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Fourier Neural Operator Surrogate Modelling of Lattice-Boltzmann Simulations

[1]A. Junk*; [1]J. M. Winter; [1]S. Schmidt; [1]N. A. Adams;

[1]*Chair of Aerodynamics and Fluid Mechanics, School of Engineering and Design, Technical University of Munich (TUM), Germany*

Abstract

Understanding complex flow dynamics with extensive parameter spaces requires efficient sampling methods. Fourier Neural Operator (FNO)-based surrogates offer a promising solution, yet their performance depends heavily on the choice of hyperparameters. This study systematically examines the impact of hyperparameters on FNO-based surrogate models for lattice Boltzmann simulations of the 2D Kármán vortex street and analyzes their temporal prediction capabilities for up to 120 recursive uses, which equal more than four vortex shedding periods. The study relies on datasets created with an in-house lattice-Boltzmann solver, that contain the flow field information of the Kármán vortex street for various resolution levels at a Reynolds number of 150. The models are trained on single and mixed resolution datasets and validated on both lower and higher resolution data, introducing additional validation parameters such as the Mean Squared Error (MSE) and the Pearson Correlation Coefficient (PCC) of the circulation of the velocity field. A detailed hyperparameter study on the impact of the FNO architecture on the models' long term prediction capabilities is conducted, demonstrating the vast potential for optimization of FNOs via hyperparameter tuning. Additionally, the impact of a mixed-resolution training dataset compared to a single-resolution dataset is investigated on both low and high resolution inference data, showing the potential of optimizing the FNOs zero-shot super-resolution capabilities for up to 40 recursive predictions.

Keywords: Fourier Neural Operator; Surrogate Modelling; Lattice Boltzmann Method

Introduction

Fluid mechanical problems, such as multiphase flows, have historically been computationally expensive and require sophisticated numerical methods. Their simulation involves a trade-off between coarse grids for faster computation and fine grids for more accurate but slower solutions. Many complex flows, however, necessitate fine grids to achieve physically accurate results. Consequently, accelerating numerical solvers through data-driven machine learning models offers an opportunity to deliver precise solutions without high computational costs, while simultaneously increasing the potential to accurately sample complex parameter spaces of complex flows. [1-6]

While classical neural networks are often limited to resolution-bound solutions, mesh-invariant neural operators (NOs) enable a promising approach to tackling fine-grid complex fluid mechanical problems. Mesh-invariance allows NOs to be trained on lower-resolution grids and subsequently applied to higher-resolution problems, thus offering flexibility and efficiency. This property stems from the NOs ability to map between function spaces, effectively reconstructing the solution operator for the underlying partial differential equations (PDEs). NOs can deliver solutions orders of magnitude faster than traditional solvers, and outperform classical neural networks, since they can generate solutions for different mesh resolutions through a single forward pass without the need for retraining. However, NOs face challenges related to the computational cost of solving integral operators, which has prevented them from surpassing convolutional and recurrent neural networks in finite-dimensional settings with fixed resolutions. [4,6-12]

This limitation is addressed with the introduction of the Fourier Neural Operator (FNO) with quasi-linear complexity in the Fourier transform and state-of-the-art approximation capabilities by Li et al. [4]. By applying the Fourier transform on the integral operator, convolutions are performed via simple multiplications, significantly reducing the computational burden associated with the integral operators found in classical NOs. This technique, which has long been employed in spectral methods for solving differential equations, represents a major advancement for NOs and has sparked further advancements in the field such as U-FNOs [14]. [4,13]

This study explores the potential of the FNO to act as surrogate for a numerical lattice-Boltzmann method (LBM) solver, with a particular focus on its ability to predict the temporal evolution of the Kármán vortex street over four periods at a Reynolds number of 150, recursively. All FNO models presented are created and trained using the open-source NVIDIA Modulus deep-learning framework [15]. First, an in-house LBM solver is used to generate numerical data of the vortex street at different resolutions. The resulting data is processed into training and inference datasets. A hyperparameter study is then conducted to examine the impact of FNO layer depth and latent channels on the model's

*Corresponding Author, A. Junk alexandra.junk@tum.de

prediction capabilities over 120 recursive uses, corresponding to four full periods of the flow field. The resolution-invariance of the best-performing FNO configurations is investigated on the high-resolution data with additional investigations concerning the impact of mixed-resolution datasets on high-resolution prediction accuracy.

Numerical Method

The single precision data used in this study is created by an in-house LBM simulation framework for the weakly compressible Navier-Stokes Equations (NSE). The LBM has been introduced and refined based on the lattice-gas automaton proposed by Frisch et al. [16] in 1987 and solves the evolution of discrete particle distribution functions. A detailed derivation of the LBM is presented by Krüger et al. [17]. In this study, the resulting 2D density and velocity fields at a Reynolds number of 150 are used for training. Additional information on the LBM solver setup is given in Table A1.

The aim of this study is to investigate the FNOs potential to act as surrogate for the LBM solver, specifically in temporal prediction scenarios. FNOs have been introduced by Li et al. [4] as a mesh-invariant deep learning architecture, that learns mappings between infinite-dimensional function spaces. The general architecture of the FNO is identical to the Neural Operator proposed by Li et al. [6], except for the kernel integral operator that is replaced by a convolution in Fourier Space. This leads to the FNO learning parameters directly in Fourier Space and subsequently to its potential of zero-shot super-resolution predictions [4].

This study employs FNOs as surrogates for the temporal evolution of the velocity components and density flow field of the Kármán vortex street. Each FNO model is trained with an Mean Squared Error (MSE) training loss to predict all of the three mentioned fields simultaneously. We validate the physical accuracy of the prediction using the MSE and Pearson Correlation Coefficient (PCC) on the density and velocity magnitude field $|\bar{v}|$, and the circulation Γ of the flow field. We consider 300 trajectories for four periods of the vortex street to average the validation metrics. A hyperparameter study of the number of FNO Layer (L) and Latent Channels (LC) impact on long term stability is conducted. Additionally, a super-resolution test case with a resolution of 1024x512 as well as the impact of mixed-resolution datasets on the prediction accuracy is investigated. This study employs the FNO implementation provided by the open source NVIDIA Modulus deep-learning framework [15]. The parameters concerning the different training datasets and FNO architectures can be found in Table A2 and Table A3. All FNO hyperparameters not explicitly specified in Table A3 are set to their default values in Modulus.

Results

Figure 1 shows the impact of different FNO hyperparameters on the long term prediction accuracy, starting with inference data of the same resolution as the low resolution training data. All investigated architectures with less than 6 Layers show unstable behaviours for the low resolution test case. While the density is predicted with a near identical MSE by all configurations for more than 6 Layers, slight differences in accuracy can be seen for the velocity magnitude as well as the circulation.

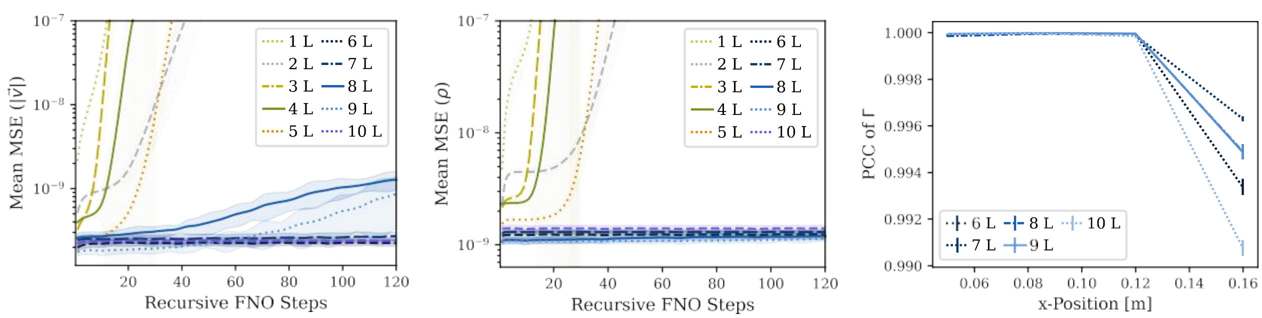

Figure 1 MSE of $|\bar{v}|$ and ρ and PCC of Γ for all 10 FNO architectures with 1-10 L and 14 LCs evaluated on the training resolution data.

Figure 2 shows all stable LC variations. While a clear pattern for the influence of the Layer configuration on stability could be observed in Figure 1, a more random behavior is observed for the variation of Latent Channels in Figure 2. Nevertheless, both hyperparameter variations show the same trend of a slightly higher, yet also more constant, MSE

*Corresponding Author, A. Junk alexandra.junk@tum.de

for the density compared to the velocity field. Similar to the Layer variation, the PCCs of the circulation of the stable LC configurations show a high capability to capture the circulation of the flow at different domain positions, but lose accuracy towards the end of the flow field. This is most likely caused by the circulation decreasing towards the outflow, which causes the FNO to be less capable of capturing the correct individual values and oscillation throughout time. An exemplary visualization of the predicted velocity magnitude field $|\bar{v}|$ for the low resolution case is depicted in Figure 3.

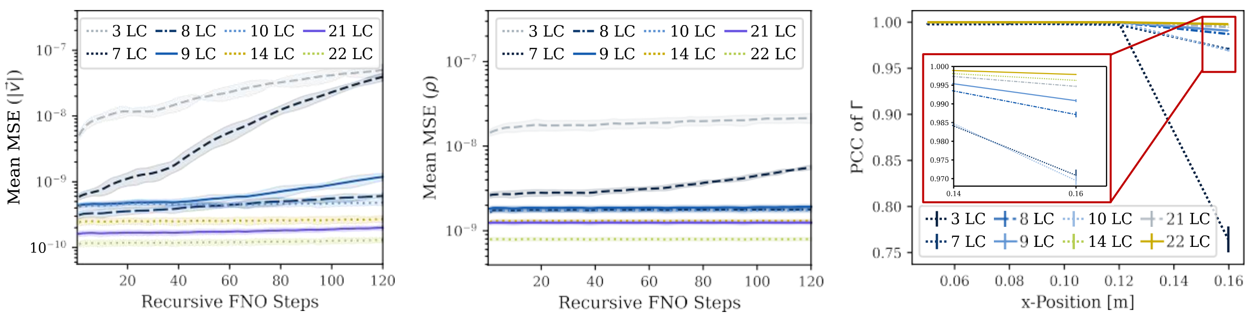

Figure 2 MSE of $|\bar{v}|$ and ρ and PCC of Γ for all stable FNO architectures with 7 L and 2-24 LCs evaluated on training resolution data.

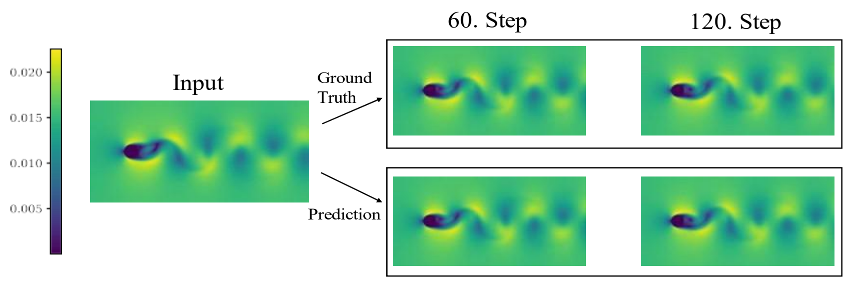

Figure 3 Exemplary low resolution prediction (7L 14LC).

Next, we investigate the zero-shot super-resolution capability and apply the six FNO configurations with the highest PCCs of the circulation to high resolution data. Comparing Figure 4 to Figure 1 and Figure 2 it becomes apparent, that higher resolution predictions from the first FNO use onwards have an increased MSE compared to the predictions on the actual training resolution. This can be caused by structures being more accurately resolved with the high resolution and therefore hard to capture for the FNO trained on low resolution. As visualized by the PCC of $|\bar{v}|$, only the 7L 22LC configuration is able to predict the high resolution vortex street with acceptable accuracy for more than 20 recursive FNO uses, though all depicted architectures are capable of performing an accurate one-step zero-shot super-resolution prediction. The circulation is overall predicted less accurately and only the 7L 22LC model achieves results with a PCC greater than 0.8. An exemplary visualization of a 7L 22LC model prediction is depicted in Figure 5, demonstrating the decreased accuracy compared to Figure 3 with visible artefacts in the flow field, yet capturing an intact vortex street with correct shedding frequency and cylinder positioning.

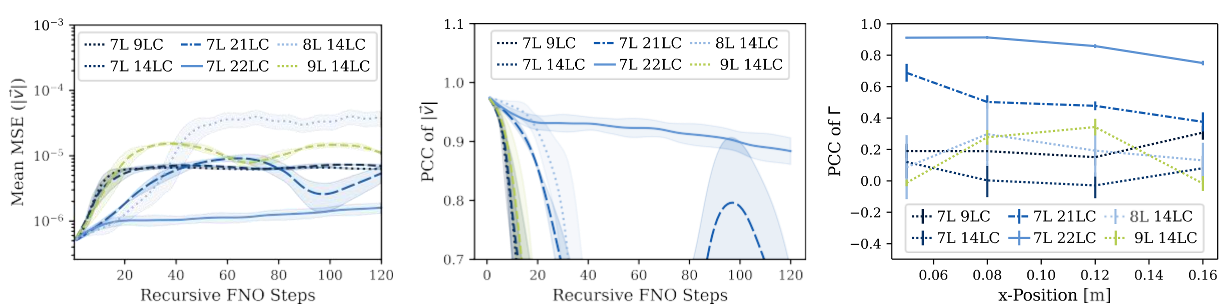

Figure 4 MSE of $|\bar{v}|$, PCC of Γ and $|\bar{v}|$ for all the 6 best performing architectures with 1-10 L and 2-24 LCs evaluated on high resolution data.

*Corresponding Author, A. Junk alexandra.junk@tum.de

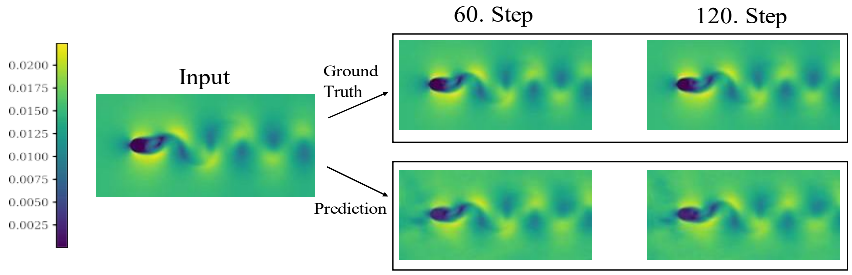

Figure 5 Exemplary high resolution prediction (7L 22LC).

Lastly, the 7L 22LC configuration is trained on several mixed resolution datasets, that combine the low resolution data with 0, 64, 128 and 256 middle resolution samples (M), see Table A2. Again, the trained FNOs are evaluated on the low and high resolution inference data to investigate the potential improvement of the high resolution prediction via dataset fine-tuning. When comparing their low resolution prediction accuracy, see Figure 6, it becomes apparent, that training with mixed resolution data slightly decreases the long-term prediction accuracy of an FNO, however, only the 256M case shows a decidedly unstable behaviour. High resolution predictions, as depicted in Figure 7, on the other hand show slight improvements in accuracy for the first recursive FNO uses, yet all mixed configurations develop unstable behaviours in their long-term stability. Overall, mixed resolution datasets can improve high-resolution predictions, though only for a limited amount of recursive FNO uses.

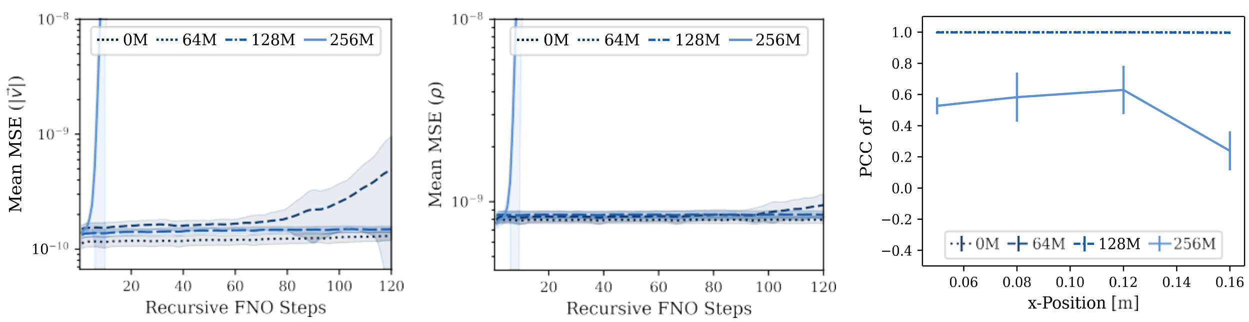

Figure 6 Low resolution predictions of the 7L 22LC trained on Mixed Resolution Datasets with different Middle Resolution Sample Numbers (M).

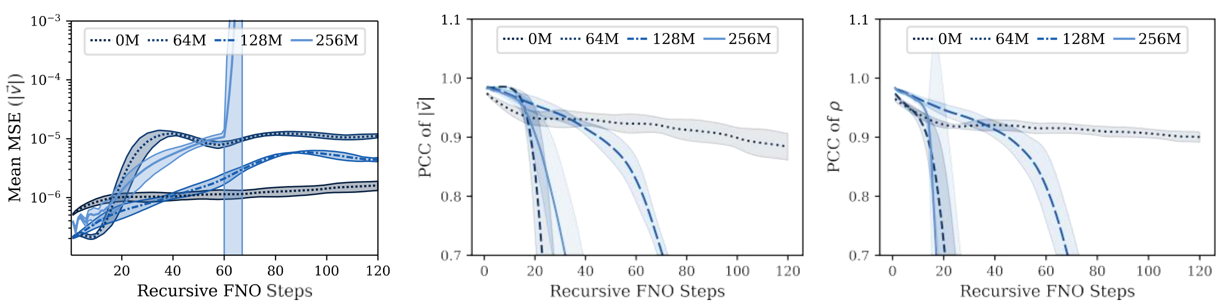

Figure 7 High resolution predictions of the 7L 22LC trained Mixed Resolution Datasets with different Middle Resolution Sample Numbers (M).

Conclusion

The investigation of the temporal prediction capabilities of different FNO architectures has demonstrated a high potential of FNOs to act as surrogate models for LBM simulations. The temporal evolution of a periodic flow field can be captured with sufficient accuracy on training resolution for over 4 periods. Zero-shot super-resolution can be achieved, though requiring advanced hyperparameter tuning and entailing a loss in accuracy if a recursive application of the FNO is intended. Additionally, if high resolution applications are the main objective, mixed resolution datasets can improve the FNOs performance for a limited amount of recursive uses at the cost of decreasing long-term stability.

*Corresponding Author, A. Junk alexandra.junk@tum.de

Appendix

Table A1 LBM Simulation Setup

Boundary Conditions	Physical Parameters	LBM Algorithm
Inlet: Moving Wall	Ma = 0.2	Single Precision
Sides: Zero Gradient	Re = 150	D2Q9
Outlet: Fixed Pressure Outlet		Collision: SRT

Table A2 Single and Mixed Resolution Dataset Parameters

	Training Data (Low Resolution)	Validation Data (Low Resolution)	Training Data (Mixed Resolution)	Validation Data (Mixed Resolution)
Sample Size	640	256	640 low; 0, 64, 128 and 256 middle resolution	256 low resolution
Batch Size	64	64	64	64
Resolution	512x256	512x256	Low: 512x256, Middle: 768x384	Low: 512x256

Table A3 FNO Hyperparameters

Decoder	FNO	Scheduler	Training & Validation
Out Features: 3	In Channels: 3	Initial Learning Rate: 1.e-2	Epochs: 100
Layers: 1	Latent Channels: 2-24	Decay Rate: 0.85	Validation Frequency: 8th epoch
Layer Size: 32	Layers: 1-10	Decay Frequency: 8th epoch	
	Fourier Modes: 32	Type: LambdaLR	
	Padding: 9	Optimizer: Adam	

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*Corresponding Author, A. Junk alexandra.junk@tum.de

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*Corresponding Author, A. Junk alexandra.junk@tum.de