CV processes that have not been measured because of technical difficulties, such as concentrations of actinide metals and ions at the electrode surfaces.

In a separate task, analytical tools are being developed for characterization of emission signatures at different points in pyroprocessing (high-temperature) methods. A computational non-destructive safeguards study has been conducted using the Monte Carlo N-particle (MCNP6) radiation-transport code to examine "delayed" nuclear decay activity ratio (AR) signatures for a conceptual electrorefining and pyroprocessing model. ("Delayed" decay means that very short-lived isotopes are ignored.) Spent-fuel inventories were prepared using MCNP6 burnup calculations for a generic Westinghouse fuel assembly with 3% and 5% ^{235}U enrichments and various burnups and cooling times. The model was patterned after the INL Mark IV electrorefiner, and it evaluates the distribution of active metals, noble metals, lanthanides, uranium, and transuranic elements. Radiation signatures were determined before and after electrorefining. Delayed gamma ARs for $^{134}Cs/^{137}Cs$, $^{134}Cs/^{154}Eu$, and $^{154}Eu/^{137}Cs$ were developed and assessed. The work suggests that delayed neutron and gamma signatures can be useful for electrorefining and pyroprocessing forensic analysis. [LANL]

Waste IPSC

The Waste team completed the groundwork needed to start building production-level software for modeling long-term performance of a radioactive waste disposal system in an engineered/geologic environment. This work consisted of three thrusts: a 1-D model with high fidelity, a 3-D high-resolution model with low fidelity, and an assessment of existing software to help design a path forward for the DOE-NE Office of Used Nuclear Fuel Disposition (UFD).

The 1-D work produced a software package called the Advanced Performance Assessment Code (APAC) based on SNL's Trilinos solver capabilities. The 3-D effort produced a software package called the Generic Performance Assessment Model (GPAM) based on SNL's "agile" Albany suite of software components. (Agile refers to an ongoing SNL code development effort to create reusable code that will accelerate the creation of new application codes.) The Waste team developed a plan to combine APAC and GPAM to provide the computation engine required by UFD. The design will ultimately provide new interfaces to connect additional features, including uncertainty quantification, graphical user interface, database, and chemistry. [SNL]

Fundamental Methods and Models

Modeling of defect sinks at grain boundaries in Fe-Cr and Fe-He systems

A framework was developed to quantify the migration (segregation) of point defects/elements to grain boundaries and to quantify uncertainty in atomic-level simulations, in particular for segregation of Cr and He to grain boundaries in irradiated steels (Fe-Cr systems with produced He). The approach was first applied to the interaction between point defects and grain boundaries in simple body-centered cubic Fe and then extended to more complex Fe-He and Fe-Cr systems.

Molecular statics simulations were used to generate a grain boundary structure database that contained about 170 grain boundaries with varying tilt and twist angles. Then, over 200,000 simulations were run to calculate formation and binding energies at all potential grain boundary sites within 15 Å of the boundary; the formation energies supply information about the likelihood of certain defect types to form, while the binding energies supply information about the force driving defect segregation.

The results indicated that both low- and high-angle grain boundaries were effective sinks (attractors) for point defects, but a few low-Σ grain boundaries were less effective sinks (Σ is a descriptor for interface fit). The formation energies depend on the local atomic structure and the distance from the boundary center. The strongest correlation for point defects occurred between the grain boundary energy and mean formation energy. The length scale of interaction between point defects and He and Cr segregation was found to be over a full lattice unit larger for self-interstitial atoms than for vacancies (mean of 6-7 Å vs. 10-11 Å for vacancies and interstitials, respectively). [PNNL]

Coupled Potts/phase-field modeling of gas bubble evolution

The evolution of Xe gas bubbles during post-irradiation annealing of UO_2 fuels can occur both by (1) migration and coalescence (M&C) driven by surface diffusion at the bubble/matrix interface when the bubbles are relatively small and (2) by Ostwald ripening (OR) via bulk diffusion as larger bubbles become larger at the expense of smaller bubbles. Previously, the Potts model was successfully used to simulate the evolution of Xe bubbles in a UO_2 matrix

by the M&C mechanism (see the Feb. 2012 *NEAMS Update*). However, the accuracy of the results can be further improved if concurrent processes—bulk diffusion and OR—could be modeled concurrently with the M&C mechanisms. The phase-field method is efficient for modeling bulk diffusion and OR and may also account for the effect of internal elastic stresses better.

Thus, a coupled Potts/phase-field simulation technique was developed for bubble evolution that can deal with both bulk diffusion and internal stresses. Initial coupled simulations were carried out using 2-D simulations using a 128 × 128 site grid. Fig. 5 shows six snapshots of bubble evolution with the coupled Potts/phase-field model. The image sequence corresponds to the order in which each method was alternately applied. Growth by bubble M&C is apparent in the Potts model results (a, c, and e), while the phase-field results show bubble growth by OR (b, d, and f). [ORNL]

Aging in Fe-Cr alloys

The aging behavior of Fe-Cr alloys was studied with phase-field modeling using relevant thermodynamic data and quantitative physical parameters. Fe-Cr alloys were chosen because they have a simple binary structure, reliable thermodynamic data, and widespread application in nuclear power plants. The evolution of dislocations was modeled with an eigenstrain approach in two dimensions; relevant thermodynamic data was derived from Thermo-Calc™.

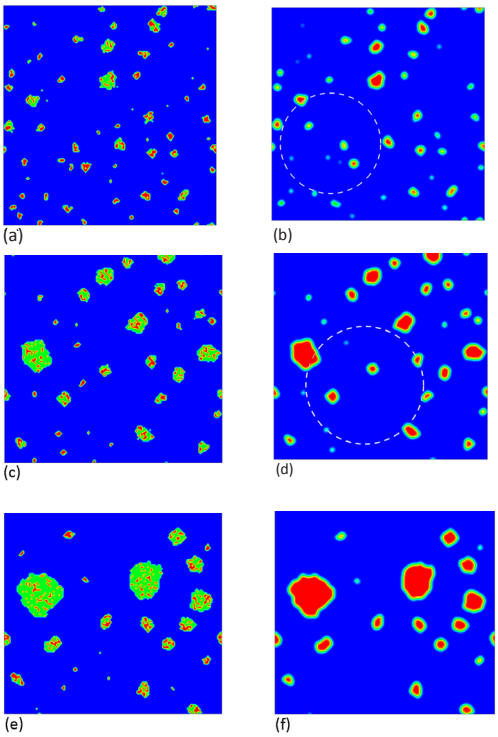


Fig. 5. Bubble evolution as simulated by the coupled Potts/phase-field model. The Potts model produced images a, c, and e, and the phase-field model was applied after each Potts iteration to produce images b, d, and f. The circles in images b and d identify locations where OR bubble growth is especially prominent.

Fig. 6 illustrates the predicted aging of Fe with 20 atomic % Cr due to the presence of two dislocation walls. The simulation treated the alloy as homogenous, that is, comprising only Fe and Cr. The early nucleation and growth of Cr precipitates at the wall dislocations, caused by heterogeneous nucleation and concentration flux, can be seen in (a) and (b) of Fig. 6. In time (c and d), further growth causes the formation of platelet Cr precipitates, and wall precipitates begin to coalesce. [INL]

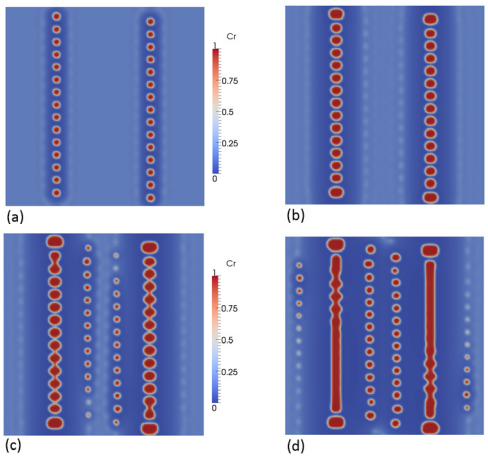


Fig. 6. Microstructural evolution behavior of Fe-Cr alloy with 20 atomic % Cr at 535K with two dislocation walls.

Development of a strength model for Fe-Ni-Cr alloys

A physics-based strength model for Fe-Ni-Cr alloys was completed. It accounts for grain boundary segregation and irradiation effects. The novel feature of this model is that it predicts the deformation behaviors of single crystals using dislocation density evolution mechanisms and continuum dislocation dynamics (CDD). The model was then extended to polycrystalline iron alloys by coupling CDD with polycrystalline crystal plasticity (CP).

Single-crystal Fe was modeled first and the results validated by experimental data and then compared with results from single-crystal constitutive equations developed for texture analysis (SCCE-T) and SCCE based on dislocation density (SCCE-D). The CDD model demonstrated higher fidelity than the other methods that describe anisotropic behaviors. The accuracy of CDD over the other models (Fig. 7) is due primarily to its use of physics-based laws for dislocation density evolution but also its ability to simulate dislocation defect interactions and cross-slip, which is very important when loading conditions activate only one primary slip mechanism. [PNNL]

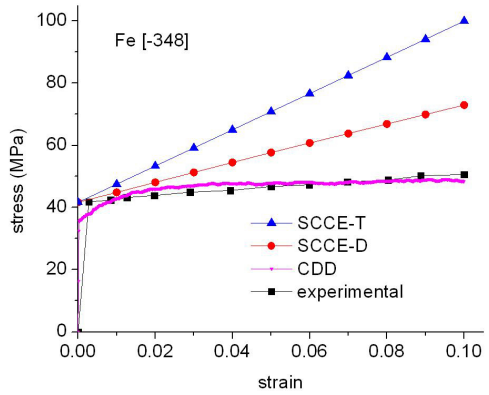


Fig. 7. Experimental and simulated stress/strain curves for single-crystal iron with uniaxial tensile loading along [-348] directions.

Verification, Validation, and Uncertainty Quantification

Uncertainty quantification

Inference addresses one of the critical problems for achieving predictive capabilities in NEAMS codes – the process of drawing conclusions about system performance given prior knowledge, code outputs, and experimental data. The VU team has focused on addressing rare event inference, which refers to making predictions about the probability of rare events often found in safety analyses.

One approach uses importance sampling, which preferentially draws samples from "important" regions of the input space and appropriately weights them to obtain unbiased estimates of statistics of interest, such as means or failure probabilities. The VU team completed and reported studies of importance sampling for black-box simulations, where the user has no a priori knowledge about where the important regions lie. Two approaches were developed: (1) percentile/quantile estimation and (2) Gaussian process adaptive importance sampling (see the May 2012 *NEAMS Update*). [LANL, SNL]

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. A comprehensive demonstration was recently completed.

The assessment of validation experiment datasets included:

- Flow in a cylinder array (Utah State University),
- High Reynolds number pipe flow (Bettis),
- Bluff bodies and cross flow (Bettis),
- VHTR lower plenum flow data (INL),
- European data on flow turbulence and combustion,
- Code verification benchmarks, and
- ANL CFD Max data. [ANL, Bettis Laboratory, INL, SNL]

The demonstration was based on the ANL CFD MAX experiment, including experimental data, associated design documents, metadata, videos of experiment and data measurement techniques, etc. The *GEN-IV Materials Handbook* infrastructure was leveraged to develop the following:

- Data warehouse structure,
- Network design and backup system,
- Relational database schema (from ANL MAX),
- System security and user account privileges,
- Homepage and user interface,
- User manual (ready for distribution),
- Warehousing of ANL MAX CFD data, and
- Initial data quality assessment. [INL, ORNL]

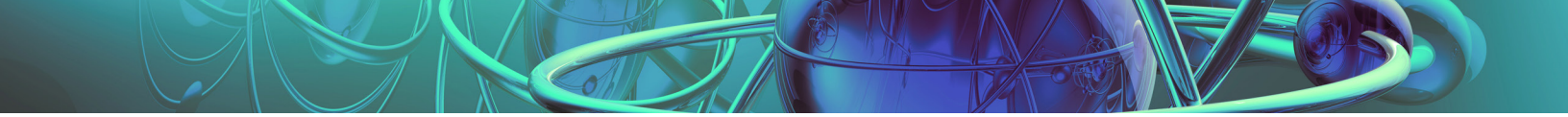
Capability Transfer

Early user program participants and other team members completed their evaluation activities and delivered reports summarizing their work during FY2012. The program succeeded in placing NEAMS software products (the BISON/MOOSE and AMP fuel performance codes and Nek5000 CFD code) into the hands of seven teams of users willing to provide constructive feedback to the development teams on the scientific and computational performance of the codes, their usability, and other factors. The early users focused their activities on a variety of validation problems, including a number of cases from the International Fuel Performance Experiments database. [ANL, INL, LANL, ORNL, TAMU]

A relationship between the NEAMS program and the Nuclear Regulatory Commission (NRC) was initiated. Recommendations for program-wide policies for software licensing, release, and distribution were provided in a final report. The report on software policies is expected to be completed in November. [ORNL]

Enabling Computational Technologies

The NEAMS Common Software Stack (NEAMS-CSS) was developed and tested on several Linux variants. NEAMS-CSS improves usability of NEAMS application codes by simplifying the process of obtaining, configuring, compiling, and installing supporting libraries and tools. NEAM-CSS was used to build MBM, AMP, and Nek5000, demonstrating that a single, common software installation can support multiple NEAMS application codes and that the installation process can be simplified to a single user command. [INL]



Static analysis was use to improve four codes relevant to NEAMS: AMP, MOAB, HDF5, and VisIt. Hundreds of defects were discovered and triaged. Over 250 of the most critical defects were fixed. Defects in AMP were fixed by AMP developers. Defects in MOAB, HDF5, and VisIt were fixed by the ECT team. In addition, the cyclomatic complexity measure was used to make an initial assessment of percent of functions of unusually high cyclomatic complexity (cyclomatic score >20).

Table 1 summarizes all analysis results. Note that defect rates of 1-2 defects per 1,000 lines of code (0.1-0.2%) are considered very good, particularly for Risk Level 4 codes, as defined in the NEAMS Software Quality Assurance Plan (SQAP). [LLNL]

The release of the NEAMS Integrated Computational Environment (NiCE) 2.0 was completed. The focus of this release was on developing and refining infrastructure to simultaneously support many users and codes with a common code base. Notable new capabilities are single and multiple simultaneous job launch with chained dependencies, problem setup with chained dependencies, and coupling of NiCE with VisIt. Several videos explaining how to use NiCE were also developed. [ORNL]

The NEAMS web site was completed and moved to a new domain name, neams.ne.anl.gov. The site content was partially re-organized in response to feedback from key stakeholders. A number of new features were added to the site back-end to facilitate the process of content update as the NEAMS program evolves.

The NEAMS SQAP was revised to version 1.6 to include NQA-1 compliance at all rigor levels. In addition, the compliance flow-down was adjusted to demonstrate compliance directly with DOE Order 414.1D, the Fuel Cycle Technologies QA Program Description, and NQA-1. The overarching NEAMS/ASCEM SQAIP was completed, demonstrating the potential for cost sharing of SQA processes. Review of the RELAP-7 SQA documentation suite was completed and work to combine the documents into a NEAMS-compliant SQAP was begun. [LLNL]

Preparations for an open source release of Cubit under the modified general public license are nearing completion. The initial release is planned for early FY2013. [SNL]

Technical Spotlight: Modeling precipitate nucleation

Nucleation in solid-state phase transitions, which describes the formation of a nuclei of a product phase in the parent phase, is a very difficult process to model. The formation of a critical nucleus is controlled by competition among several energies—bulk free energy decreases proportional to the nucleus' volume, interfacial energy increases proportional to the nucleus' interfacial area, and long-range interaction energies, such as elastic interactions—as well as thermal fluctuations (kinetic energy) that overcome the nucleation barrier. A critical nucleus is mathematically defined as a fluctuation of the concentration and/or order parameter that minimizes the free energy increase among all fluctuations leading to nucleation, i.e., the "saddle point" along the minimum energy path between the metastable initial phase represented by a local minimum in the free energy landscape and the equilibrium phase represented by the system minimum.

Thus, the formation of a critical nucleus requires overcoming a thermodynamic barrier. According to classical nucleation theory, the nucleation rate, which determines the particle density as well as the resultant microstructure, depends on the magnitude of the nucleation barrier. This barrier usually changes with time and space, as it is associated with the free energy of the system. Therefore, a nucleation model needs to correctly describe the energetic competition, nucleation barrier, and nucleation rate.

Table 1. Summary of error analyses for 4 NEAMS codes.

Code	No. of Lines	No. of Defects	Rate (%)	False Positives[a]	No. Triaged	No. Fixed	Complexity (%)[b]
MOAB	104,566	190	0.182	19 (10%)	94	40	6.93
HDF5	340,993	512	0.150	68 (13%)	367	70	28.1
AMP	103,727	296	0.199	17 (8%)	206	62	3.5
VisIt	1,195,082	2,756	0.185	≈20%	N/A	84	4.31
Total	1,744,368	3,754	0.179	–	667	256	–

[a] Problems identified by static analysis that were determined not to be actual defects.
[b] Percentage of functions with high cyclomatic complexity, an indicator of code maintenance difficulty.

The phase-field approach can correctly describe the energetic competition during microstructure evolution and predict the morphology and concentration profile or the order parameter profile of a critical nucleus. The morphology describes the nucleus structure (such as shape and size), the concentration profile describes the concentration distribution inside the nucleus, and order parameter profile describes the structure distribution. For structural phase transition, one order parameter can describe the information of a critical nucleus. For precipitation, two variables (concentration and order parameter) may be needed.

However, since the phase-field model assumes that energy minimization is the driving force of microstructure evolution, any nuclei smaller than the critical size will shrink. To overcome this, critical nuclei are randomly added into the simulation cell in the phase-field model. So a key question is, when and where should a critical nucleus be introduced during the simulation?

To answer this question, a general nucleation scheme based on the nucleation probability was employed. To test the scheme, the nucleation and growth of Cr-rich precipitates were simulated in Fe-Cr alloys. First, atomistic simulations determined the free energy density of Fe-Cr alloys, Cr mobility, and the interfacial gradient coefficient. Fig. 8 displays the free energy surface obtained from the atomistic simulations.

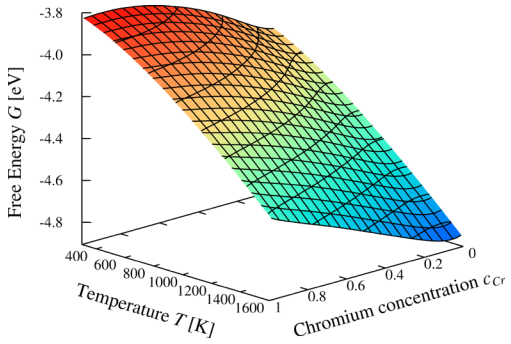


Fig. 8. Chemical free energy of Fe-Cr alloys.

Next, the interfacial energy of a flat interface and critical nucleus size were examined. Table 2 lists the interfacial energies of the flat interface calculated from the phase-field model. For comparison, the corresponding values from atomistic simulations are listed as well. The interface energies from the atomistic and phase-field simulations have the same temperature dependence, i.e., decrease with increasing temperature. However, the interfacial energy predicted from the phase-field model is larger than that from the atomistic simulations.

Table 2. Interfacial energies from simulations.

Temperature (K)	Phase field (J/m^2)	Atomistic (J/m^2)
300	0.58	0.405
400	0.56	0.391
500	0.53	0.376
600	0.50	0.361
700	0.49	0.344

The dependence of critical nucleus size on Cr concentration was obtained in a series of 3-D simulations. The simulations were performed in a 128 × 128 × 128 cubic simulation cell with periodic boundary conditions in all three directions. The grid size was 0.43 nm. In the simulations, Cr nuclei with a predetermined range of sizes were introduced randomly into the simulation cell. An added nucleus shrank when its size was smaller than the critical size but grew when its size was larger than the critical size. Fig. 9 summarizes the microstructure from the simulations, and Table 3 presents the predicted critical nucleus sizes from the modeling and from atomistic calculations. The critical nucleus sizes predicted by the phase-field model are in good agreement with those from atomistic simulations.

Table 3. Critical size of Cr precipitates in Fe-Cr alloys at 600 K.

Cr concentration	Diameter (nm)	
	Phase-field model	Atomistic theory
0.11	1.72	2.04
0.13	1.72	1.54
0.15	1.29	1.29
0.17	1.29	1.14
0.19	<1.08	1.02

The following assumptions were made in order to introduce nuclei into a 2-D 512 × 512 simulation cell:

- The phase transition driving force is proportional to local super-saturation.
- Nucleation takes place at the point of maximum super-saturation in the representative volume with a probability calculated by the classical nucleation rate.
- The representative volume is a circle of a size sufficient to allow Cr to reach its center, as determined by the Cr diffusivity and nucleation time.
- The probability of nucleation is zero once a Cr precipitate (nucleus) already exists or the amount of Cr in the representative volume is insufficient to form a critical nucleus.

The nucleation scheme was implemented as follows for each nucleation time:

1. Randomly choose a representative volume.
2. Calculate the nucleation probability at the point with the maximum Cr super-saturation in the volume.
3. Determine whether a nucleus should be generated at the potential nucleation site based on the probability (step 2), and introduce a nucleus if nucleation is likely.
4. Repeat steps 1 through 3 for n = V/Ω_0 times, where V is the volume of simulation cell and Ω_0 is the representative volume.

Nucleation and growth were simulated for different Cr concentrations at 600 K. In the simulations, the sizes of the introduced nuclei depended on the local Cr concentration (Table 3). Fig. 10 presents the spatial evolution of Cr precipitates over time. Fig. 11 plots the total volume of precipitates over time for three Cr concentrations (C_{Cr}). Nucleation rates over time are plotted in Fig. 12 for the same concentrations. The results show a clear trend: as the Cr concentration decreases, the nucleation rate decreases, but the nucleation period increases.

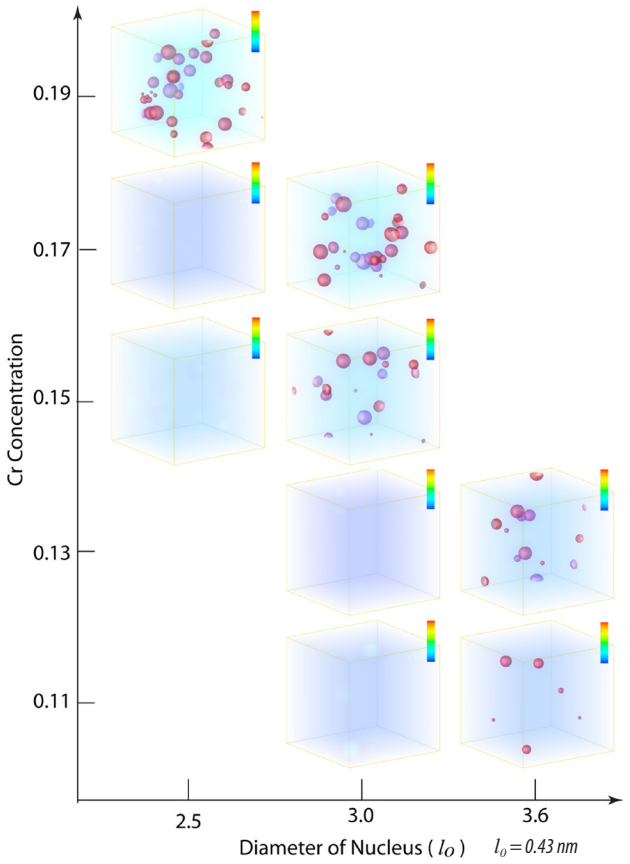


Fig. 9. Dependence of the microstructure on the nucleus size and average Cr concentration (expressed as a ratio where blue = 0 and red = 1). The red particles are Cr precipitates.

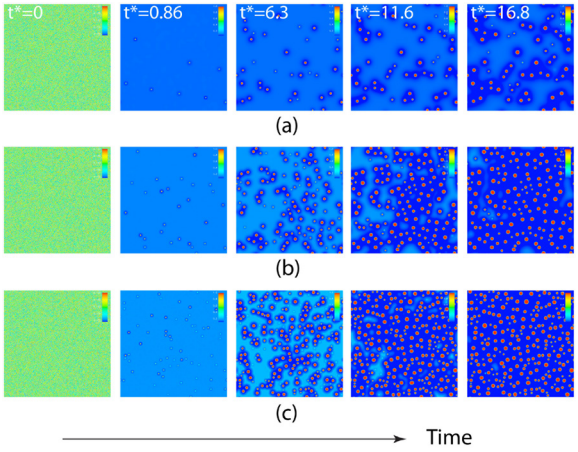


Fig. 10. Evolution and growth of Cr-rich precipitates in 2-D simulation, where (a) $C_{Cr} = 0.11$, (b) $C_{Cr} = 0.15$, and (c) $C_{Cr} = 0.19$. See Fig. 9 for key to coloring.

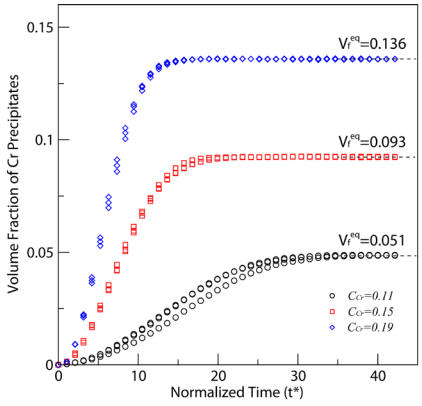


Fig. 11. Precipitate volume over time for three average C_{Cr} values.

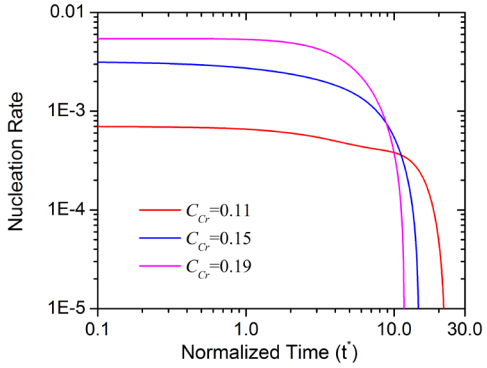


Fig. 12. Nucleation rate over time for three average C_{Cr} values at 600 K.

The Cr precipitate coarsening kinetics were also analyzed. The average precipitate radius and evolution time had a linear relationship, in agreement with the Lifshitz-Slyozov-Wagner theory, which describes the boundary between

small, shrinking particles and large, growing particles in slow-diffusion systems undergoing Ostwald ripening (see side bar on this page for further discussion of OR).

For the heterogeneous nucleation, the effect of the dislocation stress field on Cr segregation and nucleation was studied. The results show that edge dislocations are favored sites for Cr precipitate nucleation. Fig. 13 shows the predicted microstructural evolution behavior of Fe with 20 atomic % Cr at 535 K with the presence of an edge dislocation dipole.

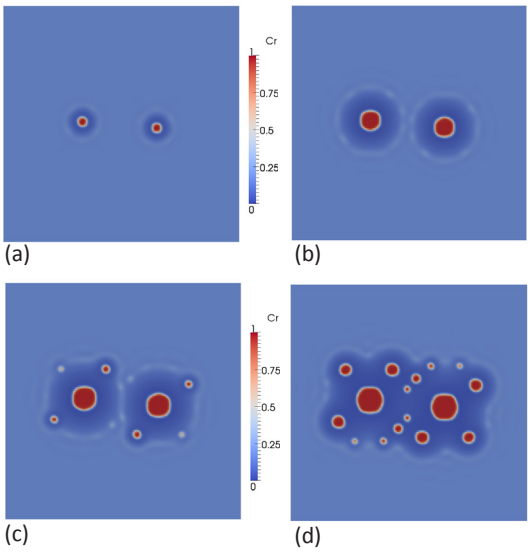


Fig. 13. Microstructural evolution of an Fe-Cr alloy with 20 atomic % Cr at 535 K with the presence of an edge dislocation dipole.

In summary, the simulations demonstrate the ability of phase-field models to simulate homogeneous and heterogeneous nucleation processes with minor modification to permit the initial formation of nuclei. Future work on benchmarking these results with experimental measurements and kinetic Monte Carlo simulations are needed to further validate and verify the mechanism-based generic phase field methodology.

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Nucleation Concepts

Ostwald ripening describes the tendency of atoms in an inhomogeneous structure to migrate from small to large clusters because atoms on the surface of a large cluster share bonds with more atoms than do atoms on the surface of a smaller cluster and are thus more stable.

Lifshitz-Slyozov-Wagner (LSW) theory of Ostwald ripening describes where the boundary is between small, shrinking particles and large, growing particles in slow-diffusion systems.

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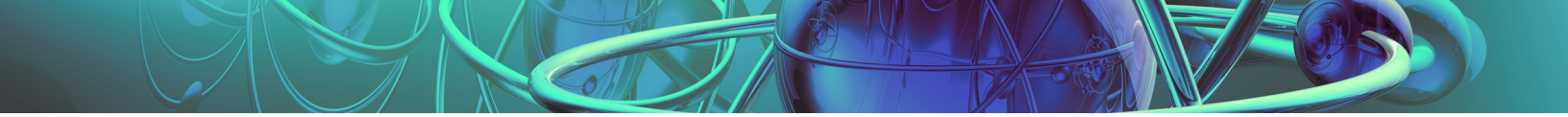

Recent and Upcoming Level 1 and 2 Milestones

Completed during this Quarter (July - September 2012)			
Milestone ID	**Description**	**Due Date**	**Finish Date**
M2MS-12AN0601123	Develop NEAMS project schedule for FY2013 and beyond	7/31/2012	9/28/2012*
M2MS-12IN0603338	Plan for RELAP-7 support of Mark 1 BWR major power level increase application	7/31/2012	7/26/2012
M2MS-12LL06090613	Perform static QA analysis of three NEAMS codes, including BISON	8/30/2012	8/28/2012
M2MS-12LA0602071	Demonstrate implementation of atomistic results into MBM simulation	8/31/2012	8/31/2012
M2MS-12OR0608117	Report recommendations for NEAMS engagement with the NRC	9/1/2012	9/1/2012
M2MS-12OR0604041	Complete separations plant-level model, including voloxidizer, dissolver, solvent extraction, and analysis	9/26/2012	9/28/2012
M2MS-12AN0601061	Complete extensible code for integrating separations system models	9/28/2012	9/28/2012
M2MS-12AN0603092	Implement Nek5000-based uRANS module	9/28/2012	10/1/2012
M2MS-12AN0603118	Complete initial development of the PROTEUS-2D1D module	9/28/2012	9/30/2012
M2MS-12IN0602111	Report on progress in phase field methods development	9/28/2012	9/27/2012
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	9/28/2012
M2MS-12LA0604021	Issue report on integrated separations plant model	9/28/2012	9/28/2012
M2MS-12OR0602032	Deliver AMP 2.0 to RSICC for release	9/28/2012	7/31/2012
M2MS-12PN0602121	Issue joint Fuels/FMM report on development of phase-field methods	9/28/2012	9/28/2012
M2MS-12PN0606016	Complete strength model for Fe-Ni-Cr system with grain boundary segregation and irradiation effects	9/28/2012	9/28/2012
M2MS-12SN0605061	Demonstrate simulations collaboratively defined with UFD Program	9/29/2012	9/27/2012
M2MS-12IN0603108	Demonstrate SHARP/PRONGHORN interoperability by modeling a prismatic core with the MOOSE platform	9/30/2012	9/26/2012
M2MS-12IN0602041	Release BISON to users for nominal simulation of UO_2 in an LWR	9/30/2012	9/7/2012
M2MS-12IN0602183	Demonstrate application of BISON to an accident-tolerant fuel design	9/30/2012	9/17/2012
M2MS-12IN06033310	Release RELAP-7 1.0	9/30/2012	6/4/2012
M2MS-12OR0609091	Release NiCE 2.0	9/30/2012	9/28/2012

*Completed on originally scheduled due date.

Coming Due during the Next Quarter (October–December 2012)			
Milestone ID	**Description**	**Due Date**	**Status**
M2MS-12AN0605116	Use the transportation logistics tool to conduct and report on simulations identified by UFD integration team	10/31/2012	On schedule
M2MS-12LL06031213	Report final results of seismic gap analysis workshop for SHARP	10/31/2012	Delayed (new due date)
M2MS-12AN0603081	Demonstrate SHARP framework support for a coupled physics problem	11/30/2012	Delayed (new due date)
M2MS-12AN0603279	Complete integrated multi-physics simulations of a BWR fuel assembly with PROTEUS, Nek5000, and AMP	11/30/2012	Delayed (new due date)*
M2MS-12OR0603021	Complete multi-physics simulation of fuel assembly with AMP	12/31/2012	On schedule
M2MS-12OR0605081	Demonstrate AMP for modeling UFD	12/31/2012	On schedule

*Delayed by unanticipated performance issues when using parallel computing platforms.