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COUPLED MULTI-PHYSICS OF ADVANCED MOLTEN SALT NUCLEAR REACTORS

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EXECUTIVE SUMMARY

The Advanced Reactors and Fuel Cycles Group (ARFC) conducts modeling and simulation in the context of nuclear reactors and fuel cycles and toward the improved safety and sustainability of nuclear power. In the context of high-performance computing, this work requires the coupling of multiple physics models at multiple scales to model and simulate the design, safety, and performance of advanced nuclear reactors. In particular, thermal–hydraulic phenomena, neutron transport, and fuel performance couple tightly in nuclear reactors. Detailed spatially and temporally resolved neutron flux and temperature distributions can improve designs, help 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 and thermal hydraulics in an advanced, molten-salt-fueled nuclear reactor.

RESEARCH CHALLENGE

Nuclear power provides 19 percent of the total electricity generation in the United States and is our largest source of clean energy. The current state of the art in advanced nuclear reactor simulation (e.g., the CASL DOE innovation hub) is focused primarily on more traditional light-water reactor design types. 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 safety and sustainability of nuclear power. High-fidelity simulation of dynamic reactor performance of these designs requires development of models and tools for representing unique materials, geometries, and physical phenomena.

The current work is a finite-element-based physics application, Moltres, that extends the open source MOOSE framework to appropriately model coupled thermal–hydraulics and neutronics of molten salt flow in high-temperature liquid-fueled reactor designs. By developing the Moltres application in the open, ARFC seeks to enable both transparency and distributed collaboration on nuclear reactor concepts that promise advanced safety or sustainability.

METHODS & CODES

ARFC has developed Moltres [1], a collection of physics kernels material definitions, to extend the ecosystem of applications built upon the highly scalable, fully implicit, Multiphysics Object-Oriented Simulation Environment (MOOSE) framework from Idaho National Laboratory [2]. These physics kernels enable Moltres to solve arbitrary-group neutron diffusion, temperature, and precursor governing equations in anywhere from one to three dimensions and can be deployed on an arbitrary number of computational processing units. Moltres is devoted to previously unmatched fidelity in coupled neutronics and thermal hydraulics MSR simulation.

MOOSE and LibMesh handle translation of Moltres-defined weak PDE forms into residual and Jacobian functions that are the inputs into PetSc Newton–Raphson solution routines. All codes use MPI for parallel communication and are easily deployed on massively-parallel cluster-computing platforms. By default, MOOSE applications use monolithic and implicit methods that are ideal for closely coupled and multiscale physics.

To solve these large systems of partial differential equations on a finite element mesh in a fully coupled, implicit way, the MOOSE framework was designed to take advantage of high-performance computing capability. Accordingly, it employs a hybrid shared and distributed memory parallel model. These simulations are memory intensive, so the exceptional memory capability of the Blue Waters resource will be essential to performant simulation times. It is also important to note that rendering visualizations of the results can be computationally intensive and that a MOOSE tool exists for taking advantage of HPC resources for conducting those rendering tasks. Explorations of the use of the *yt* visualization toolkit [5] for this purpose have also been pursued in collaboration with the Data Exploration Lab, led by Prof. Matthew Turk.

RESULTS & IMPACT

Blue Waters has enabled ARFC to develop and test a first-of-its-kind, scalable, finite element model of the transient neutronics and thermal hydraulics in a liquid-fueled molten salt reactor design. Moltres is a physics application for multiphysics modeling of fluid-fueled molten salt reactors (MSRs). It couples equations for neutron diffusion, thermal hydraulics, and delayed neutron precursor transport. Neutron diffusion and precursor transport equations are set up using an action system that allows the user to employ an arbitrary number of neutron energy and precursor groups respectively with minimal input changes. Moltres sits atop MOOSE, which gives Moltres the capability to run seamlessly in massively parallel environments. To date, Moltres has been used to simulate MSRs in 2D-axisymmetric and 3D geometric configurations. As these simulations increase in fidelity, their results will be able to inform the safety and sustainability case for deployment of advanced commercial nuclear reactors.

Moltres solves arbitrary-group neutron diffusion, temperature, and precursor governing equations in anywhere from one to three dimensions and can be deployed on an arbitrary number of processing units. The model problem presented here has a 2D-axisymmetric geometry with heterogeneous group constants for fuel and moderator regions. Fuel volume fraction and fuel salt composition are based on the MSR experiment design. Neutron fluxes show expected cosinusoidal shapes in radial and axial directions with visible striations between fuel and moderator regions. Additionally, the fast group neutron flux is enhanced in fuel regions while the thermal group flux in enhanced in moderator regions. Due to advection, the temperature profile increases monotonically in the direction of salt flow. The role of advection is also seen in precursor concentrations. Long-lived precursors exhibit maximum concentrations at the core outlet. As the decay constant increases across precursor groups, the maximum concentrations move toward the reactor center where the precursor production rate is maximum. Future Moltres work includes generating a high-fidelity, 3D model as well as investigating various transient accident scenarios, additional reactor configurations, and numerous design concepts.

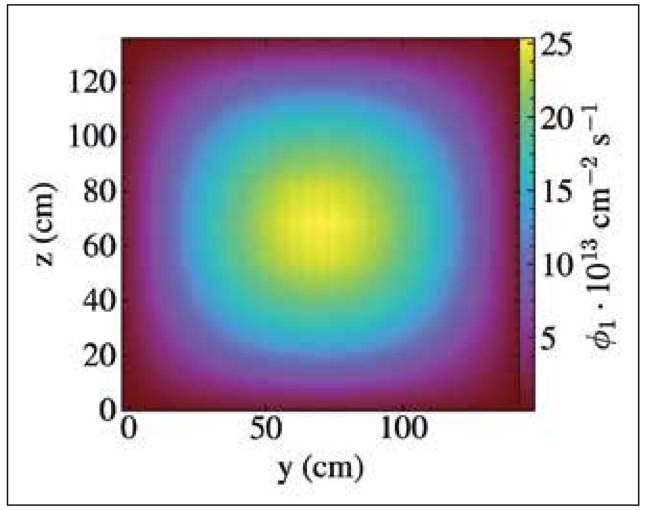

Figure 1: This image shows the neutron flux in a 2D cylindrical axisymmetric model of a molten-salt reactor. This flux has the anticipated magnitude and canonical cosine shape (r = 0 is center of core) and is undergoing validation against experimental results from the Molten-Salt Reactor Experiment.

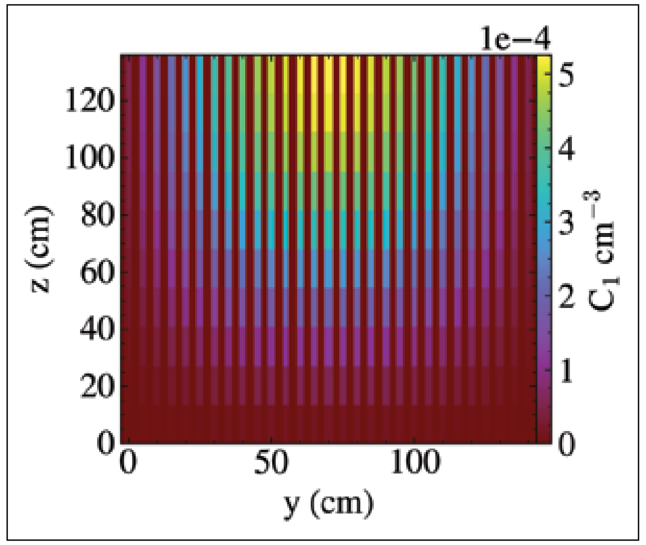

Figure 2: This image shows the temperature in a 2D cylindrical axisymmetric model of an MSR. The reactor core temperature peaks near the reactor outlet in this model because of fuel advection (r = 0 is center of core).

WHY BLUE WATERS

To assess nuclear reactor performance under a variety of conditions and dynamic transients, the ARFC group must conduct myriad two-dimensional and three-dimensional 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 AND DATA SETS

[1] Lindsay, A., K. Huff, and A. Rykhlevskii, *ARFC/Moltres: Initial Moltres release*, Zenodo (2017), DOI: 10.5281/zenodo.801823