ANL/NEAMS-14/3

NEAMS Update

Quarterly report for April – June 2014

Published October 2014

Overview

- BISON's thermo-mechanical contact algorithm was significantly improved (page 2).
- MOOSE and PETSc were enhanced to improve the convergence of the contact solver (page 2).
- A temperature-based creep model for zircaloy cladding was added to BISON (page 3).
- Progress was made in the BISON model for fuel microstructure, in particular for the evolution of the average grain size (page 3).
- Improvements to MOOSE interfaces and data structures have made the framework more user-friendly and significantly increased execution speed (page 4).
- Computational speed of the SFR System Analysis module has significantly improved by the addition of a finite-element flow model (page 5).
- Various improvements were made to MeshKit and the Reactor Geometry Generator (page 5).
- PROTEUS has been updated and tested on a two-dimensional model of the Advanced Test Reactor core (page 6).
- RAVEN control logic software has become a permanent component of RELAP-7 (page 8).
- RAVEN's ability to determine cladding failure probability has been assessed with a reactor station blackout model (page 9).
- Development teams continue to enhance the NiCE user environment and VisIt visualization toolkit (pages 10 and 11).

Thomas Named RPL Lead

Justin W. Thomas has been named the new Reactor Product Line (RPL) lead for NEAMS. Justin received his Ph.D. in nuclear engineering from Purdue University, where he contributed to the development of a multiphysics LWR modeling capability that was among the first to perform full-core simulations featuring high-resolution predictions of within-pin neutron fluxes and temperature profiles.

At Argonne, Justin has supported the NEAMS program by extending this capability for prismatic-block very-high-temperature reactors, and contributing to a multiscale sodium-cooled fast reactor transient safety analysis modeling capability. Justin also contributes to the Advanced Reactor Technology program and hopes to seek further collaboration with this key customer for the RPL.

Fuel Product Line (FPL) Accomplishments

Engineering Scale (BISON)

The thermo-mechanical contact algorithm used by BISON was significantly improved during this quarter. Thermo-mechanical contact problems are of central importance in fuel performance simulations, most notably for accurately modeling pellet-cladding interaction in nuclear fuel rods. BISON has long modeled such contact problems with a high degree of fidelity, although doing so can lead to run-time issues of less than desirable robustness of solution convergence. In cooperation with the development teams for MOOSE and PETSc (the solver library underlying MOOSE), BISON developers greatly improved the robustness of the contact algorithm. [INL]*

Taken individually, the elastic and thermal diffusion problems for the independent fuel pellet and cladding system are elliptical problems that are generally well-behaved numerically; optimal convergence of iterative linear solvers for these problems can be achieved using a variety of preconditioners. Once contact between elastic or thermally conducting structures begins (see ***Fig. 1***), however, preconditioning and convergence can become increasingly difficult and often lead to divergent thermoelastic solutions.

To improve the convergence of the contact solver, three improvements to MOOSE and PETSc have been made: (1) the MOOSE constraint system was used to implement contact, (2) dynamic sparsity modification of the Jacobian constraint rows was added to the constraint system, and (3) exact matrix elimination and assembly of the reduced system was added to PETSc.

Testing of these improvements on a variety of model problems have been performed with the goal of incorporating them into production BISON simulations. Results to date have been outstanding and have confirmed that a major advance in the robustness of the contact algorithm has been achieved. Convergence is generally ensured and is much less sensitive to both mesh refinement and an increased number of contact nodes. [INL, University of Chicago]

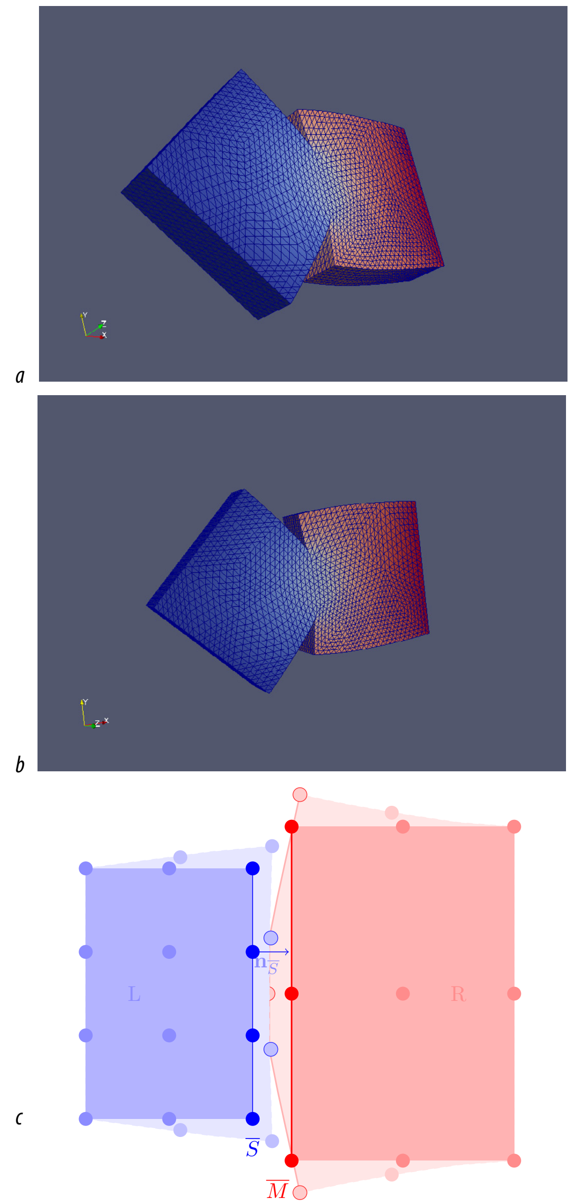

Fig. 1. BISON simulation of two contacting tetrahedral meshes: (a and b) two views of the full mesh and (c) detail showing node-to-node interaction.

*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).

In the area of transient/accident simulations, a temperature-based transition creep model was implemented in BISON for zircaloy cladding under normal to loss-of-coolant-accident (LOCA) conditions (***Fig. 2***). Last year's LOCA demonstration problem has been re-run using the new capability; although a detailed comparison of results is still in progress, the new model appears to be an improvement. The new capability will be further validated with the Rosinger creep tests, and the results will be incorporated into an update of the BISON Assessment Report. [INL]

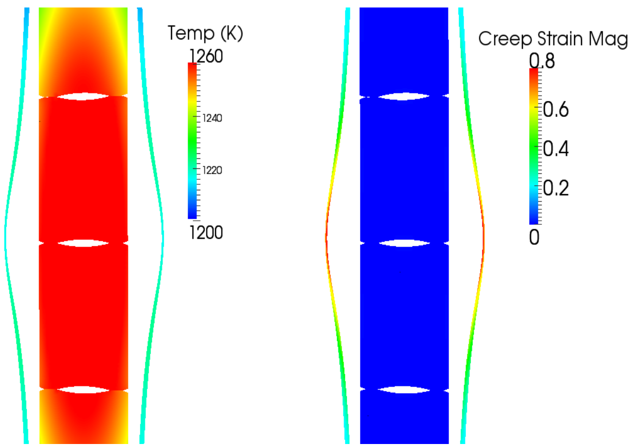

Fig. 2. Ballooning of zircaloy cladding under LOCA conditions using an enhanced creep model.

Subcontinuum Scale (MARMOT and Atomistic Simulations)

One of the primary goals of the FPL is to develop mechanistic materials models that model material behavior under irradiation based on the state of microstructure rather than fuel burnup, which does not reflect the actual history of the material. These models are developed at the mesoscale, as informed by atomistic simulations; however, up-scaling such models will enable a more predictive fuel performance capability at the engineering scale (BISON). [INL]

In this approach, the current state of the microstructure is represented by a series of microstructure variables within the BISON fuel performance code, such as the average grain size or the intragranular porosity. Models must be developed to describe the evolution of these variables as a function of temperature, stress, and neutron flux, as well as other microstructure variables. In addition, models are required to define how the various material properties vary with respect to the microstructure variables. This approach bases the model on the current state of the microstructure rather than the burnup. Finally, these relationships defining the microstructure must developed as physics-based models rather than empirical fits to experimental data in order to allow them to make accurate predictions outside of the bounds of data used for validation.

An important aspect of this activity is developing a mechanistic and accurate grain size model that can be used in BISON. The average grain size in UO_2 fuel pellets typically begins at about 10 µm. However, during reactor operation, the temperature near the center of the pellet rises above 1,500 K. At these temperatures, the mobility of the grain boundaries (GBs) rises sufficiently for them to migrate and reduce the overall free energy of the system. Smaller grains tend to disappear and larger grains tend to grow, such that the average grain size increases over time (see ***Fig. 3***). The increasing grain size within the fuel is important because it significantly affects fuel swelling, fission gas release, and creep; a recent study found that the fuel swelling model in BISON is quite sensitive to the grain radius. For this reason, it is critical to accurately predict the average grain radius. Other competing irradiation effects also contribute to changes in grain size and are also the subject of investigation and model development.

Work this year has resulted in the development of a mechanistic material model for the evolution of the average grain size in UO_2 fuel. The model predicts the change in grain size as a function of GB mobility (determined using molecular dynamics [MD] simulations), the curvature driving force (developed using MD and

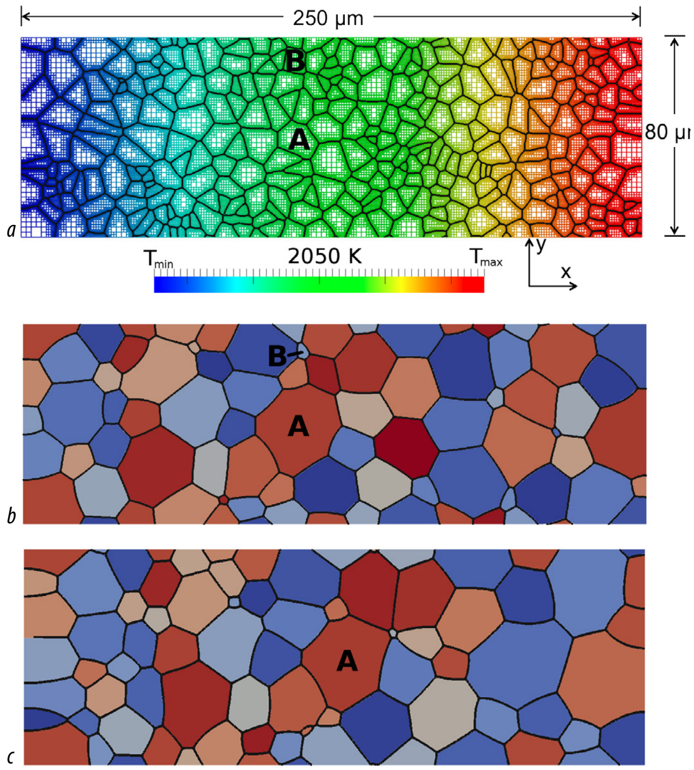

Fig. 3. MARMOT simulations of grain growth: (a) initial fine microstructure, (b) growth under isothermal conditions, and (c) growth under a thermal gradient. Note the growth of grain A at the expense of other grains, such as B.

MARMOT simulations), and a resistive force due to pores (which was taken from the literature, but validated against UO_2 data) and fission gas bubbles (described by a new analytical model informed by MARMOT simulations). [INL]

Continuing work is focusing on understanding the impact of GB anisotropy on the average grain size and quantifying the importance of fission gas bubble dragging. The completed model will be implemented in BISON and coupled to the fission gas release and sintering models. A number of BISON assessment cases will be rerun using the new model to quantify its impact. [INL]

MOOSE Framework

The interfaces in MOOSE have always been optimized to minimize development time. During the past quarter, several new features have been added to make model development even easier.

The Input Parameters system now contains methods for performing automatic range checking of user-supplied inputs, default coupling parameters, and parameter deprecation routines. Each of these features improves the robustness while simplifying the application development. Developers can now supply simple mathematical expressions for any user-supplied parameter to verify that it is within the proper expected range for the model. The framework performs error checking, freeing the developer from the need to write tedious and often duplicate routines for this purpose.

Default coupling values allow users to supply simple expressions or even functions wherever a normal variable would normally be expected. This allows models to be decoupled during development without any code changes, which simplifies troubleshooting and debugging. Finally, deprecated parameters allow developers to evolve their input parameter sets without breaking backwards compatibility. [INL]

Data structures have been streamlined to reduce MOOSE's memory footprint for many applications. These improvements now allow significantly larger simulations – by two orders of magnitude in some cases – to be run using the same resources as before. ***Fig. 4*** shows the memory usage for a mesoscale simulation run on several hundred processors. [INL]

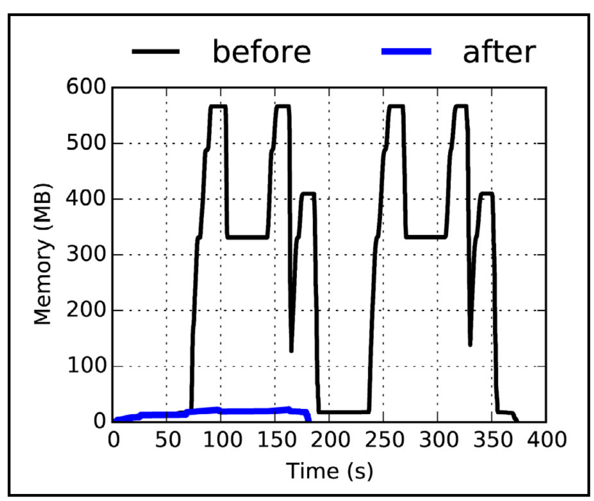

Fig. 4. Comparison of MOOSE memory use and processing speed before and after optimization.

Finally, MOOSE has added support for reading an image or stacks of images to produce initial conditions for simulations. This feature has practical applications in running validation cases against postirradiation samples or any other 3D dataset. Currently, this capability is being used by MOOSE's phase-field module and the MARMOT mesoscale simulator. [INL]

RPL Accomplishments

SFR System Analysis

The SFR System Analysis team continued to develop this MOOSE-based module using the primitive variable-based formulation finite-element flow model (FEM). Significant code improvements have been made through the demonstration simulation of the Advanced Burner Test Reactor (ABTR) protected-loss-of-flow transient (see ***Fig. 5***). The primary SFR system simulation capabilities based on the new set of components and the new FEM have been demonstrated, while the execution speed has been greatly improved when compared to the simulations performed last year using a density-based flow model (from about 2 hours to about 8 minutes). [ANL]

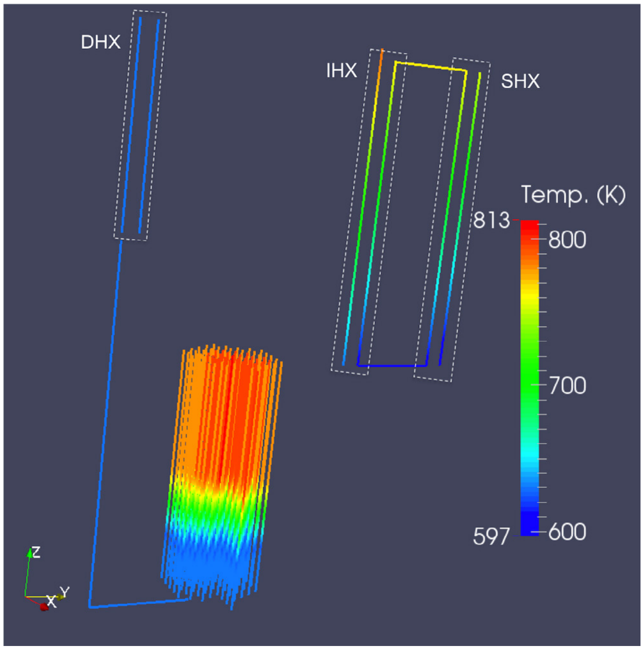

Fig. 5. Temperature distribution in the ABTR during a protected-loss-of-flow transient.

A new capability of modeling the fluid equations using the Boussinesq approximation has been developed and incorporated into a test suite. Although this model has been verified, code performance cannot be significantly improved because only the Jacobian-free Newton-Krylov solution method is available now. The performance can actually deteriorate for some tests due to the worsening of the matrix condition number. However, this development will be useful when the segregated-type solvers are implemented with MOOSE. [ANL]

The thermal hydraulic SFR Module development team has successfully presented a novel fluid model that has been developed and implemented in the SFR Module. The presentation at the 2014 ANS Annual Meeting was titled "A Fully-Coupled Finite Element Formulation for One-Dimensional Incompressible Thermally Expandable Flow." The paper received high scores from reviewers and the program committee, which recommended it for publication in Nuclear Technology. [ANL]

MeshKit

The MeshKit team moved MeshKit to Git on Bitbucket, a free hosting service. Git is a distributed revision control and source code management system with an emphasis on speed, data integrity, and support for distributed, nonlinear workflows. The team released MeshKit 1.2 as a part of the SIGMA 1.0 release. This release fixed various bugs and issues with different MeshKit builds and adopted features from the University of Wisconsin–Madison and Kitware. [ANL]

A new common.inp file was added to the AssyGen/CoreGen flow of the Reactor Geometry Generator (RGG). This change made the user input much simpler. Other changes in the RGG 1.0 release by Kitware included a new CoreGen scheme for shifting material and boundary conditions numbers for creating meshes, such as the ABTR core, and a new load balancing scheme for copy/move task distribution. [ANL]

The paper "Generating Unstructured Nuclear Reactor Core Meshes in Parallel" was accepted for International Meshing Roundtable 23. MeshKit training is being offered at Argonne (***Table 1***). See page 8 for the addresses of NEAMS framework websites. [ANL]

Table 1. Syllabus for MeshKit/RGG training.

- Introduction
- Design philosophy
- Graph-based mesh generation
- MeshKit algorithms and tools
- RGG 3-stage reactor core geometry and mesh generation
- AssyGen program
- CoreGen program
- Using the RGG interface:
  - Load existing RGG models (KAIST PWR, 1/6th VHTR, etc.)
  - Create a rectangular assembly and core model
  - Create a hexagonal assembly and core model
  - Create a mesh and explore available material and boundary conditions

NEAMS Structural Mechanics (Diablo)

Diablo was installed on three Linux clusters at Argonne, and two structural mechanics early adopters began learning the code and running example simulations. SHARP integration efforts included adding Diablo support for fully parallel read/write of MOAB databases and design discussions on in-memory parallel mesh transfers and CouPE extensions to support structural mechanics. The Diablo team also collaborated with ORNL on integrating a copy of Diablo into the SHARP repository and build system. [LLNL]

NEAMS Neutronics (PROTEUS)

The MC^2-3/PROTEUS training was held on April 22 onsite at Argonne. The full-day training consisted of presentations about the methodology and use of the MC^2-3 cross section generation and PROTEUS neutron transport codes. Twenty-two participants attended the training, including eight people from Purdue, ORNL, and TerraPower (***Fig. 6***). [ANL]

The updated version of PROTEUS along with its detailed methodology and user manuals has been completed. The update includes the enhanced transient options and the cross section application programing interface (API), which has the subgroup and resonance table cross section options. The new transient options contain an inhomogeneous fixed-source capability to support DOE's Global Threat Reduction Initiative in simulating the Russian IBR-2 reactor with a moving reflector. New cross section libraries are under verification using the cross section API. [ANL]

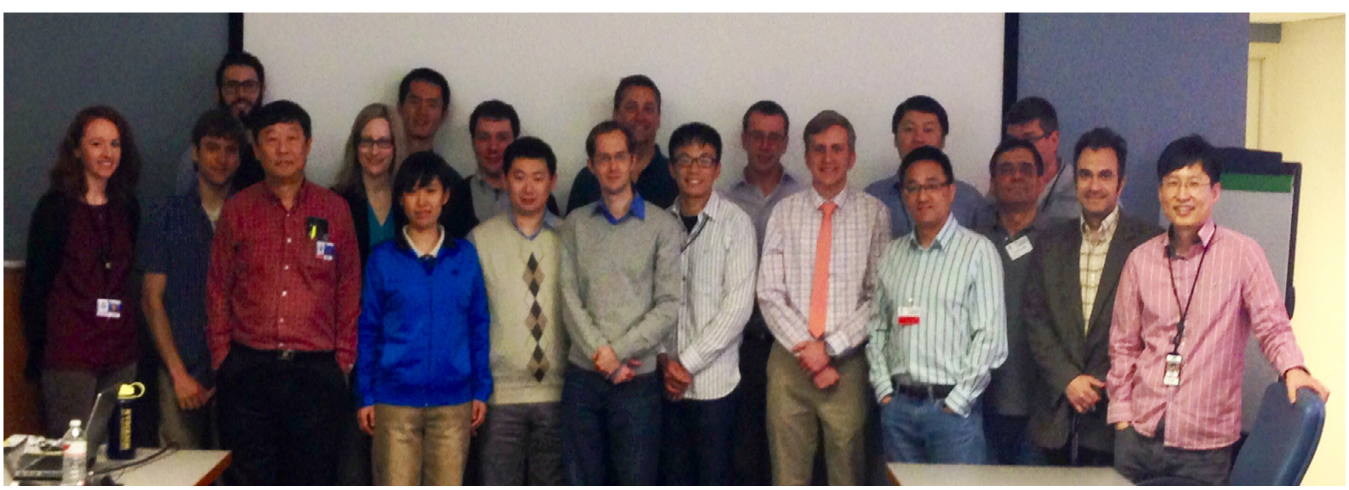

Fig. 6. Participants in the MC2-3/PROTEUS Training on April 22.

As a verification effort for PROTEUS, the two-dimensional Advanced Test Reactor (ATR) core was simulated by PROTEUS and the Monte Carlo N-Particle (MCNP) code using the same 23-group multigroup cross sections. With use of an angular quadrature of Legendre-Tchebyshev L3T15 and 3 million elements, the PROTEUS solutions agreed well with MCNP within 300 pcm for eigenvalue and 4.6% for region-averaged group fluxes in the fuel meat regions (i.e., the fissile part of a fuel rod) (***Fig. 7***). A further improvement could be made with mesh refinements, especially in non-fuel regions. [ANL]

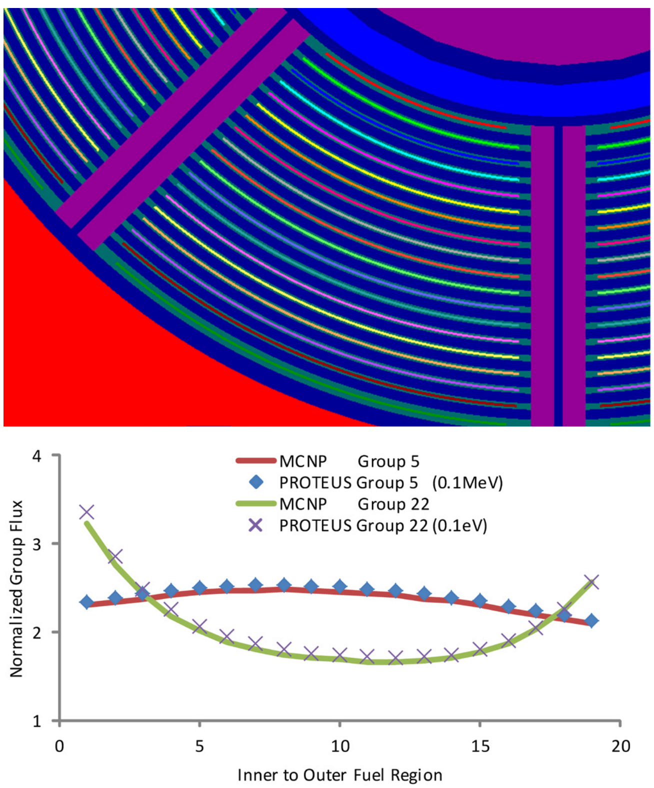

Fig. 7. Comparison of region-averaged group fluxes between PROTEUS and MCNP in fuel meat regions for the ATR.

Thermal Hydraulics (Nek5000)

The SHARP team continues to address the applicability of a fully coupled, three-physics, high-fidelity toolkit to the problem of reactivity feedback dependent on assembly deformations. This past quarter, the team has focused mostly on continuation of the validation-driven development of the thermal-hydraulics module Nek5000 for low-Mach-number multispecies capability. The latest implementation for large-eddy simulations (LES) involved the use of CVODE library for the numerically stable setup that has been successfully tested on the 2014 OECD/NEA PANDA benchmark geometry. In addition to the use of an accurate but computationally more expensive low-Mach number formulation, the team finished a long-transient validation simulation test with a relatively inexpensive Boussinesq approximation that is faster to compute. ***Figs. 8*** and ***9*** show the computational results with the corresponding formulations at different simulation times for slightly modified geometries. The comparison of the results is underway. [ANL]

An abstract – “Large-eddy Simulations of Stratification Layer Erosion by a Jet” – was submitted to the 67th Annual Meeting of the APS Division of Fluid Dynamics. The team also prepared and presented several well-received talks at the 2014 ASME 4th Joint US-European Fluids Engineering Summer Meeting, including “A Novel Variant of the k-ω - URANS Model for Spectral Element Methods – Implementation, Verification, and Validation in Nek5000” and “Implementation and Validation of a Hybrid RANS/LES Model in the Spectral Element Solver Nek5000.” [ANL]

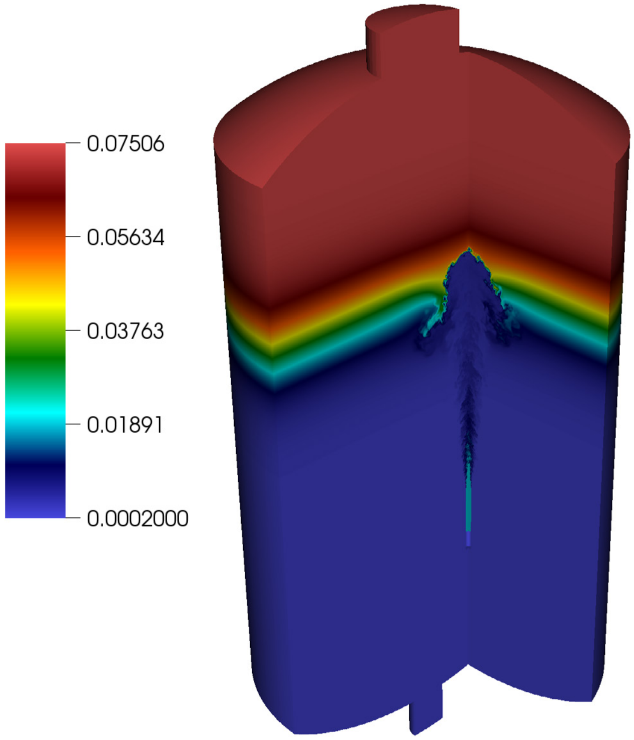

Fig. 8. Pseudocolor plot of helium mass fraction at early times of PANDA simulation with low-Mach number approximation. A vertical jet of larger helium fraction (light blue) has penetrated the initial stratification layer separating the helium-rich region (red) from the air-rich region (blue) of the vessel.

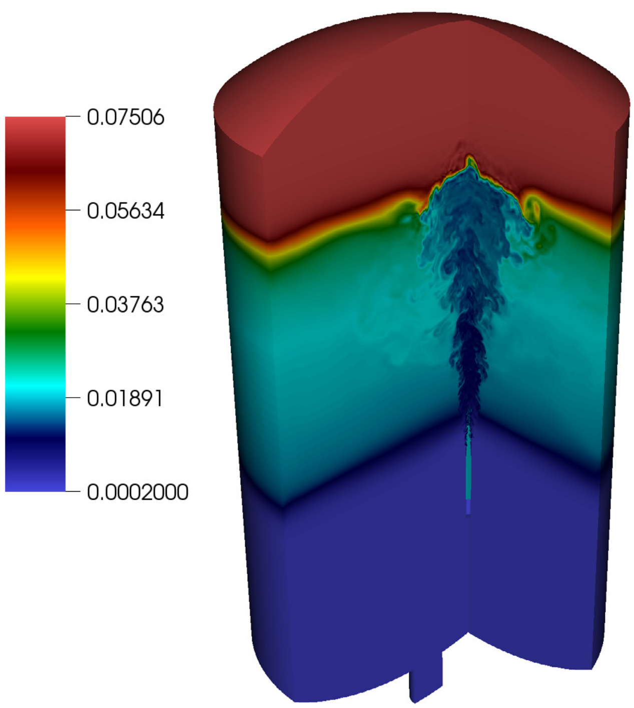

Fig. 9. Pseudocolor plot of helium mass fraction at the final simulation time of PANDA simulation with Boussinesq approximation. Helium from the pipe inlet (light blue) has filled a significant portion of the vessel, eroding the initial stratification layer. The geometry is simplified to speed up the simulation.

Plant Simulation (RAVEN)

Software Development

RAVEN control logic software has been moved to become a permanent component of RELAP-7. The reason of this choice was to give RELAP-7 the capability to perform nuclear plant simulations even in absence of the RAVEN driver. Generally speaking, RAVEN allows the software infrastructure to open a python interface where variables get evaluated at each time step; eventually, this will become a general feature of the MOOSE environment. [INL]

The data management infrastructure that manages, stores, and recovers the mapping between the input space and the simulation outcomes has been extended in RAVEN to integrate the information concerning the probability associated with each realization of the input space. This allows performance of a statistic postprocessing analysis to obtain mean, standard deviation, skewness, and kurtosis of the figure of merits. These values represent the output of the simulation as correlation analysis between the input and output spaces. [INL]

The postprocessing capabilities have been extended also to compute reliability surfaces. The computation of multidimensional volume and surface integrals inside and along limit surfaces, for the evaluation of risk functions, is ongoing. [INL]

Station Blackout Analysis

A boiling water reactor station blackout (SBO) scenario has been modeled and analyzed to determine cladding failure probability using different sampling techniques (Monte Carlo, Latin Hypercube, grid, and adaptive limit surface search). All methodologies show coherent cladding failure probabilities and correlations between the random variables in the input space and the failure probability of the cladding. Moreover, this demonstration successfully tested the usage of multidimensional/parametric probability functions. [INL]

Fig. 10 shows the simulation of the probability distribution function of the cladding failure temperature as a function of the burnup. ***Fig. 11*** instead shows the limit surface that is a four-dimensional plot (recovery time of the diesel generators, recovery time of the external power, burn-up, and cladding failure temperature probability) where the fourth dimension is plotted using a color map over the spheres that identify the location of the limit surface. The limit surface plot confirms the deterioration of the probability of success due to increased burnup. Moreover, as expected, a discontinuity is present in the limit surface due to the equivalence, with respect the failing probability of the cladding, of the restoration of cooling capacity either by recovery of the diesel generators or off-site power. [INL]

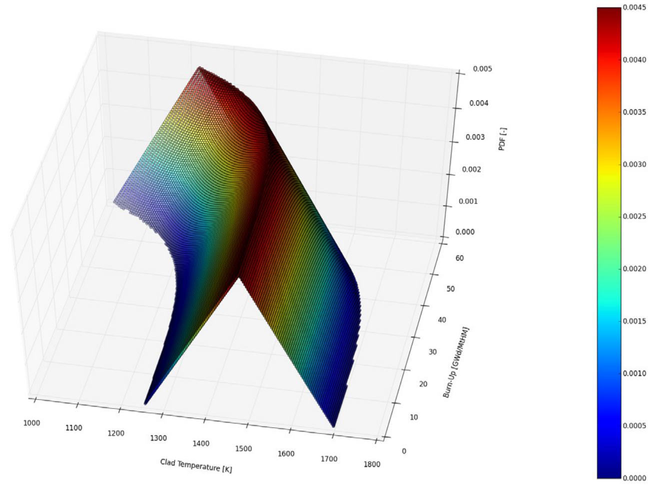

Fig. 10. Probability distribution function of the cladding failure temperature as a function of burnup.

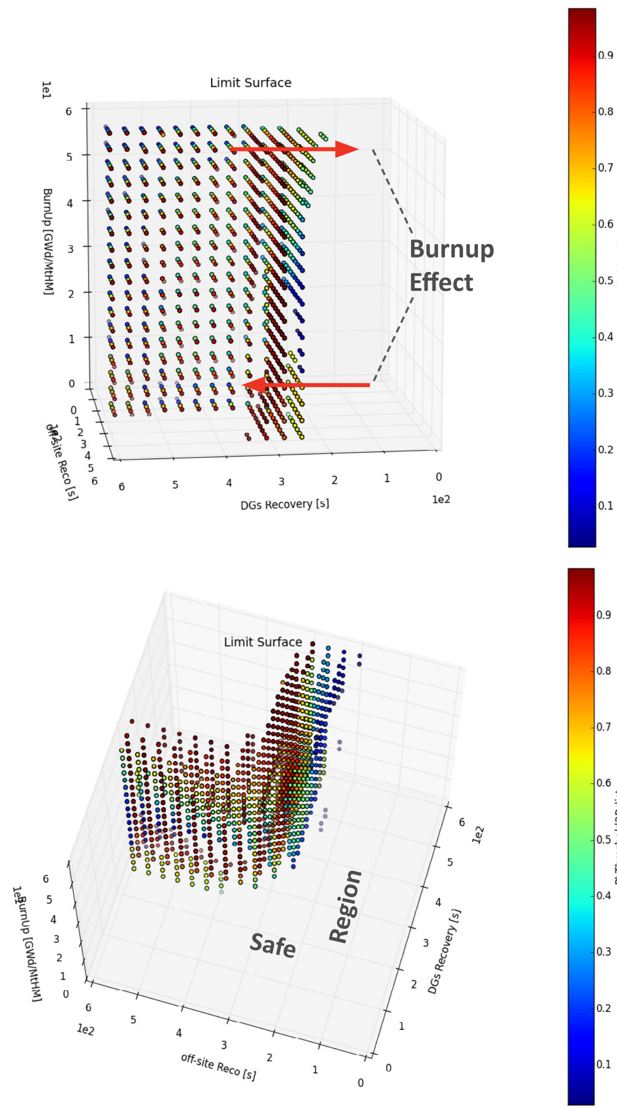

Fig. 11. Limit surface delimiting safe from unsafe region in the input space. (See text for explanation.)

User Environment (NiCE)

In June, NiCE introduced support for 3D reactor plant views in its reactor analyzer. Backed by an object-oriented plant model and built around jMonkeyEngine, the 3D view supports many plant components, including pipes, core channels, junctions, branches, heat exchangers, reactors, and various specialized subclasses. The view is interactive and can be populated from NiCE-friendly HDF5 files and supported simulation-specific input files. [ORNL]

In additional, the NiCE team released a new reactor perspective dedicated specifically to reactor simulation data analysis. This perspective streamlines the user's experience by maximizing available screen space for the interactive reactor analyzer views (***Fig. 12***). A new reactor viewer lets the user simultaneously open and browse multiple HDF5 reactor files. [ORNL]

The NiCE team also continued work on the SHARP build system, making the GNU Autotools build process for the coupled multiphysics framework an efficient, simple, and streamlined task. More work was done to improve the overall user experience of the build system, such as the ability to automatically download and build critical framework dependencies, such as MOAB, PETSc, and MPICH. Hooks were also developed for future integration with the Diablo structural mechanics code. [ORNL]

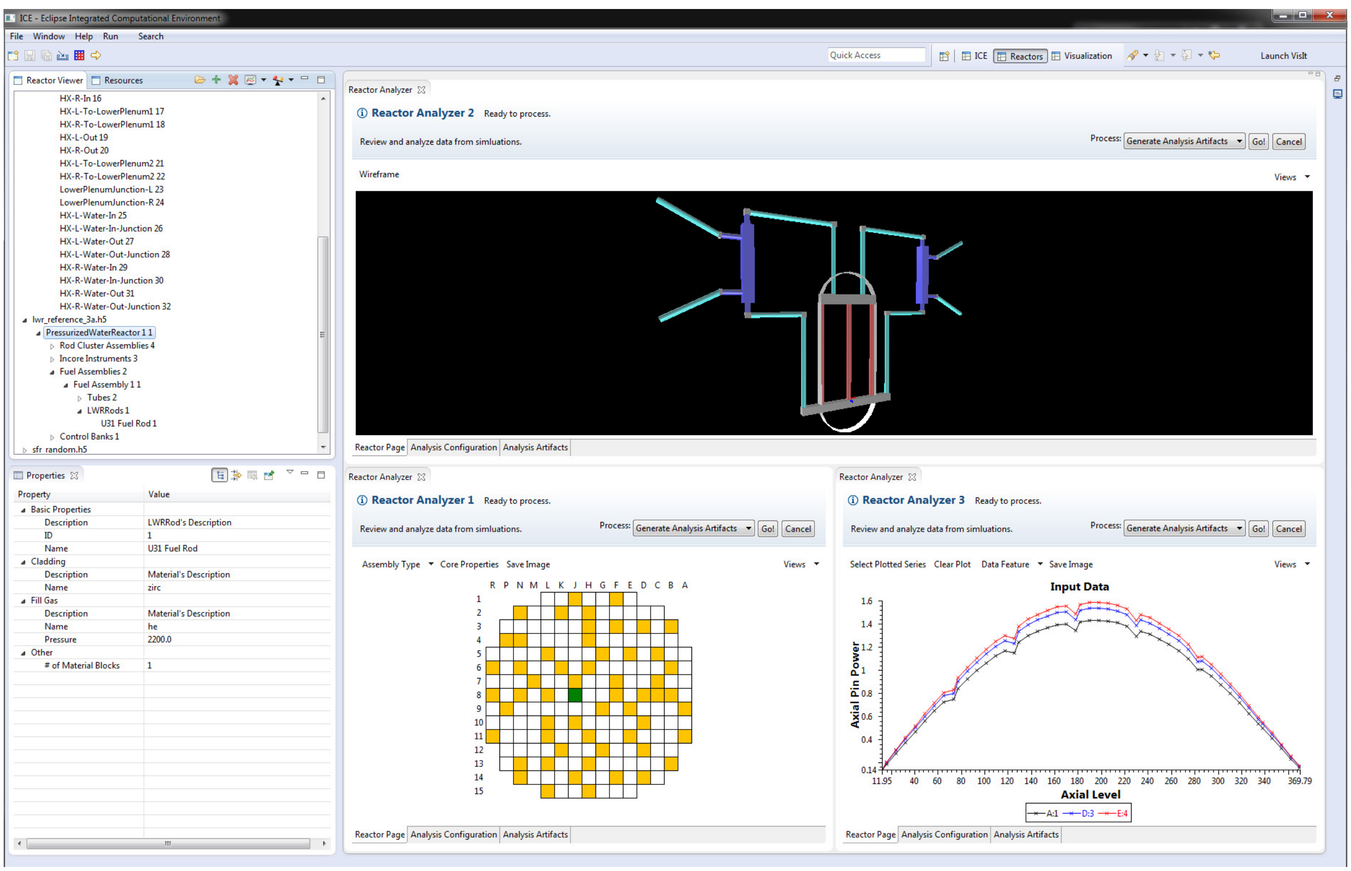

Fig. 12. Screen shot of the updated NiCE reactor analyzer with support for RELAP-7.

Visualization (VisIt)

VisIt is a high-performance visualization package used by several teams within NEAMS (***Fig. 13***). As part of VisIt development, new support for spectral element solvers is being implemented to provide in-situ visualization that can be coupled with Nek5000 for solution monitoring while simulations are in progress. This is especially challenging for the highest-resolution models. [LBNL]

The VisIt and NiCE teams are collaborating to add custom visualization capabilities for the NEAMS ToolKit user base, which includes work to extend VisIt support to the wide variety of modern operating systems that are supported by NiCE. [LBNL]

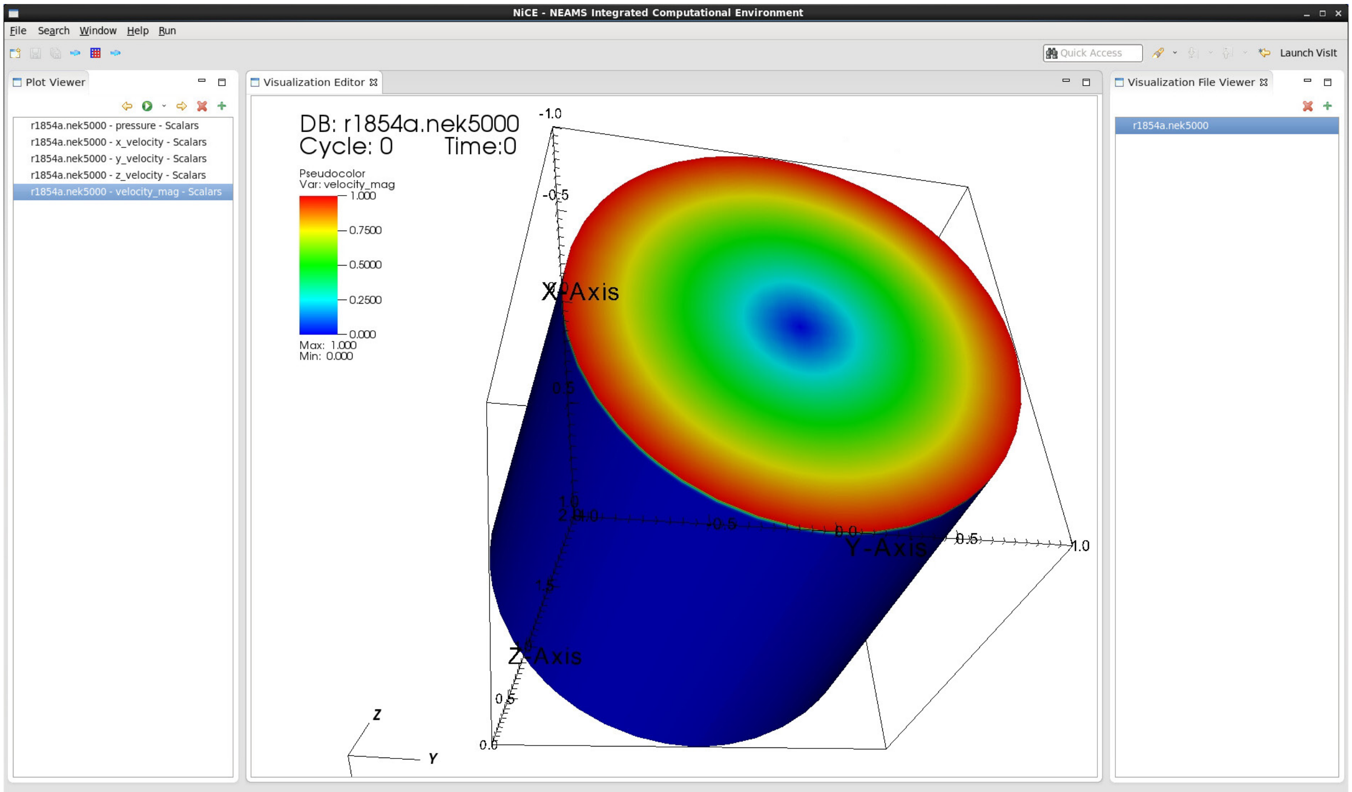

Fig. 13. Screen shot of the updated NiCE user environment with embedded VisIt visualization of multidimensional fuel pellet data.

Availability of This Report
Online Access: U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via DOE's SciTech Connect (http://osti.gov/scitech/).

About Argonne National Laboratory
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see www.anl.gov.

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Status of Level 1 and 2 Milestones

Completed Milestones

Milestone ID	Description	Due Date
M2MS-14OR06030623	Implement NiCE support for RELAP-7 and initial plant-level reactor analyzer views	5/30/2014
M2MS-14AN0603041	Deliver updated NEAMS neutronics module and user manual to support SFR transient analysis	6/30/2014
M2MS-14IN0602031	Implement a quantitative model in BISON for fuel average grain size	6/27/2014
M2MS-14IN06030510	Report techniques for reliability analysis in station blackout models	7/8/2014
M2MS-14LA0602041	Implement new MARMOT models for fission gas/product diffusion	6/30/2014

Upcoming Milestones

Milestone ID	Description	Due Date
M2MS-14AN06030210	Simulate single assembly with online mesh deformation	9/30/2014
M2MS-14AN0603022	Release version 1.0 of the CouPE coupler/driver	9/30/2014
M2MS-14AN0603024	Release MeshKit version 2.0	9/30/2014
M2MS-14AN0603038	Update and demonstrate the SFR system simulation capability	9/30/2014
M2MS-14AN0603039	Provide update on testing and development of Nek5000 thermohydraulic capability	11/30/2014*
M2MS-14IN0602022	Release BISON update for LWR fuel performance in quasi-steady-state and off-normal conditions	9/30/2014
M2MS-14IN0602023	Update BISON validation and assessment report	9/30/2014
M2MS-14IN0602032	Deliver an initial quantitative fracture model for BISON implementation	9/30/2014
M2MS-14LA0602042	Deliver a new heirarchical diffusion model for BISON implementation	9/30/2014
M2MS-14LL0603072	Update the NEAMS structural mechanics module to support FY14 demonstrations	7/31/2014
M2MS-14OR0602051	Perform a benchmark problem with Thermochimica-MOOSE/BISON/ MARMOT for oxygen potential in high-burnup LWR fuel	9/30/2014
M2MS-14OR0603062	Demonstrate PROTEUS for selected reactor benchmarks and problems	8/30/2014*
M2MS-14OR06030627	Implement and demonstrate prototype ORIGEN API for integration with other codes	9/30/2014
M2MS-14OR06030647	Complete initial review of SHARP integration interfaces and implement improvements	9/30/2014

**Revised due date.*

MeshKit V1.2 *RGG V1.0* *RGG Training*

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