COUPLED MULTIPHYSICS OF ADVANCED MOLTEN-SALT NUCLEAR REACTORS

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EXECUTIVE SUMMARY

The Advanced Reactors and Fuel Cycles Group (ARFC) models and simulates nuclear reactors and fuel cycles with the aim of improving the safety and sustainability of nuclear power. In the context of high-performance computing, this work couples multiple physics at multiple scales to improve the design, safety, and performance of advanced nuclear reactors. In particular, thermal–hydraulic phenomena, neutron transport, and fuel reprocessing couple tightly in nuclear reactors. Detailed spatially and temporally resolved neutron flux, temperature distributions, and isotopic compositions can improve designs, characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for those unique physics. In the work presented here, conducted on Blue Waters, ARFC has demonstrated the capability to simulate coupled transient neutronics, thermal hydraulics, and fuel reprocessing in multiple advanced, molten-salt-fueled nuclear reactor designs.

RESEARCH CHALLENGE

Nuclear power provides 19% of the total electricity generated in the United States and is our largest source of clean energy. The current state of the art in advanced nuclear reactor simulation focuses primarily on traditional light-water reactor designs. Our work extends that state of the art by enabling similar modeling and simulation capability for more advanced reactor designs that have the potential to improve the already unparalleled safety and sustainability of nuclear power. High-fidelity simulation of dynamic advanced reactor performance requires development of models and tools for representing unique materials, geometries, and physical phenomena.

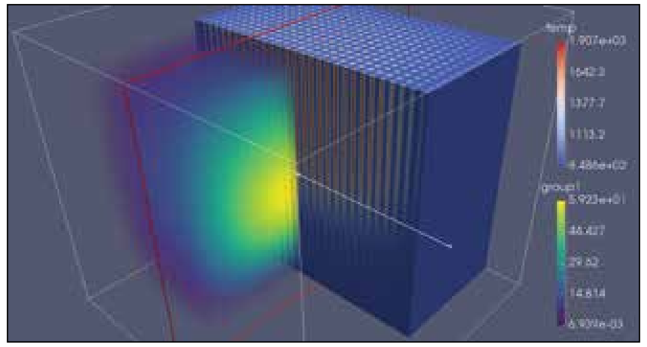

Figure 1: The coupled fast neutron flux and temperature in a 3D cuboidal model of a molten-salt reactor. Moltres coupled results have been validated against experimental results from the Molten-Salt Reactor Experiment.

METHODS & CODES

We developed two new simulation tools to enable advanced reactor and fuel-cycle simulations. First, the finite-element-based physics application Moltres [1,2] couples the thermal–hydraulics and neutronics of molten-salt flow in high-temperature liquid-fueled reactor designs. Second, we have developed a Python package for modeling fuel-salt reprocessing, SaltProc [3].

SaltProc includes fission product removal, fissile material separations, and refueling for time-dependent analysis of fuel-salt evolution. It relies on full-core high-fidelity Monte Carlo simulations to perform depletion computations that require significant computational time and memory.

Moltres is a collection of physics kernel extensions and material definitions for the highly scalable, fully implicit, Multiphysics Object-Oriented Simulation Environment (MOOSE) framework from Idaho National Laboratory [4]. These physics kernels enable Moltres to solve arbitrary-group neutron diffusion, temperature, and precursor governing equations in up to three dimensions and on an arbitrary number of processing units.

Moltres is built on top of the MOOSE framework, which itself leans on the LibMesh [5] finite element library and the PETSc [6] toolkit for solving systems of discretized partial differential equations (PDEs). MOOSE and LibMesh handle translation of Moltres-defined weak PDE forms into residual and Jacobian functions that PETSc solves simultaneously via Newton–Raphson routines. All codes use MPI for parallel communication and are easily deployed on Blue Waters. MOOSE applications like Moltres use monolithic and implicit methods that are ideal for closely coupled and multiscale physics.

Finally, these simulations are memory-intensive, so MOOSE employs a hybrid shared and distributed memory parallel model. The exceptional memory capability of the Blue Waters resource has been essential to performant simulation times.

RESULTS & IMPACT

Current interest in advanced nuclear energy systems and molten-salt reactor (MSR) concepts has illuminated a need for tools that model these systems. By developing such applications in the open, ARFC enables both transparency and distributed collaboration on promising nuclear reactor concepts. Detailed spatially and temporally resolved neutron fluxes, temperature distributions, and changing isotopic compositions can improve designs, help characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for unique physics.

ARFC has conducted simulations of the Molten-Salt Reactor Experiment (MSRE) and the conceptual Molten-Salt Breeder Reactor (MSBR) with deterministic multiphysics and Monte Carlo methods, respectively. Steady-state, transient, and fuel-cycle analysis simulations have been run in 2D as well as 3D by leveraging the Moltres and SaltProc tools developed in our group. Future work may include similarly challenging materials and geometries such as those in sodium-cooled, gas-cooled, and very-high-temperature reactor designs, which also boast improved safety and sustainability.

The model problem presented in Fig. 1 has a 3D-cuboidal geometry with heterogeneous group constants for fuel and moderator regions. Fuel-volume fraction and fuel-salt composition are based on the MSRE design. Neutron fluxes show expected cosinusoidal shapes in radial and axial directions with visible striations between fuel and moderator regions.

Meanwhile, Fig. 2 demonstrates fuel-cycle dynamics obtained from depletion and SaltProc reprocessing simulations for a 10-year time frame. An MSBR full-core safety analysis was performed at the initial and equilibrium fuel-salt compositions for various reactor safety parameters such as effective multiplication factor (shown), neutron flux distributions, temperature coefficients, rod worths, power, and breeding distributions [7,8].

WHY BLUE WATERS

Simulations that faithfully capture this coupling at realistic spatial and temporal resolution are only possible with the aid of high-performance computing resources. To assess nuclear reactor performance under a variety of conditions and dynamic transients, the ARFC group must conduct myriad 2D and 3D finite element simulations using the MOOSE framework and our in-house-developed modules. Such simulations commonly occupy tens of thousands of CPU cores at a time and vary in completion time. The MOOSE framework has been shown to scale very well up to 10,000 cores. The ARFC group has demonstrated appropriate scaling for MSR simulation above 20,000 CPU cores (600 Blue Waters nodes). Transient and multiscale simulations, which require greater capability per simulation, are on the horizon for our work. These may occupy up to 100,000 CPU cores at a time. Only a few of those larger simulations will be necessary to enable better understanding of the dynamics in these reactor systems.

PUBLICATIONS & DATA SETS

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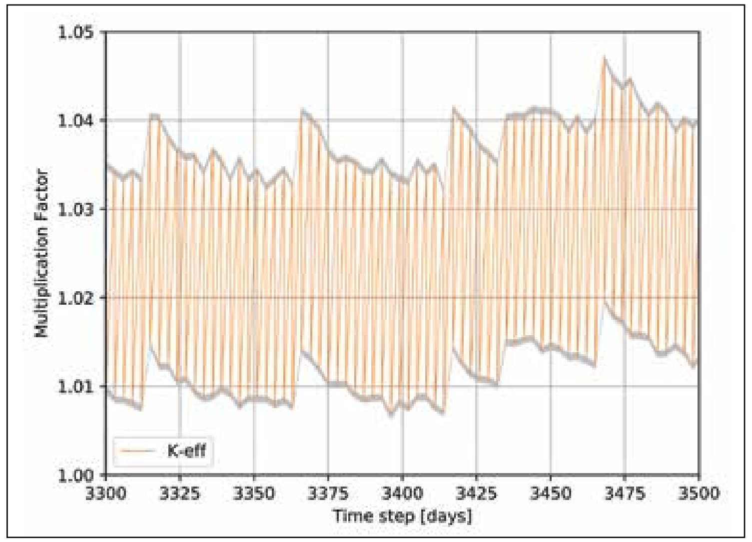

Figure 2: Simulated dynamics of reactor criticality (multiplication factor) in the Molten-Salt Breeder Reactor with SaltProc simulation of Rb, Sr, Cs, and Ba online reprocessing over 3,435 days.