Research Statement

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The world's energy future depends on improved safety and sustainability of nuclear reactor designs and fuel cycle strategies. Accordingly, I focus on modeling and simulation of reactor and fuel cycle 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.

Further, I have diversified my research to include the coupled multiphysics of advanced reactor transients. In particular, I am currently developing a multi-scale simulation of neutronics and thermal hydraulics within the Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) [6, 7]. All of my research has incorporated software practices that enable more efficient and reproducible scientific computation [8, 9]. The following subsections highlight my past research initiatives and how they were enabled by strong software practices.

Cyclus Fuel Cycle Simulator Faced with inflexibility in previous nuclear fuel cycle simulators, I led a software design effort called Cyclus [5, 10]. 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 [11], Cyder, calculates disposal-related fuel cycle metrics of prototype geologic disposal concepts in the context of alternative fuel cycles. By integrating hydrologic contaminant transport and transient thermal transport 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 [7]. To build on this, I have forged a collaboration with the

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

Future Research

To meet key challenges in the safety and sustainability of nuclear energy, I will establish a synergy between reactor design and fuel cycle analysis. To achieve this, my research program will bring modern scientific computing practices to bear on simulation at both scales. When high-fidelity simulation at the reactor technology scale reveals which physics are most dominant, those key reactor behaviors (e.g. efficient fuel utilization) can then be captured and propagated through a fuel cycle analysis at the scale of many facilities over hundreds of years. Together, modeling and simulation at such disparate levels of detail will illuminate the impacts (e.g. reduced need for reprocessing or mining) of reactor design choices (e.g. online refuelling) on the worldwide nuclear energy system (see Figure 1) and vice versa.

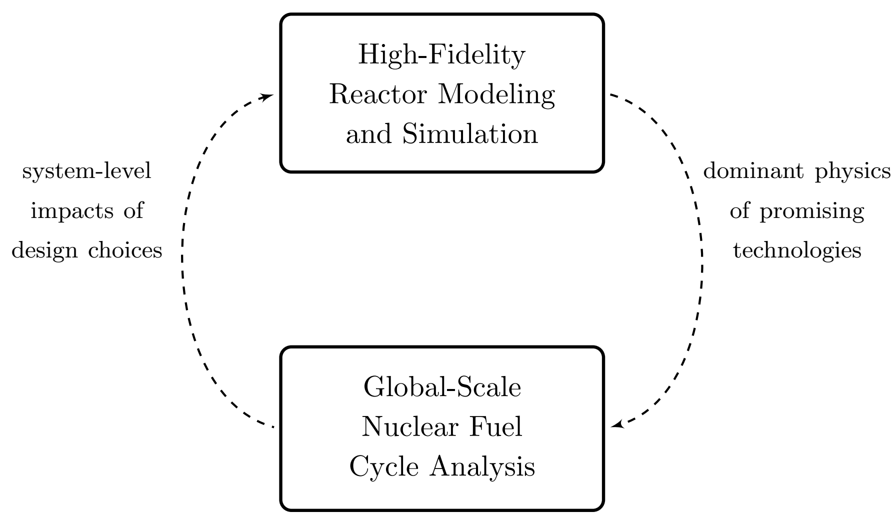

Figure 1: Complementarity of High-Fidelity Reactor Simulation with Fuel Cycle Analysis.

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, MOOSE, and the Python for Nuclear Engineering (PyNE) toolkit [12, 13], 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 and collaborations across a range of key challenges including security, energy policy, repository safety, and reactor physics. Potential questions include: 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? How do transitions to various advanced reactor designs compare in feasibility?

In the near term, one question I will address was identified as crucial to domestic energy policy in the Department of Energy (DOE) Office of Nuclear Energy Evaluation and Screening effort [14]. Technology families were identified in that effort as promising from the perspective of many metrics including sustainability. To assist DOE in selecting high-impact R&D efforts, specific reactor designs within these technology families will require more detailed comparisons within a discrete facility fuel cycle simulator.

I can make these comparisons using Cyclus by configuring a suite of reactor facility models to capture the dominant physics of each reactor design identified. Via parametric analyses of equilibrium and transition scenarios, the comparative sustainability features of reactor technologies can be assessed. Because Cyclus tracks materials and facilities discretely, the addition of these libraries will enable fuel cycle comparisons using metrics with richer detail than has historically been possible [15].

Conducting these parametric studies 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 reactor model already existing in the Cyclus ecosystem or develop their own 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 the trade-off between speed and fidelity, in which a simulation must be rapid while simultaneously detailed enough to uncover system-level responses of reactor-scale technology choices.

Modeling and Simulation 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 or online reprocessing strategies). I will conduct these analyses by developing computational methods that navigate trade-offs between accuracy and compute time. Potential areas of future inquiry in this arena include: What simulation tools can be developed support regulatory needs for reactors with mobile fuel forms (e.g. molten salt)? What lower fidelity methods can preemptively identify key physics in complex, multi-scale systems? Could machine learning algorithms similarly improve our approach to accelerated Monte Carlo?

In the near term, I am interested in the potential to derive new insights in reactor design optimization by fully coupling neutronics with thermal hydraulics. The potential to eliminate coupling distortions may be a breakthrough capability that could reveal important details in reactor behavior. For example, transient simulations are essential to the advancement of nuclear reactor safety. Faithful assessments of reactor response in transient scenarios require coupled simulation of neutronics, thermal hydraulics, and structural performance. However, fully coupling those physics, rather than loosely coupling them, requires specialized computational methods.

Accordingly, my research group will investigate reactor technology design optimizations by conducting simulations using tools such as MOOSE that implement such methods. In the case of MOOSE, the Jacobian-Free Newton-Krylov (JFNK) solution method [16], combined with physics-based preconditioning, enables extraordinary parallel scalability. To wield this capability, my research group will develop dimension-agnostic physics 'kernels,' combine them with validated kernels developed by others, and construct them into coherent simulations targeted at informing advanced reactor design optimizations. In the example of transient scenarios, my simulations could explore parameters that might reduce the need for large safety margins by increasing Beyond-Design-Basis Event (BDBE) survivability.

External Research Funding My research ambitions fit well into current DOE Nuclear Energy University Programs (NEUP) funding areas. In particular, Fluoride-Salt-Cooled, High-Temperature Reactors (FHRs) research, transient simulation, Cyclus developments, and MOOSE applications have all been supported in recent workscopes.

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 contributions to computational nuclear toolkits from programs such as the National Science Foundation (NSF), Google Summer of Code, the Alfred P. Sloan Foundation, and the Gordon and Betty Moore Foundation.

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

I have co-authored grant proposal submissions to numerous institutions including NEUP, NSF, INL, and National Energy Research Scientific Computing Center (NERSC). While only two of those proposals were ultimately 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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