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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 October - December 2011 | February 2012

Quarterly Highlights

- Version 1.0 of AMP, the fuel assembly performance code, was tested on the JAGUAR supercomputer and released on November 1, 2011. See page 2 for a detailed discussion of this new simulation tool.
- A coolant sub-channel model and a preliminary UO_2 smeared-cracking model were implemented in BISON, the single-pin fuel code. Page 2 provides more information on how these models were developed and benchmarked.
- The Object Kinetic Monte Carlo model was implemented to account for nucleation events in meso-scale simulations. See page 3 for a discussion of the significance of this advance.

Blue Gene supercomputer.

- The SHARP neutronics module, PROTEUS, was expanded to be applicable to all types of reactors. See page 3 for a discussion of the importance of PROTEUS.
- A plan has been finalized for integrating the high-fidelity, three-dimensional reactor code SHARP with both the systems-level code RELAP7 and the fuel assembly code AMP. This is a new initiative (page 4).
- Work began to evaluate the applicability of AMP to the problem of dry storage of used fuel and to define a relevant problem to test the applicability. See page 5 for more discussion of this critical issue.
- A code to obtain phonon spectra from the force-constant matrix for a crystalline lattice has been completed. Page 6 describes this important bridge between sub-continuum and continuum phenomena.
- Benchmarking was begun on the meso-scale, finite-element fuels code MARMOT to validate its new variable splitting algorithm. See page 6.
- A very computationally demanding simulation of diffusion-driven nucleation of new microstructural features has been completed. Page 7 provides an explanation of the difficulty of this simulation.
- Experiments were conducted with deformed steel to validate a crystal plasticity finite-element code for body-centered cubic iron. See page 7.
- The Capability Transfer Roadmap was completed and published as an internal laboratory technical report. See page 8.
- The AMP fuel assembly code input generator was integrated into the NEAMS Integrated Computational Environment (NiCE). Page 9 provides more details on the planned NEAMS computing environment.
- The NEAMS program website (neams.energy.gov) is nearly ready to launch (page 9).

Coming Events

- **February 27-28 |** Reactor IPSC seismic initiative gap analysis workshop, LLNL
- **April 24-26 |** Principal investigator meeting, Washington, DC

Accomplishments

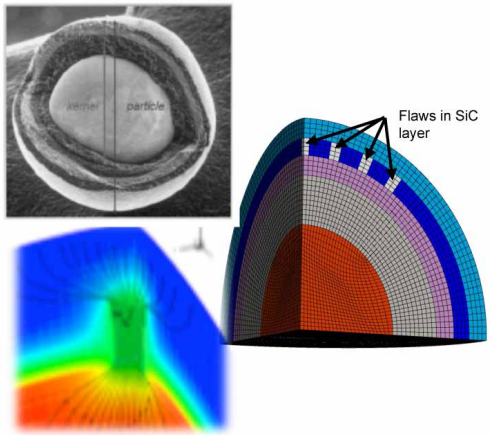
Fuels IPSC

Assembly-scale code development

AMP-1.0 was released through the Radiation Safety Information Computational Center on November 1, 2011; for this release, the Center independently tested the software on the JAGUAR supercomputer, a first. A presentation at the American Nuclear Society Winter Meeting demonstrated the solution transfer capabilities within AMP for accurately coupling structured and unstructured meshes for fuel pins and assemblies, which is necessary for AMP to interface with neutronics, thermal-hydraulics, and structural mechanics simulations in the future. Finally, one-way coupling of Denovo (neutron transport) and AMP (fuel performance) was completed and tested for a single fuel pin; testing at the fuel assembly scale is underway. [ORNL] [1]

Pin-scale code development

A single-pin coolant sub-channel model was implemented in BISON, the pin-scale simulation code. This enables BISON to compute the heat transfer coefficient and coolant temperature as a function of axial position along the fuel pin (rather than requiring this information to be supplied by the user). At present, the model is only applicable to pressurized water reactor coolant conditions, but modifications to include boiling water reactor (BWR) coolant conditions are in progress. A preliminary UO_2 thermal and irradiation creep model has been implemented in BISON and is undergoing testing and comparison with independent calculations; the model appears to be working as expected. Implementation of VPSC into BISON was initiated, which will allow for a more fundamental prediction of cladding creep.



Modeling of tristructural-isotropic fuel with BISON

A preliminary UO_2 fuel smeared-cracking model has been implemented in BISON. An initial test of the cracking model, integrated with the other fuel performance models already in BISON, included a simulation of the RISO GE7 bump test on rod ZX115. BISON results agreed well with experimental measurements of fuel centerline temperature, final fuel pin profile, and end-of-life fission gas release values. The results of this benchmarking were presented at the FUMEX III Benchmarking Meeting (Vienna, Austria) in December 2011, where results from other fuel performance codes performing the same calculation on the same pin were also presented; BISON results were extremely close to predictions made from other proven codes (e.g., TRANSURANUS, ENIGMA) for this experiment. [INL]

Meso-scale model development

Results from molecular dynamics (MD) simulations were used to calibrate the cohesive zone model under development for predicting discrete cracking in UO_2. The percolation model developed for fission gas release from grain boundaries, previously executed in two dimensions, was enhanced to allow the investigation of 3-D grain boundary networks. Composition-dependent mobility has been introduced into the phase field methodology and is now implemented within MARMOT.

Density functional theory (DFT) calculations were performed to parameterize a point defect model derived by CEA Cadarache (France) in order to describe diffusion of U in UO_2 samples that are close to the stoichiometric composition. The model captures diffusion via both vacancy and interstitial mechanisms. The DFT results show that the lowest migration barrier is obtained for a single vacancy mechanism along the <110> direction, which also provides the lowest total activation energy. The model predictions compare favorably to existing experimental data.

Molecular dynamics simulations for four different grain boundary (GB) orientations were completed for multiple temperatures, and Kapitza resistances have been calculated. This information is needed by meso-scale models that calculate thermal conductivity based on microstructure.

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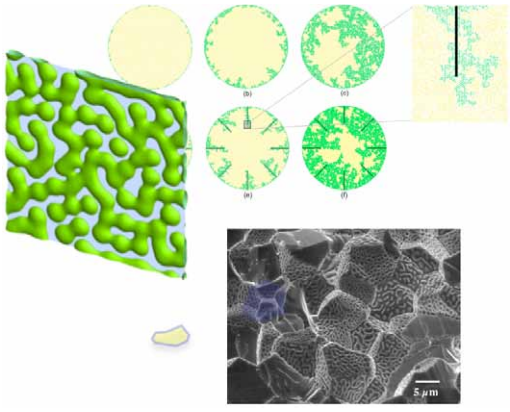
[1] The laboratories responsible for each task are identified in brackets at the end of its discussion. The NEAMS laboratories are Argonne National Laboratory (ANL), Idaho National Laboratory (INL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL).

Generic phase-field methods

At the November 2-3, 2011, coordination meeting, the Fuels IPSC and FMM teams developed a detailed plan for collaborating on generic phase field methods. The Fe-Cr system was selected for developing phase field methodologies for incorporating the effects of vacancy, gas bubble nucleation, variable cluster mobility, and lattice defects.

The Object Kinetic Monte Carlo approach has been implemented into a finite-difference phase-field code that includes cluster-size-dependent diffusivities and algorithms to model cluster coalescence. These efforts are expected to enable an efficient inclusion of the nucleation events into the phase-field modeling. Testing of a new implementation of a variable splitting algorithm, implemented in MARMOT, indicates that although the variable splitting algorithm offers faster execution time, the use of higher order Hermite elements converges faster. [INL]

Results have already been obtained from lower length scale calculations of Xe and vacancy diffusion coupled to meso-scale simulation of fission gas redistribution. A new approach was implemented in MARMOT to deal with singularities using the application of natural logarithms to describe the entropy of mixing for the Xe-U and Xe-U-Va fission gas redistribution models. Furthermore, as part of the development of algorithms for determining interfacial structures, a parallel search strategy to speed up Grand-Canonical Simulated Quenching simulations was implemented; the usefulness of the method has been demonstrated by recovering crystalline structures from initially amorphous configurations for an EAM metal (e.g., Cu or Fe). [LANL]



Simulation of gas bubble dynamics with MARMOT

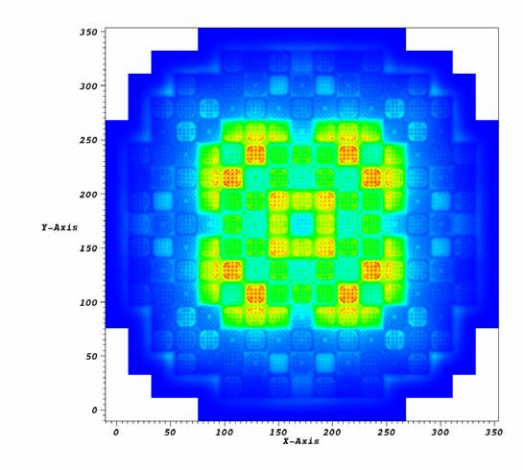
Reactor IPSC

The Reactor IPSC team is developing SHARP, a virtual reactor simulation suite of high-fidelity physics models and framework components that enables the user to evaluate the impact of design decisions on the performance and safety of nuclear reactors or nuclear reactor components.

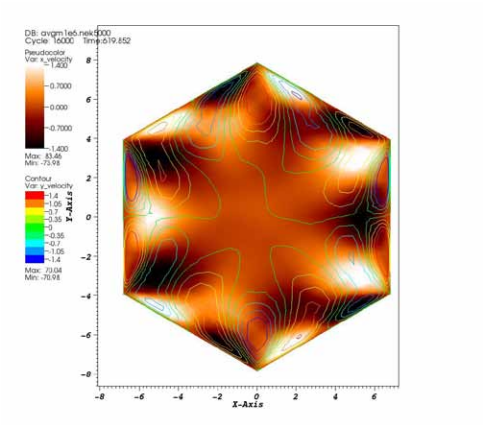
SHARP neutronics module development

The SHARP neutronics module, PROTEUS, includes neutron and gamma transport solvers and cross-section processing tools as well as the capability for depletion and fuel cycle analysis. The existing high-fidelity solver package was extended to be independent of reactor technology and demonstrated with 2-D MOC and Sn method simulations of LWR core configurations. Efforts to support verification and validation of the DeCART code, used as one reference solution method by the SHARP code development team, continued as part of an I-NERI collaboration with the Korean Atomic Energy Research Institute.

The development of an intermediate fidelity 2D-1D capability using 2D fully heterogeneous MOC in the radial direction coupled to 3D coarse-mesh transport was initiated. This module, called PROTEUS-2D1D, will provide heterogeneous geometry power distributions and local reaction rates at reduced computational cost in comparison to the fully 3-D exact geometry methods. Initial development of the underlying toolsets needed to construct the 2D-1D model directly from 3D CAD or mesh descriptions derived from the SHARP framework module, MOAB, has been completed. An initial 2D MOC capability, derived from the high-fidelity MOC solver of PROTEUS, was also implemented as the basis for PROTEUS-2D1D.



Fully heterogeneous predictions of thermal neutron flux in a hypothetical metal-oxide-fueled PWR



Predicted secondary (in-plane or transverse) flow velocity profiles in one of two MAX thermal mixing facility jets

SHARP thermal fluids module development

The SHARP thermal fluids module, Nek5000, provides solvers for multi-dimensional heat transfer and fluid dynamics. The Nek5000 module is an open source development project, with the current release available for download from the project web site. An improved checkpoint and restart capability has been introduced which retains sufficient data history to recreate the full state of an unsteady simulation. This reduces vulnerability of long-running simulations to unplanned machine outages, and reduces overall computational costs for long-running jobs which require job resubmission. Additionally, code documentation has been expanded to reflect frequently asked questions since its release in December 2010, and verification tests have been expanded to cover newly added capabilities.

Validation continues to be a high priority for the thermal fluids module. Additional experimental velocity profile measurements were collected in the MAX thermal mixing facility prior to shutdown for instrumentation upgrades to provide additional information on secondary flows in the two inlet jets. These data have been used to identify regions in which predictions and experiments do not agree for further analysis. Computational models describing the Russian SIBIRIA shear stress experiment were also constructed using the tools provided by the SHARP framework to support the next phase in the U.S.-Russian collaboration on advanced fluid dynamics code validation.

SHARP supporting elements development

The SHARP supporting elements include tools used for model development and libraries used to facilitate code coupling. The development of the MeshKit parallel mesh generation toolset continued, with MeshKit tools being used to generate initial mesh representations of the EBR-II fuel assembly that will be considered in coupled multi-physics demonstration calculations. Building on success from the previous quarter, the implementation of the MOAB framework module within the Nek5000 thermal fluids module was improved based on lessons learned from initial applications. As part of the overall transition from the research phase to the development phase, a prototype POD-based uncertainty quantification capability was demonstrated using a simple fluid flow solver. The methodology will be applied to Nek5000 simulations in the coming months.

New initiatives

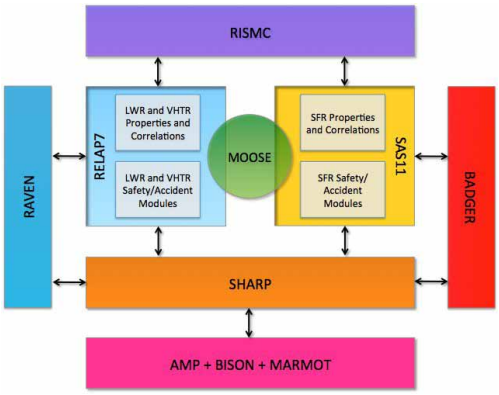
The Reactor IPSC has focused significant effort in the first quarter on the development of detailed work plans that reflect changes in scope and schedule and the introduction of several collaborative initiatives.

In December, SHARP and RELAP7 reactor system simulation code teams met in Denver to define plans for integration between SHARP components and RELAP7 and for collaborative development of system code components. The primary outcome of this meeting was a collaborative vision for the development of a suite of code components, which can be used for multi-scale simulation of reactor system

thermal hydraulics. Contributors to these joint efforts were identified and an initial group of SHARP developers will participate in a MOOSE framework workshop in early January to kick off the collaboration. More detailed collaboration plans will be included in the revised software development plans of both SHARP and RELAP7.

Meetings were held in November and December to accelerate plans for integration of the SHARP reactor simulation code suite and the AMP fuels performance code. The demonstration of the integrated capability is planned in two phases. The first phase will focus on an instrumented SFR fuel assembly from experiments completed in EBR-II to take advantage of immediate availability of data. The second phase will focus on a BWR fuel assembly identified in collaboration with industry collaborators.

The work scopes for all five labs participating in the NEAMS Seismic Initiative have been finalized, and development of a simplified but technically interesting model reactor design is in progress. A gap analysis workshop has been scheduled for February 27 and 28.



Data exchange paths between Reactor IPSC components

Separations and Safeguards IPSC

The Separations IPSC team has focused on continuing the development of the integrated plant model and the electrochemical model. The integrated plant model is being developed with input from the FCT Sep/WF campaign. For the electrochemical modeling effort, the team is using a template for collecting and aggregating information on various activities in the United States and in other countries. The template has been circulated among U.S. labs to obtain input for establishing a baseline of current capabilities, which will then be used to inform the development of a roadmap for future modeling efforts. The team is in discussions with the MPACT campaign as well as with related NNSA-managed activities. [ORNL, LANL]

Waste Forms IPSC

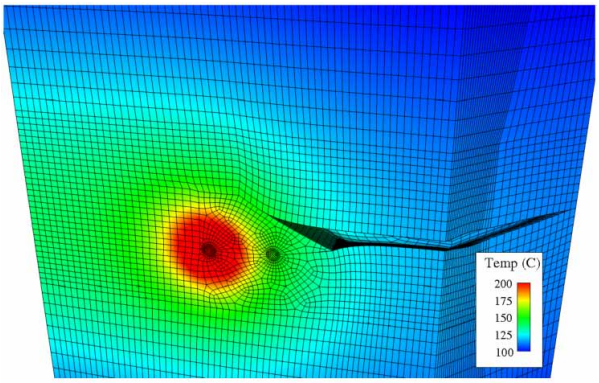
Very long-term storage of used fuel

Members of the Waste IPSC team attended the Used Fuel Disposition (UFD) Cladding Test Plan workshop in Las Vegas, NM. Presentations and discussions at the workshop included a tentative plan for the use of AMP to understand the sensitivity of parameters in a hydride model to the mechanical state of used nuclear fuel after centuries of dry-storage, definition of a demonstration test problem for very long-term storage of used nuclear fuel, and a proposed subsequent workshop to discuss NEAMS simulation plans and specific experiments that could be used to inform and gain an understanding of hydride models available from previous experiments.

Separately, team members participated in a 2-day meeting with ENERCON Federal Systems staff in Duluth, GA, on issues surrounding storage and transport of nuclear fuel.

Other Waste IPSC tasks

Funding changes to the Waste IPSC have reduced the work scope, with initial focus on development of a performance assessment scale model for coupled multiphysics processes in an engineered repository. An initial software framework is mostly complete, with some work remaining to fix minor bugs. Waste IPSC team members contributed to a software requirements document with a three-phase implementation plan; the plan is being reviewed by stakeholders in the UFD campaign. Implementation of the first phase of the plan has been initiated. The NEAMS deliverable report, "Progress toward Bridging from Atomistic to Continuum Modeling to Predict Nuclear Waste Glass Dissolution," was printed and distributed. [SNL]



Thermo-mechanics of salt

Fundamental Methods and Models

The FMM program element continues to focus on developing physics-based multi-scale material models and modeling methodologies for predicting how radiation affects the way that advanced fuels and structural materials respond to changes in temperature.

Ab initio atomic-scale and MD models

The FMM team is developing atomic-scale models to determine mechanistic-based quantitative values, such as formation energies and diffusion coefficients, for use at the continuum scale to predict the evolution of radiation-induced microstructure kinetics.

A new method is being developed for seamlessly coupling atomistic-scale models to continuum-scale (bulk) models using time-dependent Green's functions to accurately predict the dynamic response of the continuum region to any perturbation inside the atomistic region. During the first quarter of FY2012, the FMM team finished implementing a code whereby the force-constant matrix for a crystalline lattice was calculated and diagonalized to obtain phonon spectra, which were then applied to body-centered cubic (bcc) iron. The team has started to implement an iterative technique for obtaining the lowest energy eigenvectors of the sparse force constant matrix, which is applicable to larger supercells. [LLNL]

MD simulations are being focused on determining the atomic structures and stress field distributions of coherent twin (Σ3) GBs. The formation energies and binding energies of vacancy, interstitial, and He defects are also calculated using molecular static methods. The dimer method is being used to determine the migration barriers, the energy surfaces of the pathways of vacancies, interstitials, and He defects in GBs, which will provide an initial insight into the diffusion of defects in GB. The dimer method can accurately find transition states and does not require the end configurations, but it is a trial-and-error method and thus time-consuming. As soon as the saddle point searches are carried out, the rate for each transition mechanism will be estimated using harmonic transition state theory. These results are compared with those in bulk Fe, and will provide important atomic-level input for the phase field mode of the sink strength of GBs. [PNNL]

Continued MD simulation runs are filling the table of the critical stress vs. angle in the case of the interaction of edge dislocation with tilt grain boundaries for integration into the dislocation dynamics simulations in the hierarchical model framework. Some test structures with screw dislocations were produced to study the interaction of a screw dislocation with grain boundaries. [PNNL]

Meso-scale models

The overall objective of this task is to develop a suite of meso-scale modeling methods that can predict spatial and temporal evolutions of microstructure upon irradiation. Specifically, these models evaluate materials behavior at scales between molecular and bulk. The FFM team is collaborating with the Fuels IPSC team on generic phase field methods and models, and a coordination meeting was held at PNNL on November 2-3, 2011, to develop a detailed plan. [PNNL, INL, LANL]

The composition-dependent mobility in the formulism of the phase-field modeling is implemented into the MARMOT phase-field algorithm. Benchmarking was done for the MARMOT, finite element (FE)-based phase-field framework that utilizes the new implementation of the variable splitting algorithm. The results indicate that while the variable splitting algorithm executes about eight times faster, the use of higher-order Hermite elements offers faster convergence. A manuscript summarizing these results has been submitted for publication. Work is also continuing on implementing a J2 von-Mises' time-dependent and independent plasticity into the MARMOT phase-field algorithm. The current studies do not include adoptive meshing, which will be incorporated later. [INL]

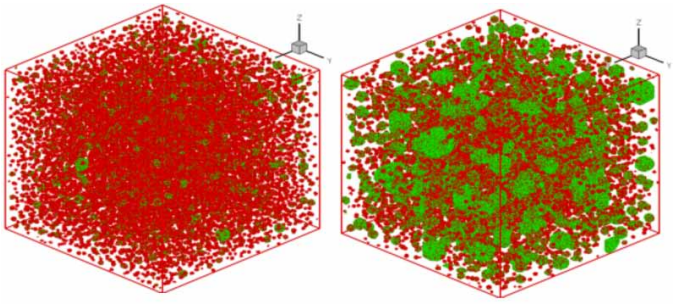
A phase-field model is being developed to predict the sink strength of GBs for interstitials and vacancies in

irradiated bcc Fe. The model takes into account (1) spatially dependent chemical-free energy for the grain boundaries; (2) one-dimensional random walk for describing higher diffusivity of Fe interstitials compared to vacancies; and (3) void nucleus generation, in addition to the common consideration of point defect (vacancy/interstitial) generation, diffusion and recombination, and long-range elastic interaction. The rate theory for comparison of GBs was surveyed. [PNNL]

A meso-scale benchmark problem on UO_2 post-irradiation annealing was identified for comparing the predictions of a stand-alone Potts model, a hybrid Potts-phase field model, a fast-Fourier transform based phase field model, and an FE-based phase field method. This future work will involve several laboratories. [PNNL, INL, SNL, ORNL]

The capability to model nucleation of new microstructural features, such as graining or a new phase, has been developed. This is a very significant accomplishment, as simulation of nucleation in the phase-field is computationally very demanding. While nucleation is robust in the Potts models, nucleation driven by diffusive processes is difficult. The FMM team has simulated a two-phase system undergoing a phase transition consisting of nucleating the lower-energy phase followed by growth of this new phase. The kinetics of this nucleation is controlled by the change in free energy due to formation of the new phase. The kinetics of the subsequent growth of the new phase is controlled by diffusion to obtain the stable compositions. The hybrid model treats this process very easily, and temperature gradients are being introduced into the hybrid model. [SNL]

The evolution of multiple gas bubbles is being extended to polycrystals with isotropic boundary energy and mobility to capture the influence of grain boundaries on the breakaway growth. The simulations were carried out in a 208 x 208 x 208 cell containing the polycrystalline grain structure with an initial gas content of 5%. The results clearly show that the presence of grain boundaries enhances the onset of breakaway growth. [ORNL]



Modeling of gas bubble nucleation

Hierarchical up-scaling methodology

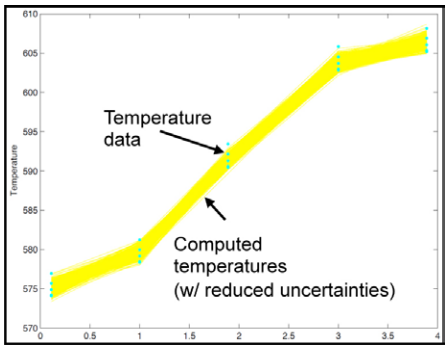
Development and validation continue on a hierarchical up-scaling methodology for predicting mechanical properties and deformation behavior of nuclear structural materials. In particular, work focused on including MD-generated mobilities into subsequent dislocation dynamics (DD) and crystal plasticity (CP) analyses, with a focus on modeling plastic deformation and strength in Fe-Ni-Cr systems and the effect of grain boundaries and strengthening mechanisms with irradiation effects. The objective here is to construct a deformation map for the flow stress as a function of composition, defect density irradiation dose (defect density: Frank-loops and or helium bubbles), and temperature. So far, 10 cases have been run for a-Fe, Fe-5%Ni, Fe-10Ni, Fe-15%Ni, and Fe-20Ni at 300 K, with one set of irradiation defect density (Frank Loops) of $2.4 \times 10^{22}/m^3$. [PNNL]

Development of a CP FE code for bcc Fe (UMAT in ABAQUS) was completed and runs were begun using either 12- or 24-slip systems. To verify the code, a series of electron backscatter diffraction (EBSD) experiments were run on IF steel deformed in tension to 12 or 17%. The simulation results were compared with the IF steel experimental data to show von Mises effective stresses as compared with GND density measurements from EBSD data. The team began to develop a DD CP model with long-range and GB effects and to introduce additional activation energy into the rate equation for mobile dislocations in the vicinity of internal interfaces. This energy barrier is derived from the assumption of a thermally activated dislocation penetration event through a GB with a specific geometry. [PNNL]

Various optimization methods were implemented, including simulated annealing with a different cooling schedule and generic algorithm on a statistically stable representative volume element buildup, enabling reconstruction of a large 3-D domain image. A multi-regression nonlinear

simulated annealing is also being developed and implemented. The team has identified the framework on hierarchical up-scaling of mechanical deformation of Fe-Cr stainless steel using CP informed by DD. Hierarchical up-scaling of He diffusion in Fe-Cr steel at a GB resolution was developed and implemented by combining the discrete MD and continuous FE methods. [PNNL]

Recent progress includes publishing the VVUQ-for-Subcontinuum milestone report (SNL Report SAND2011-9257), which describes strategies for developing verification and validation plans tailored to subcontinuum-scale activities. Initial meetings were held with FMM modelers to discuss the structure of the calculations, lay the groundwork for preparing the plans, and coordinate efforts. [SNL, PNNL]



Model Calibration

Verification, Validation, and Uncertainty Quantification (VU)

To support the NE-KAMS project, the VU team assessed existing databases that might be leveraged. A meeting held at PNNL to evaluate VELO concluded that numerous components of VELO can be used for NE-KAMS, particularly with respect to workflow. Evaluations were also performed of the NDMASS (NGNP) knowledge/collaboration suite for modeling and simulation and the GEN-IV Materials Handbook; both tool sets have numerous applications for NE-KAMS. [PNNL]

The VU team provided support to the Fuels IPSC team in several areas. First, a journal article is being drafted that summarizes sensitivity, calibration, and validation studies conducted with the LIFE-4 and FRAPCON codes. Work began on an initial sensitivity study with the FEAST-Metal code. The purpose is to reduce the initial parameter set for follow-on calibration and validation studies. The team's priority for FY2012 is to work with the MOOSE/BISON code suite and applications for development of new VU capabilities in two areas: (1) rare event inference and (2) predictive maturity assessments. Initial activities have included establishing access to MOOSE/BISON and identification of other applications needed for the effort.

Other accomplishments include progress in developing new "importance sampling" methods that exhibit improvements (i.e., much fewer number of samples required) over traditional approaches in rare event inference applications and participation in the LWR Sustainability Risk-Informed Safety Margin Characterization (RISMC) working group meeting held in Albuquerque, NM, on November 8-10, 2011, to discuss the role of NEAMS support of R7 and UQ algorithms that may be of interest to the RISMC group.

Capability Transfer (CT)

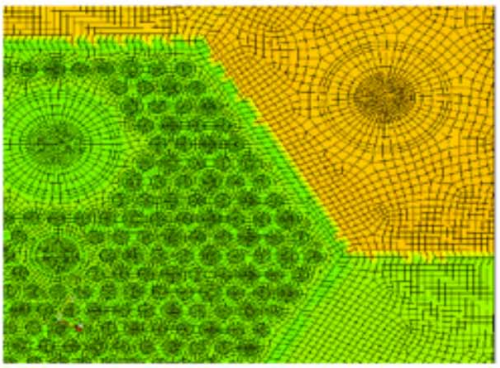
The CT team completed work on the CT roadmap and published it as an ORNL technical report for archival purposes. New work begun in FY2012 included initiating the contracting process for Texas A&M University's Early User activities, discussions related to eventual software distribution, and discussions to engage the Nuclear Regulatory Commission, the key regulator of commercial nuclear energy systems. The CT team has contacted staff in the Office of Regulatory Research, where most of the Commission's modeling and simulation activities are based, as well as the ORNL Export Control Office to gain a better understanding of how export control issues will affect software distribution. [ORNL]

Enabling Computational Technologies (ECT)

The purpose of the ECT element is to leverage and share with the IPSC elements common software investments, such as frameworks (NiCE), mesh generation (CUBIT), and visualization (VisIt); common software development know-how, such as DOE-compliant software quality assurance (SQA) processes and tools; and common resources, such as computer platforms, collaborative web interactions, and a NEAMS web presence.

The NiCE development team worked with the Fuels and Reactors IPSCs to develop NiCE 2.0 plug-ins for their respective codes and strategies for handling geometries and meshes. The NiCE team is also developing extensive

documentation and deployment infrastructure to make NiCE easier to use. NiCE 2.0 is on schedule for its planned June 2012 release. Demonstration releases are planned between now and June, starting in late January 2012. In early February, the team plans to release a demonstration copy to the NEAMS community with plug-ins for the export control codes.



Simulation of complex meshes

In preparation for NE-wide adoption of the NEAMS SQA plans (SQAPs), the NEAMS SQAP was revised based on input from engaging DOE NE and FCT stakeholders and a new version, 1.5, was prepared. An overall NEAMS/ASCEM SQA document was drafted to describe how program-specific practices guide software development and promote compliance with their respective SQAP.

A strategic plan for a NEAMS program website (neams.energy.gov) was developed, reviewed, and approved by various stakeholders. A Redmine site for collaborative web development was set up and accounts were established for key stakeholders, with the option to possibly include all NEAMS teams. An ECT-specific web site based on the FY11 work scope was launched as neamsweb.ne.anl.gov to serve primarily as a test-bed for new content and functionality destined for neams.energy.gov.

Management and Integration

During the first quarter of fiscal year (FY) 2012, the management team:

- Conducted the annual program review meeting during mid-December to present technical progress to a broad audience of stakeholders, including national laboratory staff, federal staff, and industry representatives. [ANL]
- Developed FY2012 plans for exploiting an end-of-year in-flux of FY2011 funds. The revised FY2012 work scope includes several 1-year initiatives
- Revised the FY2012 work scope to mitigate the unavailability of FY2012 funding. Changes in work scope are complicated by interdependencies among the various tasks and milestones. In many cases, tasks have been delayed because of the lack of spending authorization. Management is reviewing delayed tasks to identify those on the critical path.
- Participated in the first of a series of reviews by an external ad-hoc subcommittee of the Nuclear Energy Advisory Committee commissioned by the Assistant Secretary Nuclear Energy.
- Oversaw the transition of technical progress tracking and reporting to a new project management system, Program Information Collection System: Nuclear Energy (PICS:NE). Because of funding authorization dependencies, the technical work is somewhat disconnected from the system designed to track it. This will improve as cost account managers learn PICS, the budget cycle approaches mid-year, and leadership provides improved guidance for entering and extracting PICS:NE data.
- Oversaw the writing and production of this report, which will be issued quarterly.

Technical Spotlight: What Do Mongolian Barbeque and Software Quality Have in Common?

In the NEAMS program, the software quality philosophy is to make the software "experience" better on three levels—the software itself, the user and stakeholder experiences with the software, and the experiences of the scientists building the software.

Past experiences and lessons learned have shown that prescriptive one-size-fits-all software quality approaches fail to achieve wide-spread adoption. For research codes,

a risk-based, graded approach works best to balance agility with discipline. Risk grading allows appropriate software process rigor to be applied based on the severity of the potential consequences of failure.

In NEAMS, risk grading of a given software code is accomplished by using a graded scale with inputs from the IPSC team leads. The risk grading process is straightforward—a member of the Software Quality Engineering (SQE) team conducts a 30-minute interview and uses the responses to produce a risk score for the software. The higher the risk score, the more rigorous the required software development and management processes. Risk grading is repeated as the codes mature and may also be used for higher-consequence decision-making, licensing, or safety-related applications. However, risk grading is only part of the story.

Prescribing that simulation scientists use a particular software process or tool is considered a "push" strategy of requirements adoption. Conversely, allowing scientists to choose from a number of software development tools and process solutions that are compliant with a given risk level is the preferred "pull" strategy of adoption. The pull strategy enables the simulation scientists to choose from among the best, and probably more attractive, contemporary processes and tools that meet their needs. It also institutionalizes the commitment to software quality. If the tool or process is not going to make the scientist's development experience better, it is likely to be resisted or bypassed.

Pull strategies have been very successful in other industries, such as the music and restaurant industries. Many consumers have demonstrated a preference to choosing individual songs to download to their MP3 player, as opposed to having to purchase complete, more expensive albums that include the songs that they want. A similar experience is offered by the Mongolian Grill™, where you pick the ingredients that best suit your taste to create your meal. In other words, greater freedom of choice is an effective way to improve your listening or dining experience. With software processes and tools, involving the scientists in the selection process helps ensure their commitment to the outcome and increases their satisfaction levels.

Therefore, the SQE team is taking a pull approach to software quality, which is more challenging to implement than simply requiring people to follow rules, monitoring compliance, and imposing penalties for noncompliance (commonly referred to as "audit and punish"). To be successful, the pull approach requires a strong commitment from NEAMS management and NEAMS hands-on practitioners. Predictive uses of the codes, high-performance computing, and uncertainty quantification are all putting higher demands on software quality. Software quality approaches that were acceptable even five years ago would fall short by today's software quality standards.

The SQE team provides support and tools for continuous improvement of NEAMS software. However, most of the key commitment comes from the NEAMS code teams. The SQE team recently completed work on an on-line expert system to help NEAMS developers find and select practices and tools. The name of the website–www.silverbuckshot.net –is derived from the fact that there is not a single silver bullet for building better software. Instead, better software involves a number of processes and tools that, when used by competent practitioners on software problems, tend to make big improvements.

The NEAMS SQA effort also brings contemporary software quality tools to the table. For instance, the Klocwork® static analyzer scans source code for 1,600 types of known problems and identifies them so they can be fixed. Klocwork uses heuristics and finds problems like uninitialized variables, array out of bounds, memory leaks, tainted inputs, and unreachable code. A report visualization is shown in Figure 1.

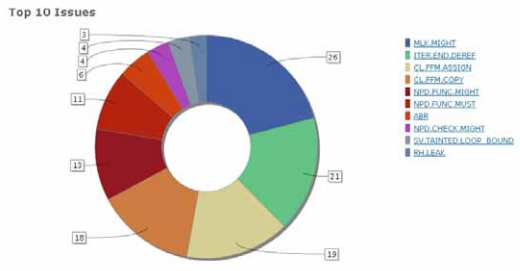


Figure 1: Visualization of results from a static analysis of a NEAMS code using Klocwork

Another new tool the SQE team has rolled out is Infer, which runs proof-of-correctness separation logic specifications against code memory manipulations to literally provide a one-page insight, called an x-ray diagram,

into the code's quality, as shown in Figure 2. Not only can the tools be used on new code, but they also are effective for legacy and open-source codes that support NEAMS simulation tools.

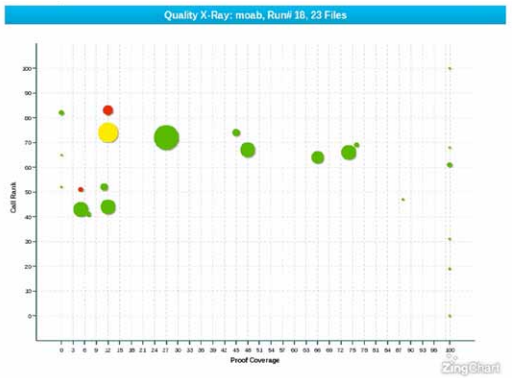
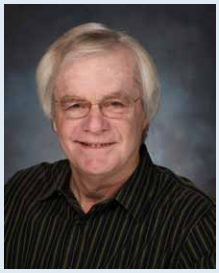


Figure 2: An X-ray visualization of memory utilization of a NEAMS code



About the author: Greg Pope has more than 40 years of experience developing software in the commercial and government sectors. Prior to joining LLNL in 2001, Greg founded and ran a software testing company, patented automated software testing tools, and held management and technical positions involving mission-critical testing of military systems and development of software code for avionics and aerospace. Greg has given industry keynote addresses, written technical papers, and taught internationally on software quality.

Recent and Upcoming Level 1 and 2 Milestones

Completed during this Quarter			
Milestone ID	Milestone Title	Due Date	Actual Finish
M2MS-12AN0601013	Hold fall principal investigator (PI) meeting	11/1/2011	10/13/2011

Coming Due during the Next Quarter			
Milestone ID	Milestone Title	Due Date	Status
M2MS-12OR0602031	Demonstrate AMP coupling to neutronics code on full LWR assembly	1/31/2012	On schedule
M2MS-12LL0603123	Submit seismic analysis interim status report	3/1/2012	On schedule
M2MS-12AN0603201	Establish representative assembly for multi-physics demonstrations	1/31/2012	On schedule

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NEAMS Overview

The Advanced Modeling and Simulation Office within the DOE Office of Nuclear Energy (NE) has been charged with revolutionizing the design tools used to build nuclear power plants during the next 10 years. To accomplish this, the DOE has brought together the national laboratories, U.S. universities, and the nuclear energy industry to establish the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program.

The mission of NEAMS is to modernize computer modeling of nuclear energy systems and improve the fidelity and validity of modeling results using contemporary software environments and high-performance computers. NEAMS will create a set of engineering-level codes aimed at designing and analyzing the performance and safety of nuclear power plants and reactor fuels. The truly predictive nature of these codes will be achieved by modeling the governing phenomena at the spatial and temporal scales that dominate the behavior. These codes will be executed within a simulation environment that orchestrates code integration with respect to spatial meshing, computational resources, and execution to give the user a common "look and feel" for setting up problems and displaying results.

NEAMS is building upon a suite of existing simulation tools, including those developed by the federal Scientific Discovery through Advanced Computing and Advanced Simulation and Computing programs. NEAMS also draws upon existing simulation tools for materials and nuclear systems, although many of these are limited in terms of scale, applicability, and portability (their ability to be integrated into contemporary software and hardware architectures).

NEAMS investments have directly and indirectly supported additional NE research and development programs, including those devoted to waste repositories, safeguarded separations systems, and long-term storage of used nuclear fuel.

NEAMS is organized into two broad efforts, each comprising four elements.

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Integrated Performance and Safety Codes (IPSCs)

Fuels IPSC: develop models for fuel pins and assemblies that simulate and predict how their mechanical properties and chemistry evolve over time in a reactor core's extreme environment.

Reactors IPSC: develop component, full-core, and systems-level simulation tools to evaluate overall reactor performance and safety. Important phenomena include thermal hydraulics, neutronics, and structural mechanics in both normal and off-normal conditions.

Separations and Safeguards IPSC: develop models to simulate spent nuclear fuel processing to reduce volume, recover useful fuel, isolate dangerous by-products, and prevent loss and diversion of fissile material.

Waste Forms IPSC: develop tools to evaluate the transportation and storage logistics options for nuclear waste, as well as the long-term performance of nuclear waste forms in engineered and geologic environments.

Cross-cutting Methods and Tools

Fundamental Methods and Models (FMM): develop physics-based multi-scale modeling methods for predicting how advanced fuels and structural materials respond to irradiation.

Verification, Validation, and Uncertainty Quantification (VU): develop tools for assessing the predictability of NEAMS products and assuring their robustness.

Capability Transfer (CT): engage the user community to promote and refine NEAMS products, as well as the regulatory community to gain acceptance of data generated with NEAMS products.

Enabling Computational Technologies (ECT): enable common simulation components, such as mesh generation and visualization; develop web-based collaboration tools, including a NEAMS web site; and facilitate compliance with software quality assurance (SQA) requirements.