Blue Waters Professor Report: Advanced Reactors and Fuel Cycles

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1 Project Information

Project title: Advanced Reactors and Fuel Cycles

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Co-PIs and Collaborators: Postdoctoral Scholar Alexander Lindsay was a key part of my research group in 2016-2017: Alexander Lindsay, Postdoctoral Scholar, Nuclear Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign

2 Executive Summary

The Advanced Reactors and Fuel Cycles Group (ARFC) conducts modeling and simulation in the context of nuclear reactors and fuel cycles toward improved safety and sustainability of nuclear power. This work requires high performance computing capabilities to couple multiple physics at multiple scales to model and simulate the design, safety, and performance of advanced nuclear reactors. In particular, thermal-hydraulic phenomena, neutron transport, and fuel performance couple tightly in nuclear reactors. Detailed spatially and temporally resolved neutron flux and temperature distributions in particular can improve designs, help characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for those unique physics. In the work presented here, ARFC has demonstrated the capability to simulate coupled, transient neutronics and thermal hydraulics in an advanced, molten-salt-fueled nuclear reactor.

Highlight: The coupled multiphysics capabilities in two computational tools developed for and demonstrated on Blue Waters helped Prof. Huff to secure significant ($999,694) grant funding this year. The award, “Enabling Load Following Capability in the Transatomic Power MSR” is part of ARPA-E’s Modeling-Enhanced Innovations Trailblazing Nuclear Energy Reinvigoration (MEITNER) initiative.

3 Description of research activities and results

ARFC Blue Waters activity began in November 2016 when access to the ARFC allocation was initiated for PI Huff. In the two years since the start of this allocation, Blue Waters has enabled ARFC to develop and test two significant new capabilities. First, Moltres is a first-of-its-kind finite element model of the transient neutronics and thermal hydraulics in a liquid-fueled molten salt reactor design [1, 2, 3, 4]. Second, SaltProc is a highly capable tool for fuel salt reprocessing simulation [5, 6, 7].

3.1 Key Challenges

The current state of the art in advanced nuclear reactor simulation (e.g. the CASL DOE innovation hub) is focused on more traditional light water reactors. This work extends that state of the art by enabling similarly high fidelity modeling and simulation of more advanced reactor designs which have the potential to improve the already unparalleled safety and sustainability of nuclear power. High fidelity simulation of performance in these designs requires development of models and tools for representing unique materials, geometries, and physical phenomena. The current work includes extension of the MOOSE framework to appropriately model coupled thermal-hydraulics and neutronics of molten salt flow in a high temperature liquid-fueled reactor design. Future work will include similarly challenging materials and geometries such as those in sodium cooled, gas cooled, and very high temperature reactor designs which promise advanced safety or sustainability.

3.2 Why it Matters

Nuclear power is an emissions free, safe source of electricity with unparalleled energy density, baseload capacity, and land-use effiency. As we together face energy poverty, climate change, and simultaneous increase in worldwide energy use, the world's energy future increasingly depends on improved safety and sustainability of nuclear reactor designs and fuel cycle strategies. Advanced reactor and fuel cycle systems are sufficiently complex that sophisticated scientific software and high-performance computing resources are essential to understanding and improving them.

In particular, insights coupling feedback between the reactor scale and the fuel cycle scale are essential to the deployment and scalability of these innovations in the real world. The work conducted in this allocation seeks exactly those insights and builds a research program that trains future reactor and fuel cycle designers in best practices for large scale engineering modeling and simulation. Additionally, development and demonstration of high fidelity software for multi-physics in advanced reactor types builds a foundation for future funding through the Department of Energy Office of Nuclear Energy.

3.3 Why Blue Waters

To assess nuclear reactor performance under a variety of conditions and dynamic transients, the ARFC group must conduct myriad 2-dimensional and 3-dimensional finite element simulations using the MOOSE framework and our in-house developed modules. This class of simulations commonly occupy tens of thousands of CPU cores at a time and vary in completion time. The MOOSE framework is shown to scale very well up to 10,000 cores. The ARFC group has demonstrated appropriate scaling for MSR simulation above 20,000 CPU cores (600 Blue Waters nodes). Transient and multi-scale simulations, which require greater capability per simulation, are on the horizon for our work. These may occupy up to 100,000 CPU cores at a time. Only a few of those larger simulations will be necessary to enable better understanding of the dynamics in these reactor systems.

3.4 Accomplishments

Moltres [8] is a physics application for multiphysics modeling of fluid-fuelled molten salt reactors (MSRs). It couples equations for neutron diffusion, thermal hydraulics, and delayed neutron precursor transport. Neutron diffusion and precursor transport equations are set up using an action system that allows the user to use an arbitrary number of neutron energy and precursor groups respectively with minimal input changes. Moltres sits atop the Multi-physics Object-Oriented Simulation Environment [9] which gives it the capability to run seamlessly in massively parallel environments. To date, Moltres has been used to simulate MSRs in 2D-axisymmetric and 3D geometric configurations. As these simulations increase in fidelity, their results will be able to inform the safety and sustainability case for deployment of advanced commercial nuclear reactors.

Moltres solves arbitrary-group neutron diffusion, temperature, and precursor governing equations in anywhere from one to three dimensions and can be deployed on an arbitrary number of processing units. The model problem presented here has a 2D-axisymmetric geometry with heterogeneous group constants for fuel and moderator regions. Fuel volume fraction and fuel salt composition are based on the Molten Salt Reactor Experiment design. Figure 1 demonstrates that neutron fluxes show expected cosinusoidal shapes in radial and axial directions with visible striations between fuel and moderator regions. The fast group flux is enhanced in fuel regions while the thermal group flux in enhanced in moderator regions.

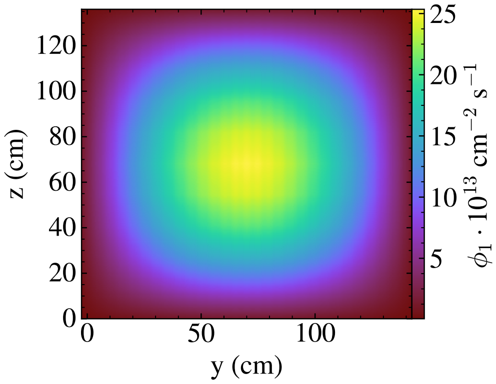
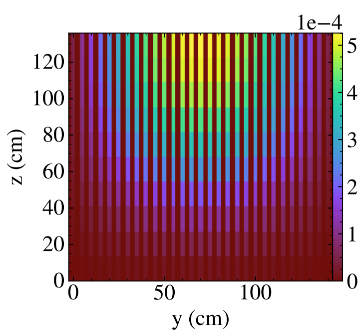
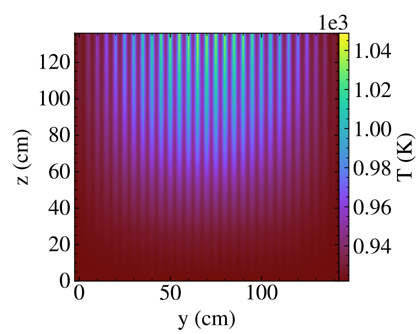


Figure 1: This image shows the neutron flux in a 2-D cylindrical axisymmetric model of an MSR. This flux has the anticipated magnitude and canonical cosine shape (r = 0 is center of core) and is undergoing validation against experimental results from the Molten Salt Reactor Experiment.

In Figure 2b, it can be seen that the temperature profile increases monotonically in the direction of salt flow. This is due to advection. The role of advection is also seen in precursor concentrations. Long lived precursors exhibit maximum concentrations at the core outlet, as seen in Figure 2a. As the decay constant increases across precursor groups the maximum concentrations moves towards the reactor center where the precursor production rate is maximum. Future Moltres work includes generating a high-fidelity 3D model as well as investigating various transient accident scenarios.



(a) This image shows the concentration of some particularly important fission-product nuclides called delayed neutron precursors. The concentration of the group of longest lived precursors ($\lambda = 1.24 \times 10^{-2} s^{-1}$) peaks near the reactor outlet in this 2-D axisymmetric model (r = 0 is center of core).



(b) This image shows the temperature in a 2-D cylindrical axisymmetric model of an MSR. The reactor core temperature peaks near the reactor outlet in this 2-D axisymmetric model because of fuel advection (r = 0 is center of core).

Additionally, we have developed an online reprocessing model, SaltProc which includes fission product removal, fissile material separations, and refuelling for time dependent analysis of fuel-salt evolution. This tool relies on full-core high-fidelity Monte Carlo simulations perform depletion computations. Simulations which faithfully capture this coupling at realistic spatial and temporal resolution are only possible with the aid of high performance computing resources.

These fuel cycle simulations have occupied up to many hundreds of nodes simultaneously and have resulted in rich datasets for use in reactor design and analysis. Fuel cycle dynamics and quasi-equilibrium compositions were obtained from depletion and reprocessing simulations for a 10-year time frame. The MSBR full-core safety analysis was performed at the initial and equilibrium fuel salt compositions, for various reactor safety parameters such as effective multiplication factor, neutron flux distributions, temperature coefficients, rod worths, power and breeding distributions.

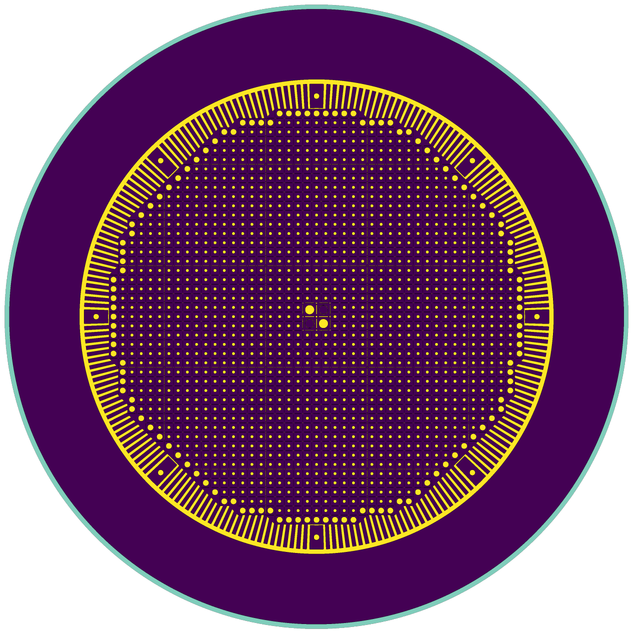
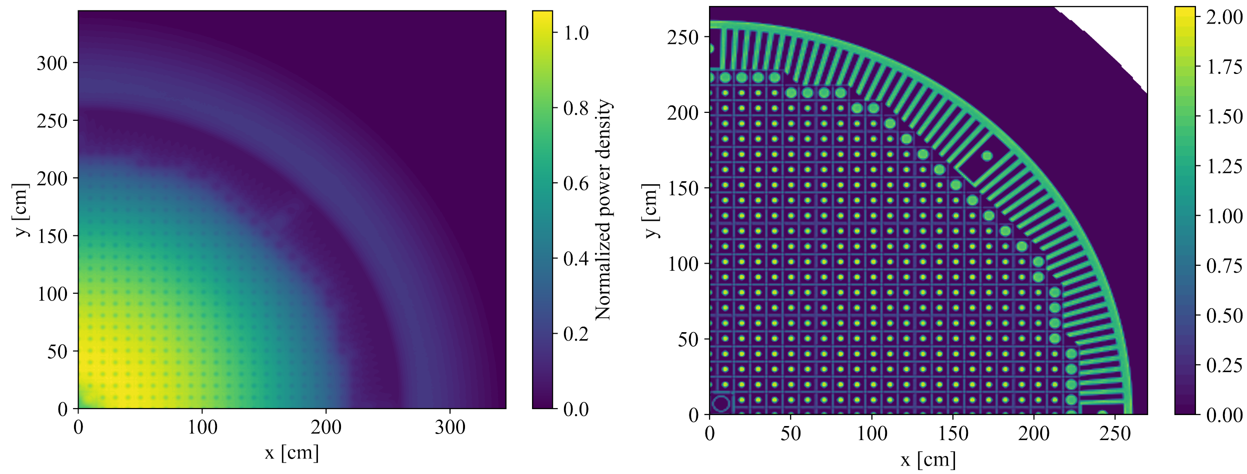


Figure 3: High fidelity monte carlo neutron transport solutions in the Molten Salt Breeder Reactor are at the heart of fuel cycle analysis on Blue Waters. Above, yellow represents the fuel salt, purple represents the graphite moderator, and blue is the outer vessel.



(a) Normalized power density

(b) ^{232}Th neutron capture reaction rate normalized by total flux

4 List of publications associated with this work

4.1 Publications and Products

- A. Lindsay, G. Ridley, A. Rykhlevskii, and K. Huff, "Introduction to Moltres: An application for simulation of Molten Salt Reactors," Annals of Nuclear Energy, vol. 114, pp. 530540, Apr. 2018.

- A. Rykhlevskii, "Advanced online fuel reprocessing simulation for Thorium-fuled Molten Salt Breeder Reactor," Masters thesis, University of Illinois at Urbana-Champaign, Apr. 2018.

- A. Rykhlevskii, J. W. Bae, and K. Huff, "arfc/saltproc: Code for online reprocessing simulation of molten salt reactor with external depletion solver SERPENT," Zenodo, Mar. 2018.

- A. Lindsay and K. Huff, "Moltres: finite element based simulation of molten salt reactors," The Journal of Open Source Software, vol. 3, pp. 12, Jan. 2018.

- Ridley, G., 2017. Multiphysics Analysis of Molten Salt Reactor Transients (Undergraduate Report No. UIUC-ARFC-2017-01), Advanced Reactors and Fuel Cycles Group Report Series. University of Illinois at Urbana-Champaign, Urbana, IL. `https://github.com/arfc/publications/tree/2017-ridley-msrTransients`.

- A. Rykhlevskii, A. Lindsay, and K. D. Huff, "Full-core analysis of thorium-fueled Molten Salt Breeder Reactor using the SERPENT 2 Monte Carlo code," in Transactions of the American Nuclear Society, (Washington, DC, United States), American Nuclear Society, Nov. 2017.

- G. Ridley, A. Lindsay, and K. Huff, "An Introduction to Moltres, an MSR Multiphysics Code," in Transactions of the American Nuclear Society, (Washington D.C.), American Nuclear Society, Oct. 2017.

- G. Ridley, A. Lindsay, M. Turk, and K. Huff, "Multiphysics Analysis of Molten Salt Reactor Transients," Undergraduate Report UIUC-ARFC-2017-01, University of Illinois at Urbana-Champaign, Urbana, IL, Aug. 2017. DOI 10.5281/zenodo.1145437.

- Lindsay, A., Huff, K., Rykhlevskii, A., 2017. arfc/moltres: Initial Moltres release. Zotero. doi:`dx.doi.org/10.5281/zenodo.801823`.

4.2 Highlighted Keynotes

PI Huff gave two keynote talks in 2017. One was to PyCon 2017, with an audience of over 3000 people. The second was at SciPy 2017, with an audience of 700 people. Each keynote mentioned my affiliation with NCSA, my position as a Blue Waters Professor, and the work being conducted on Blue Waters in my group.

- Kathryn Huff, "Academic Open Source" Scientific Python Conference (SciPy2017), Austin, TX. July 12, 2017. Presentation: `http://katyhuff.github.io/2017-07-12-scipy`. Video: `https://www.youtube.com/watch?v=Nqzvnqg4OJ8`.
- Kathryn Huff, "Do it for Science" Python Conference (PyCon2017), Portland, OR, May 20, 2017. Presentation: `http://katyhuff.github.io/2017-05-20-pycon`. Video: `https://www.youtube.com/watch?v=kaGS4YXwciQ`.

4.3 Highlighted Presentations

The work conducted on Blue Waters using Moltres appeared in detail within three presentations during the course of the allocation.

- Andrei Rykhlevskii, "Computational Tools for Molten Salt Reactor Simulation," presented at the Blue Waters Symposium, Sun River, OR. June 4, 2018. Presentation: `http://arfc.github.io/pres/2018-04-07-comp-tools-msr.pdf`
- Kathryn D. Huff, "Modeling and Simulation at Disparate Scales: Molten Salt Reactor Physics and International Fuel Cycle Transitions," presented at the NERS Colloquium, Ann Arbor, MI. February 16, 2018. Presentation: `https://katyhuff.github.io/2018-02-16-ners`
- Alexander Lindsay and Kathryn Huff, "Moltres: a MOOSE Application for Simulation of MSRs." Workshop on Multi-physics Modeling and Simulation of Molten Salt Reactors, Berkeley, CA.June 15, 2017. Presentation: `arfc.npre.illinois.edu/img/pres/2017-06-15-msr-pres.pdf`.
- Kathryn Huff, "Modeling and Simulation of Advanced Reactors and Fuel Cycles," Invited Seminar, UC Davis Mechanical and Aerospace Engineering Seminar, Davis, CA. April 20, 2017. Presentation: `http://katyhuff.github.io/2017-04-20-davis`. Video: `https://www.youtube.com/watch?v=YqTxZC1i-B0#t=6m28s`
- Kathryn Huff, "Advanced Nuclear Reactors and Fuel Cycles: Simulation of Multiple Physics at Disparate Scales" Computational Science and Engineering Seminar Series, 1030 National Center for Supercomputing Applications, Urbana, IL. February 2, 2017. Presentation: `http://katyhuff.github.io/2017-02-02-cse`. Video: `https://www.youtube.com/watch?v=fWlUW_CFo3M`.
- Gavin Ridley. "Transient Simulations of Next Generation Nuclear Reactors." Illinois Summer Research Symposium, Session: Improving Big Data Algorithms for Food and Energy Security, Urbana, IL. July 21, 2017 (Awarded Honorable Mention for Outstanding Oral Presentation). `http://www.grad.illinois.edu/sites/default/files/PDFs/ISRS-program-booklet-2017.pdf`

5 Plan for next year

The development of the Moltres software began in September 2016 and has now been demonstrated on hundreds of nodes on Blue Waters. We haved scaled that up to include very (spatially) large reactor core simulations of the Molten Salt Breeder Reactor design and the Transatomic Power reactor. This year we will continue to emphasize transient accident scenarios (Moltres) and fuel salt reprocessing analysis (SaltProc) in both of these reactor designs.

The following updates will continue to support our research productivity this year.

- **Larger Scale Problems** The software we developed in house (moltres) is now capable of 3D simulation and can be used by many students. Accordingly, we expect this portion of our activity to be strong this year.

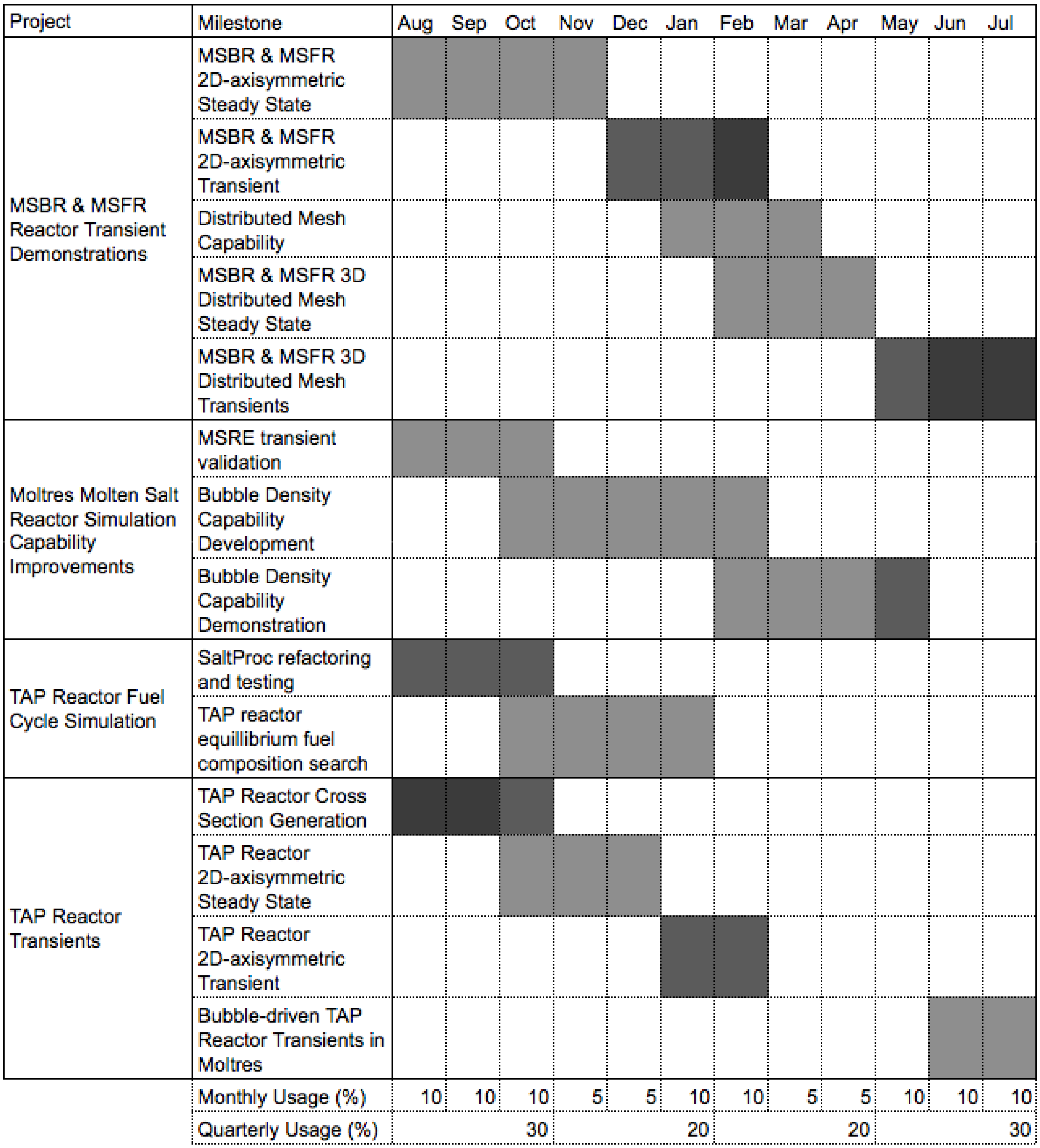


Figure 5: Planned project schedule for molten salt reactor related activities in 2018-2019.

- **Monte-Carlo Cross-Section Generation** The ARFC group began working with monte-carlo software for cross section generation last year. The Serpent 2 software is fully parallelizable, very memory intensive, and produces very high fidelity results. We will continue this activity in 2018-2019 and the computational intensity of our work will remain stable.
- **Group Size** The number of graduate students in the Advanced Reactors and Fuel Cycles group rose to 7 in 2017 and will remain approximately this size through 2019..
- **Expansion into Agent Based Modeling** The scope of the work within ARFC will continue to include some capacity computing work. While this is not the bulk of ARFC work, we have a project in statistical optimization methods for agent based modeling (the Cyclus application [10]) that benefits from a few hundreds or thousands of independent single-node runs.

System nodes needed per run: 20 - 5,000. Many simulations will be run on 100-200 nodes, while a few much larger simulations will be run on 5,000 nodes. While it is possible, it is unlikely that we will run larger runs this year.

Anticipated memory usage: Unknown.

Expected numerical operations: Unknown.

Expected local and remote memory accesses: Unknown.

Total Node Hours: Approximately 100,000 node hours.

Anticipated data transfer: Data transfer will be in the "few gigabytes" per run for most runs. Large runs may be in the "tens of gigabytes."

5.1 Usage Schedule:

See Figure 5.

References

[1] A. Lindsay, G. Ridley, A. Rykhlevskii, and K. Huff, "Introduction to Moltres: An application for simulation of Molten Salt Reactors," *Annals of Nuclear Energy*, vol. 114, pp. 530–540, Apr. 2018.

[2] A. Lindsay and K. Huff, "Moltres: finite element based simulation of molten salt reactors," *The Journal of Open Source Software*, vol. 3, pp. 1–2, Jan. 2018.

[3] G. Ridley, A. Lindsay, and K. Huff, "An Introduction to Moltres, an MSR Multiphysics Code," in *Transactions of the American Nuclear Society*, (Washington D.C.), American Nuclear Society, Oct. 2017.

[4] G. Ridley, A. Lindsay, M. Turk, and K. Huff, "Multiphysics Analysis of Molten Salt Reactor Transients," Undergraduate Report UIUC-ARFC-2017-01, University of Illinois at Urbana-Champaign, Urbana, IL, Aug. 2017. DOI 10.5281/zenodo.1145437.

[5] A. Rykhlevskii, A. Lindsay, and K. D. Huff, "Full-core analysis of thorium-fueled Molten Salt Breeder Reactor using the SERPENT 2 Monte Carlo code," in *Transactions of the American Nuclear Society*, (Washington, DC, United States), American Nuclear Society, Nov. 2017.

[6] A. Rykhlevskii, J. W. Bae, and K. Huff, "arfc/saltproc: Code for online reprocessing simulation of molten salt reactor with external depletion solver SERPENT," *Zenodo*, Mar. 2018.

[7] A. Rykhlevskii, "Advanced online fuel reprocessing simulation for Thorium-fuled Molten Salt Breeder Reactor," Master's thesis, University of Illinois at Urbana-Champaign, Apr. 2018.

[8] A. Lindsay, K. Huff, and A. Rykhlevskii, "arfc/moltres: Initial Moltres release," *Zenodo*, June 2017.

[9] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie, "MOOSE: A parallel computational framework for coupled systems of nonlinear equations," *Nuclear Engineering and Design*, vol. 239, pp. 1768–1778, Oct. 2009.

[10] K. D. Huff, M. J. Gidden, R. W. Carlsen, R. R. Flanagan, M. B. McGarry, A. C. Opotowsky, E. A. Schneider, A. M. Scopatz, and P. P. H. Wilson, "Fundamental concepts in the Cyclus nuclear fuel cycle simulation framework," *Advances in Engineering Software*, vol. 94, pp. 46–59, Apr. 2016.