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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 January – March 2012

Published May 2012

Quarterly Highlights

- The integration of Denovo and AMP was demonstrated in an AMP simulation of the thermo-mechanics of a complete fuel assembly (page 2).
- Bison was enhanced with a mechanistic fuel cracking model (page 2).
- Mechanistic algorithms were incorporated into various lower-length-scale models to represent fission gases and dislocations in UO2 fuels (page 3).
- Marmot was improved to allow faster testing of meso-scale models using larger problem domains (page 3).
- Component models of reactor piping were developed for use in Relap-7 (page 3).
- The mesh generator of Proteus was updated to accept a mesh specification from Moose and equations were formulated for the intermediate-fidelity Proteus-2D1D module (pages 3 and 4; also see the technical spotlight starting on page 9).
- A new pressure solver was implemented in Nek5000 and demonstrated to work 2.5 times faster than the previous solver (page 4).
- Work continued on volume-holdup models for two fuel reprocessing operations: voloxidation and dissolution (pages 4 and 5).
- Progress was made on a pyroprocessing model and the characterization of pyroprocessing emission signatures (page 5).
- A new 1D groundwater waste transport code was delivered to the used fuel disposition (UFD) campaign (page 5).
- Efforts on waste form modeling included empirical simulation of sodium-borosilicate glass compositions (page 5).
- The Waste team developed three prototypes for modeling hydride reorientation in fuel cladding during very long-term fuel storage (page 5).
- A benchmark demonstration problem (fission gas bubble growth) was modeled to evaluate the capabilities of different meso-scale numerical methods (page 6).
- Work continued on a hierarchical up-scaling framework to model structural materials by directly coupling dislocation dynamics and crystal plasticity (page 6).
- New “importance sampling” methods were developed and demonstrated to reduce the computational cost of rare-event inference (page 7).
- The survey and evaluation of existing data and knowledge bases was updated for NE-KAMS (page 7).
- The NEAMS Early User Program was launched (page 8).
- The Nuclear Regulatory Commission (NRC) Office of Regulatory Research was introduced to the NEAMS program (page 8).
- The NEAMS overall software quality assurance plan (SQAP) was revised to version 1.5 (page 8).
- Work continued on NiCE and its plug-ins and other utilities, such as Cubit and VisIt (page 8).

Coming Events

- **May 22 -23 |** Nuclear Energy Advisory Council review of NEAMS, Washington, DC

Accomplishments

Fuels IPSC

Assembly-scale code development

The Fuel IPSC team tested the integration of a radiation transport code (Denovo) with AMP by modeling a full-size 17×17 Westinghouse pressurized water reactor (PWR) fuel assembly. The tests demonstrated the ability to model the thermo-mechanics of an entire fuel assembly using the three-dimensional power distribution provided by a separate, concurrent simulation. In this demonstration, the coupling of the two codes was "one-way" in that AMP used real-time information supplied by Denovo, but Denovo did not use AMP results. The key to the integration is a novel scheme for mapping Denovo's coarse power distribution mesh to the fine mesh needed for the thermo-mechanics calculation in AMP while limiting Denovo's use of computing resources. The results (Fig. 1) give important insight into locations within the fuel assembly where the assumption of axisymmetric power used in many existing fuel performance codes inaccurately represents the power distribution. [ORNL]*

Pin-scale code development

A mechanistic, smeared fuel cracking model for UO_2 has been implemented in Bison and tested with simulations of IFA-432 Rod 1, an experiment conducted in the Halden reactor. ("Smeared" refers to the fact that cracks are represented in aggregate, rather than as discrete, individual cracks.) Failure to account for fuel cracking can result in temperature predictions that are off by as much as 200°C at beginning-of-life. Excellent agreement between prediction and measurement is obtained when an empirical correlation for fuel relocation is used (as in the NRC's FRAPCON), which was expected, since the empirical correlation was fit to data that included this experiment; this result is important, however, in that it indicated that Bison predictions are at least as good as those of FRAPCON for the same empirical models but without the need to calibrate the model to experimental data. [INL]

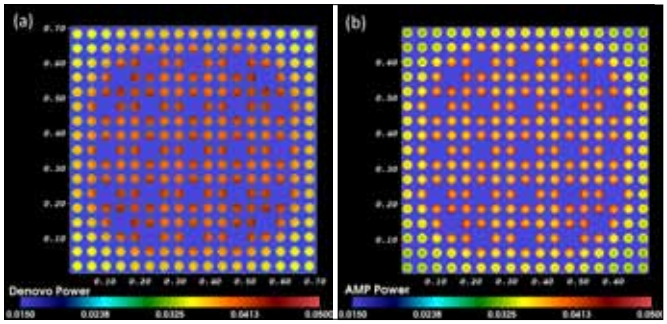
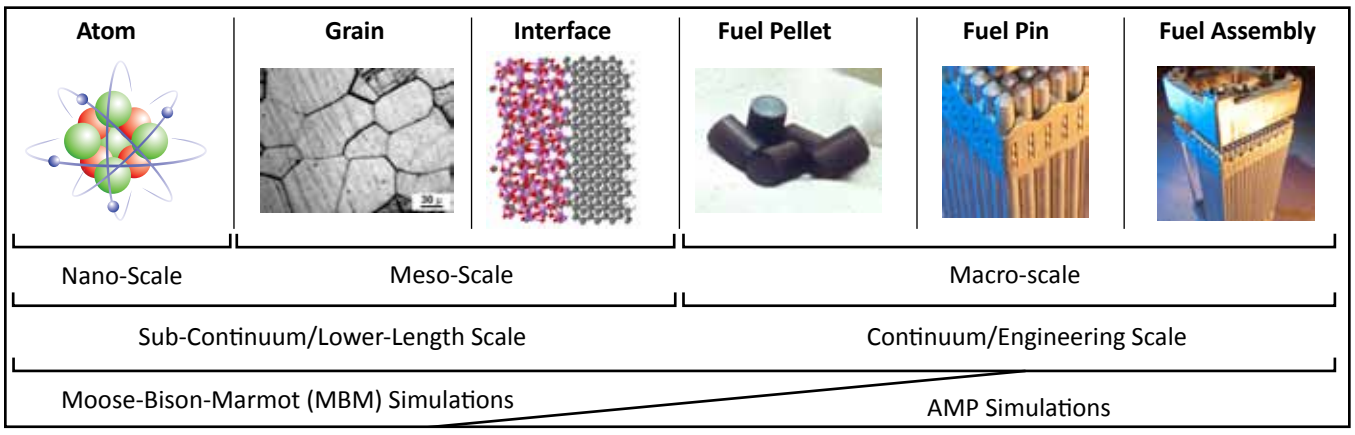


Fig. 1. Translation of Denovo output to AMP: (a) Cross section of fuel assembly showing Denovo-calculated power distribution. (b) The same data represented in the AMP mesh

A model for calculating the radial power profile in a fuel pin, local burnup, and local concentrations of important fission products was also completed in Bison. This model is critical for making accurate fuel temperature predictions in thermal reactor fuels of all types, since a failure to account for the flux depression inside a fuel pin can amount to over-prediction of temperature by several hundred degrees. Knowledge of local concentrations of important fission products is vital input for modeling many fuel behavior models, especially swelling and gas release. [INL]

*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 fuel simulations



Finally, models for thermal and irradiation creep of UO_2 fuel were implemented in Bison. [INL]

Lower-length-scale model development

To develop mechanistic models for fuel thermal conductivity, the Fuel team used supercells up to 55 nm long to determine the thermal conductivity of UO_2 with Xe incorporated. Atomistic simulations were used to determine thermal resistance values for four different types of grain boundaries, and these values have been used in meso-scale simulations of heat transport through representative fuel microstructures. [LANL]

Density functional theory techniques, previously applied to diffusion of Xe in UO_2, have now been extended to Kr. Thus, both major gaseous fission products are now included in the simulations, which have identified the transport mechanism as being vacancy mediated. Activation energies have been calculated for each gas element, and these values are now used in Marmot. [LANL]

A phase-field model was used to perform parametric studies of fuel restructuring due to void and grain boundary migration under temperature and stress. These studies are elucidating the roles of bulk diffusion, surface diffusion, grain boundary mobility, and grain size on microstructure evolution. Atomistic studies are underway to understand the interaction of dislocations with He bubbles of varied sizes and pressures. Results indicate that, except for very large bubbles under high pressure, bubbles are not obstacles for screw dislocations. [INL]

The following modifications to Marmot were initiated: the fully-coupled solution algorithm in the phase-field code is being replaced with a staggered solution algorithm, the new algorithm was tested for Allen-Cahn formalism (in which the order parameters are not conserved) and is being extended to Cahn-Hilliard formalism, and the overall structure of Marmot was modified to make it easier to develop and implement new models. Now, generic kernels for the split solution to the Cahn-Hilliard formalism have been introduced so that a model can be created by only coding in the problem-specific chemical potential. [INL]

Reactor IPSC

The NEAMS Reactor IPSC team is developing two major modeling tools, Relap-7 and Sharp. Either code suite can be used as a standalone analysis tool, or Sharp can be used to augment experimental data to increase the accuracy and broaden the applicability of Relap-7.

Relap-7 development

Relap-7 provides engineering-scale models of basic reactor components for full plant system performance and safety analysis. Relap-7 utilizes one-dimensional and zero-dimensional models for the prediction of fluid flow with phase change, conjugate heat transfer, core power with reactivity feedback, and structural response to pressure and heat.

During the second quarter, the Reactor team drafted software development guidance documents and a software quality assurance plan and developed component models for pipe flows, pipe junctions, and basic reactor core channels using the Moose code development framework. These components are now being tested for inclusion in a simplified reactor model.

Sharp development

The Sharp toolset includes modules for prediction of neutronics (neutron behavior), fluid flow, conjugate heat transfer, and structural mechanics, as well as libraries and components to support module development and integration.

Proteus development

The Sharp neutronics module, Proteus, includes neutron and gamma transport solvers, cross-section processing tools, and tools for depletion and fuel cycle analysis. Efforts in the second quarter focused on three major priorities: multi-physics integration, intermediate-fidelity tool development, and demonstrations of applicability.

Integration of the second-order, discrete ordinates (Sn method) solver of Proteus with the latest version of the MOAB framework (which represents and evaluates mesh data) was initiated to enable its use for multi-physics analysis. With these updates, Proteus can obtain the mesh specification from the MOAB framework and store its data on the MOAB mesh representation so that MOAB can manage the various meshes used by the physics modules.

The intermediate-fidelity Proteus-2D1D module will represent power distributions and local reaction rates reduced computational cost in comparison to fully 3D methods. The equations to be solved have been

formulated and are being implemented using components of the existing Proteus-UNIC module (to accelerate development).

Application of the code set to advanced reactor types continued, currently in support of upgrades to INL's Advanced Test Reactor (ATR). The ATR's complex serpentine plate-fuel geometry (Fig. 2) presents a particularly challenging problem to analysts.

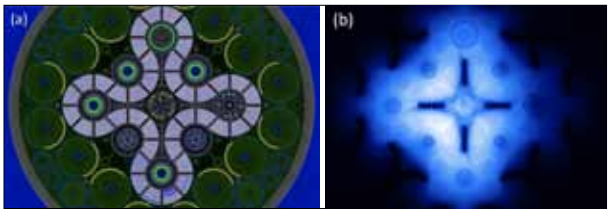


Fig. 2. Modeling the ATR core: (a) Sharp representation of core geometry. (b) Proteus prediction of thermal neutron flux.

Nek5000 development

Nek5000, Sharp's thermal fluids module, provides solvers for multi-dimensional heat transfer and fluid dynamics. In the second quarter, an updated pressure solver was released, multi-physics integration capabilities were restored to the code, and initial benchmark analyses of the Russian SIBIRIA experiment were completed.

The new pressure solver contains a spectral element multi-grid pre-conditioner that supports the Pn-Pn formulation, which has become the discretization method of choice for large eddy simulation. This pre-conditioner significantly reduces iterations and run time compared to the previous pre-conditioner: the pressure solver is 2.5 times faster, and the overall module is 1.5 times faster. For some simulations of complex geometry, such as the detailed wire-wrapped sodium fast reactor (SFR) fuel assembly, the new solver makes the difference between solvability and intractability. Nek5000 has been re-integrated with the MOAB framework.

The updated Nek5000 module was used to perform initial simulations of experiments carried out in the Russian SIBIRIA facility have been completed (Fig. 3). In the experiments, local shear stresses were measured in a fluid flowing within a narrow annulus with and without partial blockage. The detailed stress measurements provide an important dataset for future validation efforts.

Fig. 3. Predicted flow pressures and velocities in a partially blocked pipe.

Other Sharp developments

The Sharp structural mechanics module, Diablo, provides solvers for multi-dimensional structural mechanics. In the second quarter, work was initiated to integrate the existing Diablo code with the most recent release of the MOAB framework.

Other efforts this quarter have included updating the MOAB framework module to provide compatibility with the updated solvers of Proteus and Nek5000, supporting the integration of AMP into the MOAB framework, and developing the MeshKit toolset for complex reactor geometries. In particular, MeshKit has been applied to development of the SFR assembly model for future multi-physics demonstration activities and to the development of the ATR model from existing models based on the Monte Carlo N-particle transport code.

NEAMS seismic initiative

A recent seismic workshop (February 27-28) identified six priorities for simulating the seismic response of nuclear power plants:

- Nonlinearities associated with the structure/ soil interface
- Arbitrary, spatially-distributed wave fields
- Nonlinear hysteretic models of structural elements
- Seismic isolators
- Nonlinear soil
- Internal fluid-structure interaction

The first two are part of the Reactor IPSC work scope; the others are not.

Safeguards and Separations IPSC

During the second quarter, work continued on two fuel reprocessing operations: voloxidation and dissolution. Because voloxidizers do not operate in discrete physical stages, the Separations team is applying volume-holdup model to each unit as a network stage (vertex) (see Fig. 4). Fig. 5 illustrates some of the material volumes that are the outputs of these models. Testing of the prototype models provided realistic results. Ongoing work includes development of visualization tools and "translation"

efforts to adapt the models to existing tools and programs, such as the Fuel Cycle Technologies program and the SNL Safeguards Performance Model. [ORNL, LANL]

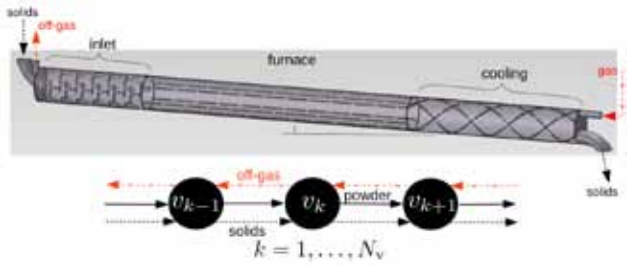


Fig. 4. Voloxidization calciner with network representation of flows and holdup.

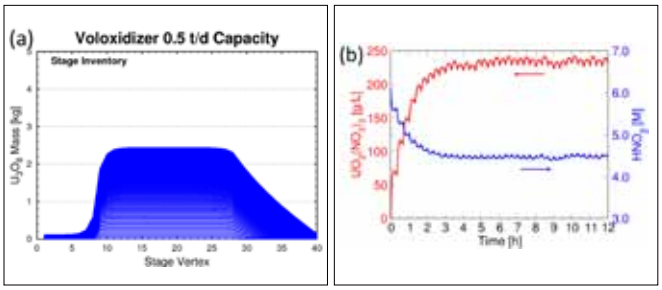


Fig. 5. Representative output data from reprocessing simulations: (a) Voloxidizer U_3O_8 inventory profile. (b) Uranium and nitric acid outlet concentrations during dissolver startup transients.

The pyroprocessing model under development is based on diffusion control and couples dissolution at anode with deposition at the cathode. Key thermochemical properties include potentials, activity coefficient, and diffusion coefficient. Available experimental data are used to develop predictive correlations for the properties of fission products in molten KCl-LiCl. The physical and chemical properties of actinides in a liquid cathode (cadmium) were also modeled. [LANL]

Progress on the characterization of pyroprocessing emission signatures during the second quarter include (1) development of a library of source terms for various values of initial enrichment, burnup, and cooling time; (2) completion of code for automatically generating the passive neutron and photon source signatures for the source term; (3) computing and examining the passive emission signatures as a function of element and burnup; (4) developing and utilizing tools to visualize and quantify the results; and (5) further progress toward developing a representation of the pyroprocess geometry. [LANL]

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 IPSC

A new one-dimensional groundwater waste transport code was delivered to the used fuel disposition (UFD) campaign. This code supports more rigorous physics coupling and is intended to serve as the basis for a replacement of GoldSim, a performance assessment code that was used in analyses for the Yucca Mountain licensing application. With additional direct support from the UFD campaign, new work is beginning on a higher-fidelity 3D code for waste disposal analysis. [SNL]

Efforts on waste form modeling included simulation of two sodium-borosilicate glass compositions using empirical force field potentials (which account for chemical bonding energies, van der Waals forces, etc.). Calculated glass densities and other key parameters matched experimental results reasonably well. These calculations were performed using simulation cells of >1,000 atoms. [SNL]

The Waste team developed a prototype application programming interface (API) for modeling hydride reorientation in fuel cladding during very long-term fuel storage. The prototype includes three alternative APIs and tests that exercise them. The first API simply calls a MatPRO subroutine to calculate cladding stress. A second, more general API supports SNL's Library of Advanced Materials for Engineering (LAME). A third API is intended to support more advanced hydride modeling under development. When complete, the hydride reorientation model will be implemented in AMP. [ORNL, SNL]

Fundamental Methods and Models

Benchmarking of meso-scale modeling

In the past quarter, a meso-scale benchmark demonstration problem was modeled to evaluate the capabilities of different numerical methods used to simulate meso-scale microstructure evolution in UO_2 during post-irradiation thermal annealing. The purpose of the meso-scale benchmark problem was to provide a common basis for assessing several meso-scale models (phase-field, Potts, and kinetic Monte Carlo [kMC]) developed by different groups to calculate the evolution kinetics of intra-granular fission gas bubbles. [INL, LANL, ORNL, PNNL, SNL]

An important aspect of defining a common benchmark problem was to establish a consistent set of initial, boundary, and thermodynamic conditions across the selected meso-scale methods. The benchmark problem was constructed to include important microstructural evolution mechanisms of the kinetics of intra-granular fission gas bubble behavior, such as the atomic diffusion of Xe atoms, U vacancies, and O vacancies; the effect of vacancy capture and emission from defects; and the elastic interaction on non-equilibrium gas bubbles. An idealized set of assumptions and a common set of thermodynamic and kinetic data were imposed on the benchmark problem to simplify the mechanisms considered. The modeling capabilities of different methods are compared against selected experimental and simulation results. For example, Fig. 6 shows the Marmot-predicted bubble growth during the thermal annealing process for the 10-nm thick 2D simulation. [INL, LANL, ORNL, PNNL, SNL]

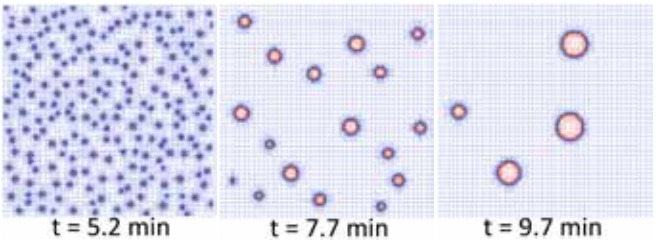


Fig. 6. Marmot 2D simulation of fission gas bubble growth during fuel annealing.

The comparison of simulation results with experimental bubble behavior data showed that, while all methods incorporate the same mechanisms that influence intra-granular bubble growth and coarsening, the Potts model and kMC method are challenged by the low solubility and long-range diffusion necessary to simulate this problem correctly. The statistical-mechanical nature of the Potts and kMC methods require large ensembles with long computational times to solve this problem. Increasingly more complex meso-scale benchmark problems are needed to further verify and validate the predictive capabilities of these meso-scale modeling methods. [INL, LANL, ORNL, PNNL, SNL]

Up-scaling framework

The FMM team continued building a hierarchical up-scaling framework to predict the strength of structural materials by directly coupling dislocation dynamics and crystal plasticity. Results from a series of large-scale dislocation dynamics simulations (Fig. 7) were used to calculate the parameters used in the dislocation dynamics code and develop a computational framework to directly couple dislocation dynamics and continuum mechanics. The traditional viscoplasticity simulation is enhanced with this framework by using science-based assumptions about dislocation growth and annihilation rates instead of the empirical exponential hardening law. Methods to represent the effects of cross-slip and an interaction matrix of slip systems are being developed. The final model will also account for anisotropic elastic and Peierls stress, polycrystalline structures, and irradiation effects. [PNNL]

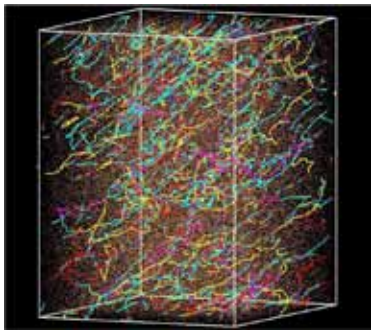


Fig. 7. Simulated dislocation-defect structure after plastic deformation in Fe-Cr-Ni steel.

Verification, Validation, and Uncertainty Quantification (VU)

Rare-Event Inference

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 a particularly challenging class of problems, rare event inference, which refers to

making predictions about the probability of rare events (many safety-related problems are in this category). Significant progress was made in developing new statistical approaches based on importance sampling. In general, this approach attempts to focus sampling on values of the input random variables that result in particular outputs of interest, such as the mean probability of failure. This can result in tremendous computational cost savings over traditional approaches, such as Monte Carlo or Latin-hypercube sampling (LHS). [SNL, LANL]

Results for one importance sampling method, Gaussian process adaptive importance sampling (GPAIS), are compared with LHS results in Table 1 for a virtual reactor. The analysis was performed on the simulation of pressurizer failure in a simplified reactor system, where the metric of interest is the probability that the peak coolant temperature (PCT) is higher than a certain threshold temperature (given in column 1). The second column in the table shows the "reference" probabilities computed using 10,000 LHS samples. The GPAIS results (column 3) were obtained using only 240 samples and agree reasonably well with the LHS results at a fraction of the computational cost.

Table 1. Comparison of failure probability estimation with LHS and GPAIS.

Failure Threshold Temperture (°F)	Probability that PCT > Threshold		Average Fraction of Important Samples (GPAIS)
	LHS Estimate (10,000 Samples)	GPAIS Estimate (240 Samples[a])	
680	0.0101	0.0090	0.29
690	0.0071	0.0058	0.34
700	0.0036	0.0034	0.36
710	0.0012	0.0011	0.25
720	0.0001	0.0002	0.12

[a] 60 initial samples plue 180 "adaptive" samples selected using results from the samples already processed.

The last column in the table shows why this happens: the GPAIS approach has directed a large fraction of the samples into the "important" region of interest, that is, those samples that indicate failure. LHS typically would only put 0.1% of the samples into this region. [SNL, LANL]

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 that provides verification and validation, uncertainty quantification, and other resources for advanced modeling and in nuclear reactor design and analysis. In the second quarter, the VU team updated its survey and evaluation of existing data and knowledge bases. This resulted in a better understanding of how these existing capabilities can be used to leverage the development of NE-KAMS. A coherent strategy for linking NE-KAMS to other DOE databases has been developed. [INL, Bettis Laboratory]

Predictive Maturity

Many programs have struggled to ensure that the VU elements are implemented in a manner consistent with the intended use of the simulations. To help address this issue, the VU team has been developing a system of governance and guidance processes called discovery, accumulation, and assessment (DAA) to plan, track, assess, and communicate VU activities and results. The DAA process is being applied to a fuel rod validation problem with the Bison code. This process is providing appropriate contexts for the Bison validation work in terms of VU elements, as well as in terms of simulation ensembles, physical experiments, and math models. Although the effort is immature, application of DAA early in the process has accrued a number of benefits. The VU team is currently developing prototype software (called "Synopsis") to help manage the execution of DAA. [SNL, LANL, INL]

In a related study, the VU team has demonstrated a new methodology that orders experiments to better inform the calibration of the LIFEIV nuclear fuel performance code. The study showed that the predictive maturity index (PMI) is an effective measure of convergence of the calibration process. This measure will soon be applied to the calibration of Bison. [SNL, LANL, INL]

Capability Transfer

The Early User Program is designed to put software developed by the IPSC teams into the hands of a small group of users outside of the program for evaluation and feedback. During the second quarter, users at Texas A&M University (TAMU) and INL began to work with Nek5000 from the Reactors IPSC and users at ORNL and INL began to work with AMP and Bison from the Fuels IPSC. An INL

user applied Bison to a UO_2 fuel irradiation experiment (Risoe AN-4) in PWR test reactor DR3. In the experiment, a refabricated and instrumented fuel rod is subjected to slow ramp and hold tests to investigate fission gas release and microstructural changes. Initial Bison results are being compared with the measured fuel temperature and fission gas release. [INL, ORNL, TAMU]

Another important activity is to introduce NEAMS approaches and products to the NRC, to gain regulatory acceptance of science-based modeling and simulation capabilities for demonstrating safety and performance. This acceptance is essential if NEAMS products are ever used in a licensing-related context. To that end, members of the NEAMS program recently provided an initial briefing to representatives of the NRC Office of Regulatory Research. Ongoing periodic briefings are planned.

Enabling Computational Technologies

The NEAMS overall SQAP was revised to version 1.5 with NE-5 input and approved. The FMM SQAP was started with a study to verify that traditional SQA practices and tools apply to FMM modeling activities, which involve extensive use of such things as MATLAB experiments and Excel spreadsheet calculations. [LLNL]

Static analysis of AMP and its third party libraries (TPLs) was started. The ECT team found and fixed about 300 defects in HDF5, a fundamental input/output library used by AMP and other NEAMS codes and TPLs. After evaluation of several static analyzers for Fortran source code, Intel Fortran Studio XE was selected for use in NEAMS. The team started development of an iGeom-based database plugin for VisIt; it is based loosely on an existing iMesh plugin. The Redmine collaborative project management site launched in December, together with monthly half-hour teleconferences, has improved communications and productivity. [LLNL]

Website development focused on the division of content between the AMSO and NEAMS sites. To avoid conflict and duplication, the scope of website development was expanded to include an overhaul of existing AMSO pages. The ECT team is gathering content from NEAMS stakeholders and existing sites and continuing development of the backend of the site, to add features such as pop-up definitions. [LLNL and subcontractors]

Work to support the TetGen tetrahedral mesher in Cubit has continued. Cubit has been updated to build with either a commercial mesher or the TetGen mesher. A list of CMake support activities for AMP has been identified and preparations for providing support are underway. [SNL]

NiCE development has focused on enhancements to the workflow engine and on integration with external tools such as VisIt. The workflow engine was enhanced to support AMP and Nek5000 as well as to provide a means to capture documentation relating to these codes in XML and NiCE PSF format. The infrastructure to simplify persistent storage of simulation data was substantially improved. Significant progress in the real-time monitoring library, the NiCE Updater, was also made, and an initial prototype is nearing completion (Fig. 8). Integration of VisIt with NiCE was started. [ORNL]

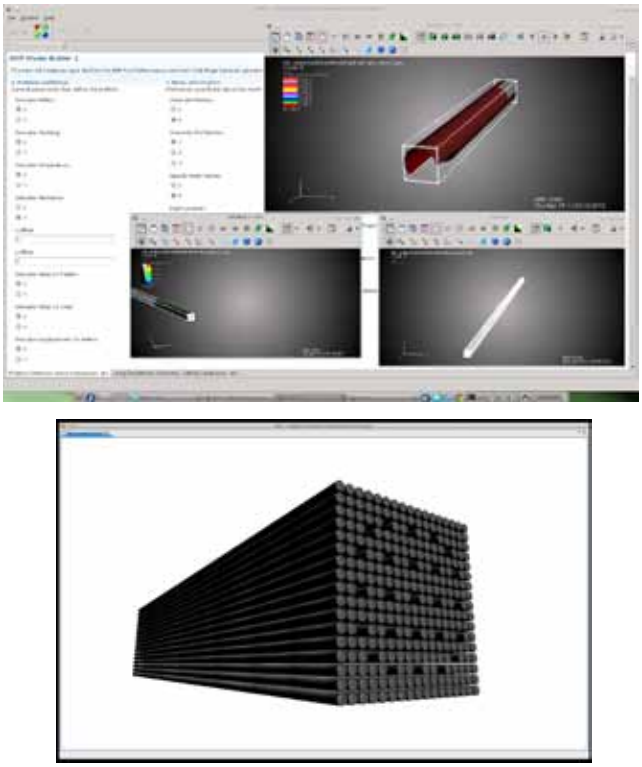


Fig. 8. NEAMS tools: (top) AMP model builder and (bottom) NiCE geometry viewer

AMP, Moose-Bison-Marmot, and Nek5000 codes as well as all of their TPLs were acquired, built, and tested for quality assurance. Required TPLs were inventoried and management requirements were evaluated. A report was drafted to identify and discuss management challenges and proposals for minimizing costs. [INL]

Technical Spotlight: Making high-resolution neutronics models practical

Of the processes and systems being simulated with NEAMS tools, one of the most challenging, especially in terms of computational resources, is neutronics, that is, the motions and interactions of neutrons and gamma rays with materials in the reactor core. Neutronics modeling depends on solutions of the neutral particle Boltzmann transport equation for neutrons and gamma rays and solutions of the Bateman equations for fuel depletion. The transport equation is a function of space, direction of travel (angle), and speed (energy). In deterministic methods, the energy representation is cast into a multi-group formulation and the angular domain is discretized using an angular cubature (set of directions). Using a finite element method, this can quickly lead to 10,000 degrees of freedom (DOF) per mesh vertex. Given that a detailed mesh of the reactor core can require 10^9 vertices, the problem size is well over 10^{13} DOF per time step.

To reduce the DOF to a more manageable size, most existing neutronics tools use spatial homogenization, which relies upon a superposition principle where the complex geometrical solution within repeating structures (such as fuel assemblies) can be replaced with a homogeneous representation on a coarser grid. The energy representation is also homogenized, where a "thousand"-group calculation on a single pin-cell is used to generate effective "hundred"-group data. Once the physics equations for the coarse grid are solved, solutions for progressively finer grids can be superimposed to obtain the solution to the original 10^{13} DOF problem. This technique has performed excellently in the past and some of the effort in NEAMS has provided updates to existing neutronics tools.

The drawback to spatial homogenization is that it introduces error into the multi-step solution scheme, so the intermediate steps must be representative of the actual conditions in the detailed calculation to minimize this error. Fig. 9 shows a typical reactor geometry that conforms to the spatial homogenization methodologies in existing tools (Monju reactor) and one that does not conform (ATR). The Monju core simulation can be done well with existing tools for most analysis needs, while simulation of the ATR core has almost exclusively relied upon Monte Carlo modeling tools. However, recent successes with Attila have demonstrated the viability of fine-mesh neutronics tools. Similarly, heterogeneous modeling capabilities like those in DeCART have also demonstrated that fine-mesh calculations of PWR, boiling water reactor (BWR), and very high-temperature gas-cooled reactor (VHTR) cores are possible.

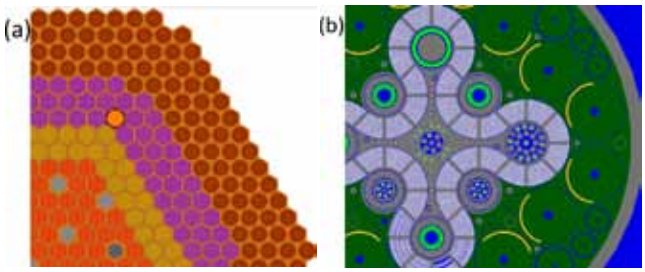


Fig. 9. Comparison of reactor core geometries: (a) Monju and (b) ATR.

Because of the large problem size of PWR simulations, the DeCART tool has demonstrated particular effectiveness in performing these calculations without relying upon spatial homogenization. While the energy group "homogenization" is still being used via the sub-group methodology, the primary advantages of DeCART are (1) the restriction of the complex 3D geometry into a semi-structured, 2D geometry and (2) a coarse grid solution algorithm with a transverse integration approach in the axial direction (2D1D). The 2D-based geometry significantly reduces the user effort required to generate large, complex 3D geometries and is easily replicated using 2D-conformal, unstructured finite-element meshes to handle novel geometries (like the ATR, which cannot currently be modeled with DeCART). The primary advantage of DeCART is a solution algorithm that does not require full convergence of the fine mesh solution to achieve a highly accurate coarse grid solution (pin-cell solutions in the case of DeCART).

For a coupled physics calculation, "pin-level" reaction rates, such as pin-power, are needed, whereas the spatial reaction distribution within each fuel pin is not. DeCART has demonstrated an exceptional ability to perform these types of calculations on typical PWR, BWR, and VTHR cores, several of which were done using coupled neutronics and thermal-hydraulics. However, users have complained about excessive computational run-time, the

inability to model novel core geometries, and an inability to treat small axial mesh sizes.

Figure 10 shows example solutions obtained using the tools under development in NEAMS, where the focus has been on detailed 3D solutions of the transport equation via the second-order, even-parity, discrete ordinates methodology and the method of characteristics. The work has focused on building solvers capable of efficiently solving problems with 10^{12} or more DOF on parallel computers. While the routine analysis of problems so large remains impractical, the experiences gained from that work have guided the development of tools, such as DeCART, that have a reduced computational burden.

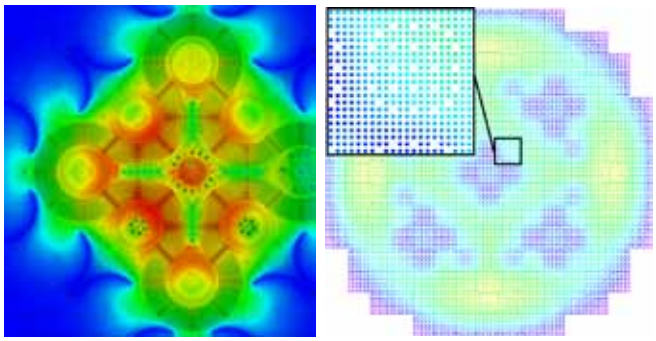


Fig. 10. Visualization of thermal flux and power solutions obtained with NEAMS tools.

The DeCART methodology is being implemented in a 2D1D solver that resolves the outstanding issues in DeCART. The 2D-based geometry concept is maintained, but the use of a 2D, unstructured finite-element approach allows easy application to complex, irregular core geometries. Also, the 2D1D methodology uses a 3D discretization of the transport equation to address the issues with axial mesh size. A full space-angle-energy parallelization strategy is being employed to improve computational performance. Finally, the key focus on solving on a coarse grid level is being maintained, although the coarse grid solver does not require the existence of a structured grid-based sub-geometry.

Part of the NEAMS effort is devoted to setting up new benchmark and validation problems derived from experimental data for comparison with results from the new neutronics tools. The results of comparing one such calculation with data from a fast reactor experiment at the Zero Power Reactor showed that the tools developed under NEAMS improved the prediction of the reaction rates from 5-10% error to less than 4% error (Fig. 11).

Future development will focus on replacing the second-order even-parity methodology, which has seen the most success, with a least-square, continuous finite-element formulation, including a spatial multi-grid preconditioner. This formulation eliminates the previous problems with spatial mesh size and low-density mediums, without affecting computational performance. Also, we are researching the multi-group-based cross section libraries and methodologies that are applicable to both thermal and fast systems.

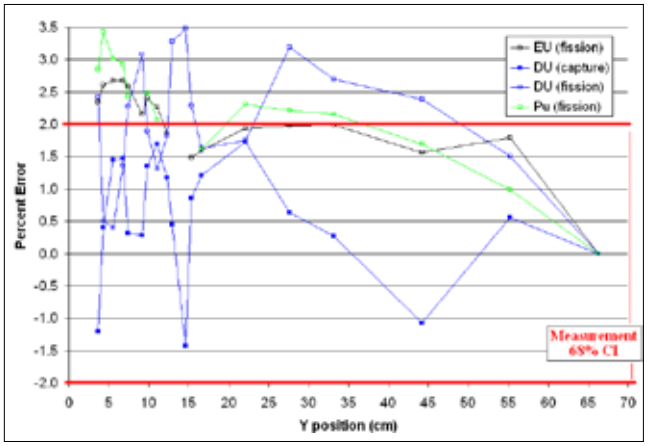


Fig. 11. Calculated foil reaction rate errors obtained using NEAMS tools.

Selected NEAMS Abbreviations

AMSO	Advanced Modeling and Simulation Office (NE-71)
ATR	Advanced Test Reactor
BWR	boiling water reactor
DAA	discovery, accumulation, and assessment
DOF	degrees of freedom
GPAIS	Gaussian process adaptive importance sampling
kMC	kinetic Monte Carlo [method]
LES	large eddy simulation
LHS	Latin-hypercube sampling
MCNP	Monte Carlo N-particle
PMI	predictive maturity index
PWR	pressurized water reactor
SEMG	spectral element multi-grid
SFR	sodium fast reactor
SQA	software quality assurance
TPL	third party [software] library
UFD	used fuel disposition
VHTR	very high-temperature gas-cooled reactor

Recent and Upcoming Level 1 and 2 Milestones

Completed during this Quarter			
Milestone ID	Milestone Title	Due Date	Actual Finish
M2MS-12OR0602031	Demonstrate AMP coupling to Denovo on full LWR fuel assembly	1/31/2012	1/30/2012
M2MS-12AN0603201	Establish representative fuel assembly for multi-physics demonstrations	1/31/2012	1/31/2012

Coming Due during the Next Quarter			
Milestone ID	Milestone Title	Due Date	Status
M2MS-12IN0602061	Demonstrate implementation of atomistic results into a combined MOOSE-BISON-MARMOT simulation	5/31/2012	On Schedule
M2MS-12AN0603018	Expand collaboration plan for SHARP modeling and simulation area	6/30/2012	On Schedule
M2MS-12AN0603278	Complete multi-physics simulations of a sodium fast reactor fuel assembly using the PROTEUS, Nek5000, and AMP	4/30/2012	On Schedule
M2MS-12IN0603336	Simulate steady-state single-phase PWR (normal operations) with RELAP7	5/15/2012	On Schedule
M2MS-12IN0603337	Complete RELAP7 SQAP	5/31/2012	On Schedule
M2MS-12IN0603339	Complete RELAP7 development plan	6/30/2012	On Schedule
M2MS-12SN0605074	Develop and demonstrate final hydride reorientation model for UNF-VLTS	6/30/2012	On Schedule
M2MS-12PN0606017	Benchmark gas bubble nucleation and growth in irradiated UO2 in concert with other mesoscale models	4/11/2012	On Schedule

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Computer Tools Used in NEAMS

Name	Purpose or Description
ABAQUS	Fuel assembly structural analysis code
AMP	Advanced Multi-Physics code for modeling continuum-scale fuel assembly performance
Bison	Continuum-scale, single-pin fuel performance code
Cubit	Mesh generation code
DeCART	Full-core, pin-resolved, transient neutronics code with thermal-hydraulic feedback; used in Sharp
Denovo	Neutronics (radiation) transport code
Diablo	Structural mechanics solver used in Sharp
HDF5	Fundamental input/output library for AMP
iGeom	Web-based tool for creating and using geometric constructions
LAME	Library of Advanced Materials for Engineering
Marmot	An object-oriented finite element framework for multiphysics phase-field (meso-scale) simulations; used in NEAMS as a single-pin fuel performance code for modeling microscopic response of nuclear fuel to irradiation
MATLAB	MATrix LABoratory; programming environment for algorithm development, data analysis, visualization, and numerical computation
MatPRO	Commercial material properties database
MBM	Integration of Moose, Bison, and Marmot that enables atomistically informed multi-scale simulations of nuclear fuel microstructure
MeshKit	Parallel mesh generation toolset
Moose	Multiphysics Object-Oriented Simulation Environment; a parallel computational framework for coupled systems of nonlinear equations
Nek5000	Multi-dimensional heat transfer and fluid dynamics module in Sharp
NiCE	NEAMS integrated Computing Environment; the NEAMS user interface and application management tool
PICS:NE	Program Information Collection System: Nuclear Energy; a web-based project management tool.
Proteus	The neutronics (radiation) transport module in SHARP
Relap-7	Reactor Excursion and Leak Analysis Program; single-zone (0-D/1-D) code for managing and coupling other simulation codes to model a complete nuclear power plant under a variety of operational and accident conditions
Sharp	High-fidelity, 3-D reactor core simulation framework for evaluating the impacts of design changes on reactor performance and safety
TetGen	Tetrahedral mesh generator in Cubit
UMAT	Crystal plasticity, finite-element code for body-centered cubic iron
VisIt	Visualization code

NEAMS Overview

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 SQA requirements.