## Research Statement

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I aim to improve the safety and sustainability of nuclear power through advanced nuclear reactor designs and fuel cycle strategies. Accordingly, I focus on modeling and simulation of such systems, which are sufficiently complex that sophisticated scientific software and high-performance computing resources are essential to understanding and improving them. A background in both physics and nuclear engineering underpin my computational expertise and uniquely prepare me to develop a research program that advances modeling and simulation of both reactors and fuel cycles.

## Past and Current Research

In the physics domain, I laid a foundation in the physics of particles through research that involved numerical methodologies for accelerator physics 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 which has grown from an individual project to a multi-institution, international collaboration. Finally, in my current work, I have extended my research focus to include the coupled multiphysics of advanced reactor transients. In particular, I have simulated coupled 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] which 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 I am also poised to produce a transient, three-dimensional, multi-scale PB-FHR analysis with fully coupled thermal-hydraulics and deterministic neutronics.

## Future Research

If selected by this committee, I expect to bring modern scientific computing practices to bear on both advanced reactor design and fuel cycle analysis.

My research program 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 can illuminate the impacts of design choices on the worldwide nuclear energy system (see Figure 1) and vice versa.

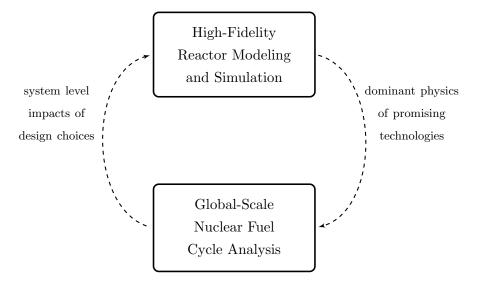


Figure 1: Complementarity of high fidelity reactor simulation and fuel cycle analysis.

To this end, my research will emphasize application-driven software development, but will minimize duplication of efforts by incorporating open source projects such as Cyclus [13], MOOSE [19], and the Python for Nuclear Engineering (PyNE) toolkit [20, 21] which are fertile ground for contributions with a wide impact potential.

Technology-Level Comparisons of Sustainable Fuel Cycles I have had enough experience in fuel cycle analysis to develop many of my own 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 equillibrium 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 My research program will be driven by 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 computational methods that navigate trade-offs between accuracy and compute time. Long-term methodological questions in this computational 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 can be derived from fully coupled simulations. 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 change the face of reactor modeling entirely.

For example, Design- and 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 and fully-coupled solu-

tions to systems of neutron transport and thermal hydraulic equations. MOOSE, from INL, which relies on this exceptional numerical method as well as adaptive mesh refinement for structured and unstructured meshes, is beginning to be used in earnest for nuclear engineering applications (e.g., [25, 26, 27, 28, 29] among others).

Simulations of particular advanced reactor designs in the MOOSE paradigm will require developing dimension-agnostic, application-driven physics 'Kernels,' combining them with validated kernels developed by others, and constructing them into coherent simulation objects.

**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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