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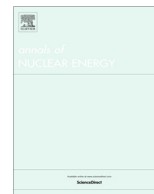
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Physics-based multiscale coupling for full core nuclear reactor simulation



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ABSTRACT

Numerical simulation of nuclear reactors is a key technology in the quest for improvements in efficiency, safety, and reliability of both existing and future reactor designs. Historically, simulation of an entire reactor was accomplished by linking together multiple existing codes that each simulated a subset of the relevant multiphysics phenomena. Recent advances in the MOOSE (Multiphysics Object Oriented Simulation Environment) framework have enabled a new approach: multiple domain-specific applications, all built on the same software framework, are efficiently linked to create a cohesive application. This is accomplished with a flexible coupling capability that allows for a variety of different data exchanges to occur simultaneously on high performance parallel computational hardware. Examples based on the KAIST-3A benchmark core, as well as a simplified Westinghouse AP-1000 configuration, demonstrate the power of this new framework for tackling—in a coupled, multiscale manner—crucial reactor phenomena such as CRUD-induced power shift and fuel shuffle.

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1. Introduction

Nuclear reactors are archetypal multiscale, multiphysics systems. Atomistic reactions ultimately drive very large-scale energy generation processes through micro- and mesoscale phenomena. Across the range of scales, a myriad of physical processes impact the system: microstructural evolution of materials, nucleate boiling, plasticity, creep, conjugate heat transfer, neutronics, fluid flow, and others. Traditionally, domain-specific software has been developed to tackle individual pieces of this problem (Ransom et al., 1982; Berna et al., 1997; Lyon et al., 2004; Joo et al., 2004) and several development efforts have attempted to utilize such extant software in conjunction with data exchange to simulate entire reactors. Several related US Department of Energy sponsored programs (Weber et al., 2007; NEAMS, 2013; CASL, 2013) have met with varying levels of success in this endeavor.

These nuclear reactor simulation efforts hinge on the ability to efficiently transfer data between different pieces of software. The fact that each constituent program has different data representations, requirements, and parallel partitionings greatly complicates the overall effort. Additionally, the code for exchanging data between n programs scales as $\mathcal{O}(n^2)$, eventually impeding progress and negatively impacting correctness and maintainability. Maintenance of legacy software often occupies more time than the development of new codes and new simulation capability.

Further complications arise because of the need to orchestrate the solution processes of multiple, independently developed codes running at different time and length scales. For instance, software that simulates microstructural grain evolution within fuel and software that simulates engineering-scale fuel performance are frequently designed to run well on timescales of seconds and years, respectively. Furthermore, most existing software is not designed to be controlled or run by an external driver program. Such software may include hard-coded time-stepping routines or may abort when an error condition arises rather than gracefully allowing the error to be handled at a higher level in the software stack. Therefore, modifications to existing codes are frequently

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necessary: new software must be written to drive the solution process and keep the menagerie of independent codes in sync.

The Multiphysics Object Oriented Simulation Environment (MOOSE) developed at Idaho National Laboratory (Gaston et al., 2009) represents an alternative path toward reactor simulation. MOOSE utilizes a modular approach, allowing scientists and engineers to create new fully coupled, multiphysics applications. A number of different physics simulation capabilities have been developed based on the MOOSE framework, including geomechanics (Podgorney et al., 2010), chemical transport (Guo et al., 2013), and superconductivity (Karpeev et al., 2013) applications. Of particular interest in the present work is a set of nuclear-related applications for simulating fuel performance, neutronics, thermal-hydraulics, fuel microstructure, and the effect of CRUD (Chalk River Unidentified Deposits) on fuel performance.

Recent MOOSE framework developments have enabled the efficient combination of multiple, independently developed applications with the goal of achieving massive, multiscale calculations. These developments, which include both a flexible execution strategy and a sophisticated data exchange facility, allow MOOSE-based applications to run concurrently while exchanging data, a process we have termed “multicoupling.” We believe the multicoupling technique will make an impact on a number of challenging numerical problems, both within the nuclear field and in the broader scientific community. Truly understanding these problems, which in the nuclear field include stress corrosion cracking, radiation void swelling, and irradiation creep, requires data from the atomistic length scale to be efficiently utilized on the engineering scale, as informed by the mesoscale (Short et al., 2014). The MOOSE framework, and others like it, represent a new and computationally efficient pathway to this end.

2. Methodology

The MOOSE framework was developed to simplify the creation of fully coupled, nonlinear, multiphysics applications. Here, “fully coupled” refers to solving all of the coupled partial differential equations (PDEs) simultaneously within one Newton-based solve. More than 30 MOOSE-based applications have been created under the fully coupled paradigm over the last five years. Each MOOSE-based application is made up of physics “modules” that describe the PDEs to be solved, material properties, boundary and initial conditions, postprocessed quantities, etc. Multiple MOOSE-based applications can be “composed” to create applications that comprise the physics from the constituent applications (Zhang et al., 2013a; Tonks et al., 2013a). While fully coupled multiphysics is useful for dealing with problems where the physics are strongly interacting, not all multiphysics problems are (or need to be) fully coupled. Examples include systems with multiple time scales and codes which couple with external software.

These situations can be described as “loosely coupled systems of fully coupled equations.” For instance, one MOOSE-based application may be used to compute the microstructural evolution of a material, while another engineering-scale application computes its macroscopic linear elastic response. Each of those two applications is treated as a fully coupled system of nonlinear equations that can be solved independently and later exchange data. In order to enable this solve structure within MOOSE, two new class hierarchies (families of C++ objects) have been developed: *MultiApps* and *Transfers*.

A *MultiApp* object allows multiple MOOSE (or external) applications to run simultaneously in parallel. A single *MultiApp* might represent thousands of individual solves (for example, thousands of individual microstructure calculations in a multiscale simulation). Each subsidiary application (or “sub-app”) within a

MultiApp is considered to be an independent solve. There is always a “master” application at the top level and a hierarchy of *MultiApps* beneath it, as shown in Fig. 1. A sub-app can have its own *MultiApps*; indeed, arbitrarily nested levels of solves are possible. In parallel, all sub-apps are distributed across the available processors and executed simultaneously.

While a *MultiApp* allows for arbitrary levels of hierarchical solves to be computed efficiently in parallel, those solves still require the exchange of data. The *Transfer* system within MOOSE implements this exchange. Although several libraries for mapping solution fields between meshes exist (Mahadevan et al., 2013; Slattery et al., 2013), there are many other types of data that applications must send and receive in order to implement a coupled solve. Thus, there are three main categories of *Transfers* within MOOSE:

1. *Field mapping*: L_2 -projection, interpolation, evaluation, etc.
2. *Postprocessed spatial data*: Layered integrals and averages, assembly-averaged data, etc.
3. *Scalar values*: Integrals, averages, point evaluations, etc.

“Field mapping” is simply taking a mesh-supported finite element solution field variable and transferring it (in some way) to another mesh. “Postprocessed spatial data” *Transfers* are designed to move spatially varying data that has been postprocessed (typically from a solution field). For example, transferring the average fuel temperature in axial slices along a fuel rod into a neutronics application (where it could be used to determine fuel temperature feedback in a cross-section calculation). “Scalar values transfers” are primarily useful for transferring data between domains of disparate physical size. An example would be computing the macroscale thermal conductivity from microstructure solves for use within a nuclear fuel performance calculation. The heat conduction solve can receive a “field” comprised of an interpolation of the thermal conductivity sampled from each of the microstructure simulations.

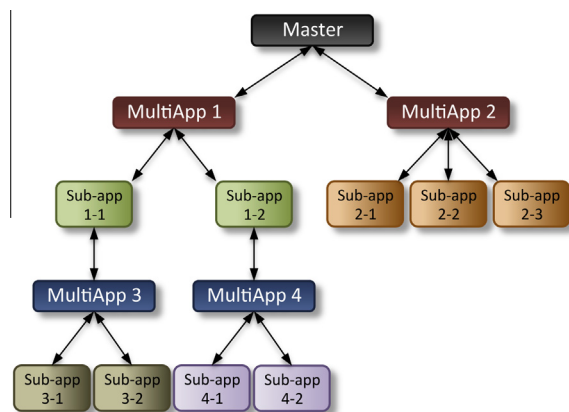


Fig. 1. General MOOSE *MultiApp* hierarchy for multicoupling applications.

Table 1
BISON fuel pellet dimensions.

| | |
|------------------------|---------------------------|
| Pellet quantity | 350 |
| Pellet height | 9.906×10^{-3} m |
| Pellet outer radius | 4.1275×10^{-3} m |
| Clad thickness | 6.35×10^{-4} m |
| Clad gap width | 8.85×10^{-5} m |
| Clad bottom gap height | 1.0×10^{-3} m |
| Plenum fuel ratio | 0.074541 |

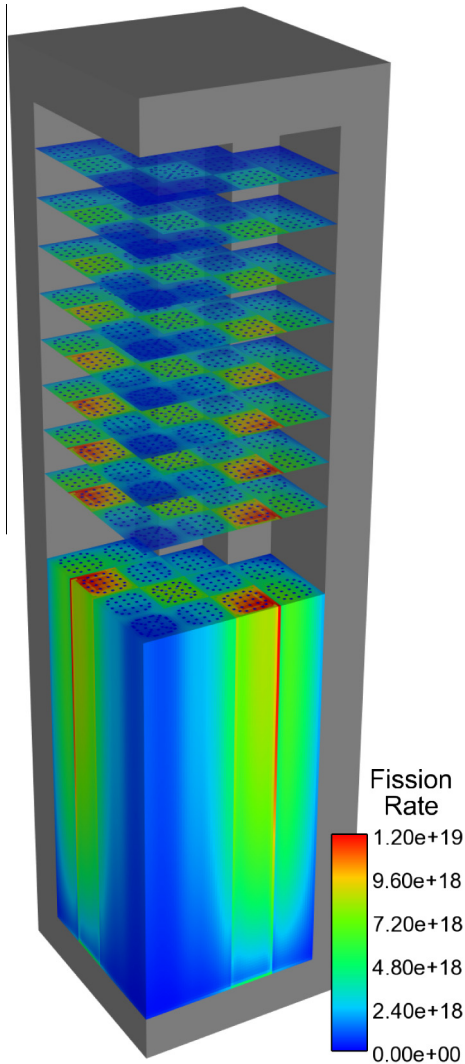


Fig. 2. Extended KAIST-3A benchmark reactor quarter core. The surface and slices show the fission rate (in fissions/cm³/s) after an 18-month fuel cycle as computed using RattleS_Nake.

Users need not write new C++ code to take advantage of the MultiApps and Transfers capabilities. Rather, the quantity and type of Transfers and MultiApps to be used in the simulation are specified in a text-based input file. The code necessary to achieve a multiscale, multiphysics calculation (such as a full reactor core simulation) stays constant while simulation complexity is increased. The result is that software quality and maintainability remain high, while at the same time, further (potentially independent) development efforts are unhindered. Finally, we note that both MultiApps and Transfers are dimension-agnostic and support mixed-dimensional solves. For instance, (r,z)-axisymmetric fuel performance calculations can be embedded within a three-dimensional neutronics calculation. The Transfer system accounts for coordinate system transformations when data exchanges are required.

3. Results

Three primary physics capabilities are required to model light water reactors (LWRs): neutron transport, fuel performance, and thermal fluids. These physics map to the MOOSE-based applications known as RattleS_Nake (Wang, 2013; Wang et al., 2014), BISON (Williamson et al., 2012), and RELAP-7 (Zou et al., 2013),

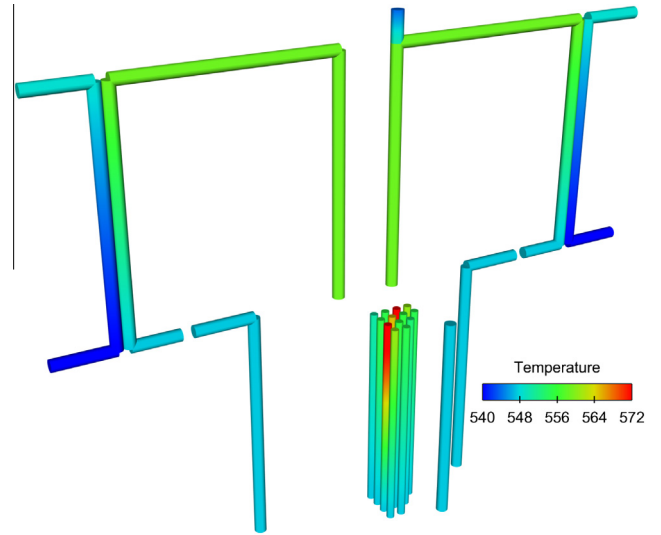


Fig. 3. Temperature (Kelvin) in the RELAP-7 piping network utilized for modeling cooling channels for the benchmark KAIST-3A simulation.

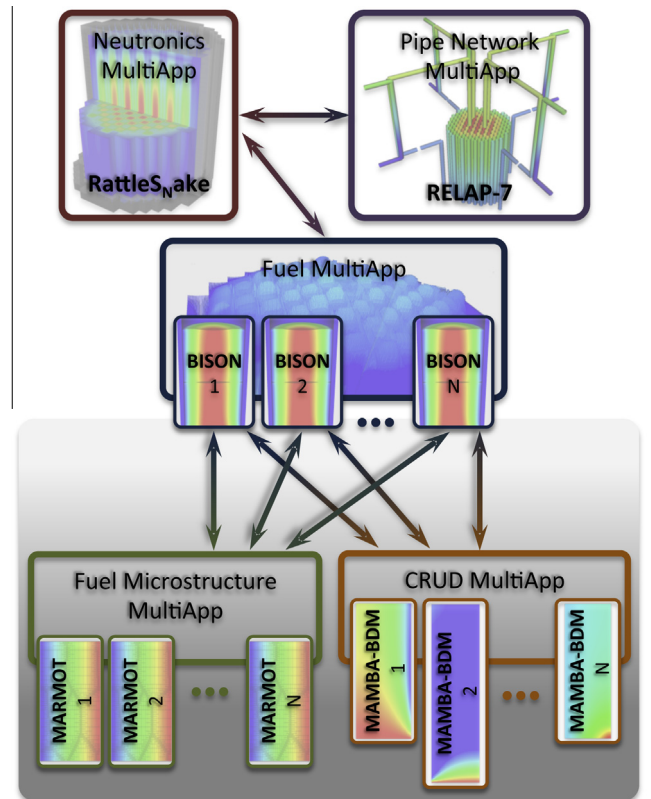


Fig. 4. Simulation data flow chart for RattleS_Nake, RELAP-7, and BISON used in the calculations described in Sections 3.1, 3.2, and 3.3. Microstructure calculations conducted with the MARMOT and MAMBA-BDM applications (shaded region) were used only in the simulation detailed in Section 3.2.

respectively. The MultiApp and Transfer systems are used to simultaneously solve all three physical systems and transfer data between them, producing a hierarchical, multiscale, multiphysics simulation of a light water reactor. Before discussing the simulation results, we briefly describe the aforementioned MOOSE-based applications in greater detail.

RattleS_Nake is a MOOSE-based application that solves the multigroup linear Boltzmann equation for modeling neutron

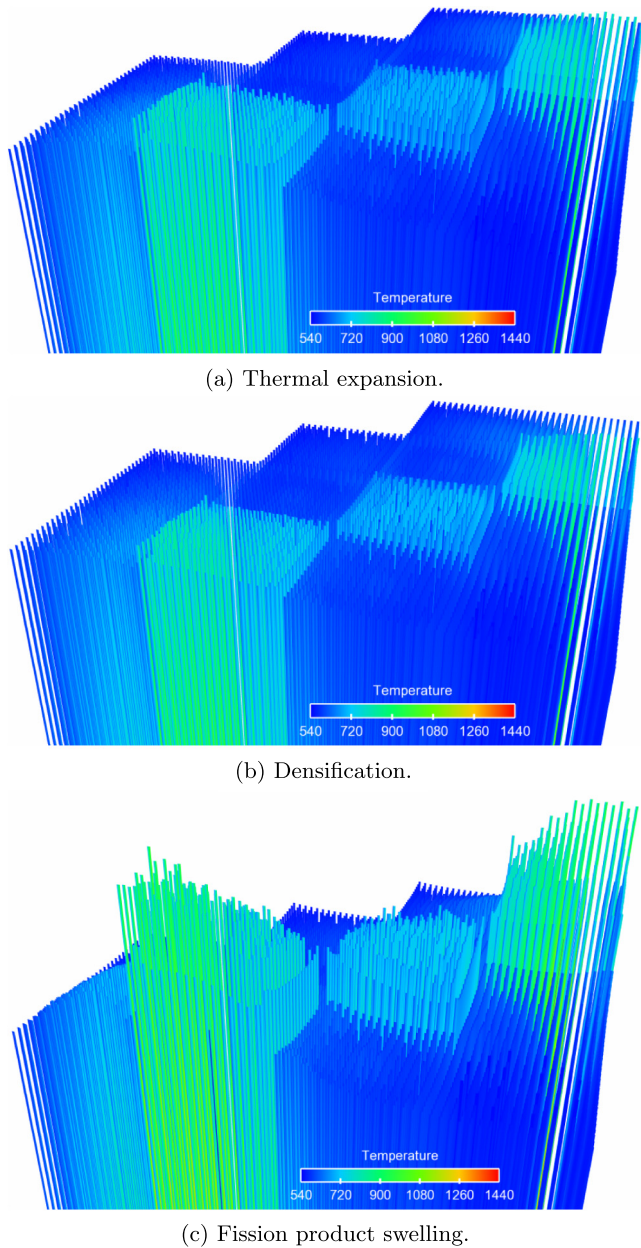


Fig. 5. KAIST-3A benchmark results. Fuel displacement (computed in meters and exaggerated by a factor of 10 for visualization) and temperature (in Kelvin) of 3432 rods computed with BISON during the (a) thermal expansion, (b) densification, and (c) fission product swelling phases.

transport. It solves both transient and eigenvalue primal/adjoint problems, and implements a variety of numerical discretizations including S_N (Wang, 2013), P_N , and a number of continuous finite element formulations (Wang et al., 2014; Wang and Gleicher, 2014; Hansen et al., 2014). RattleS_Nake has also been verified against several well-known benchmarks (Lewis et al., 2001; Biron et al., 1977; Gleicher et al., 2012; Ellis et al., 2014). In the present work, we employ the diffusion solver and assume the multigroup cross sections are properly generated. Finally, although RattleS_Nake supports both microscopic depletion (tracking interesting or important isotopes) and macroscopic depletion (using lumped variables such as burnup and look-up tables), we only use the macroscopic depletion approach here. The isotope densities can be unfolded for fuel performance analysis if desired.

BISON is a finite element-based nuclear fuel performance code applicable to a variety of fuel forms such as light water reactor fuel rods, TRISO particle fuel, and metallic rod and plate fuel. It solves the fully coupled equations of thermomechanics and species diffusion, for either 1D-spherical, 2D-axisymmetric or 3D geometries. BISON provides models for temperature- and burnup-dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. BISON is currently being verified (Hales et al., 2014; Williamson et al., 2014; Perez et al., 2013) and validated against a wide variety of fundamental fuel rod experiments.

RELAP-7 (Reactor Excursion and Leak Analysis Program, version 7) is a MOOSE-based nuclear reactor system safety analysis code being developed at Idaho National Laboratory. The overall design goal of RELAP-7 is to take advantage of thirty years of advances in computer architecture, software design, numerical integration methods, and physical models to improve upon previous implementations (Ransom et al., 1982), and extend the analysis capability for all reactor system simulation scenarios. RELAP-7 employs a stabilized continuous Galerkin finite element formulation to solve both single and two-phase compressible flow equations in 1D “pipes” connected by zero-dimensional “components” such as junctions, turbines, and pumps. It has a graphical user interface which allows users to develop simplified reactor models, and will eventually be leveraged to conduct probabilistic risk assessment studies in conjunction with other MOOSE-based codes.

3.1. Benchmark Quarter Core Simulation: KAIST-3A

As a proof of concept for the new MultiApp and Transfer capabilities within MOOSE, a fictitious, three-dimensional reactor quarter core with 13 assemblies and 3432 fuel rods based on the KAIST-3A benchmark problem (Cho, 2000) was created by extending the original configuration in the axial direction to a height of 385.56 cm, and adding reflector regions to the top and bottom, as shown in Fig. 2. In addition, a two-loop piping network containing heat exchangers, pumps, and pressurizers was constructed, as pictured in Fig. 3. Within this model, one “core channel” pipe is utilized for each assembly, representing a homogenization of the

Table 2

Details of Transfers used in the simulations discussed in Sections 3.1, 3.2 and 3.3. The shaded rows describe the transfers for the MARMOT and MAMBA-BDM microstructure calculations, which were only used in the simulation described in Section 3.2. The final column shows the category (based on the list in Section 2) for each type of Transfer.

| Application | SubApp | Data | Category |
|--------------------------|-------------|-----------------------|----------|
| RattleS _N ake | → BISON | Coolant Temp. | 1 |
| RattleS _N ake | ← BISON | Fission Rate | 1 |
| | | Fuel Temp. | 2 |
| | | Clad Temp. | 2 |
| | | Burnup | 2 |
| RattleS _N ake | → RELAP-7 | Clad Temp. | 2 |
| RattleS _N ake | ← RELAP-7 | Coolant Temp. | 3 |
| BISON | → MARMOT | Fuel Temp. | 1 |
| BISON | ← MARMOT | Fission Rate | 1 |
| BISON | → MAMBA-BDM | Thermal Cond. | 2 |
| | | Clad Temp. | 1 |
| | | Coolant Temp. | 1 |
| BISON | ← MAMBA-BDM | BO ₃ Conc. | 2 |
| | | CRUD Temp. | 2 |

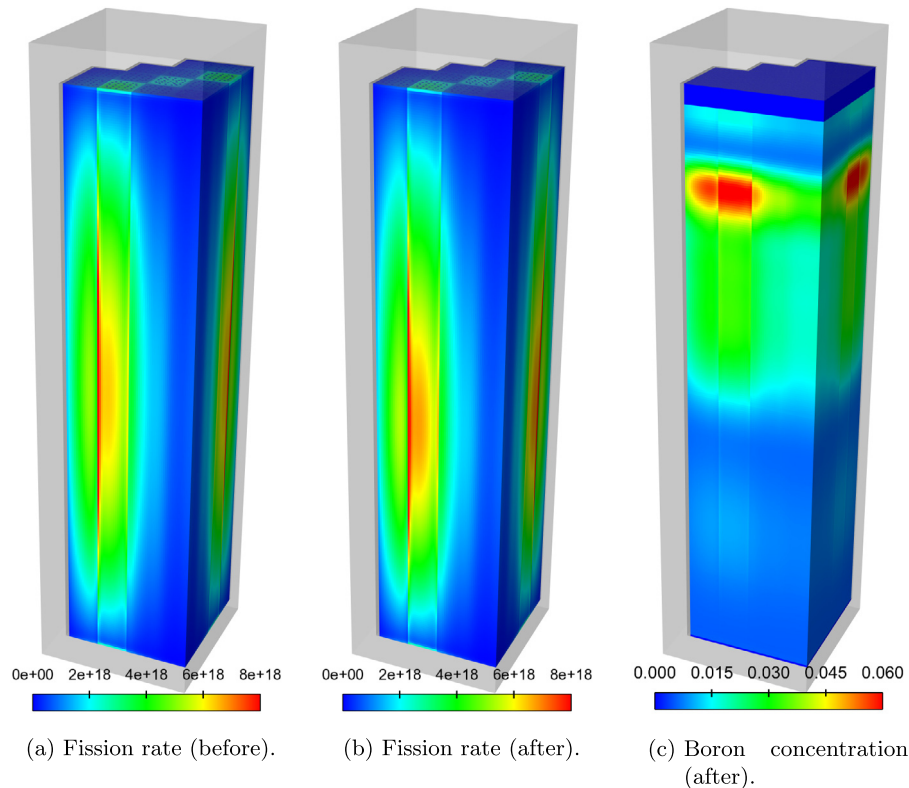


Fig. 6. Results of the KAIST-3A CIPS simulation: (a) and (b) are the fission rates (in fissions/cm³/s) before and after CIPS, respectively, and (c) is the (dimensionless) boron concentration.

flow through the total cross-sectional area of an assembly, an approach which has been used previously (Ransom et al., 1982) with success. Typical LWR fuel and clad dimensions were used to develop an axisymmetric “smeared pellet” fuel representation (a single fuel column is utilized; individual pellets are not meshed) as in Table 1.

The MultiApp system shown in Fig. 4 (other than the shaded microstructure portion of the figure) was used to execute these simulations simultaneously. In this system, RattleSnake acts as the “master” application and forms a conduit for transferring information back and forth between BISON and RELAP-7. The BISON MultiApp is composed of 3432 separate BISON calculations (run concurrently) to model the fuel behavior through the 18-month fuel cycle. The RELAP-7 MultiApp solves a single system for the thermal-fluid response in the two-loop piping system. This simulation demonstrates the flexibility of the MultiApp approach: many simultaneous simulations, a few, or just one are possible, depending on the characteristics of the problem.

In order to link together the various solves, Transfers were employed as shown in Fig. 4 to move data between the MultiApps and the master. At each timestep of the master RattleSnake application, the following events occur:

1. Using the previous timestep’s fuel, cladding, and coolant temperatures (from BISON and RELAP-7, respectively), RattleSnake computes an updated fission rate solution field.
2. RattleSnake transfers the fuel cladding temperature to RELAP-7.
3. RELAP-7 computes an updated coolant temperature solution field, and transfers it back to RattleSnake. The RELAP-7 solver generally takes much smaller timesteps than either the BISON or RattleSnake solvers, and therefore it executes an entire sequence of smaller sub-timesteps, treating the fuel cladding temperature as constant, to synchronize itself with the solution time of the RattleSnake application.

4. RELAP-7 transfers the updated coolant temperature field back to RattleSnake.
5. RattleSnake transfers fission rate and coolant temperature to BISON.
6. BISON computes updated fuel and cladding temperatures, and transfers them back to RattleSnake.

This solution scheme demonstrates a core concept of multicoupling: multiple Transfers are employed to move data in parallel, and when transferring to/from a MultiApp containing many sub-apps, the transfers for all sub-apps are completed simultaneously, and in parallel.

The results of this simulation are shown in Figs. 2, 3, and 5. Each fuel rod has its own (unique) power profile and power history; therefore the fuel rods are able to grow and shrink (due to thermal expansion, fuel densification, fission product swelling, creep, and other effects) individually, as shown in Fig. 5. Assemblies with higher fission rates yield warmer fuel and cladding, leading to cross-section modifications in RattleSnake and higher coolant temperatures in RELAP-7 in the nearby flow channels. The simulation ran for 4 hours and 15 minutes on 3432 processors of the “Fission” cluster at Idaho National Laboratory. In total, Fission consists of 12512 2.4-GHz processors, and was ranked #138 on the November 2011 Top500 list.

3.2. Multiscale effects simulation

The LWR model described in Section 3.1 allows us to explore operational issues relevant to the nuclear power industry. As previously mentioned, a nuclear reactor is an inherently multiscale system. Engineering-scale reactor physics, such as CRUD Induced Power Shift (Deshon et al., 2011) or “CIPS,” clad hydride formation and embrittlement (Guo et al., 2008), and fuel thermal conductivity degradation (Bagger et al., 1994), are the direct result of

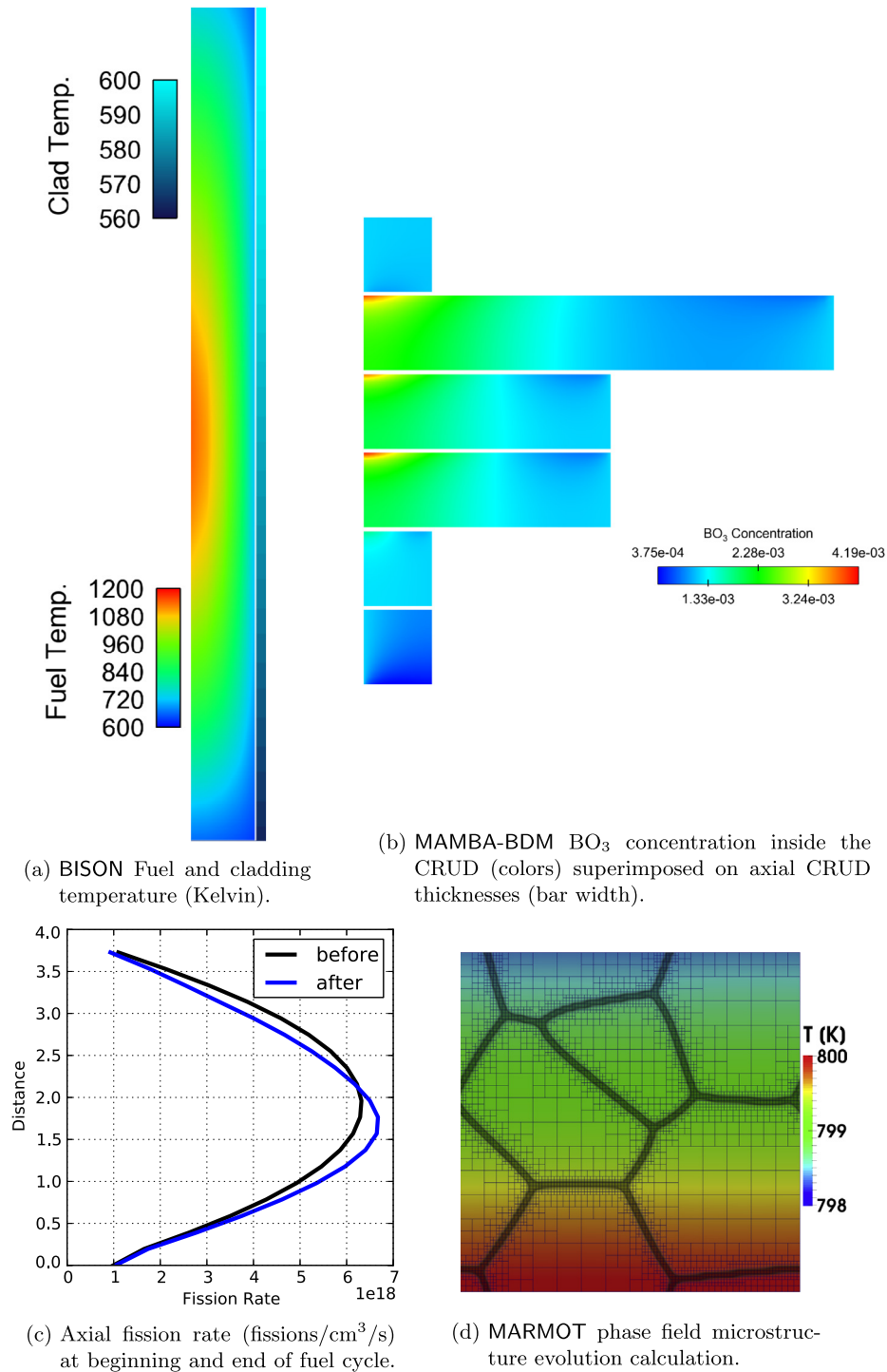


Fig. 7. Multiscale effects simulation results: (a) shows fuel and cladding temperature in Kelvin, (b) shows BO_3 concentration (dimensionless) at six positions along the fuel rod, (c) is a plot of axial fission rate (fissions/ cm^3/s), and (d) shows the temperature gradient and grain boundary configuration. The presence of boron at the top of the quarter core shifts the axial flux profile downward.

microstructural effects. Due to the hierarchical nature of the *MultiApp* system, these effects can be integrated into a multiscale LWR simulation without modification to the source code of any of the constituent applications. To demonstrate the hierarchical capability of *MultiApps* and move toward high-fidelity modeling of CIPS, MOOSE-based microstructure simulations based on the MAMBA-BDM and MARMOT applications were added to each BISON rod of the KAIST-3A 3D benchmark problem described

previously. These two applications are now briefly described in further detail.

MAMBA-BDM is a MOOSE-based CRUD microstructure simulator which incorporates models for porous flow, heat transfer, boiling, and boron deposition (Short et al., 2013). Although MAMBA-BDM is capable of solving for soluble and precipitated boron, both of which contribute to the axial power shift in LWRs, the present simulation considers only the soluble phase. These CRUD deposits

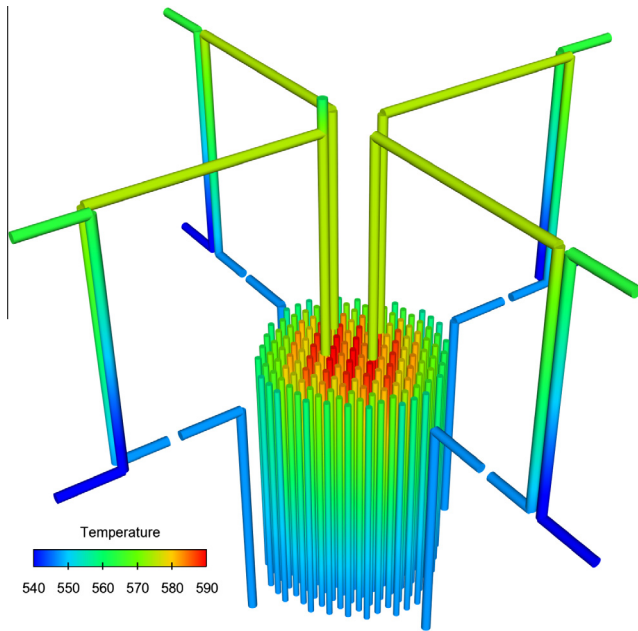


Fig. 8. Temperature (Kelvin) in the RELAP-7 piping network of cooling channels for the AP1000 full reactor simulation.

form at sites of sub-cooled nucleate boiling, typically on the upper spans of the fuel rods where the coolant is the warmest. The disproportionate amount of boron in the upper part of the reactor absorbs neutrons, damping fission rates in that area. The effect is to “shift” the axial power profile toward the bottom of the reactor (Deshon et al., 2011).

MARMOT is a MOOSE-based mesoscale modeling code that predicts the co-evolution of microstructure and material properties due to applied load, temperature, and radiation damage (Tonks et al., 2012) using the phase field method. MARMOT has been used to model void/bubble dynamics (Zhang et al., 2012), phase separation (Zhang et al., 2013b), grain boundary migration (Tonks et al., 2013c; Tonks et al., 2014), crystal plasticity (Chockalingam et al., 2013), and the impact of microstructure on material properties such as thermal conductivity (Tonks et al., 2013b; Millett et al., 2013). In the present work, fuel temperature and fission rate are transferred from the BISON fuel simulation into MARMOT, and MARMOT transfers thermal conductivity values back into BISON.

Six CRUD microstructure simulations were added to each of the 3432 BISON simulations in the KAIST-3A benchmark problem. A prescribed CRUD growth rate based on the work of Walter et al. (2013) is employed to compute the boron deposition over time throughout the quarter core. The boron concentration in the microstructure models is then returned to RattleSnake (via BISON), where the extra boron impacts spatially dependent macroscopic cross-sections, causing CIPS to occur. As with the KAIST-3A benchmark problem described in Section 3.1, the multiscale effects simulation also ran on 3432 processors of the “Fission” cluster.

The coupling scheme used in this simulation is described in Table 2. The CRUD simulations are effectively inserted “in-between” the cladding in the BISON simulation and the coolant temperature from the RELAP-7 simulation (meaning heat must flow out of the cladding in BISON and through the CRUD microstructure to get to the coolant). The boron concentration, as calculated in the CRUD microstructure simulation, is passed back up the chain to RattleSnake. The results of an 18-month fuel cycle are shown in Figs. 6 and 7: boron tends to build up in the upper part of the reactor and is more pronounced in assemblies with higher fission rates (and thus warmer fuel, cladding, and coolant). This

large concentration of boron has the effect of depressing the fission rate in those areas, effectively shifting the axial power profile toward the bottom of the reactor.

In addition to the CRUD simulations already described, three MARMOT microstructure simulations per BISON fuel rod were also run. As discussed in Table 2, the BISON simulation transferred temperature and fission rate to MARMOT, while MARMOT computed and transferred thermal conductivity values back to the BISON simulation, thereby inducing a two-way coupling from the engineering scale fuel calculations to the microstructure calculations. While individual MARMOT and MAMBA-BDM application objects are capable of running on multiple processors, the large overall number of BISON rods, the relatively small size of each 2D microstructure simulation, and the fact that the microstructure applications were not directly coupled to one another made it less efficient to distribute the individual microstructure calculations across multiple processors. Instead, multiple microstructure simulations were assigned to each processor and executed simultaneously: a simple (but effective) algorithm for harnessing large-scale computational resources to solve relatively small subproblems.

This simulation demonstrates the process of incorporating MOOSE-based applications, in this case for CRUD, into an existing LWR model. Note that, in order to run this simulation, no code had to be added or changed in any of the RattleSnake, BISON, RELAP-7, or MAMBA-BDM simulations. The teams developing these codes have been working independently (for years in some cases) but, because they are all based on MOOSE, the applications can be seamlessly combined with multicoupling. More capabilities and fidelity can be added to the MOOSE LWR model in this manner. For instance, grain-scale microstructure simulations of fuel thermal conductivity with MARMOT (Tonks et al., 2013a) have also been performed. Similarly, HYRAX (Jokisaari and Thornton, 2013) simulations could be added to model brittle hydride formation in the cladding of each rod. As the number of MOOSE-based applications grows, so does the variety of possible science-based full core simulations.

3.3. Full reactor simulation: AP1000

Sections 3.1 and 3.2 employed a small 3D benchmark quarter core to provide a convenient testbed for the multicoupling idea. We now extend this new capability to model a contemporary reactor design, specifically the Westinghouse AP1000 (Schulz, 2006). The public design documents for this reactor were retrieved from the NRC website (NRC, 2007). From these documents, a neutronics mesh was developed, cross-sections were computed using DRAGON-4 (Marleau et al., 1994), a RELAP-7 piping network containing four loops was created (see Fig. 8), and a BISON fuel rod model was generated. The resulting AP1000 simulation was comprised of 41448 BISON fuel rods and 157 assemblies, with one RELAP-7 flow channel per assembly.

The capability to physically move and “reset” sub-apps within a MultiApp was exercised in the AP1000 simulation. The process of moving assemblies and inserting fresh fuel is known as a “shuffle” and occurs approximately once every 18 months in a working reactor (NRC, 2007). In the present simulation, a fuel shuffle was performed at the 12-month mark, and a shuffle pattern in which high-burnup fuel from the interior of the reactor was swapped with low-burnup fuel closer to the core periphery was selected. (Access to a “real” fuel shuffle pattern was not available at the time the simulation was performed; the outermost assemblies were not moved during the shuffle, and therefore remain at low power/burnup throughout the course of the simulation). In addition to moving assemblies around, a new fuel assembly was inserted into the center position of the reactor.

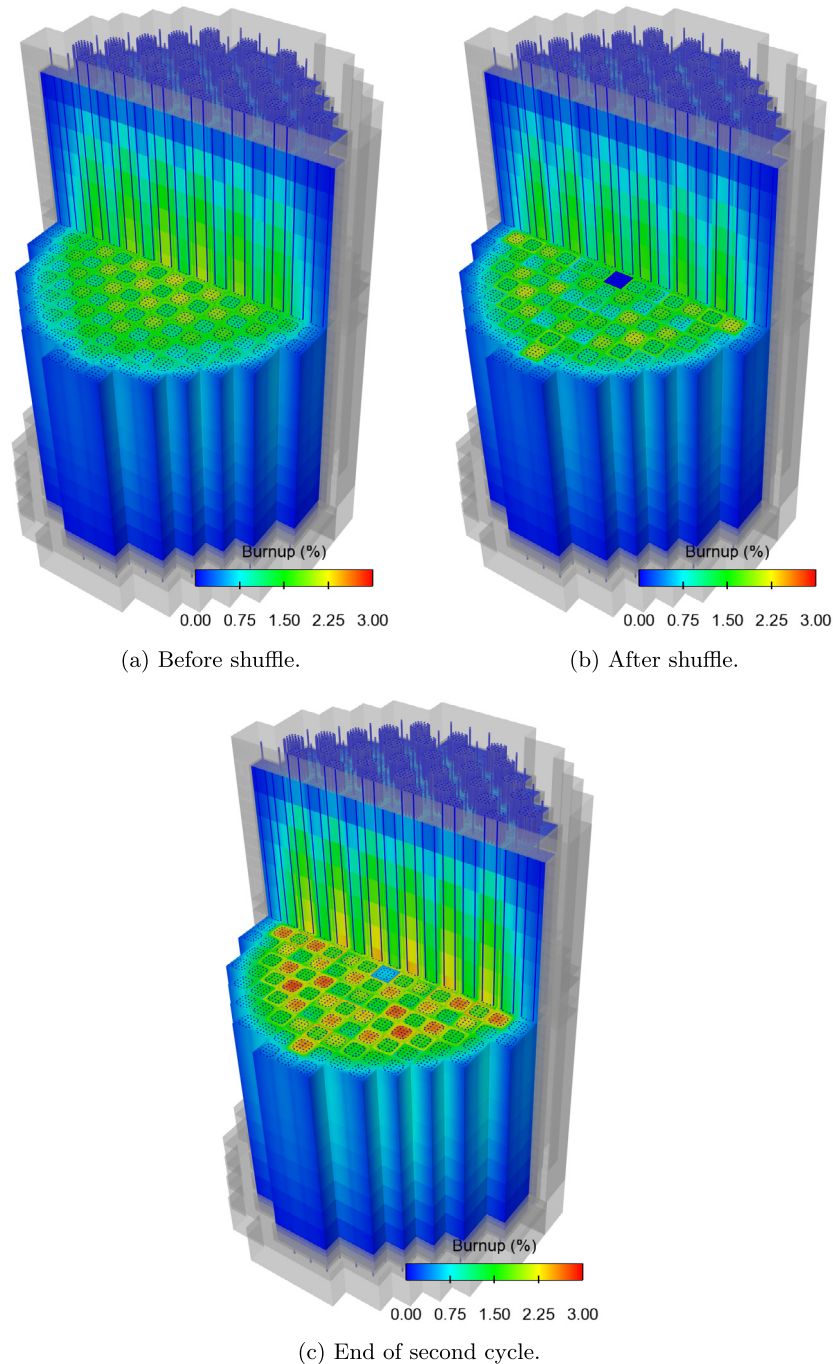
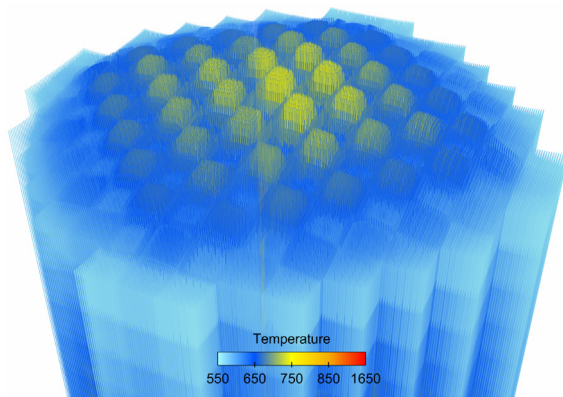


Fig. 9. Results of AP1000 simulation showing burnup (a) prior to the shuffle, (b) after the shuffle, and (c) the end of the second cycle.

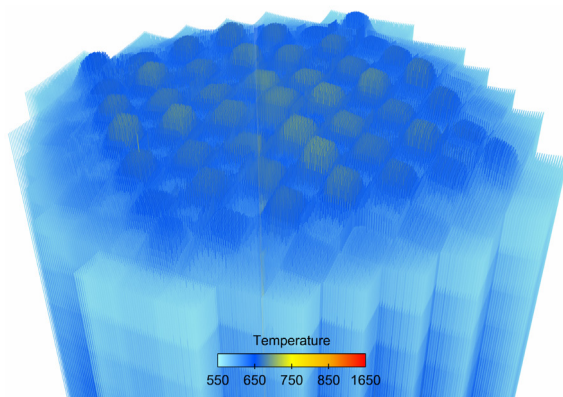
Fig. 9 shows the burnup, as computed by each of the BISON simulations, and transferred back to the neutronics mesh, just before and just after the shuffle event. In addition, Fig. 9 shows the burnup toward the end of the second cycle, where it has somewhat equilibrated across the core. Fig. 10 shows the fuel stacks at the same three times. Note that the “state” of the rods is not changed during the shuffle; rather, the actual simulation representing each rod is moved within the computational space. The AP1000 fuel shuffle calculation ran for 24 hours and 20 minutes on 2160 processors of the “Fission” cluster. These results represent an entirely new capability to track the complete history of every rod within a nuclear reactor from the time it is placed in the reactor until the time it is removed.

4. Implications

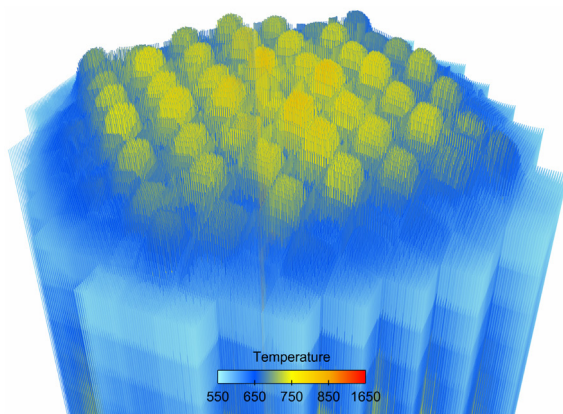
Multicoupling, as implemented in MOOSE using the `MultiApp` and `Transfer` systems, fundamentally alters the process of developing complex, multiphysics software. Rather than creating a single, monolithic program or attempting to “hard-wire” several physics projects together via large coupling frameworks, smaller individual simulations can first be created using a general framework, then numerically verified, and finally validated against experimental data before being linked together using the `MultiApp` and `Transfer` systems. The multicoupling method also allows for simultaneous validation of smaller codes with single-effect experiments in parallel with multiscale simulation and



(a) Before shuffle.



(b) After shuffle.



(c) End of second cycle.

Fig. 10. Results of AP1000 simulation showing the displacement (computed in meters and exaggerated by a factor of 20 for visualization) and fuel temperature (in Kelvin) as computed using BISON (a) prior to the shuffle, (b) after the shuffle, and (c) the end of the second cycle.

larger, integrated experiments. New information gleaned from any length scale can be incorporated seamlessly and the master simulation re-run to reflect any changes. The end result is a better testbed for scientific discovery.

Each component MOOSE-based application used in the simulations described here required, on average, approximately 10–15 lines of new code in order to implement the multicoupling approach. The `MultiApp` and `Transfer` systems were initially committed to the MOOSE source code repository February 18, 2013, and the full core simulation results were first presented

May 6, 2013 (Gaston et al., 2013), approximately two and a half months later. The relatively short time period between the creation of the software and the presentation of initial results underscores the efficacy and feasibility of the method.

The multicoupling concept has the potential to revolutionize the ability of small groups to perform industrially relevant, multi-scale simulations. Problems of large technological significance do not always require high precision or fidelity at the outset, but rather the ability to investigate and substantiate large changes to early-stage designs. The degree of full coupling versus loose coupling can therefore be tuned as the design process moves forward, increasing in accuracy as major design decisions are made.

Multicoupled simulations such as these exhibit both the potential to build a bridge of higher bandwidth between the communities of science and industry, and to make a number of formerly intractable or difficult problems easier to tackle. These problems, which are inherently multiscale, represent large- (sometimes global-) scale simulations whose results are inextricably linked to highly localized behavior. These include the multiscale full core simulation discussed here, as well as use in nuclear fuel disposition, continental-scale geomechanics, complex processing plants like refineries and chemical manufacturing facilities, and multi-scale material science problems like irradiation-assisted stress corrosion cracking or radiation-induced microstructural change over timescales of years.

5. Conclusions

A new method for coupling independent multiphysics simulations was developed within the MOOSE framework, and its effectiveness was demonstrated on a number of realistic problems in which burnup, radiation swelling, and CIPS due to boron accumulation in CRUD were computed. This method, herein called multicoupling, allows the user to seamlessly tie together separate codes, specifying whether they are loosely or fully coupled. The “multicoupling” method establishes a new paradigm for performing engineering-scale numerical simulations which take into account localized information from lower length scales. The “framework first” model, in contrast to building monolithic or piecemeal codes, is more efficient in the long run and represents a new way of approaching large-scale problems. This model is made possible by an efficient framework and high performance computational resources.

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