Topological Machine Learning for Predicting Spatiotemporal Evolution in 1D Magnetohydrodynamics

Gabriel Wendelll Celestino Rocha[1*], Gandhimohan Madras Viswanathan[1],
[1]Dept. of Physics, Universidade Federal do Rio Grande do Norte
[*]Corresponding author: gabrielwendell@fisica.ufrn.br

Introduction

Brio–Wu MHD Shock Tube

- The Brio–Wu shock tube is a 1D Riemann problem in ideal magnetohydrodynamics consisting of a discontinuity separating two constant states. Its evolution generates a rich wave structure—including fast and slow shocks, rarefaction fans, and a contact discontinuity—making it a challenging benchmark for data-driven prediction.

Why Topological Data Analysis

- Traditional numerical error metrics (MSE, RMSE) provide limited information about structural correctness. Persistent homology captures the shape of data across scales, identifying features such as the number of connected components (β_0) and loops (β_1). By applying TDA to spatial profiles through **Takens delay embeddings**, we obtain a robust multiscale descriptor of the evolving wave morphology—allowing us to detect when ML surrogates violate the physical structure of the solution.

Objectives

- Characterize the ground-truth MHD dynamics via persistent homology.
- Train a baseline 1D CNN to perform next-step temporal prediction of density and pressure fields.
- Analyze how well the CNN preserves the topological structure of the true evolution.
- Identify failure signatures (e.g., artificial oscillations, topology collapse, incorrect wave speeds) using Betti curves and persistence diagrams.

Methodology

1. Simulation Data

- 1D ideal MHD Brio–Wu shock tube.
- 41 snapshots from $t = 0$ to $t = 2$ with $\Delta t = 0.05$.
- Spatial grid: $N_x = 1000$.
- Fields used: density and pressure.

2. Spatial Takens Embedding

- For each time t_k, a spatial signal $f(x)$ is mapped to

$$\Phi_{m,\tau}(x_i) = \left[f(x_i), f(x_{i+\tau}), \ldots, f\left(x_{i+(m-1)\tau}\right)\right].$$

- We use $m = 4$, $\tau = 2$, and stride $= 2$.

3. Persistent Homology & Betti Curves

- Vietoris–Rips filtration applied to the embedded point cloud.
- Betti numbers $\beta_0(\varepsilon)$, $\beta_1(\varepsilon)$ computed over scales $\varepsilon \in [0, 6]$.
- Time-resolved Betti heatmaps provide $\beta_0(\varepsilon, t)$ and $]\beta_1(\varepsilon, t)$.

CNN Temporal Predictor

- **Input:** concatenated normalized $\rho(t_k)$ and $p(t_k)$, shape $(2, N_x)$.
- **Network:** 1D CNN with three convolutional layers (kernel size 5).
- Trained on 40 input–target pairs.
- Multi-step rollout: predictions fed recursively into the model.

Normalization

We'll use global z-score normalization per variable: For each scalar field $f \in \{\rho, p\}$

$$\mu_f = \frac{1}{N_t N_x} \sum_{k=0}^{N_t-1} \sum_{i=0}^{N_x-1} f_k(i),$$

$$\sigma_f^2 = \frac{1}{N_t N_x} \sum_{k,i} \left[f_k(i) - \mu_f\right]^2,$$

$$\tilde{f}_k(i) = \frac{f_k(i) - \mu_f}{\sigma_f}.$$

Input

$$X_k(x) = \begin{pmatrix} \tilde{\rho}(t_k, x) \\ \tilde{p}(t_k, x) \end{pmatrix} \in R^{2\times N_x},$$

Target

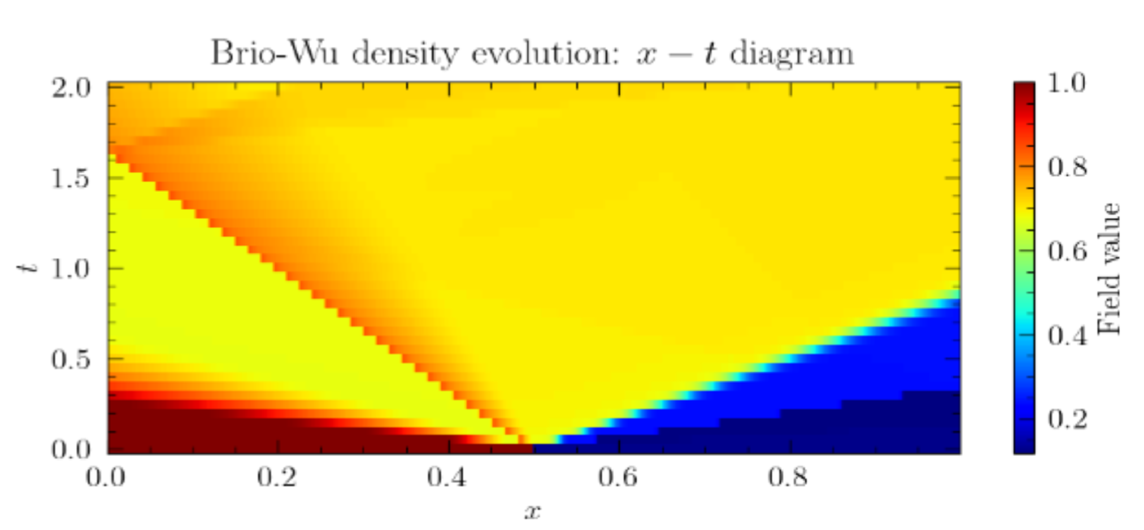
$$Y_k(x) = \begin{pmatrix} \tilde{\rho}(t_{k+1}, x) \\ \tilde{p}(t_{k+1}, x) \end{pmatrix}.$$

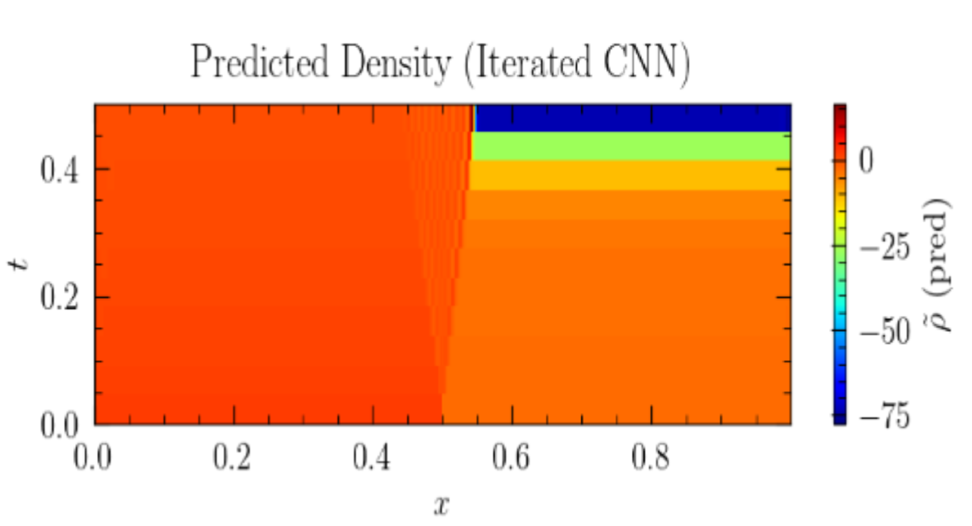
Stacking all pairs, we get tensors:

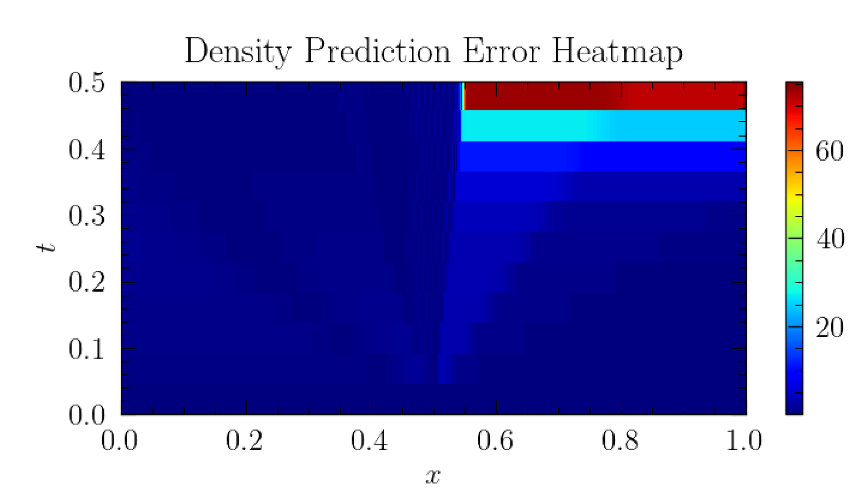
$$\mathbf{X} \in R^{(N_t-1)\times 2\times N_x}, \quad \mathbf{Y} \in R^{(N_t-1)\times 2\times N_x}.$$

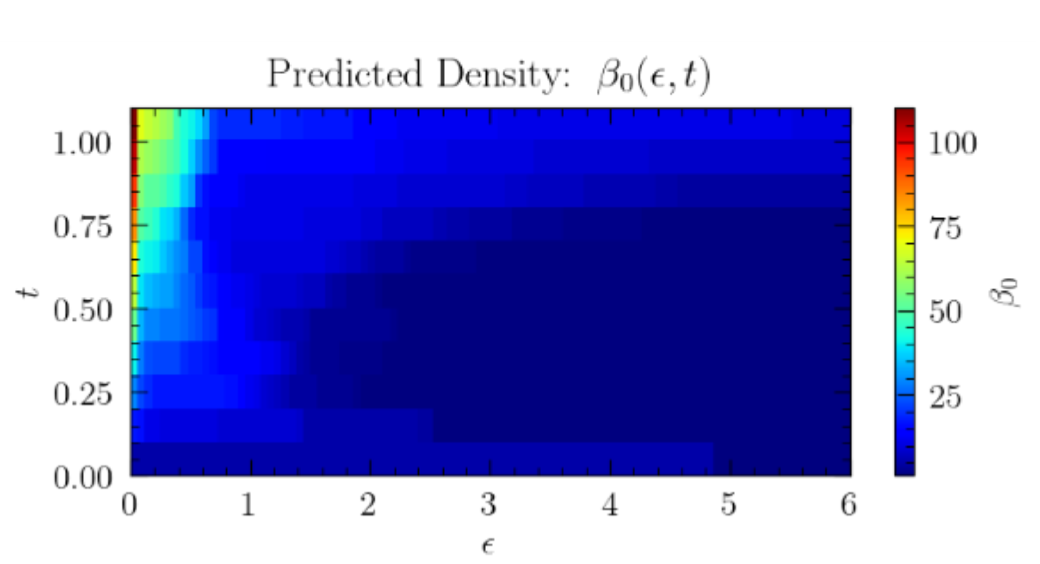
- Inputs to the neural network are approximately zero-mean and unit-variance, which stabilizes optimization.
- TDA is invariant under translation and scale in many constructions, but using normalized fields helps when we later compare different variables or experiments.

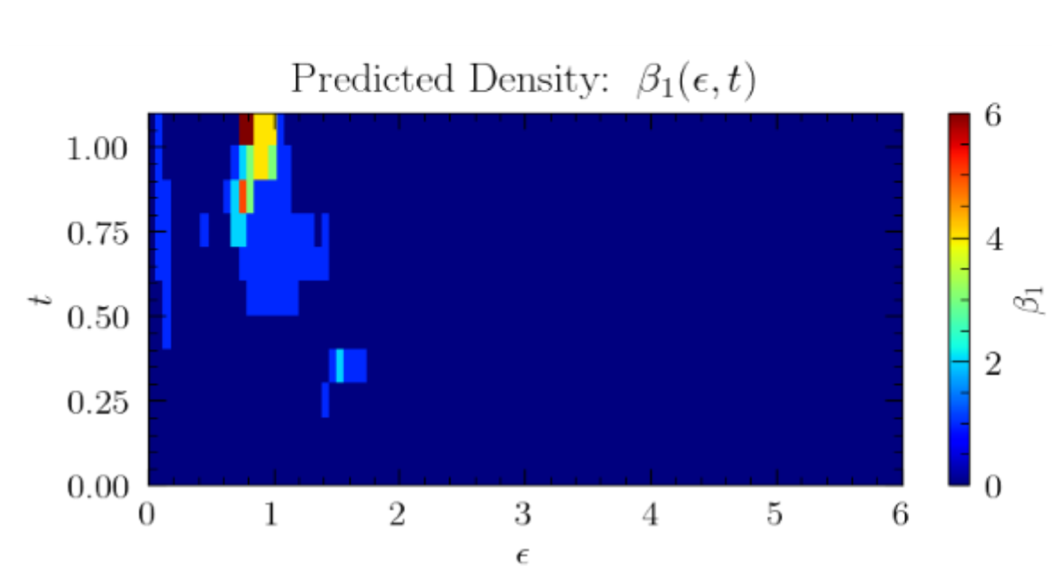
Results & Analyses

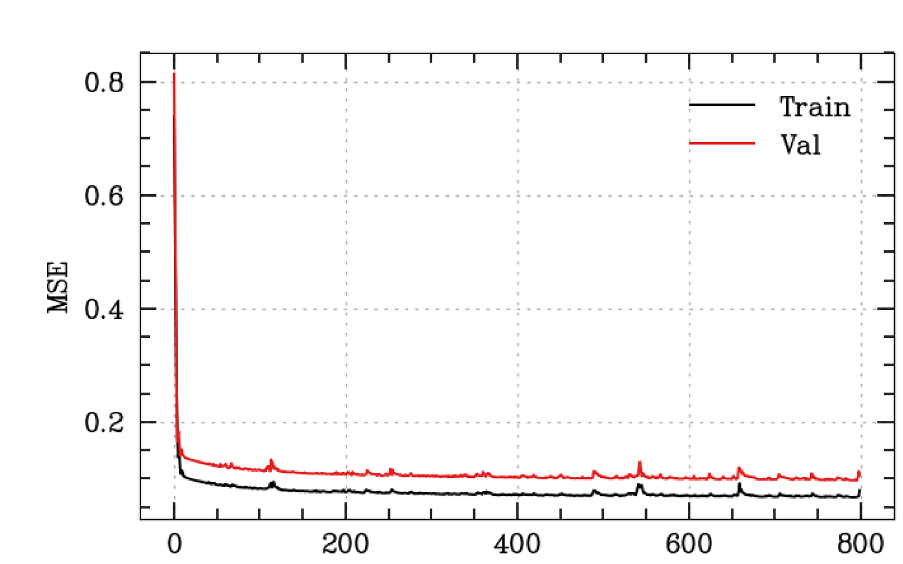












Summary

- The Brio–Wu shock tube provides a stringent test for ML surrogates due to its discontinuities and nonlinear wave interactions.
- A simple CNN baseline fails to reproduce key dynamical and structural features under multi-step forecasting.
- Topological Data Analysis effectively exposes failure mechanisms, including shock smearing, incorrect propagation, and spurious oscillations.
- TDA offers a robust, physics-informed diagnostic framework for evaluating ML models in scientific computing, beyond traditional pointwise metrics.

QR Code