

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 modeling and simulation of both 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]. This agent-based nuclear fuel cycle simulator has now grown from an individual project to a multi-institution, international collaboration. Finally, I have diversified my research focus to include the coupled multiphysics of advanced reactor transients. In particular, I am currently pursuing 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] 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 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 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.

(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 be 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, 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 fully-coupled solutions to systems of neutron transport and thermal hydraulic equations. Accordingly, design-driven simulations 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.

References

- [1] **Kathryn D. Huff.** Excess Single Event Effects in the Second Chip of a Series. Technical Report 0, Los Alamos National Laboratory Report, Los Alamos, NM, United States, August 2003.
- [2] **Kathryn D. Huff.** Digital filtering applications to the lead slowing-down spectrometer. Technical Report 0, Los Alamos National Laboratory Report LA-UR-04-8757, 2004, Los Alamos, NM, United States, 2004.
- [3] **Kathryn D. Huff.** *QUIET Celestial Gain Calibrations*. Undergraduate, University of Chicago, Chicago, IL, United States, May 2008.

- [4] M. G. Clerc, P. Cordero, J. Dunstan, **Kathryn D. Huff**, N. Mujica, D. Risso, and G. Varas. Liquid-solid-like transition in quasi-one-dimensional driven granular media. *Nature Physics*, 4(3):249–254, March 2008.
- [5] **Kathryn D. Huff**, Paul PH Wilson, and Matthew J. Gidden. Open Architecture and Modular Paradigm of Cyclus, a Fuel Cycle Simulation Code. In *Transactions of the American Nuclear Society*, volume 104, page 183, June 2011.
- [6] UC Berkeley Facilitators and UC Berkeley Assistants. Fluoride-Salt-Cooled, High-Temperature Reactor (FHR) Methods and Experiments Program White Paper. 2013.
- [7] UC Berkeley Facilitators and UC Berkeley Assistants. Fluoride-Salt-Cooled, High-Temperature Reactor (FHR) Subsystems Definition, Functional Requirement Definition, and Licensing Basis Event (LBE) Identification White Paper. 2013.
- [8] M. I. T. Facilitators, UW Madison Facilitators, and UC Berkeley Facilitators. Fluoride-Salt-Cooled, High-Temperature Reactor (FHR) Development Roadmap and Test Reactor Performance Requirements White Paper. 2013.
- [9] UW Madison Facilitators, M. I. T. Facilitators, and UC Berkeley Facilitators. Fluoride-Salt-Cooled High Temperature Reactor (FHR) Materials, Fuels and Components White Paper. *Fluoride-salt-cooled High-Temperature Reactor Workshop White Papers*, 2013.
- [10] **Kathryn Huff**. PyRK: Python for Reactor Kinetics, 2015. <https://github.com/pyrk/pyrk>.
- [11] Greg Wilson, D. A. Aruliah, C. Titus Brown, Neil P. Chue Hong, Matt Davis, Richard T. Guy, Steven H. D. Haddock, **Kathryn D. Huff**, Ian M. Mitchell, Mark D. Plumbley, Ben Waugh, Ethan P. White, and Paul Wilson. Best Practices for Scientific Computing. *PLoS Biol*, 12(1):e1001745, January 2014.
- [12] Anthony Scopatz and **Kathryn D. Huff**. *Effective Computation in Physics*. O’Reilly Media, S.I., 1 edition edition, May 2015.
- [13] Robert W. Carlsen, Matthew Gidden, **Kathryn Huff**, Arrielle C. Opotowsky, Olzhas Rakhimov, Anthony M. Scopatz, Zach Welch, and Paul Wilson. Cyclus v1.0.0. *Figshare*, June 2014. <http://dx.doi.org/10.6084/m9.figshare.1041745>.
- [14] **Kathryn D. Huff**, Matthew J. Gidden, Robert W. Carlsen, Robert R. Flanagan, Meghan B. McGarry, Arrielle C. Opotowsky, Erich A. Schneider, Anthony M. Scopatz, and Paul P.H. Wilson. Fundamental Concepts in the Cyclus Nuclear Fuel Cycle Simulator. *Submitted*, 2015.
- [15] **Kathryn D. Huff**. *An Integrated Used Fuel Disposition and Generic Repository Model for Fuel Cycle Analysis*. PhD thesis, THE UNIVERSITY OF WISCONSIN - MADISON, October 2013.

- [16] **Kathryn D. Huff**. Cyclus Fuel Cycle Simulation Capabilities with the Cyder Disposal System Model. In *Proceedings of GLOBAL 2013*, Salt Lake City, UT, United States, October 2013.
- [17] **Kathryn D. Huff** and W. Mark Nutt. FY12 Sensitivity Studies Using the UFD Clay Generic Disposal System Model. Technical Report FCRD-USED-2012-000141, Argonne National Laboratory (ANL), Argonne, IL, United States, July 2012.
- [18] **Kathryn Huff** and Theodore H. Bauer. Numerical Calibration of an Analytical Generic Nuclear Repository Heat Transfer Model. In *Transactions of the American Nuclear Society*, volume 106 of *Modeling and Simulation in the Fuel Cycle*, pages 260–263, Chicago, IL, United States, June 2012. American Nuclear Society, La Grange Park, IL 60526, United States.
- [19] Derek Gaston, Chris Newman, Glen Hansen, and Damien Lebrun-Grandi. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. *Nuclear Engineering and Design*, 239(10):1768–1778, October 2009.
- [20] Anthony Scopatz, Paul K. Romano, Paul P. H. Wilson, and **Kathryn D. Huff**. PyNE: Python for Nuclear Engineering. In *Transactions of the American Nuclear Society*, volume 107, San Diego, CA, USA, November 2012. American Nuclear Society.
- [21] Cameron Bates, Elliot D. Biondo, **Kathryn D. Huff**, Kalin Kiesling, and Anthony M. Scopatz. PyNE Progress Report. In *Transactions of the American Nuclear Society*, Anaheim, CA, United States, November 2014. American Nuclear Society.
- [22] R. Wigeland, T. Taiwo, M. Todosow, H. Ludewig, W. Halsey, J. Gehin, R. Jubin, J. Buelt, S. Stockinger, K. Jenni, and others. Nuclear Fuel Cycle Options Evaluation to Inform R&D Planning. Technical report, Idaho National Laboratory (INL), 2014.
- [23] Anthony M. Scopatz, Arrielle C. Opotowsky, and Paul P.H. Wilson. Cymetric - A Fuel Cycle Metrics Tool for Cyclus. In *Transactions of the American Nuclear Society*, volume 112 of *Fuel Cycle Simulators*, pages 81–84, San Antonio, TX, June 2015. American Nuclear Society.
- [24] D. A. Knoll and D. E. Keyes. Jacobian-free NewtonKrylov methods: a survey of approaches and applications. *Journal of Computational Physics*, 193(2):357–397, January 2004.
- [25] H. Park, D. Gaston, S. Kadioglu, D. Knoll, R. Martineau, W. Taitano, D. Lebrun-Grandie, and Damien Lebrun. Tightly coupled multiphysics simulation for pebble bed reactors. In *American Nuclear Society 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics*, 2009.
- [26] Michael Philip Short, Brian K. Kendrick, Theodore Besmann, Chris R. Stanek, Sidney Yip, Barclay Jones, and Jim Henshaw. Multiphysics Modeling of Porous CRUD Deposits in Nuclear Reactors. *Journal of Nuclear Materials*, 443(1-3):579–587, 2013.

- [27] Stephen R. Novascone, Jason D. Hales, Benjamin W. Spencer, and Richard L. Williamson. Assessment of PCMI Simulation Using the Multidimensional Multiphysics BISON Fuel Performance Code. Technical report, Idaho National Laboratory (INL), 2012.
- [28] S. R. Novascone, R. L. Williamson, J. D. Hales, M. R. Tonks, D. R. Gaston, C. J. Permann, D. Andrs, and R. C. Martineau. A Multidimensional and Multiphysics Approach to Nuclear Fuel Behavior Simulation. In *PHYSOR 2012 Advances in Reactor Physics Linking Research, Industry, and Education*, Knoxville, Tennessee, USA, 2012. American Nuclear Society, La Grange Park, IL 60526, United States.
- [29] D. Gaston, G. Hansen, S. Kadioglu, D. A. Knoll, C. Newman, H. Park, C. Permann, and W. Taitano. Parallel multiphysics algorithms and software for computational nuclear engineering. *Journal of Physics: Conference Series*, 180(1):012012, July 2009.