SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Thomas King
FACULTY ADVISOR:	Dr. Ryan McClarren
PROJECT PERIOD:	Fall 2023
PROJECT TITLE:	Developing Metadata for Nuclear Fusion Models
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	**( ) Energy Conversion and Efficiency** **(X) Sustainable and Secure Nuclear** **( ) Smart Storage and Distribution** **( ) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels** **( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Determine Scope of Data	With focus on large quantities, further exploratory progress could be made	100%
Produce Data	~1GB of data produced with varying methods and initial conditons	100%
Develop Description	Information is gathered and will be made available on IAEA Blog	50%
Develop Machine Learning	A unique, physics based, loss function, and several models were developed.	95%

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	N/A
EXTERNAL AWARDS RECEIVED	N/A
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	N/A
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	N/A
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	N/A
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	N/A
INTERNAL COLLABORATIONS FOSTERED	N/A
EXTERNAL COLLABORATIONS FOSTERED	N/A
WEBSITE(S) FEATURING RESEARCH PROJECT	Pending
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	N/A

RESEARCH EXPERIENCE

Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

My experience provided invaluable insight into the world of research and enabled me to develop skills outside of the typical curriculum. Both my faculty advisor, Dr. McClarren, and graduate student I worked closely with throughout the project, Bill Bennet, were more than helpful throughout the process. The both of them instructed me on the basics of the models I was using to produce data and taught me some of the physics behind the problems while also directing my progress, ensuring smooth sailing. An overall very positive experience.

FINAL WRITTEN REPORT

(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

Machine learning is becoming an integral part of technology development. With fusion energy research, the use of machine learning tools is hampered by the lack of publicly available data that adhere to the FAIR data principles (https://www.go-fair.org/fair-principles/). This work in collaboration with Prof. McClarren, an affiliate of ND Energy, and the International Atomic Energy Agency (IAEA) is to build an example database of simulations of inertial confinement fusion experiments.

The first goal of the project was to determine the scope of data to produce, such that the existing methods capabilities developed at ND could render increased global impact. The primary set of methods considered in this project were a series of semi-analytic equations for the isotropic particle transport equation. These equations vary in terms of source, initial conditions, and dimensions – with a number of methods requiring significantly larger computation times. Given the extremely large amounts of data required for most machine learning applications, and the limited duration of the project, a computationally fast method was chosen.

For this method, the time at which the equation would be solved to, the number of points, and the scattering ratio (a physical parameter with regard to atomic collisions) were variable. In order to develop ideal data for machine learning uses, Latin hypercube sampling was employed. This allows the user to produce a near random distribution of parameters while ensuring coverage of the full domain.

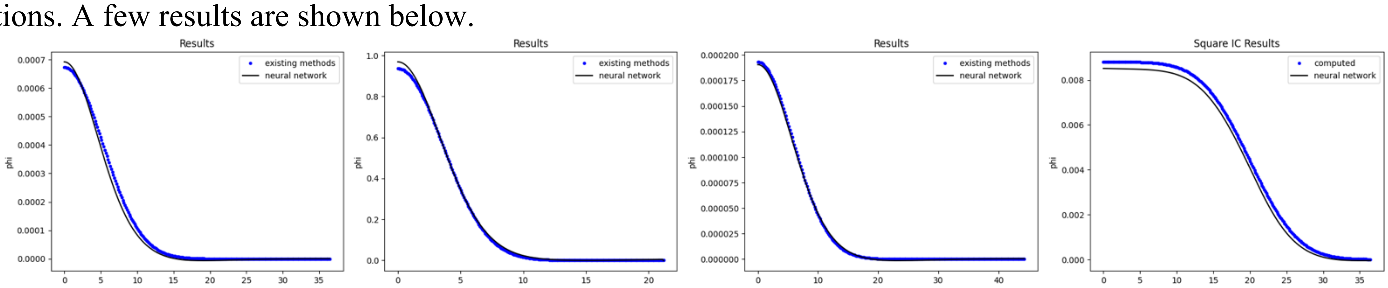
Upon modifying the methods to produce data in user-friendly files according to FAIR data principles, a tensor-flow neural network was developed as a use-case example of machine learning applications. Interestingly, the neural network model faced significant difficulties in fitting the metadata, and moreover in addressing cases that were slightly beyond or "in the gaps" of the data that the model was trained upon. As such, several strategies were applied to the model in attempts to improve accuracy.

By taking advantage of known physical constrains of the isotropic particle transport equations, a customized loss function was developed that drastically improved the fidelity of the model to the physical laws it describes. In addition to the standard mean squared error in which the machine learning model used to improve upon itself in iterative fashion, the function also considered the conservation of energy and momentum in the system and punished results that produced negative values.

```
loss = tf.cond(tf.math.less(tf.math.reduce_min(y_pred), 0), lambda: float(10**3) * tf.square(y_true - y_pred), lambda:
(0.1) * tf.square(tf.math.reduce_sum(y_pred) - tf.math.reduce_sum(y_true)) + 0.89*tf.square(y_true - y_pred) +
0.01*(tf.square(tf.math.multiply(xvals**2,y_pred) - tf.math.multiply(xvals**2,y_true))))
```

Eq (1) Loss function for neural network model utilizing physical constraints of isotropic particle transport.

The weights of the function proved to be highly sensitive to model success. In addition, stochastic gradient descent was employed in order to optimize the learning rates for speed of training models. Ultimately, these strategies enabled several models to achieve acceptable levels of accuracy, even for parameters outside of the scope the models training. Furthermore, machine learning produced data was proved to be integrable to obtain results for different source functions. A few results are shown below.



Figures: Several results of neural network produced data in comparison with the methods the models were trained on. The right most figure provides an example of the leftmost figure, produced from a plane source, integrated to a square source.