## Research Statement

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The future of nuclear power depends on improved safety and sustainability of nuclear reactor designs and fuel cycle strategies. Accordingly, I focus on modeling and simulation of both systems, which are sufficiently complex that sophisticated scientific software and high-performance computing resources are essential to understanding and improving them.

## Past and Current Research

A background in both physics and nuclear engineering underpin my computational expertise and prepare me to develop a research program that advances the modeling and simulation of reactors and fuel cycles.

My previous work in physics tackled numerical methodologies for accelerator applications [1, 2], experimental cosmological telescope calibration [3], and experimental condensed matter physics [4]. In nuclear engineering, my most novel contribution to the field has been Cyclus [5], an agent-based nuclear fuel cycle simulator that has now grown from an individual project to a multi-institution collaboration.

I have further diversified my research focus to include the coupled multiphysics of advanced reactor transients. In particular, I am currently developing a simulation of multi-scale neutronics and thermal-hydraulics within the Pebble-Bed, Fluoride-Salt-Cooled, High-Temperature Reactor (PB-FHR) [6, 7, 8, 9, 10]. All along, my work has incorporated software practices that enable more efficient and reproducible scientific computation [11, 12].

Cyclus Fuel Cycle Simulator Faced with inflexibility in previous nuclear fuel cycle simulators, I led a software design effort called Cyclus [5, 13, 14]. Cyclus enables both scientific and policy analyses by following transactions of discrete quanta of material among discrete facilities arranged in a geographic and institutional framework and trading in flexible markets. As a direct result of Cyclus' incorporation of modern software development practices and capabilities such as openness, modularity, and scalable fidelity, it has now grown into a multi-institution collaboration with dozens of users and contributors.

Cyder Repository Model My dissertation work [15], Cyder, calculates disposal-related fuel cycle metrics of prototype geologic disposal concepts in the context of alternative fuel cycles [16]. By integrating hydrologic contaminant transport [17] and transient thermal transport [18] with the Cyclus fuel cycle simulation framework, this geologic disposal model illuminates the distinct dominant physics of candidate repository geologies, designs, and engineering components.

Coupled Multiphysics for Advanced Reactor Analysis To improve understanding of accident transients in the PB-FHR, I have developed a generic simulator for coupled lumped parameter thermal hydraulics and point kinetics [10]. To build on this, I have forged a collaboration with the Multiphysics

Object-Oriented Simulation Environment (MOOSE) team at Idaho National Laboratory (INL) [19] through which we will produce a transient three-dimensional multi-scale PB-FHR analysis with fully coupled thermal-hydraulics and deterministic neutronics.

## Future Research

My research program will bring modern scientific computing practices to bear on nuclear power at two scales both advanced reactor design and fuel cycle analysis. To achieve this, I will establish a synergy between reactor design and fuel cycle analysis to meet key challenges in the safety and sustainability of nuclear energy. When high-fidelity simulation at the reactor technology scale reveals dominant physics, those dominant features of reactor behavior can then be captured and propagated through a fuel cycle analysis at the global system scale. Together, modeling and simulation at such disparate levels of detail will illuminate the impacts of reactor design choices on the worldwide nuclear energy system (see Figure 1) and vice versa.

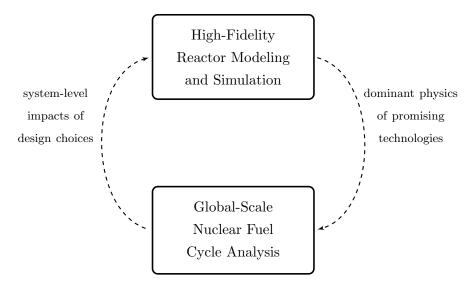


Figure 1: Complementarity of High-Fidelity Reactor Simulation with Fuel Cycle Analysis.

To this end, my research will emphasize application-driven software development. To maximize impact and accelerate the path from idea to publication, I will incorporate open source projects such as Cyclus [13], MOOSE [19], and the Python for Nuclear Engineering (PyNE) toolkit [20, 21], with which I already have strong collaborative relationships.

Technology-Level Comparisons of Sustainable Fuel Cycles I have had enough experience in fuel cycle analysis to develop many of my own potential research questions, such as: How can discrete material tracking improve resolution of "shadow" fuel cycle analyses and improve detection of material diversions? Can the provenance of fuel cycle materials identify technology bottlenecks in transitions between fuel cycles?

In the near term, one question I would like to address was identified in the Department of Energy (DOE) Office of Nuclear Energy Evaluation and Screening effort [22]. A need to distinguish sustainability performance of specific technology choices within promising families identified in that effort will require reactor technology comparisons within a discrete facility fuel cycle simulator.

Cyclus can address this question if I develop a suite of dynamically loadable libraries representing reactor facility models, each capturing the dominant physics of those common, advanced, and novel reactor designs. Via parametric analyses of equilibrium and transition scenarios, the comparative sustainability features of reactor technologies can be assessed. Due to discrete material and facility tracking, Cyclus will even able to conduct comparison using metrics with richer detail than has historically been possible [23].

Development of these libraries will be an exceptional area for early graduate student contributions. I envision, for example, advising a student interested in a particular innovative reactor design to investigate the sustainability of that design at many scales. Such a student, informed by higher-fidelity simulations, could parameterize a spectral model in Cyclus to approximate that reactor's burnup and transmutation physics at an appropriate speed and fidelity for fuel cycle simulations. This approach will benefit from my experience navigating this trade-off between speed and fidelity, in which a model must be rapid while simultaneously detailed enough to uncover system-level responses to technology choices.

Simulation Methods For Reactor Design and Analysis At its core, my research program will focus on analysis of novel reactor designs, with particular focus on those boasting inherent safety features (i.e. accident tolerant fuels or non-voiding coolants) and sustainable fuel cycles (i.e. high fuel utilization, online reprocessing strategies). These analyses will rely on developing computational methods that navigate trade-offs between accuracy and compute time. Potential areas of future inquiry in this arena include: What method improvements can speed up multi-scale multiphysics while preserving dominant physics? Can information theoretic methods improve accuracy of coupling between physics at multiple scales? Could machine learning algorithms improve our approach to accelerated Monte Carlo?

In the near term, I am particularly interested in the extent to which new insights in reactor design optimization can be derived from fully coupled multiphysics. The ability to eliminate or nearly eliminate the scaling and coupling distortions seen in simulations that are only loosely or tightly coupled may be a breakthrough capability that could reveal important details in reactor behavior. For example, Designand Beyond-Design-Basis Accident simulations are essential to the advancement of nuclear reactor safety. Faithful assessments of reactor response in these scenarios often require fully coupled, transient simulation of neutronics, thermal hydraulics, and structural performance, necessitating specialized computational methodologies.

In particular, the Jacobian-Free Newton-Krylov (JFNK) solution method [24], combined with physics-based preconditioning, enables extraordinary parallel scalability and fully-coupled solutions to systems of neutron transport and thermal hydraulic equations. Accordingly, design-driven simu-

lations within the MOOSE JFNK simulation environment may provide insights necessary for reactor technology design optimizations. Such MOOSE simulations will require my research group to develop dimension-agnostic physics 'Kernels,' combine them with validated kernels developed by others, (e.g., [25], [26], [27], [28], [29]), and construct them into coherent simulations targetted at informing advanced reactor design optimizations. In the example of accident scenarios, simulations could explore parameters that might increase Loss of Forced Cooling (LOFC), Loss of Heat Sink (LOHS), and Reactivity Insertion Accident (RIA) survivability.

**External Research Funding** My research ambitions fit well into current DOE Nuclear Energy University Programs (NEUP) funding areas. In particular, both Cyclus and MOOSE applications have been supported in recent workscopes, with Cyclus having garnered more than six NEUP awards.

Nonproliferation applications of fuel cycle analysis can be supported through the National Nuclear Security Administration (NNSA), Nuclear Regulatory Commission (NRC), and Department of Homeland Security Domestic Nuclear Threat Detection Office (DHS-DNDO). Such pursuits in combination with my focus on safety may strengthen my applications to junior faculty development awards available from the National Science Foundation (NSF), DOE, DHS-DNDO, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AF-OSR).

Furthermore, I expect that collaboration with the Nuclear Engineering Advanced Modeling and Simulation (NEAMS) campaign with current and past colleagues at INL, Argonne National Laboratory (ANL), and Oak Ridge National Laboratory (ORNL) will provide additional student support. I also expect to seek additional support for methods development and contributions to computational nuclear toolkits from programs such as the NSF, Google Summer of Code, the Alfred P. Sloan Foundation, and the Gordon and Betty Moore Foundation.

I have co-authored numerous grant proposals including five to NEUP, one to NSF, and one application for computing time on National Energy Research Scientific Computing Center (NERSC). While only two of those proposals were funded (one to NEUP and one to NERSC), all of these experiences have been essential to my understanding of the funding environment.

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