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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 2012

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Idaho National Laboratory · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · Oak Ridge National Laboratory · Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories

The NEAMS Vision

A message from K. S. Bradley, NEAMS national technical director

On behalf of all the scientists and engineers who comprise the NEAMS program, I thank you for reading the *NEAMS Update*, a quarterly report that provides timely highlights of NEAMS team accomplishments. Our goal is to enhance DOE-NE's research and development portfolio through the development of advanced computational methods. The tools we are developing — known as the NEAMS ToolKit — will provide insights into the performance and safety of advanced reactor systems that we cannot obtain through experimentation alone. They will also complement experimental work by helping us design experiments that are more complex and informative and then helping us interpret the results of those experiments.

To achieve this, the NEAMS ToolKit will incorporate fundamental descriptions of the underlying physics that govern the critical behaviors we must understand and accommodate in new reactor designs. In other words, we strive to replace the empiricism and correlations typically employed in modeling and simulation tools with mechanistic descriptions that have been validated with experiments that confirm each description in isolation as well as in interaction and competition with other phenomena.

With this approach, the ToolKit will not only succeed at reproducing the results previously observed, but it will permit designers and analysts to predict performance in regimes beyond the test base, that is, where we have no direct experimental observations.

The NEAMS team is very proud of its accomplishments, and we hope you will be intrigued by what's to come in the future. This report and our newly launched website (neams.ne.anl.gov) are intended to provide insight into our challenges and achievements.

Finally, we believe strongly that the quality and utility of the NEAMS ToolKit will be only as good as the guidance we get from stakeholders. Please, reach out to the team or myself if you have advice or ideas you would like to share. We are excited to do our part to advance nuclear energy in this country, and your input is essential to that success.

Highlights

- BISON is being calibrated using data from instrumented fuel assembly experiments for two general fuel rod configurations (page 2).
- Work continued on models of fuel microstructure changes at both the atomistic and grain scales (page 2).
- The Nek5000 team is participating in separate collaborations with the Russian Federation and the U.S.-EURATOM International Nuclear Energy Research Initiative (page 3).
- Work on multi-physics coupling demonstrations advanced to simulations of neutron transport in simplified fuel assemblies (page 4).
- A two-phase flow progression was implemented in RELAP-7 to model the reactor primary loop (page 4).
- MeshKit is being extended to permit the construction of fluids boundary layer meshes within reactor geometry meshes (page 5).
- An independent quality assessment cited nine exemplary software development practices that exceed requirements of NQA-1, which governs quality assurance for nuclear power plants (page 5).
- The NEAMS project web site has been launched.

Fuels Product Line Accomplishments

Engineering Scale (BISON)

Recent enhancements to BISON, the tool for simulating nuclear fuel performance at the engineering scale, have included extending the algorithm that governs mechanical and thermal contact between independent bodies (e.g., pellet-cladding contact that results from fuel swelling and cladding creep-down). The algorithm had previously been demonstrated to be robust when simulating either frictionless or no-slip pellet-cladding contact. Now the algorithm can accept contact with friction using a variable factor, which will likely be needed to accurately model the initial phase of pellet-cladding contact. The algorithm can also allow for the separation of bodies after initial mechanical/thermal contact, which is necessary for accurately modeling fuel behavior during reactor startup, reactor shutdown, significant power changes, or accident scenarios. Ongoing efforts will refine the simulation of contact. [INL, SNL]*

Work to couple the swelling and fission gas release models for UO_2 fuel was initiated. Additionally, the fission gas release model is being enhanced to improve its predictions of fuel behavior during transient conditions, where the best current model is known to have limitations. [INL, SNL]

The fuels team continues to assess BISON simulations against experimental data from existing benchmark problems. To date, 21 benchmark problems from the FRAPCON and FUMEX-III experimental databases have been compared to BISON results. Of particular note, the DAKOTA-BISON interface established last year is being used to calibrate the threshold that activates BISON's relocation model, which simulates the movement of fuel segments and fragments after cracking. Calibrations are being performed for two general fuel rod configurations: (1) a variety of individual rods and (2) aggregates of six rods, three each from the IFA 431 and IFA 432 experiments. Since legacy performance models initially implemented in BISON for simulating UO_2 behavior were calibrated using other fuel performance codes, this represents the first time such models have been calibrated specifically as implemented in BISON. [INL, SNL]

The MOOSE and NiCE development teams initiated a collaboration to incorporate MOOSE and MOOSE-based applications into the NEAMS Integrated Computational Environment (NiCE). Specifically, the teams have begun development of a NiCE plug-in for BISON with extensions to the NiCE data structures and user interface. The capability to fully construct and execute BISON simulations from within NiCE is expected to be available later this year. [INL, ORNL]

*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).

Lower Length Scale (MARMOT)

Work continued on models to describe various aspects of mesoscale fission gas behavior, with simulations at the atomistic scale informing their development and providing key input parameters. During this quarter, molecular dynamics simulations of the effect of the fission by-product xenon (Xe) on UO_2 thermal conductivity were performed as a function of temperature, Xe concentration, and microstructure. In addition, different manifestations of anisotropic UO_2 thermal conductivity were simulated and compared to experimental data using single crystals of UO_2 (see Fig. 1).

A Kawasaki Dynamics neighbor-switching Monte Carlo scheme was implemented in the molecular dynamics package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). This enhancement provided a new method with a greatly improved ability to simulate the nucleation, resolution, and evolution of fission gases in UO_2. The new capability is being used for simulations on U-O-Xe systems, including a parametric study of the effects of grain size distribution on fission gas release behavior within the framework of the existing percolation model that is used to scale fission gas release up to the continuum level.

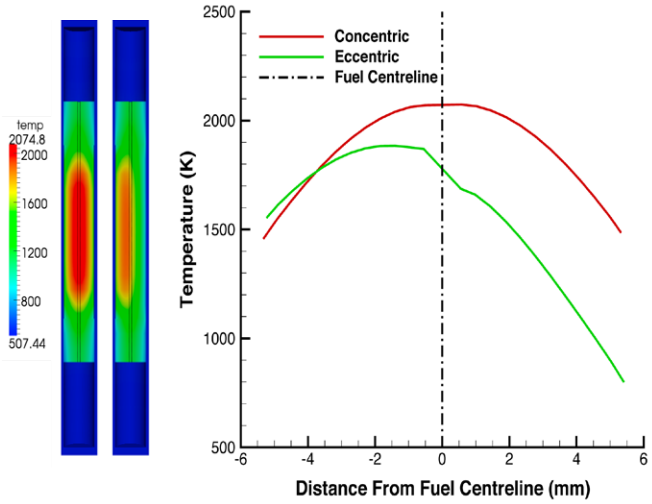

Fig. 1. Side-by-side temperature comparison for the three-dimensional (3D) concentric (left) and eccentric (right) fuel pellet simulations. Both simulations correctly locate peak temperatures within each pellet shape.

In the final molecular dynamics development, Basak empirical potentials were used to calculate the normal vibrational modes (phonons) of Xe diffusion defects and defect saddles in UO_2 in order to calculate defect entropies, which allow estimates of the pre-factors needed in Arrhenius formulations for the diffusion of fission gas atoms. This data is being incorporated into a comprehensive mesoscale fission gas diffusion model. [INL, LANL, PNNL]

The fracture behavior of UO_2 is being modeled at both the atomistic and intermediate scales to better inform the constitutive modeling of fuel failure at the engineering scale. Atomistic studies to simulate the fracture behavior in UO_2 by utilizing seven different embedded atom model potentials were extended to elucidate the role of metastable

phase transformations (i.e., rutile phase evolution) at the onset of fracture. Mesoscale investigations continued to explore how to best represent the statistical variation of fracture properties for up-scaling to the continuum level. [INL, LANL, PNNL]

Work on models needed to describe the mechanical behavior of material microstructures also continued at both the atomistic and intermediate scales. Development of a plasticity model based on continuum dislocation dynamics in a finite element framework was initiated. When complete, the model will be implemented in MARMOT. Atomistic simulations of grain boundary migration continued for UO_2 under a thermal gradient and in the vicinity of a pore. Efforts are now concentrating on twist Σ5 {310} and twin Σ3 {111} grain boundaries. Parametric values obtained from these simulations will be used in the mesoscale modeling of grain growth and fuel swelling, as well as in the engineering-scale modeling of fuel swelling and restructuring. [INL, LANL, PNNL]

Reactors Product Line Accomplishments

Code Integration (SHARP)

The effort to demonstrate coupled simulations within the reactors product line has made significant progress; Fig. 2 illustrates the current architecture. Solution transfer issues are being fixed, and pseudo-transient capability is being implemented. The team delivered pseudo-transient simulations for a single simplified sodium fast reactor (SFR) fuel assembly and for a realistic model of an EBR-II fuel assembly. The transients represented a loss of heat sink; after the steady state was calculated, the coolant inlet temperature was perturbed, leading to a change in the temperature distribution in the fuel assembly, the coolant density, and therefore the neutron flux and power density. This in turn led to a further change in overall temperature. A measurable change in reactivity was observed, consistent with expectations. [ANL]

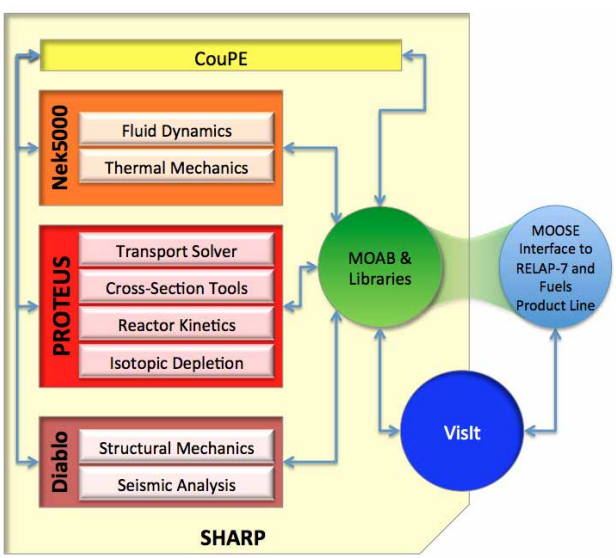

Fig. 2. SHARP architecture.

The team is currently focused on delivering a multi-assembly capability, where some of the assemblies are homogenized both from the thermal-hydraulics point of view and the neutronics point of view to provide options for simulations at reduced computational cost. These initial integrated multi-physics demonstrations of the reactors product line do not yet account for thermal expansion or other structural mechanics feedbacks, which will be included later this year. [ANL]

Thermal Fluids (Nek5000)

As part of the ongoing collaboration between DOE and the Russian Federation under the Working Group on Nuclear Energy and Nuclear Security, the NEAMS thermal fluids team is collaborating with the Russian developers of the computational fluid dynamics (CFD) codes CONV3D and CABARE at IBRAE, the Russian reactor safety institute. The collaboration supports validation of Nek5000 and the Russian codes through sharing of benchmarking and validation data and experience. Last year, the NEAMS reactors team assisted IBRAE collaborators in submission of winning proposals for compute time at U.S. leadership computing facilities. The NEAMS team has worked with the IBRAE team to help troubleshoot access to those allocations. [ANL]

The NEAMS Nek5000 and IBRAE CONV3D groups have successfully conducted their preliminary computations for the Novosibirsk fuel assembly flow blockage experiment known as "SIBERIA" (see Fig. 3) and are discussing the final experimental setup for validation runs with both CONV3D and CABARE. Benchmark problem specifications are being prepared by the NEAMS thermal fluids team for the planned comparison of predictions of thermal mixing in the ANL MAX experiment. [ANL]

The reactors team is collaborating in the U.S.-EURATOM International Nuclear Energy Research Initiative (INERI) on high-fidelity simulation of fluid flow in fuel assemblies; other participants include NRG-Petten (Netherlands), Studiecentrum voor Kernenergie (SCK, Belgium), and UGhent (Belgium). In December, the participants agreed on two first-year, code-to-code benchmarks: (1) flow in a seven-pin, wire-wrapped rod bundle and (2) flow in a pebble bed. The benchmarks will support continued development and improvement of Nek5000 and will be instrumental for the design and safety analysis of the European MYRRHA research reactor project. [ANL]

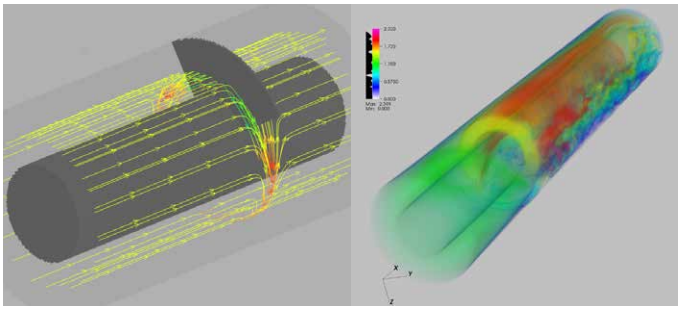

Fig. 3. Comparison of flow blockage simulations: (left) CONV3D streamlines and (right) Nek5000 velocity fields.

As a proof of concept, Rayleigh-Bénard convection was the subject of a DAKOTA uncertainty quantification study, which established that all the practical issues of running Nek5000 with DAKOTA have been resolved. In collaboration with the NEAMS thermal fluids team, work is progressing to define a DAKOTA-Nek5000 demonstration problem that best exhibits the ability to address the needs of the reactors product line. [SNL, ANL, INL]

Neutron Transport (PROTEUS)

The reactors product line multi-physics coupling demonstration involves problems with increasing difficulty, starting with simplified assemblies, moving to real EBR-II assemblies, and eventually considering real transients in the full EBR-II core. The PROTEUS neutron-transport toolset was applied to current research topics to assess potential for demonstrating causality with the limited set of physics tools available in the initial coupled code suite.

Based on standalone PROTEUS calculations, it was determined that Doppler and sodium density feedbacks are insufficient in the EBR-II reactor to produce a visible change in the radial or axial profile of the neutron flux solution. Stratification of the sodium temperature over time in the inlet plenum was chosen as the primary coupling demonstration problem to better illustrate current predictive capabilities by simulating EBR-II core transients (Fig. 4). The simulation showed that the predicted power away from the stratification is less affected than the power in the region near the XX09 test assembly. [ANL]

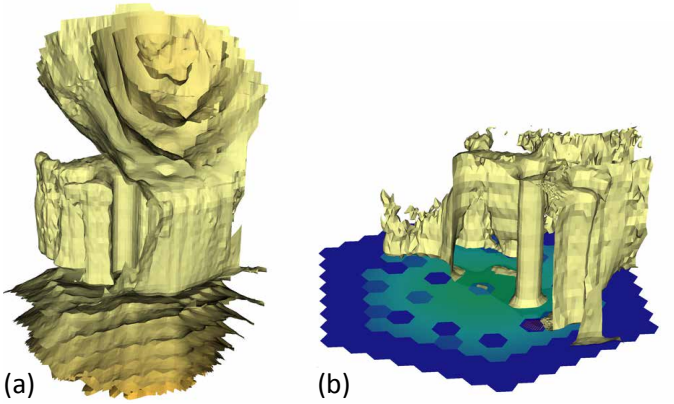

Fig. 4. Predicted change in the flux solution at an early stage of the EBR-II inlet plenum stratification transient: (a) Contour lines tilt (indicating larger error) toward increased sodium density when the temperature changes and (b) normalized radial power during the transient.

The PROTEUS development team completed initial feasibility tests for a novel subgroup method for fast spectrum reactors that could provide comparable accuracy at reduced computational cost in comparison to more conventional cross-section methods. The analysis indicates that the subgroup method can work for fast spectrum reactors when the effective multi-group library contains fewer than a hundred groups because the resonance interference errors cancel one another. In an additional study, the heterogeneity effect of a simple unit cell containing two material compositions indicated that significant error in the effective multi-group cross sections resulted when the underlying estimate of the full core neutron flux was changed. Thus, a whole-core cross section generation algorithm that accounts for the physical location of materials will be necessary when solving heterogeneous geometry descriptions. [ANL, ORNL]

Parallelization of the PROTEUS-MOC solver in plane, angle, and energy was successfully tested using the Takeda-1 benchmark. Preliminary scalability results for parallelization in angle proved to be excellent, much like previous experience with the MOCFE code and the PROTEUS-SN solver. Scalability with respect to the plane parallelization was good, as expected, while conclusions about energy parallelization cannot be drawn until investigations can be completed using more powerful computers. [ANL]

Structural Mechanics (Diablo)

The NEAMS structural mechanics module development largely focused on completing last year's exploration of seismic soil-structure interaction modeling via modern 3D nonlinear solid and structural mechanics. Final sample executions were performed, and comparisons with the corresponding results generated by the legacy SASSI approach are being documented. This culminates a large effort to assure that equivalent problems are being posed in the context of the tools' respective numerical formulations and implementations.

Reactor Primary Loop Simulation (RELAP-7)

Mathematically well-posed equations for the progression of a two-phase flow model have been defined and were implemented in the current version of RELAP-7. The progression problems start with single-phase equations and expand to two-phase flow modeling with increasing complexities in seven steps and equations. Preliminary testing has been done and further studies are ongoing to improve the robustness of the solution algorithms by implementing additional Jacobian terms (that is, more complex terms). [INL]

The code infrastructure was improved by separating the heat conduction model from the 1D fluid flow model in the CoreChannel, HeatExchanger, and PipeWithHeatStructure components to remove the "hard-coded" implementations that existed in previous versions. This improvement reduces coding redundancy, increases readability, and provides flexibility to add capabilities to the code. [INL]

A fundamental framework has been developed to couple the RELAP-7 code with the 3D kinetics code RattleSnake through another MOOSE-based application named Mammoth. Coupled RELAP-7/RattleSnake simulation results have been obtained for steady-state problems. [INL]

Advanced modeling capabilities specific to SFRs are continuing to be developed, with the focus on the accurate SFR primary system simulation under unprotected and protected loss-of-flow scenarios. Additionally, a strategy for coupling the MOOSE-based SFR module and the Reynolds Averaged Navier-Stokes (RANS)-based code STAR-CCM+ has been identified, and the initial implementation of the coupling interface was completed. Besides the code development, verification tests have been developed and examined to help ensure

that ongoing code development efforts are verified against a wide range of conditions. [ANL]

Mesh Generation (MeshKit)

Simulation of flow in a reactor often requires boundary layer meshes for better accuracy. It is often difficult to generate these meshes at the same time as the reactor mesh, so development has begun on a tool for post-mesh boundary layer (PBL) generation; the preliminary PBL code has been tested on small problems. At present, the PBL code is an algorithm in MeshKit to create new boundary layer elements on an existing mesh. Input to the program is a file containing keywords that prescribe instructions (bias, number of layers, etc.) for layer formation. The output is a mesh file (including meshed boundary layers) specified in the input file and a log file describing the intermediate steps. Future work will support tetrahedral elements and refine how elements in other bodies are affected by the boundary layer mesh (multiple bodies case). [ANL]

Integration Accomplishments

Interface between Product Lines

To successfully integrate fuels and reactors tools, analysts must be able to couple simulations that use different meshes, primarily those based on the MOOSE (fuels) and MOAB (reactors) frameworks. In other words, MOOSE and MOAB must be able to interface with each other. To this end, an activity has begun to define the relationship between MOOSE and MOAB capabilities and describe the extensions needed to ensure their compatibility. [ANL, INL]

Software Quality Assurance

In early November 2012, an independent, external team performed a software quality assurance (SQA) assessment of MOOSE, which provides the simulation framework for the fuels product line (BISON and MARMOT), as well as the reactor systems analysis tool (RELAP-7) of the reactors product line. The external assessment concluded that MOOSE has "satisfactory" compliance with organizational and QA program requirements of ASME NQA-1-2008 and -1a-2009, an outstanding result at this stage of development. Further, the independent assessors cited nine "strengths," that is, exemplary practices that exceed NQA-1 requirements. [INL]

In a separate effort, the NEAMS SQA team compiled and performed static defect analyses of the PETSc (Portable, Extensible Toolkit for Scientific Computation) and Trilinos numerical libraries, which are used in MOOSE. These libraries together comprise nearly 600,000 executable lines of source code. Initial measurements found that Trilinos had a fault density of 0.81%, and PETSc had a density of 1.3%. These are moderately higher than past measurements on nuclear production codes but are still very low defect rates and likely have no operational impact. Efforts are starting to expand to MOOSE itself and the end-application BISON. [LLNL, INL]

NEAMS Website

The NEAMS website is now operational at neams.ne.anl.gov. Visitors who sign up for a "newsletter" will receive NEAMS program announcements, including quarterly report publication, by email. [LLNL, ANL]

Technical Spotlight: Modeling and Simulation Made NiCE

It is often the little things – input or compiler flags, unfamiliar file formats, cryptic output – that make users pause before embracing new scientific software. The big things – modeling and simulation tools that run at unprecedented physical scales and resolution – might never be appreciated by the decision-makers and analysts for whom they were made without taking care of those little things that matter to the user experience. The high-performance computing (HPC) experts cannot be the only people using HPC codes if they are going to have any impact outside the NEAMS community.

The NEAMS program recognized this problem early and commissioned the development of a user-friendly integrated environment. This environment must encapsulate and abstract those activities that do not directly produce a simulation but nonetheless must be performed by users to benefit from the state-of-the-art capabilities provided by the developers. In other words, a simplified yet sophisticated user environment is an important NEAMS objective. After all, users should not have to worry about specialized file formats, runtime flags, long-term data storage, or other in-depth details of how a NEAMS product is installed, configured, and executed. Rather, users should be free to think mainly about what they want to study with NEAMS tools.

Making NiCE

The NEAMS Integrated Computational Environment – NiCE for short – is the NEAMS program's answer to the need for easy usability, accessibility, and collaboration. It complements both SHARP and MOOSE from the reactors and fuels product lines with common tools for creating input files, launching jobs locally and remotely, looking at data in 3D, and managing "assets," such as simulation input and output files.

The primary technical challenges for NiCE are manipulating the large amounts of data that high-fidelity simulations generate and both the physical scale and computational scale (i.e., number of processors) with which it will interact. The NEAMS products are petascale simulators with the potential to generate petabytes of data and run on hundreds of thousands of processing cores. NiCE must, in turn, be an extremely optimized environment that also supports those users who do not have access to the largest of machines or who want to branch out to public or private clouds; arguably, cloud users will comprise the lion's share of the user base.

NiCE is a free and open-source product available at niceproject.sourceforge.net and written in Java with a small amount of C++. It is

built on the Open Services Gateway Initiative (OSGi) framework's reference implementation (Equinox) and the rest of the widely acclaimed Eclipse platform. NiCE is both component and plug-in based and can be extended to do new things in a matter of minutes. It has plug-ins for visualization: VisIt for mesh-based output and JMonkeyEngine for 3D constructive solid geometries. The Hierarchical Data Format version 5.0 (HDF5) is used for storing information about reactors, and a relational database (Derby) is used for storing transaction data.

The most recent stable version of NiCE is 2.0, which was released on September 28, 2012.

NiCE's Feature Set and Use Cases

The value that integration and coordination provides to analysts, students, and everyday users cannot be overstated. NiCE enables users from a variety of communities to access NEAMS products uniformly and greatly simplifies training requirements for professionals or students who just want to run some simulations instead of developing code.

NiCE's design is based on requirements (user needs) and features (sets of related requirements) gathered from stakeholders and current and potential users. The requirements elicitation process for NiCE started in February 2009, and all the requirements are reviewed regularly, as often as monthly at the beginning of a development cycle. Interviews, surveys, informal discussions, and literature reviews have all been used to develop the set of functional and non-functional requirements for NiCE. (Non-functional requirements describe the qualities of a system, such as stability and scalability, as opposed to functional requirements, which describe the behavior of a system, that is, the operations it is designed to perform.) The interviews and surveys were very carefully planned and executed to remove as much bias as possible from the questions.

The feature set of NiCE is broad and covers both domain (context) and computer science (capability) concerns. The features were initially developed within the NEAMS community; input from other stakeholders was incorporated later. Currently, the NiCE requirements and features comprise the following capabilities:

- Execute simulations on a wide variety of platforms, including HPC machines, and operating systems.
- Provide tooling to set up models for input files, 3D geometries, meshes, materials, or other data for simulations.
- Provide a suite of analysis tools, including visualization, analytics, and data mining tools and algorithms.
- Provide utilities for performing uncertainty quantification.
- Provide web-, Android-, and Eclipse-based clients that connect to the same server to facilitate "universal access."
- Support the composition of new applications and workflows from existing codes and tools.
- Support the development of new computing modules in nuclear energy codes.
- Promote interoperability and loose coupling between codes.
- Provide extensive documentation for users and developers.

Some features are still being implemented.

The feature set and the results from requirements gathering interviews were used to develop seven unique use cases, which are formally defined and cover many types of interactions and scenarios between users and the system. These use cases almost completely track to the list of features. Use case is defined here as a description of the interactions between users and the system, the information that passes between the users and the system, and the before and after states of the system that define how it functions. The use cases are managed as formal specifications stored digitally and updated as needed. The use cases and scope of work they cover are as follows:

Run a simulation. Executing and monitoring simulations is often very difficult for users who are newly acquainted with a particular code and sometimes even for experienced users.

Set up a model. Specifying the input parameters that are necessary to simulate a physical system is a natural partner to executing a simulation and can be a very challenging task. In addition to supporting interactive parameter specification, NiCE includes a graphics editor for visual modification of 3D geometries (Fig. 5).

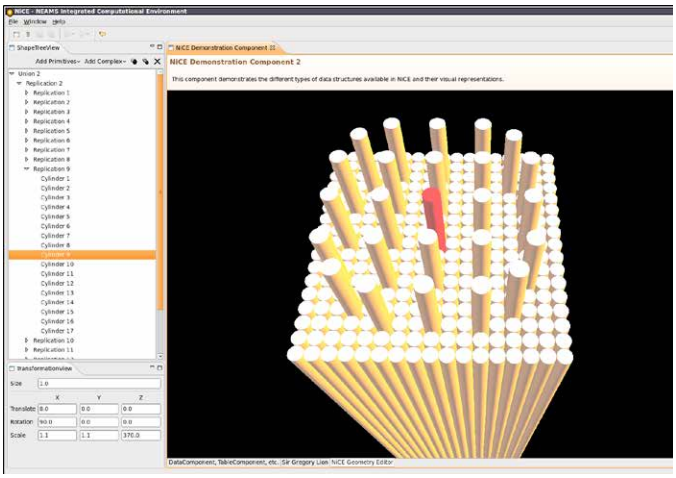

Fig. 5. NiCE geometry editor.

Analyze data. Many HPC codes provide "raw" results that are not of immediate use to an analyst. NiCE includes a dedicated "reactor analyzer" tool, which is customized for the sort of data created by a reactor simulation and can more quickly provide high-quality 3D visualizations. Mesh variables can be viewed with VisIt, and averages, such as average power per pin, can be visualized on maps at the core, assembly, and pin levels. These capabilities allow users to get to their information faster.

Create an application. Since applications and tools do not always exist to address the exact questions of an analyst, it is often necessary to create new applications, tools, or workflows by combining existing tools or developing completely new tools. NiCE is designed to help users with these tasks.

Create a module. NiCE will provide tools for extending existing NEAMS codes so that developers can easily add new modules to the product lines (via tools such as Stork for MOOSE, for example). New modules are based on existing NEAMS simulators and extend their functionality with new physics or different solvers.

Save an asset. NiCE is designed to work with software and data repositories, generically defined as catalogs, to provide both a way to share different assets between users and to store simulations and other files as needed to meet regulatory requirements, promote code re-use, etc.

Search the catalog. Since searching for a particular asset is different task than storing it and often includes retrieval, NiCE has a second data management use case specifically for searching the catalog. Separating searching from submission allows the development team to focus on the unique issues associated with viewing and retrieving data.

The features that enable these uses all point to a system that is more than a set of scripts, more than a user interface or a collection of user interfaces, and more than a file management system. They collectively describe a combined workflow and data management system that couples simple but directed input with advanced 3D visualization, execution of large complex jobs with easily accessed and analyzed output files, and performance of very complicated tasks with the ease of use of a Linux workstation or Windows PC.

Where Will NiCE Be Next?

Last year, development focused on creating the NiCE infrastructure and tools required to provide the features to enable the envisioned uses. The scope of work this year is directed at deploying NiCE for SHARP- and MOOSE-based applications, starting with BISON. The next stable release of NiCE will include persistence support via a relational database, a web client, and a revamped version of the NiCE tool set for analyzing data from reactor and fuel simulations (i.e., the reactor analyzer). The next release will also include the first versions of the fuels product line plug-ins to NiCE for users that want to set up and launch BISON jobs and limited support for other MOOSE-based applications.

Many capabilities are already available in the "nightly builds" of NiCE that can be found at the Sourceforge project page and are available to anyone who wants to try them out. However, some capabilities will remain limited while they are still in development. Feedback from test use is welcome and wanted because it allows the team to improve the product. Users can report a bug through the Sourceforge project wiki page, submit questions to the user forum or email the author directly.

The NiCE team is also developing more training videos and tutorials that will appear on the project site and YouTube (www.youtube.com/user/jayjaybillings) in the coming months. The first NiCE training seminar and webinar is being planned for later this year.

NiCE will be presented in March at EclipseCon 2013, and publications about some of its newer features have been submitted to the 2013 meeting of the American Nuclear Society and the 2nd International Workshop on Analytics for Cyber-Physical Systems.

Some computational scientists outside of NEAMS are finding uses for NiCE, including quantum computing and use in other DOE programs, such as Scientific Discovery through Advanced Computing.

Contributing Authors

The following members of the NiCE Development Team contributed to this article: Andrew Belt, Andrew Godfrey, Mike W. Guidry, S. Forest Hull, Eric J. Lingerfelt, Greg Lyon, Alex McCaskey, Ugur Mertyurek, and Neeti Pokhriyal; A. Belt and M Guidry are from the Univ. Tennessee at Knoxville, and the other contributors are from ORNL.

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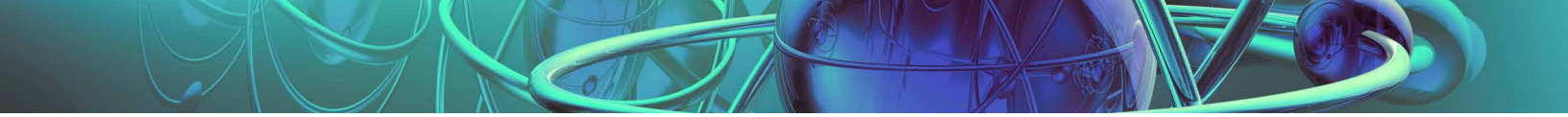
NEAMS Team in the News

AAAS Fellow. Senior computational scientist Paul Fischer (ANL) has been named fellow of the American Association for the Advancement of Science, which recognizes empirically or socially distinguished efforts to advance science or its applications. A member of the Mathematics and Computer Science Division, Dr. Fischer was elected for his outstanding technical accomplishments in computational fluid dynamics (CFD) and fluid flow simulations on extreme-scale computers.

One of Fischer's most notable achievements is his design and development of the scalable CFD code Nek5000, which he has applied to challenging problems in the hydrodynamics of nuclear reactors as well as other applications, such as modeling blood flow to aid development of advanced medical procedures. His work on Nek5000's predecessor started in the 1980s, and after commercialization of the original code, Fischer started development of the research-oriented Nek5000, which he brought to Argonne in 1998.

Fischer's work on Nek5000 has been recognized before, notably by the Association for Computing Machinery, which awarded him the Gordon Bell Prize for High-Performance Computing in 1999. He has also been recognized by Argonne and DOE for his work, and he also is a senior fellow at the University of Chicago/Argonne Computation Institute. His simulation of the Deepwater Horizon oil spill was shown on NBC Nightly News in 2010.



Recent and Upcoming Level 1 and 2 Milestones

Completed during this Quarter (October - December 2012)			
Milestone ID	**Description**	**Due Date**	**Finish Date**
M2MS-12AN0605116	Use the transportation logistics tool to conduct and report on simulations identified by UFD integration team	10/31/2012	10/29/2012
M2MS-12AN0603081	Demonstrate SHARP framework support for a coupled physics problem	11/30/2012	See note a
M2MS-13AN06030232	Provide SIBERIA shear stress simulation results to IBRAE as part of Russian Federation collaboration	11/30/2012	2/11/2013
M2MS-12OR0603021	Complete multi-physics simulation of fuel assembly with AMP	12/31/2012	10/1/2012
M2MS-12OR0605081	Demonstrate AMP for modeling UFD	12/31/2012	9/30/2012

[a] This activity was terminated by a change in scope at the program level.

Milestones Coming Due during the Next Quarter (January - March 2013)			
Milestone ID	**Description**	**Due Date**	**Status**
M2MS-13AN06030212	Update development plan for NEAMS thermal fluids module	1/31/2013	On schedule
M2MS-13AN06030215	Update development plan for NEAMS neutronics module	1/31/2013	On schedule
M2MS-13AN06030241	Complete experimental measurement of detailed inlet boundary conditions	1/31/2013	On schedule
M2MS-13LL0603074	Update development plan for NEAMS structural mechanics module	1/31/2013	Delayed (new date)
M2MS-13IN0603031	Complete INL portion of NEAMS integrated framework development plan	3/1/2013	On schedule
M2MS-13AN06030219	Complete multi-physics simulation using NEAMS structural mechanics, thermal fluids, and neutronics modules[b]	3/29/2013	On schedule
M2MS-12AN0607052	Complete experimental study of inlet boundary condition sensitivity	3/29/2013	Delayed (new date)
M2MS-12AN0607054	Complete validation comparisons	3/29/2013	Delayed (new date)
M2MS-13AN0603021	Issue NEAMS integrated framework development plan (includes deliverable from milestone M2MS-13IN0603031)	3/31/2013	On schedule
M2MS-13AN06030235	Provide MAX isothermal test specifications as part of Russian Federation collaboration	3/31/2013	On schedule
M2MS-12LL06031213	Report final results of seismic gap analysis workshop for SHARP	3/31/2013	Delayed (new date)

[b] This activity includes previously reported milestone M2MS-12AN0603279 to complete integrated multi-physics simulations with PROTEUS, Nek5000, and AMP.

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