Neural Network Applications Toward Accelerated Neutral Particle Transport Solutions

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Introduction and Motivation

- Solving the transport equation is necessary for complex non-proliferation problems, but can be very computationally costly.
- Solutions can be obtained more quickly using neural networks (NNs).
- Two methods are presented:
  - a fast but low accuracy NN model of the transport operator in the transport equation
  - a slower but more accurate method where a NN classifies the problem type to select the appropriate variance reduction techniques to accelerate the Monte Carlo simulation of the system

Mission Relevance

- The fast simulation of radiation would be useful for a variety of nuclear security problems.
- For example, when testing for the isotopic contents of a container using radiation detectors, simulations of the system will need to be performed quickly to test many different materials and match the measured radiation spectrum.

Expected Impact

- If this project is successful, the simulation time of radiation transport problems will be drastically reduced, which will speed up the time to analyze systems in a wide range of areas including source characterization.

MTV Impact

- MTV supports the development of the Hammer transport framework, which has been used as the platform for this research. Working with Hammer has given me experience with computation and particle transport methods.
- MTV provides funding for the high-performance computing resources necessary for efficient training of the neural networks.

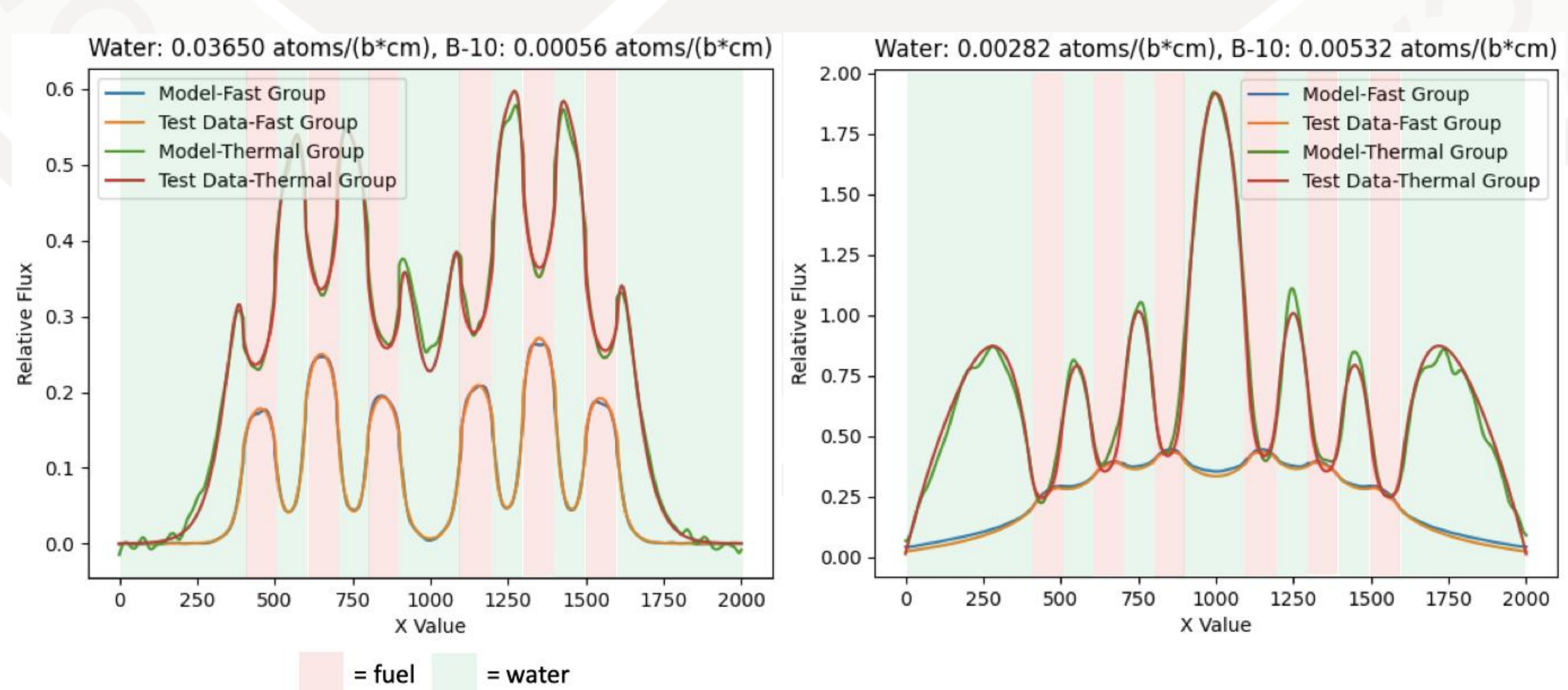
Technical Approach

- The fast approach: a NN is used to approximate the transport operator in the transport equation to rapidly obtain a solution given an input problem specification without solving the problem using conventional techniques.
  - The training is done using the PyTorch library with a framework from a method called the Fourier Neural Operator (FNO). [1]
  - The 1-D training data is converted to Fourier space to model the wave-like nature of the flux distribution and allow the model to be valid for any mesh size.
- The accurate approach: a NN is used to classify transport problems, so that the most effective variance reduction techniques that should be employed within a Monte Carlo transport code can be identified. The NN classifies based on the scalar contribution output from a discrete ordinates (S_n) solution. These are implemented using the Tensorflow library and trained using the S_n solver of the Hammer particle transport code. [2]

Results

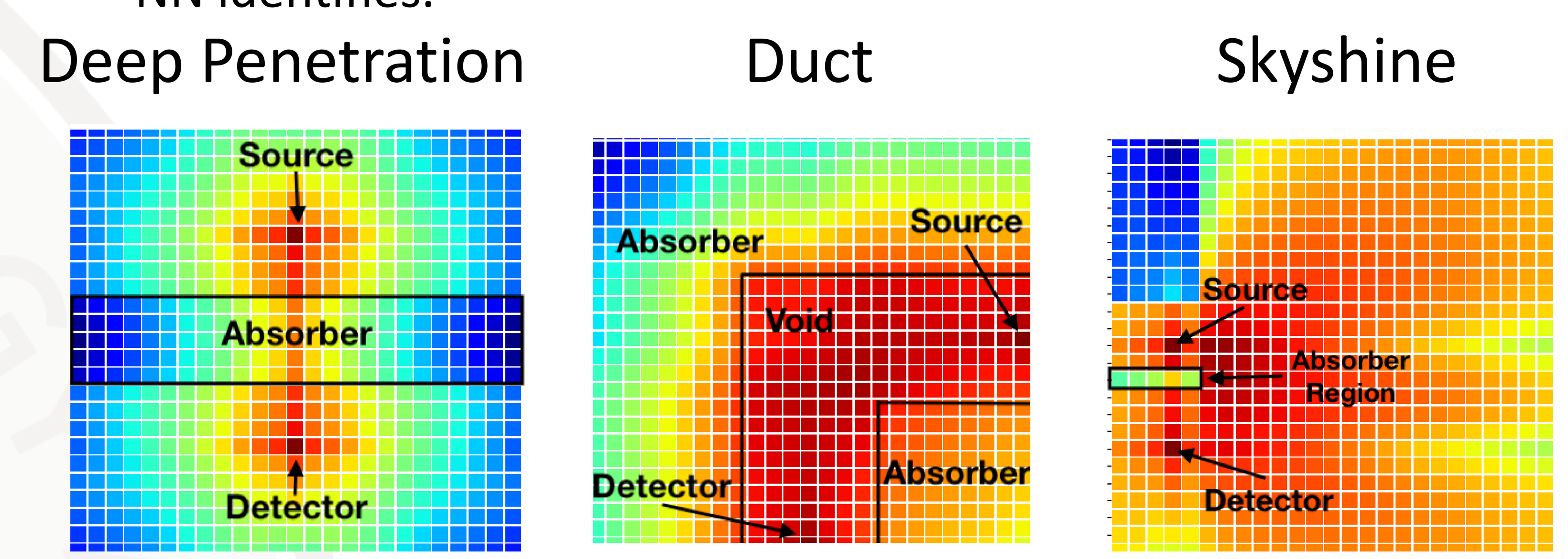
The Fast Approach

- The Fourier neural operator is able to model the steady-state flux of a 1-D reactor design with reasonable accuracy.
- The only variables on which the NN trained are the concentration of boron and water in different regions, which are a proxy for modifying absorption and scattering cross sections. Examples of the the model's prediction of the flux distributions from two sets of water and boron number density inputs are shown below.



The Accurate Approach

- The model can correctly classify basic S_n models into either a deep penetration, duct, or skyshine class with very high accuracy. The scalar contributon heatmap is shown below for example problems in each of the three classes that the NN identifies.



Conclusion

- The preliminary results show that the application of neural networks to the solution of the transport equation in these two ways has potential. But, there is still significant work needed to determine whether this will be applicable to larger, real-world problems.

Next Steps

- Expand the complexity and dimensionality of both approaches and determine how accuracy and simulation time are affected by this

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References

[1] Li, Zongyi, et al. "Fourier neural operator for parametric partial differential equations." *arXiv preprint arXiv:2010.08895* (2020).

[2] E.S. Gonzalez et al. "Hammer: An Educational and Research Platform for Neutral Particle Transport Code Development," *Trans. Am. Nucl. Soc.* **121**, 245-248 (2019).

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