ANL/NEAMS-14/2

NEAMS Update

Quarterly report for January – March 2014

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- DAKOTA-BISON was used to study the parameters that govern heat transfer across the fuel-cladding (page 2).
- Calculations of grain boundary mobility in UO_2 have been extended to high temperatures (page 2).
- Mesh adaptivity is being employed in MARMOT simulations to increase computational efficiency (page 3).
- Molecular dynamics simulations have shown correlation between atomic displacements and the anisotropic thermal conductivity in UO_2 (page 4).
- The SHARP team continues to address the application of the toolkit to assembly deformations driven by reactivity feedback (page 4).
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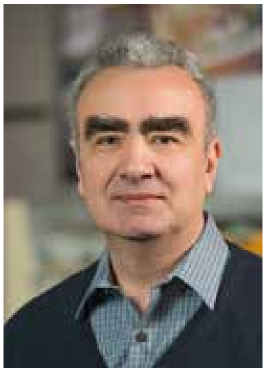
- The generalized cross section library has been tested for various fuel assemblies and reactor types (page 6).
- The subgroup cross-section interface was successfully implemented in PROTEUS-SN (page 6).



Stan Named National Technical Director

Marius Stan has been named the new national technical director for NEAMS. Stan is a senior computational energy scientist at Argonne, and he also serves as senior advisor for modeling and simulation to the assistant secretary for nuclear energy.

Stan is an internationally recognized scientist who pioneered the concept of "modeling and simulation" and the use of multiscale, multi-physics computational methods for the study of reactor fuels, materials, and coupled transport phenomena. After 13 years at Los Alamos National Laboratory, he moved to Chicago to work as a senior computational energy scientist at Argonne. He is a senior fellow with the Computation Institute at the University of Chicago and a senior fellow with the Institute for Science and Engineering at Northwestern University.

Fuel Product Line (FPL) Accomplishments

Engineering Scale (BISON)

Fuel fracture (i.e., cracking) is an important phenomenon in all types of nuclear fuels, but it is especially important in oxide fuels. Since the thermal conductivity of oxide fuels is so low, very large thermal gradients across the radius of a fuel pellet are established when the fuel pin is at power; this results in significant fuel cracking. Such cracks directly affect heat transport through the fuel, but just as importantly, they indirectly affect all fuel behaviors that are a function of stress, since cracks act to reduce the stress state in the fuel. [INL]

A fully three-dimensional smeared cracking model has been implemented and tested in BISON. The smeared cracking model is a mechanistically based model that accounts for the effects of fuel cracking by adjusting the elastic constants at material points without the added complication of making topographic changes to the mesh (as would be the case in the discrete cracking model that is under development). The smeared cracking model has been testing on a series of problems, such as the one shown in ***Fig. 1***. In this example, a uniform pressure is applied to the top surface of a composite beam (concrete on outside, steel in center) that is simply supported. In the simulation shown on top, the concrete was not allowed to crack, whereas it was allowed to crack in the simulation shown on bottom. Note that the stress levels are much lower in the cracked beam, as expected, and that the cracking occurs in the direction corresponding to the load, which means the model can represent cracks in three dimensions. It is anticipated that use of this new feature in fuel performance simulations can improve predictions by more accurately representing the stress state in the fuel. [INL]

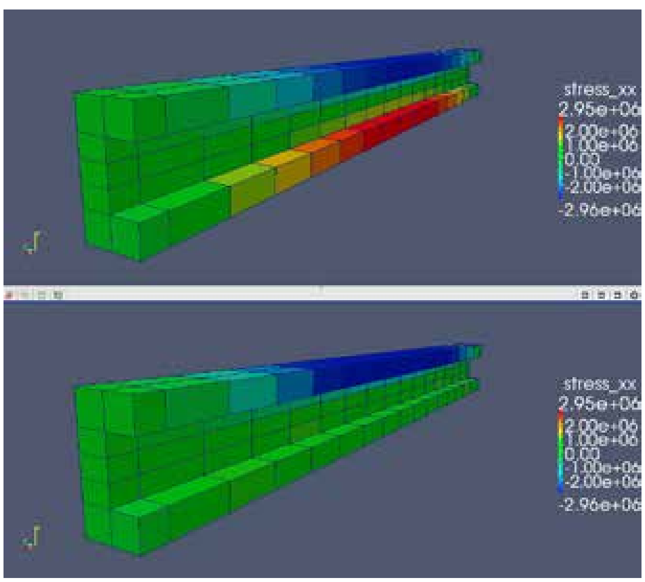


Fig. 1. BISON calculations of stress in a steel and concrete beam with (bottom) and without (top) cracking.

*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).

A journal article on BISON verification was published in Annals of Nuclear Energy (vol. 71, 2014, pp. 81-90). In addition, preparation of the first BISON verification and validation plan has been completed. The plan is expected to be a living document that will be updated annually; a copy of the validation plan is maintained on an Apache Subversion repository and is available to all BISON users. [INL]

An initial sensitivity analysis of the parameters governing heat transfer across the fuel-cladding gap has been completed using DAKOTA-BISON. The parameters assessed included roughness coefficients, the Kennard jump distance model coefficient, and the fuel thermal conductivity, looking particularly at their effects on the resulting fuel centerline temperature. The results of these analyses guide the prioritization of developing or improving mechanistic models for fuel performance. [SNL]

Subcontinuum Scale (MARMOT and Atomistic Simulations)

Calculations of grain boundary (GB) mobility in UO_2 have been extended to high temperatures (2,100-3,000 K). The results above 2,550 K are consistent with previous estimates. However, the new results, which were obtained with sufficient GB migration, suggest a transition in migration mechanisms. This transition is believed to be a result of the Bredig transition of UO_2 to a superionic phase, which is predicted to occur at about 2,300 K by the Basak potential (used in this work). The Bredig transition is a diffusional disorder of the oxygen sub-lattice, with Schottky defects generated in the anion sub-lattice enhancing self-diffusion. Further investigation regarding this hypothesis is in progress. This effort supports work toward developing a mechanistic model for restructuring in oxide fuels that will accurately predict formation and growth of the columnar grain structure and central hole under high power/temperature conditions. [INL]

Also related to a mechanistic understanding of oxide fuel restructuring has been work to develop a model of how fission gas bubbles impact grain growth within the fuel (see ***Fig. 2***). In this effort, however, fabrication porosity must also be considered and has recently been incorporated into phase field simulations. Making use of an existing analytical model, MARMOT simulations were performed and compared to previously published UO_2 grain growth data; the MARMOT results showed very good agreement with the previous work. [INL]

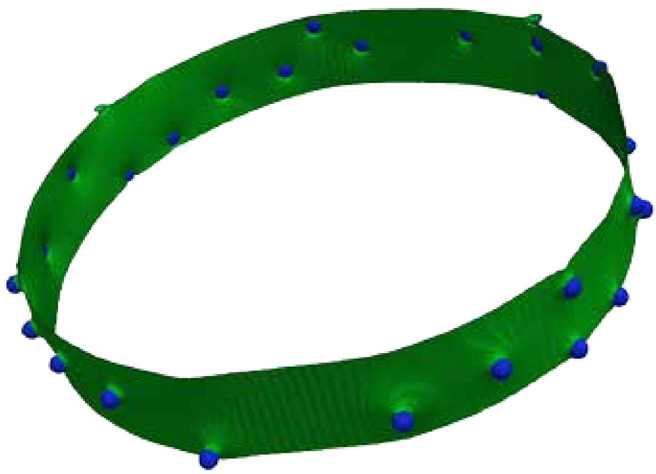


Fig. 2. MARMOT simulation of grain boundary motion in the presence of randomly distributed gas bubbles.

Finally, in preparation for developing a traction/separation law that is a function of GB porosity, mesh adaptivity has begun to be used to reduce the computational expense of the MARMOT simulations. To ensure that mesh adaptivity does not significantly impact the predicted mechanical behavior, a series of simulations with and without the use of mesh adaptivity were performed. The simulation predictions were essentially identical in all cases. Thus, the computational expense of these simulations can be dramatically reduced. [INL]

In the area of continued work on modeling the degradation of oxide fuel thermal conductivity during irradiation, the correlation between atomic displacements and the anisotropic thermal conductivity in UO_2 obtained from molecular dynamics (MD) simulations using the direct method were have been investigated. Using the Buckingham type of empirical potentials (i.e., the Basak potential), MD simulations were performed. The “local” lattice constant at different sampling regions (from “cold” to “hot” plates) in the supercell has small variations due to the applied thermal gradient, signifying anisotropic local distortions. To further understand the local distortions, an MD-calculated position profile of an oxygen ion in various simulation settings was analyzed. The shape of the distribution is an ellipsoid with the short axis along the [001] direction rather than a sphere, as would be expected for a cubic or isotropic system. This observation suggests that phonon scattering, and therefore the thermal conductivity, may be anisotropic. [LANL]

In an effort to validate this conclusion, colleagues were consulted who have performed experiments on UO_2 thermal conductivity using single crystals. Based on simulations and analysis of experimental data, these anomalous properties of UO_2 thermal conductivity were found to be largely controlled by spin-phonon interactions, including both the anisotropy and the low conductivity of UO_2 in general. Spin-phonon scattering occurs by phonons exciting the spin system. UO_2 exhibits low-lying spin excitation levels between approximately 2-3 and 10 meV for both the ordered antiferromagnetic and the paramagnetic phases, which is in the correct range to interact with phonons. [LANL]

The importance of this mechanism in reducing the overall UO_2 thermal conductivity is obvious when it is compared to the thermal conductivity of nonmagnetic ThO_2, which exhibits a 20-fold increase in the maximum conductivity. These insights are also very important for ongoing analysis of the reduction in thermal conductivity by accumulating fission gases (i.e., burnup). [LANL]

The MD predictions of anisotropic thermal conductivity in UO_2 was a new and somewhat unexpected result, and a manuscript on it is being prepared for peer review. One of the key conclusions is the importance of magnetic scattering in reducing UO_2 thermal conductivity. This contribution is difficult to estimate from simulations. However, by combining MD simulations with measurements on UO_2 single crystals, it has been possible to make accurate predictions, despite the failure to capture the magnetic scattering process explicitly. These insights will be used to improve the accuracy of molecular simulations of the impact of fission gases/products on UO_2 thermal conductivity. [LANL]

Simulations of the impact of strain on diffusion of neutral uranium vacancies have been completed, and these simulations are being extended to charged uranium vacancies, the predominant defect in stoichiometric UO_2. The initial comparison between these two defects indicates that there are some differences in how they respond to strain (shear strain in particular). This work relates to developing a mechanistic model for fuel creep. [LANL]

In the critically important area of modeling fission gas behavior, previous work has used discrete Fourier transform and atomistic simulations to calculate the diffusion coefficient of Xe under different chemical and irradiation conditions. The calculated diffusivities have been implemented into BISON, with good results compared to validation data and existing empirical fission gas diffusion models. Now the implementation of these diffusion models into MARMOT has been completed, which enables the investigation of a wide range of irradiation conditions. [LANL]

Thermochimica developers attended MOOSE training at INL in March. During this time, interaction with the MOOSE and BISON development teams allowed for important decisions to be made regarding implementation options for transport reactions in BISON. In addition, Thermochimica and MARMOT development teams made progress toward coupling the two tools. [ORNL]

Reactor Product Line (RPL) Accomplishments

Thermal Hydraulics (SHARP)

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 focused on the computational challenges introduced by deformation of the mesh offline after the computation of the displacements with Diablo. Code to account for structural mechanics deformations in coupled multi-physics simulations has been developed and demonstrated on meshes, and deformation data was used for the recent Advanced Burner Test Reactor (ABTR) benchmark. The capability has been proven on a 7-assembly core. [ANL]

More importantly, progress has been made toward online calculation of deformation. Accounting for deformations is challenging: deformations are specified only for solid portions of the structural mesh, and they must be propagated (using mesh smoothing) to fluid portions of the same mesh. Mapping deformations to the neutronics and fluid/heat transfer meshes is also challenging, as these other meshes must be located in the structural mesh before the structural mesh deformations occur.

This process has been implemented in the MOAB code and demonstrated on real deformations computed using Diablo (***Fig. 3***). This is the first application of a second-generation implementation of solution transfer; the new implementation is more versatile in how discretization operations are applied, and it should perform far better on larger numbers of processors. [ANL]

In early February, the coupled simulation team has presented its latest achievements, including the first fully coupled simulation of sodium fast reactor assemblies, to the Assistant Secretary for Nuclear Energy during a meeting at Argonne. Vijay Mahadevan (ANL) presented the multi-physics coupling using existing physics codes, along with some verification/demonstration problems and a look at parallel scalability, at the SIAM PP14 meeting in Portland, Oregon. The team has also submitted an invited paper on this topic to the "Royal Society International Proceedings A" journal. [ANL]

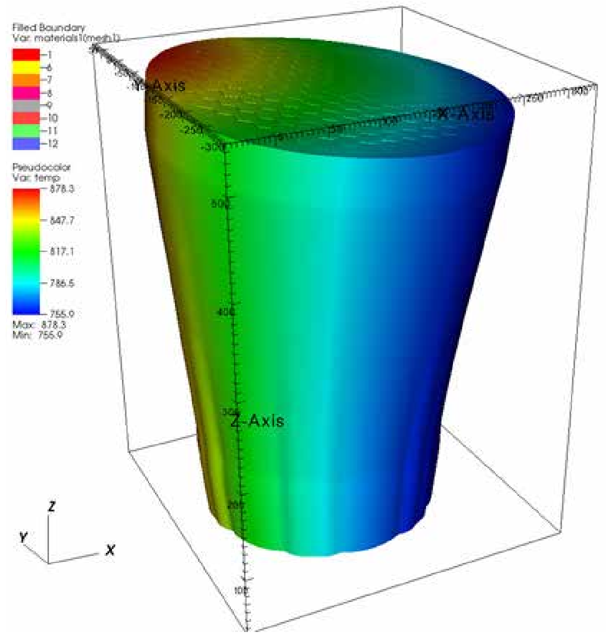


Fig. 3. Diablo simulation of thermally induced displacement (exaggerated 100×) in the 199-assembly ABTR core

Supporting Elements (SHARPER, MeshKit, MOAB)

Considerable progress has been made in assuring that SHARP is both reliable and usable. The NiCE team at ORNL has implemented a new build system called SHARPER that promises to substantially simplify installation by customers. The MeshKit team is working on a CMake-based build for MeshKit and has collaborated with Kitware Inc. to develop a graphical user interface for the Reactor Geometry Generator (RGG) and MeshKit (***Fig. 4***). The team has submitted a paper on graph-based mesh generation to the Engineering with Computers Journal. Finally, the team has added fixes to the MeshKit build system and PostBL to assist a MeshKit user at the University of Stuttgart. [ORNL]

The usefulness of flexible data backplane and mesh-based data management systems, like the MOAB libraries developed by ANL, is being recognized as a consequence of the multi-physics integration demonstration efforts of NEAMS. CD-adapco, developers of the commerical CFD code STAR-CCM+, are investing their resources in the development of code features to enable connectivity to the MOAB data backplane as a means of supporting thermofluid modeling collaboration with the SHARP and Consortium for Light Water Reactors (CASL) teams.

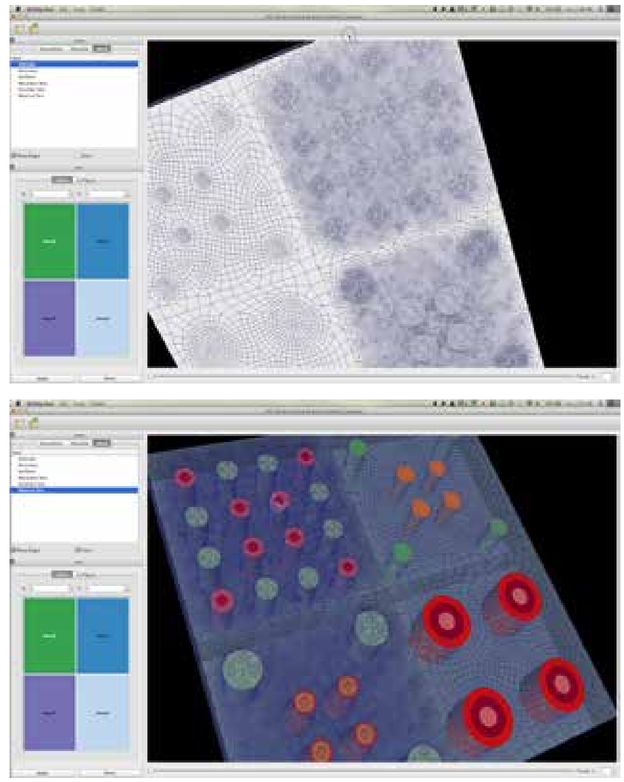


Fig. 4. Creating a reactor core mesh with the RGG: (top) establishing structural volumes; (bottom) assigning materials properties.

Thermal Fluids (Nek5000)

The Nek5000 team has extended the low-Mach-number capability to mixtures with multiple species, which will substantially increase the tool's applicability to nuclear applications. To test the implementation, the team conducted a series of validation runs for the 2014 OECD/NEA PANDA benchmark. The PANDA facility is a multi-compartment, large-scale thermal-hydraulics test rig located at the Paul Scherrer Institute, Switzerland. Initially, the experiment vessel contains well-defined gas mixture of helium/air at the top and air below with measured stratification. The benchmark transient data are requested in several positions in the vessel after a jet of air and helium is injected into it through a pipe inlet. [ANL]

A battery of tests was conducted for the different computational meshes, species diffusivities, levels of fidelity (uRANS, LES), and various formulations (hydro, Boussinesq, low-Mach-number). ***Fig. 5*** shows a mass fraction of oxygen in the LES computation with the full multiple-species setup of helium, oxygen, nitrogen, and water vapor in a low-Mach-number approximation. [ANL]

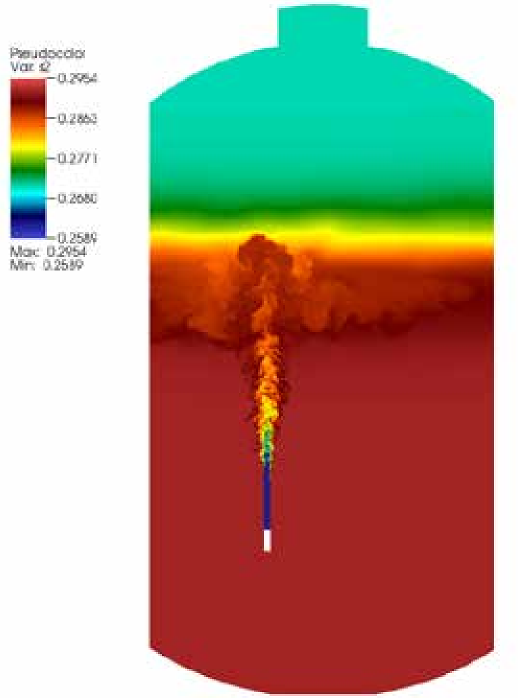


Fig. 5. Pseudocolor plot of mass fraction of oxygen in LES computation of PANDA benchmark.

Neutronics (PROTEUS)

The generalized cross section library has been tested for various fuel assemblies and 2D core cases of three primary reactor types: light-water reactors (LWRs), very-high-temperature reactors (VHTRs), and sodium fast reactors (SFRs). For most of the lattice cases, eigenvalues and pin power distributions agreed well with solutions produced by the Monte Carlo N-Particle transport code. Additional comparisons are being performed for 2D core cases: Westinghouse pressurized-water reactor (PWR), Next-Generation Nuclear Plant (NGNP) VHTR, and an ABTR-like SFR (***Fig. 6***). These tests have been conducted using the updated DeCART package while the cross-section application programming interface (API) is being implemented and tested in PROTEUS.

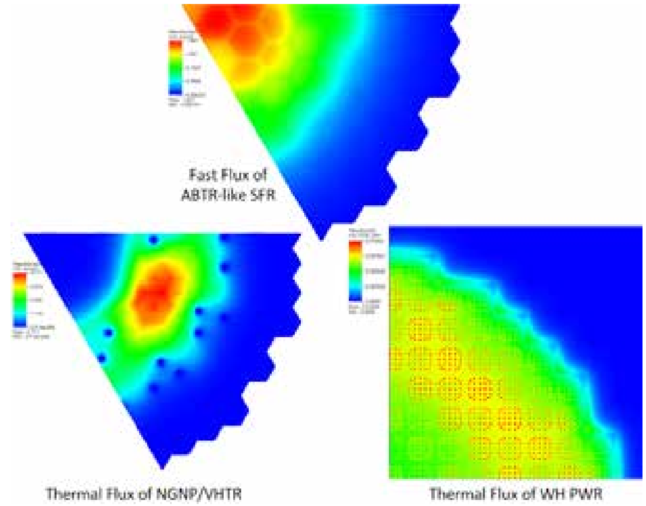


Fig. 6. 2D core benchmark problems for the generalized cross section method.

The subgroup cross-section API was successfully implemented in PROTEUS-SN and was tested for the VERA PWR pin and assembly benchmark problems. A 2D Advanced Test Reactor (ATR) core was simulated using the 47-group subgroup library on the BG/Q super computer at Argonne's Advanced Leadership Computing Facility (***Fig. 7***). During the tests, a noticeable dependency on boundary layer meshes was identified due to a very large subgroup-level flux gradient within fuel regions. This problem may be mitigated or eliminated when the generalized cross-section methodology is used in the cross-section API, as it is based on regular cross sections. [ANL]

The PROTEUS manual has been updated with methodologies and detailed input and output descriptions for the April PROTEUS/MC^2-3 training.

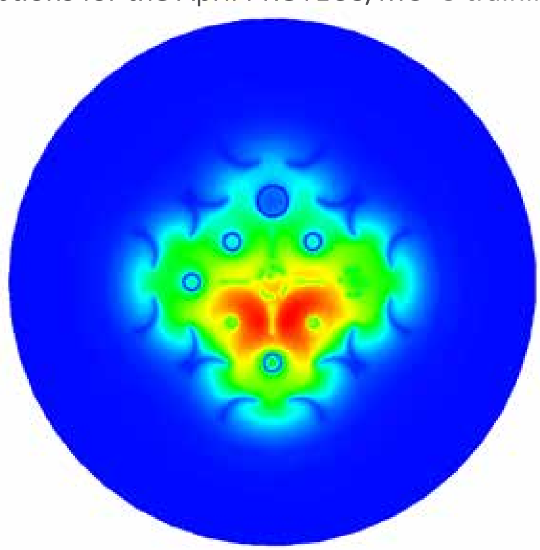


Fig. 7. 2D ATR simulation of PROTEUS using the 47-group subgroup cross section.

Status of Level 1 and 2 Milestones

Completed Milestones

Milestone ID	Description	Due Date
M2MS-14IN0603054	Deliver a "pervasive" restart capability that works for every feature in MOOSE through a sophisticated back-end "datastore"	1/31/2014
M2MS-14OR06030628	Implement and demonstrate downloadable SHARP installer	3/31/2014
M2MS-14IN0602021	Issue BISON validation plan	3/31/2014

Upcoming Milestones

Milestone ID	Description	Due Date
M2MS-14OR06030623	Implement NiCE support for RELAP-7 and initial plant-level reactor analyzer views	5/31/2014
M2MS-14AN0603039	Provide update on testing and development of Nek5000 thermohydraulic capability	6/30/2014*
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	6/30/2014
M2MS-14IN06030510	Report techniques for reliability analysis in station blackout models	6/30/2014
M2MS-14LA0602041	Implement new MARMOT models for fission gas/product diffusion	6/30/2014
M2MS-14OR0603062	Demonstrate PROTEUS for selected reactor benchmarks and problems	6/30/2014

**Revised completion date.*

Merzari receives Landis Award

Argonne nuclear engineer Elia Merzari has received the 2014 American Nuclear Society (ANS) Landis Young Member Engineering Achievement Award. The prestigious award recognizes outstanding achievement in which engineering knowledge has been effectively applied to nuclear power research and development.

Merzari was selected for his pacesetting contributions to simulation of complex turbulent flows and multiscale/multiphysics simulations of nuclear reactor designs. Merzari is a contributing member of the Nek5000 development team and is the technical lead for SHARP.

Merzari received his bachelor's and master's degrees in nuclear engineering from Polytechnic University of Milan, Italy. He received his Ph.D. in 2008 from the Tokyo Institute of Technology. He joined Argonne as a postdoctoral fellow in 2009 and was hired as a full-time staff member in 2010.

Spring BISON Sightings

While not quite as numerous as the wildlife sightings in Yellowstone National Park at this time of year, the number of BISON sightings at the recent Integration Meeting of the Advanced Fuels Campaign (AFC) (NE-5) was still impressive. Various presentations from INL, LANL, ORNL, the University of Illinois, and the University of Tennessee all highlighted on-going uses of BISON by AFC researchers as part of AFC-funded fuels activities.

For example, INL fuels researchers are using BISON to aid in postirradiation examination of metallic transmutation fuel experiments performed in the Advanced Test Reactor (ATR), especially several experimental fuel rods that experienced failure during irradiation. They are also using BISON to aid in the design of a series of double-encapsulated accident-tolerant fuel (ATF) experiments that will begin irradiation in the ATR this summer, including experiments for ATF concepts developed by Westinghouse, GE, and AREVA.

LANL fuels researchers presented their results of using BISON to investigate the use of highly corrosion-resistant FeCrAl alloys in place of traditional Zircaloy cladding, performing trade-off studies on how much thinner FeCrAl cladding could be made with respect to Zircaloy cladding. Thinner cladding could offset the neutronic penalty associated with Fe-based alloys. A NEUP project led by the University of Illinois is also making use of BISON to analyze fuel performance impacts associated with Zircaloy cladding innovations being pursued by their team.

Finally, ORNL and the University of Tennessee are making use of BISON to analyze their own ATF concept, which imbeds TRISO-coated fuel particles in a SiC matrix. All the results presented at the AFC Integration Meeting were very positive relative to the capabilities and ease of use of BISON. The overall impression by those in attendance was that BISON is becoming a real workhorse in the Advanced Fuels Campaign for analyzing a wide spectrum of fuel concepts and performance issues.

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