2023-2024 Grand Challenge Award Final Report

Awardee: **Stella Offner, Associate Professor, Astronomy**

Research Award Title: **Predicting Star Formation: Past and Future**

Overview

The Moncrief Grand Challenge funding supported a scientific machine learning study, carried out by Prof. Stella Offner, Prof. Rachel Ward, and graduate student Keith Poletti, applying different types of neural operators (NOs) to model 3D astrophysical data. This work, submitted to the American Journal of Mathematical Science (AIMS), lays the groundwork for future studies predicting direct astronomical observables. Five invited presentations were delivered on the results.

Research Results

Despite recent advances in neural operators (NOs), no studies to date have attempted to predict the temporal evolution of astrophysical systems. Accurately inferring the evolution of these systems is particularly challenging due to their long dynamical timescales and the incompleteness of the physical data. Our work investigated whether Fourier Neural Operators (FNOs) could accurately predict the dynamics for self-gravitating and supersonically turbulent astrophysical conditions.

We tested three FNO architectures: FNO-3D, which convolves across two spatial dimensions and one time dimension; autoregressive FNO-2D, which recurrently trains on the time dimension; and a U-shaped Fourier Neural Operator (UNO), which is a memory efficient alternative to the FNO-3D. We also compared to the performance of these NOs to that of a standard UNet architecture (Figure 1). We examined three cases with varying levels of missing information. In the first case modeling spherically symmetric gravitational collapse, we found the FNO trained on projected data accurately predicted the evolution over a large dynamic range. This is crucial for astrophysical problems, which are characterized by scales spanning many orders of magnitude. We further tested the FNO prediction accuracy on fully 3D supersonic, turbulent simulations without spherical symmetry. These more complex dynamics required substantially more data to train. The FNOs and UNOs performed well, achieving NRMSE of 0.01 even when the full 6D position and velocity phase space was limited to three dimensions. However, the FNOs struggled to capture small-scale structures. When reapplying the trained models to their outputs, the predictions quickly became unstable and performance deteriorated significantly. Finally, we showed that the FNOs do not require complete information about all the physical quantities that dictate the evolution of turbulent plasmas. The FNOs performed comparably in predicting the evolution of magnetized plasmas, even when no magnetic field information was included in the training. The FNO-3D architecture exhibited the best performance overall; however, our investigation showed that more training data and additional architecture adaptations are needed to reach accuracies better than a few percent for predictions over long evolutionary timescales.

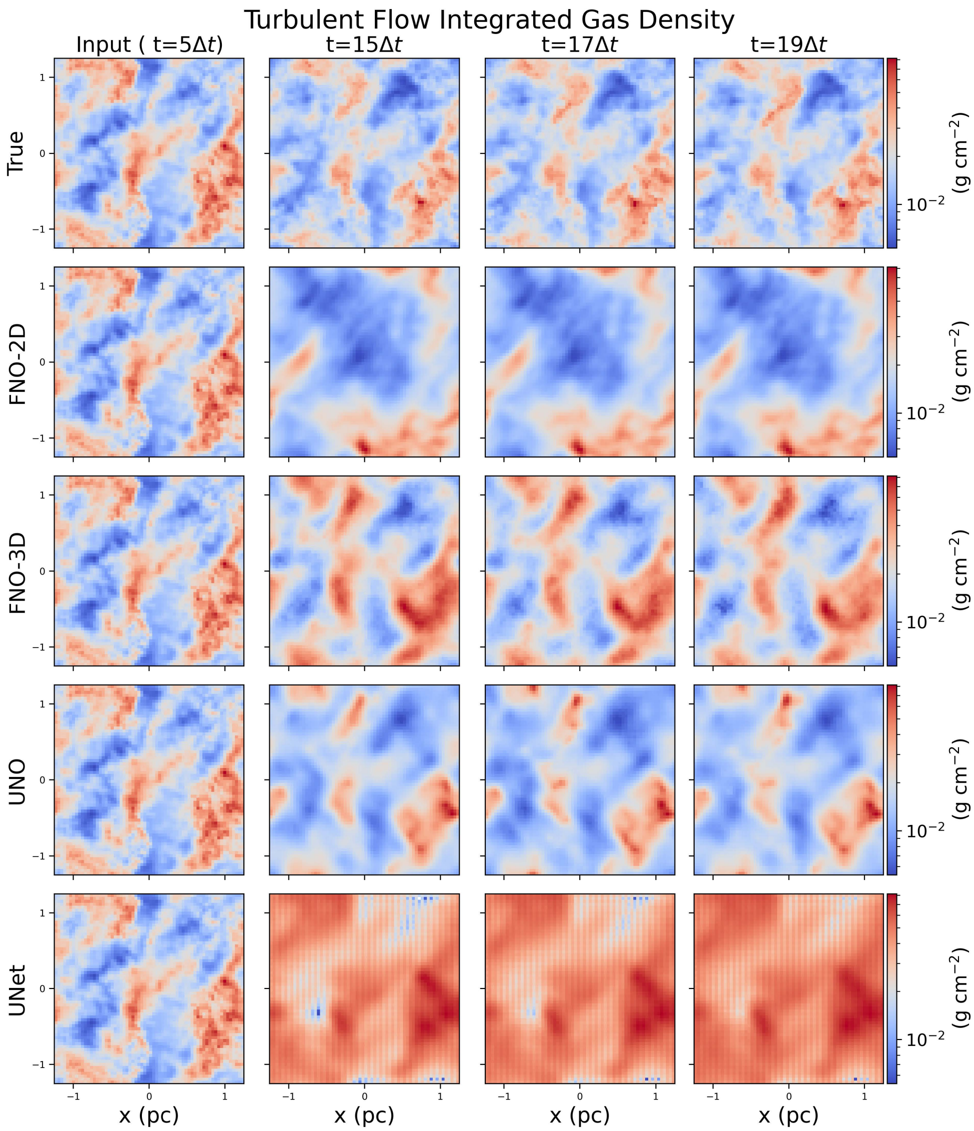

Fig. 1: . Temporal evolution from left to right of the integrated density ("column density") of a simulation of hydrodynamic turbulence. The FNO-3D achieves the best performance.

Presentations

The above research results were presented in the following talks:

1. Scientific Understanding through Data Science Conference, Pasadena, CA, Aug 2024 (planned). Speaker: Keith Poletti

2. Early Phases of Star Formation, Ringberg, Germany, May 2024. Speaker: Stella Offner (invited)

3. AI in Astronomy, Cooks Branch TX, Apr 2024. Speaker: Stella Offner (invited)
4. Great Lecture, Board of Visitors Meeting, Austin, Feb 2024. Speaker: Stella Offner (invited)
5. Astronomy / NRAO Colloquium, University of Virginia, Oct 2023. Speaker: Stella Offner (invited)

General presentations on scientific machine learning:

1. Symposium on Generative AI, Austin, TX, Apr 2024. Speaker: Stella Offner (invited)
2. Public Outreach Livestream, McDonald Observatory, Mar. 2024. Speaker: Stella Offner (invited)
3. Frontiers of Computer Science and Engineering Panel, Sept. 2023. Speaker: Stella Offner (invited)

Outcomes and Benefits

The proposed project produced the following research products:

1. An extensive training set of simulation data modeling gravitational collapse.
2. An extensive training set of simulation data modeling 3D hydrodynamic and magnetohydrodynamic turbulence.
3. A framework for making time-series predictions for the above data, including a comparison of four ML architectures.
4. An article submitted to AIMS titled "Modeling Turbulent and Self-Gravitating Fluids with Fourier Neural Operators" (under review)
5. CSEM graduate student, Keith Poletti, was trained in statistical and astronomical research methods.

The teaching release enabled by this award allowed PI Offner to write and submit a successful proposal to the NSF for a new NSF-Simons AI Institute focused on astronomy grand challenge problems. The grant will begin October 2024.

Awards and Honors

1. Best Paper, 15th International Workshop in Advances in Self-Organizing Maps, Learning Vector Quantization, Interpretable Machine Learning, and Beyond, 2024
2. Peter O'Donnell Distinguished Researcher Award, Oden Institute, May 2024
3. Plenary Lecture, American Astronomical Society winter meeting, Jan 2025

Future Work

Future work will generate a training set of synthetic data with the same characteristics and noise as actual observations. This will allow us to validate our approach in the target parameter space. Ultimately, we aim to apply our trained NOs to observational radio maps of the Taurus and Orion molecular clouds to predict their past and future evolution.