

# Research Statement

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Improving the safety and sustainability of nuclear power requires improved nuclear reactor designs, fuel cycle strategies, and waste disposal concepts. These systems are sufficiently complex that modern software methods and high-performance computing resources are essential to understanding and improving them. The importance of sophisticated scientific computing in advancing safe, sustainable nuclear power drives my research direction toward the development of computational methods and simulation tools for nuclear engineering across many scales, with special focus on the safety and security of advanced reactor designs and fuel cycles.

In the near term, I intend to continue developing computational methods for fuel cycle sustainability and reactor safety evaluation. These are the areas in which I have had sufficient experience to independently develop and pursue relevant research questions. Can nonlinear programming techniques be applied to determine appropriately critical fresh fuel compositions in a reprocessing facility model? To what extent are repository site selection decisions and fuel cycle decisions coupled? What are the comparative global fuel supply impacts of political instabilities, international fuel takeback agreements, or trade embargoes between specific pairs of nations? What deterministic methods best capture the physics of complex geometries such as pebble fuel with TRISO particles? What is the effect of this fuel choice on the bounding magnitude of a prompt reactivity insertion resulting in safe shutdown?

In the longer term, I hope to establish a research program capable of tackling a variety of challenges in nuclear energy from the technical to the political. I hope to uncover groundbreaking insights by means of simulation methods, efficient algorithms, novel computer architectures, and sophisticated design tailored to the many scales and multiple physics encountered in nuclear energy technology. The tenets of scientific endeavor (e.g., data control, reproducibility, comprehensive documentation, and peer review) suffer in projects that fail to make use of current development tools such as unit testing, version control, automated documentation and others [1, 2]. Maintenance of rigorous scientific computing standards will help my research program avoid such pitfalls [3] and incorporation of new numerical methods for reactor physics will keep my research program relevant.

## *Past and Current Research*

My past and current work in the area of nuclear fuel cycle analysis has focused on the application and development of the Cyclus nuclear fuel cycle simulator project [4] and of the Cyder used fuel disposition and disposal system model [5, 6]. Most recently, I have extended my research focus to include neutronics and coupled physics modeling of the Pebble-Bed, Fluoride-Salt-Cooled, High-Temperature Reactor (PB-FHR) [7, 8, 9, 10]. My previous research has included numerical methodologies for accelerator physics applications [11, 12], experimental cosmological telescope calibration [13], and experimental condensed matter physics [14].

**Cyclus Fuel Cycle Simulator** Faced with inflexibility in previous nuclear fuel cycle system simulation frameworks, Paul P.H. Wilson and I envisioned a more modular, encapsulated design. I led this software design effort [15, 16], called Cyclus, and was its lead developer in its first years. As a direct result of Cyclus' incorporation of modern software development practices and desired 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 Analysis Model** My dissertation work [6], a hydrologic and thermal geologic disposal model called Cyder, illuminated the distinct dominant physics of candidate repository geologies, designs, and

engineering components. By integrating hydrologic contaminant transport [17] and transient thermal transport [18] with the Cyclus fuel cycle simulation framework, Cyder calculates disposal-related fuel cycle metrics by providing a dynamic simulation environment in which to prototype geologic disposal concepts in the context of alternative fuel cycles [19].

**Coupled Multiphysics for Advanced Reactor Analysis** My postdoctoral research has begun to expand my expertise by emphasizing the development of a high-fidelity, fully-coupled, multiphysics model of the PB-FHR at the University of California - Berkeley with Professors Jasmina Vujić and Per Peterson. The objective of this work is to conduct high-fidelity simulations of transient event behavior in this complex reactor in a high-performance computing environment. In my first months at Berkeley, I forged a collaboration with the Idaho National Laboratory to conduct this development within the Multiphysics Object Oriented Simulation Environment (MOOSE) [20]. This work will result in a transient, three-dimensional MOOSE module with fully coupled thermal-hydraulics and deterministic neutronics.

## *Future Research*

Novel solutions to challenges in nuclear energy such as nuclear reactor accident response, nuclear fuel cycle strategy, and waste management will arise from the development of application-driven numerical simulation methods and incorporation of sophisticated computational tools. To this end, my work will range from individual contributions to existing toolkits to comprehensive solution libraries for specific nuclear applications (e.g., a suite of activation analysis methods for sub-critical systems). Open source projects such as Cyclus [16], MOOSE [20], and the Python for Nuclear Engineering (PyNE) toolkit [21] are fertile ground for contributing computational nuclear engineering tools with a wide impact potential. My research program will leverage the significant effort represented by those tools, rather than reinventing the wheel, and will benefit from the user and developer communities that they possess. I will briefly expand on two of my near term focus areas which exemplify these goals.

**Advanced Technology Modeling for Fuel Cycle Analysis** One of the continuing challenges in evaluating the system level impacts of nuclear technologies and policies is the need for a standardized simulation platform and library of models representing nuclear technologies and calculating fuel cycle metrics. The Cyclus simulation framework has provided this standardizing platform, but it is incomplete without a robust library of fuel cycle metric calculation methods and a versatile ecosystem of models to represent innovative nuclear technologies. My work in this area will fill this gap.

The Cyclus modeling paradigm 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. Cyclus' sophisticated design emphasizes separation of the core simulation logic from the technical nuclear process models representing the facilities of the nuclear fuel cycle. This ensures robust modularity with regard to functionality.

My work will leverage Cyclus toward the development of a library of methods for calculating fuel cycle metrics. Object-oriented methods enabled by the unique Cyclus modeling paradigm will result in metrics with richer detail than has historically been possible with previous simulators. One example is a "shadow fuel cycle" nonproliferation calculation strategy in which nuclear material is diverted by a nefarious actor within a facility to determine the minimum detectable diverted material amount. This metric is used to describe the detection sensitivity of inspections. Creative safeguards strategies may emerge from the richness of disaggregated detail

made possible by evaluating this nefarious theft scenario within the context of the discrete materials and discrete facilities of the Cyclus environment.

Additionally, my work will include both focused, single technology model development and development of concise parametric models capable of representing myriad technologies. Such models will enable assessment of a broad range of technology and policy implications related to the introduction of those technologies into the world nuclear energy market. By balancing speed with the capability to capture dominant physics, Cyclus can rapidly assess the implications of those technologies on the broader fuel cycle. Contributing advanced reactor and fuel cycle concepts to the ecosystem of available models will also increase the potential for collaboration with other domestic and international researchers in technology evaluations and community benchmarking exercises.

I envision, for example, advising a student interested in innovative reactor design to develop a parameterized spectral model to approximate burnup and transmutation physics with appropriate speed and fidelity for fuel cycle simulations. This work 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.

**Multiphysics Model Development for Reactor Design and Analysis** Another focus of my research program will include the development of multiphysics models of reactor designs, with particular focus on those boasting inherent safety features (i.e. accident tolerant fuels or non-voiding coolants). Design- and Beyond-Design-Basis Accident simulations are essential to the advancement of nuclear reactor safety. Faithful assessments of reactor response in these scenarios 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 [22], combined with physics-based preconditioning, enables extraordinary parallel scalability and fully-coupled solutions 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., [23, 24, 25, 26, 27] among others). Moreover, the MOOSE tool possesses a modular, object-oriented simulation environment approach, similar to that of Cyclus, which allows user-developers to construct applications by focusing on the unique physics of their modeling problem with minimal concern for the system solution methodology.

My future work with MOOSE, continuing a recent collaboration that I forged with the MOOSE team while at UC-Berkeley, will focus on the development of MOOSE ‘Applications’ capable of 3-dimensional, multi-scale, massively parallel analyses of promising reactor technologies. This will consist of developing dimension-agnostic, application-driven physics ‘Kernels,’ combining them with validated kernels developed by others, and constructing them into coherent simulation objects.

In particular, I am interested in the potential impacts of the fully coupled nature of MOOSE multiphysics. The ability to eliminate or nearly eliminate the scaling and coupling distortions seen in simulations that are only loosely or tightly coupled is a breakthrough capability that could change the face of reactor modeling entirely.

**External Research Funding** My future research plans fit well into the Department of Energy (DOE) Nuclear Energy University Programs (NEUP) funding scope. In particular, both Cyclus and MOOSE applications have been supported in recent workshops. Since Cyclus’ recent adoption by the DOE Office of Nuclear Energy (DOE-NE) as its flagship nuclear fuel cycle simulator, it has garnered an international, multi-institution collaboration of users and developers including more than three NEUP-funded projects.

The inclusion of the Cyclus project in previous workshops indicates that nuclear fuel energy system simulation

development with the Cyclus tool is an area of sustained interest within the DOE-NE. I have already submitted, as principal investigator, a 2014 NEUP pre-proposal to support work on advanced laser separation technology modeling for fuel cycle analysis. I expect that my intimate familiarity with Cyclus will add strength to this and future proposals.

Nonproliferation applications of fuel cycle analysis have the potential to benefit greatly from funding opportunities through the National Nuclear Security Administration (NNSA), Nuclear Regulatory Commission (NRC), and Department of Homeland Security Domestic Nuclear Detection Office (DHS-DNDO). These 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 Research (ONR), and the Air Force Office of Scientific Research (AF-OSR).

Finally, I also expect to seek additional support for methods development and contribution to computational nuclear toolkits from programs such as Google Summer of Code, the Alfred P. Sloan Foundation, and the Gordon and Betty Moore Foundation. The NSF is also interested in scientific computing and I am currently assisting in the collaborative preparation of a proposal for funding from NSF in the field of scientific computing education. Furthermore, collaboration with Nuclear Engineering Advanced Modeling and Simulation campaign with current and past colleagues at Idaho, Argonne, and Oak Ridge National Laboratories may provide additional student and collaboration support in the area of modeling and simulation.

I have had many opportunities to participate in both failed and successful grant proposals. As a graduate student, I assisted in writing grant proposals with my advisor, Paul P.H. Wilson. In 2012, one of those reached success, securing a three year, \$1.2 million, Nuclear Energy University Programs (NEUP) Research and Development grant for the expansion of Cyclus. Additionally, I was the primary author on an NEUP proposal for the 2013 call for proposals. I was pleased to have been invited to submit a full proposal, but that full proposal did not progress further. It is my hope that these early experiences with grant writing will serve me well in my own research program.

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