
Wavelet-Powered Neural Networks for Turbulence

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Abstract

Modeling fluid turbulence and explaining its associated spatio-temporal phenomena are notoriously difficult tasks. Navier-Stokes (NS) equations describe all the details of the fluid motions, but require accounting for unfeasibly many degrees of freedom in the regime of developed turbulence. Model reduction is a general methodology aiming to circumvent the curse of dimensionality. Originally driven by phenomenological considerations, multiple attempts to model-reduce NS equations got a new boost recently with development of Neural Networks (NNs), especially of the Deep Learning (DL) type, trained on the ground truth data, e.g. extracted from high-fidelity Direct Numerical Simulations (DNS). However, early attempts of building NNs to model turbulence has also revealed its lack of interpretability as the most significant shortcoming. In this paper we address the key challenge of devising reduced but, at least partially, interpretable model. We take advantage of the balance between strong mathematical foundations and the physical interpretability of wavelet theory to build a spatio-temporally reduced dynamical map which fuses wavelet based spatial decomposition with spatio-temporal modeling based on Convolutional Long Short Term Memory (C-LSTM) architecture. It is shown that the wavelet-based NN makes progress in scaling to large flows, by reducing computational costs and GPU memory requirements.

1 Challenge of Learning Spatio-temporal Physics

Multitude of research problems in physical and natural sciences are exceptionally complex to study and model with existing analysis tools because of their high-dimensionality, with thousands-to-millions degrees of freedom exhibiting *spatio-temporal* dynamics, non-linearity and chaos. One of the most pertinent problems combining all these factors is fluid turbulence, with applications to climate, earth sciences, engineering, biomedical and energy sciences. In an era where vast quantities of turbulence data are generated for studying these applications, building practically usable, physics-driven reduced order models becomes extremely challenging and important.

Recent surge in devising NN-based reduced models of turbulence [1, 2, 3] including significant efforts from the computer graphics community [4, 5, 6, 7] for flow visualization by applying powerful, but application-agnostic Deep Learning (DL) techniques, such as Generative Adversarial Networks [8] and Convolutional LSTM (C-LSTM) Networks [9] has provided valuable tools boosting research in this important field of physics. However, majority of approaches used in this emerging field are

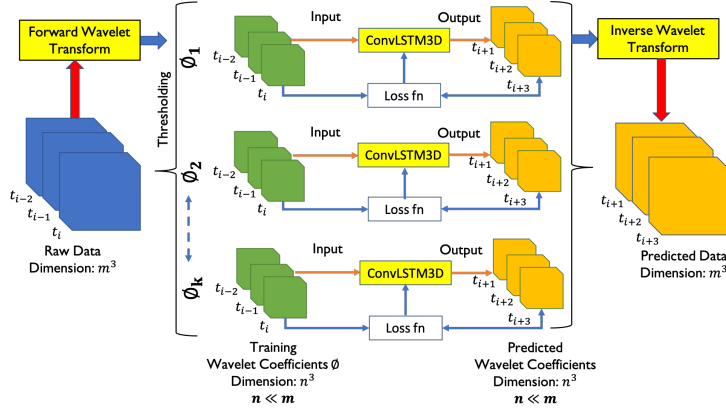


Figure 1: Wavelet-3D-C-LSTM: A schematic

limited to analysis based on two dimensional spatial projections of the originally 3+1 dimension (three-dimensional space and another dimension in time) spatio-temporal data-sets. Some of the state-of-the art spatio-temporal NN modeling architectures, like C-LSTM, have significant memory costs thus resulting in a limited utility to practical, e.g. climate and geophysical, datasets. Our main focus in this paper is on making C-LSTM tractable for large scientific spatio-temporal datasets.

2 Existing Strategy: Autoencoder 3D Convolutional LSTM

An approach to building reduced modeling of massive 3D spatio-temporal turbulence datasets is described in [10]. The main spatio-temporal modeling block, 3D-C-LSTM, was implemented in [10] through 3D extension of the 2D C-LSTM, originally proposed in [9]. To reduce dimensionality, spatial compression and decompression steps were implemented via autoencoders, sandwiched by 3D-C-LSTM layers. A sequence of 50 temporal snapshots, each of size 128^3 with 3 velocity components, was used. This imposed a significant training cost, and the solution relied on convolutional autoencoders to compress/decompress data before/after the 3D-C-LSTM block. The approach has helped to compress by factor of 125, down to $15^3 \times 15$ numbers. Knowledge of physics was utilized in Ref [10] postfactum – only to evaluate prediction quality. However, this generally successful autoencoder-based approach had two important shortcomings. First, we do not have explicit control on the features to retain in the latent space and therefore some important features may be lost. Second, autoencoders are computationally expensive for even moderate in size datasets. This manuscript suggests to resolve these complications by replacing the autoencoder NNs with explicit and physics-based model reduction guided by wavelets. Wavelets provide additional benefits of strong mathematical foundations through the wavelet selection (e.g. resulting in numerical stability) and significant reduction of the underlying computational cost.

3 Proposed Solution: Wavelet-3D-C-LSTM

In this manuscript we propose a new NN scheme, coined *Wavelet-CLSTM*, to simultaneously address the twin challenges of reducing the computational cost and injecting physics-based features into the procedure. The key idea of our *Wavelet-CLSTM* scheme consists in decomposing the 3+1 dimensional training data set with the wavelet transform, which results in a compact representation through the wavelet coefficients. The approach is superior to the previously used (auto-encoder based compression/decompression) methodology because it represents turbulence data in a compact, mathematically accurate, robust and flexible way. Moreover, we capitalize on the fact, well documented in the literature [11, 12, 13, 14, 15, 16, 17], that the wavelet coefficients capture multi-scale physics embedded in the turbulence dataset in one of the most efficient compressed formats. For example, a 3 level wavelet decomposition of a volumetric dataset of size 128^3 produces 512 coefficients of size 16^3 . This reduction in dimensionality is critical for saving memory and improving practical applicability of powerful, but expensive, architectures like C-LSTM. Additionally, a full wavelet decomposition can be used to perfectly reconstruct the original dataset i.e it is non-lossy if all coefficients are

considered. However, for reduced order modeling of practical datasets, we choose fewer coefficients to achieve maximal compression. This is an important choice to be made prior to training called **wavelet thresholding**, where the coefficients with the highest L2 norm are chosen for training - this cutoff number is determined by % of “energy” captured by the coefficients. A 3% thresholding would indicate $3/100 \times 512 \approx 15$ coefficients with the highest L2 norm. When compared with autoencoders, wavelets are advantageous because:

- Wavelet coefficients have a *dimensionality orders of magnitude lower than the original training data*, and low dimensional coefficients of a desired size can be computed for extremely large datasets [16, 18, 19]. This decouples training for each wavelet coefficient from other coefficients, thereby avoiding communication overheads and memory limitations which otherwise would plague large, distributed, parallel training tasks.
- Wavelet transform (decomposition) and inverse wavelet transform (reconstruction) can be *computed analytically*, making it orders of magnitude cheaper and faster.
- An additional benefit of the analytical formulation translates into ability to extend thresholding, i.e. the scales to be modeled can be explicitly selected *a priori* to training. (This is to be contrasted to the convolutional autoencoder handicap which lacked direct control, apart from selection of kernel size [10] *during* training.)

Our *a priori* analysis of the 3% thresholding shows that it captures all the large scales, and a majority of the intermediate scales in turbulence, however excluding sufficiently small scales. This is an acceptable trade-off, since large and intermediate scales are typical quantities of interest in majority of practical applications [20, 21, 22]. We would like to emphasize, however, that including smaller scales by increasing the thresholding percentage, is a degree of freedom to decide based on the application requirements. Increasing thresholding percentage increases the total training duration; but the adaptive, local nature of the coefficients ensures that the memory cost of training per coefficient stays *constant*, such that various coefficients can be trained *separately*, on available computer resources. This remarkable feature of the wavelet decomposition makes large scale parallelism a choice - rather than a necessity - thereby opening up this technique to extremely large datasets even with moderate computer resources available. To further increase compression efficiency we plan to investigate in the future scale based thresholding (i.e. different thresholds at different scales) as well as integer quantization (or re-quantization) to reduce the number of bits needed to represent the coefficients. A Schematic outlining this methodology is illustrated in Fig. 1.

4 Dataset and Accuracy Metrics

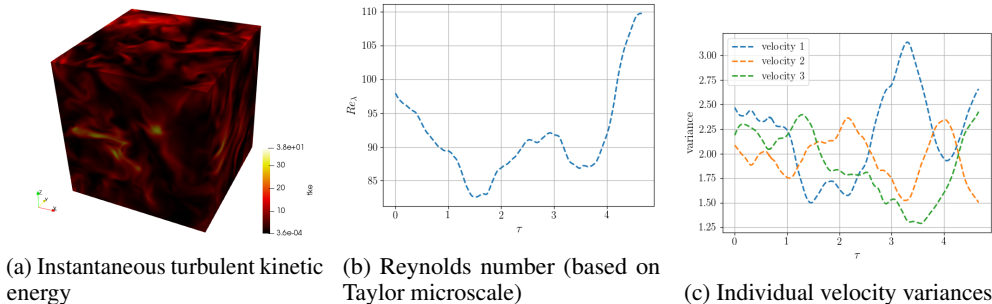


Figure 2: Representative Statistics of the Simulation

The dataset is a 3D Direct Numerical Simulation (DNS) of homogeneous, isotropic turbulence (HIT), in a box of size 128^3 . The simulation is performed using massively parallel CFDNS, by solving the incompressible Navier Stokes equations with a low band forcing restricted to small wavenumbers $k < 1.5$, using the classical pseudo-spectral approach. A combination of phase-shifting and truncation is used to achieve a maximum resolved wavenumber of $k_{max} = \sqrt{2}/3 \times 128 \sim 60$. Spectral resolution used is $\eta k_{max} \sim 1.5$, i.e. the grid spacing, Δx , is comparable to the Kolmogorov scale η . Details can be found in Ref. [23]. In this work we focus on modeling the 3 velocity components. For illustration, Figure 2a shows the turbulent kinetic energy at a time instant. Figure 2b shows the variation in the Taylor-microscale based Reynolds number with the eddy turnover time,

which characterizes the large turbulence scales. Finally, the variances in all 3 velocity components are shown in Fig. 2c.

We now briefly describe 3 basic tests of 3D turbulence which are used as “diagnostic” metrics for the accuracy of the flow predicted by the trained model.

4.1 4/5 Kolmogorov law and the Energy Spectra

The main statement of the Kolmogorov theory of turbulence is that asymptotically in the inertial range, i.e. at $L \gg r \gg \eta$, where L is the largest, so-called energy-containing scale of turbulence and η is the smallest scale of turbulence, so-called Kolmogorov (viscous) scale, $F(r)$ does not depend on r . Moreover, the so-called 4/5-law states for the third-order moment of the longitudinal velocity increment

$$L \gg r \gg \eta : \quad S_3^{(i,j,k)} \frac{r^i r^j r^k}{r^3} = -\frac{4}{5} \varepsilon r, \quad (1)$$

where $\varepsilon = \nu D_2^{(i,j;i,j)}/2$ is the kinetic energy dissipation also equal to the energy flux.

Self-similarity hypothesis extended from the third moment to the second moment results in the expectation that within the inertial range, $L \gg r \gg \eta$, the second moment of velocity increment scales as, $S_2(r) \sim v_L (r/L)^{2/3}$. This feature is typically tested by plotting the energy spectra of turbulence (expressed via $S_2(r)$) in the wave vector domain, e.g. as shown in the results section.

4.2 Intermittency of Velocity Gradient

Consequently from Eqn. 1, the estimation of the moments of the velocity gradient results in

$$D_n \sim \frac{S_n(\eta)}{\eta^n}. \quad (2)$$

This relation is strongly affected by intermittency for large values of n (i.e. extreme non-Gaussian behavior) of turbulence, and is a valuable test of small scale behavior.

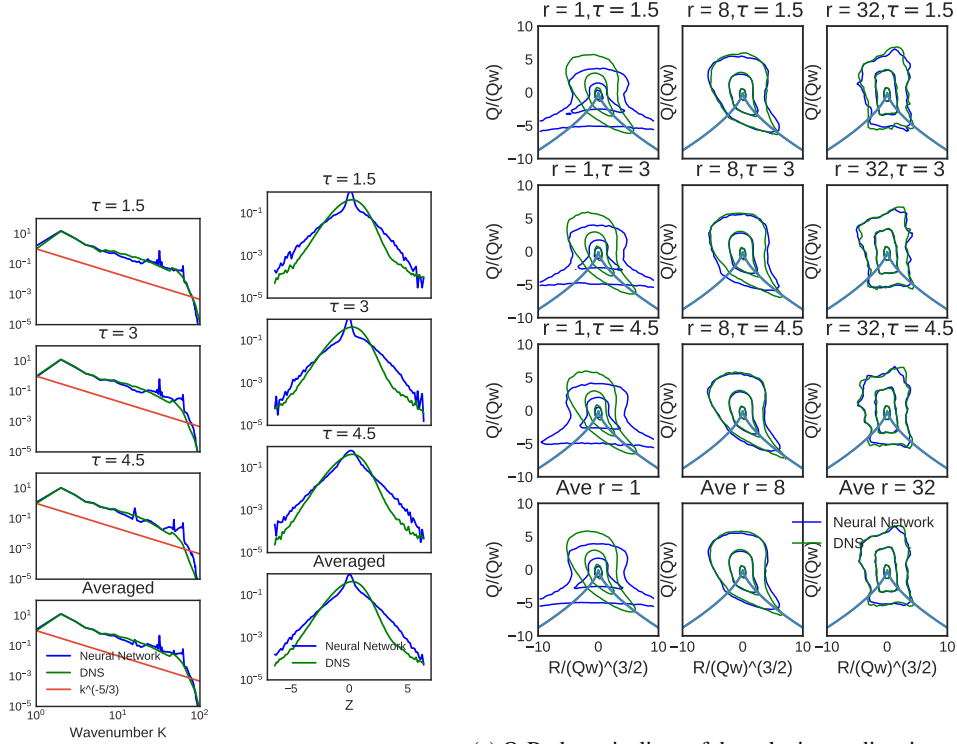
4.3 Statistics of coarse-grained velocity gradients: $Q - R$ plane.

Isolines of probability in the $Q - R$ plane, expressing intimate features of the turbulent flow topology, has a nontrivial shape documented in the literature. See Ref. [24] and references therein. Different parts of the $Q - R$ plane are associated with different structures of the flow. Thus, lower right corner (negative Q and R), which has higher probability than other quadrants, corresponds to a pancake type of structure (two expanding directions, one contracting) with the direction of rotation (vorticity) aligned with the second eigenvector of the stress. This tear-drop shape of the probability isoline becomes more prominent with decrease of the coarse-graining scale. Here, we study the $Q - R$ plane coarse-grained/filtered at different scales, to account for large scale ($r = 32$), inertial ($r = 8$), and small scale ($r = 1$) behaviors. This allows us to selectively analyze the accuracy of our predictions at different scales, since we are interested in modeling primarily the large and inertial ranges.

5 Results

The wavelet coefficients are computed with a *biorthogonal 1.3* [25] mother wavelet and 3% thresholding which we only have 15 coefficients to train, out of a total of 512. We compare accuracy of the NN predictions based on the turbulence diagnostics developed and tested in [3, 10]. We predict a sequence of flow-fields from the trained model, and analyze the flow at $\tau = 1.5, 3$ and 4.5 , which correspond to non-dimensional eddy turnover times. Analyzing the statistical properties of the predicted flow at varied time instants allows us to assess the long-term stability of our temporal predictions.

First, we analyze relative significance of different HIT scales conducting the energy spectra test. Higher wave-numbers in Fig 3a correspond to smaller scales. It is clear from the results that the large scale spectra are matched almost exactly, with good reproduction in the intermediate scale range. Comparatively, small scale spectra are not reproduced well, which is intentional because a significant portion of small scales were removed (set to zero) during the thresholding. Effects of the small scale



(a) Energy Spectra. (b) PDF of velocity gradients. (c) Q-R plane: isolines of the velocity gradient invariants coarse-grained at small, $r = 1$, inertial, $r = 8$, and large, $r = 32$ scales.

Figure 3: *Wavelet-CLSTM* Neural Network Turbulence vs Physical Simulation (DNS)

absence is also seen in the Probability Distribution Function (PDF) of the velocity gradient (Fig 3b), which tests solely the smallest scales of HIT. This is expected, since we are building a reduced order model for applications where large and inertial scales are of primary interest. The third test is the Q-R plane diagnostic in Fig 3c, which offers an arguably more stringent test of three-dimensional structure in turbulence [24, 26, 27, 28], as described in the previous section. We observe in Fig. 3c that the *Wavelet-CLSTM* reproduces the large scale behavior almost perfectly, while reproduction of turbulence geometry start to deteriorate as we move down-scales, to intermediate ($r = 8$) and small ($r = 1$) scales. The small scale behavior is not reproduced due to the 3% thresholding favoring large scales. The symmetric structure seen in the small scale prediction is likely linked to the noise added by the model. The bottom graphic "Ave" in Fig. 3c shows the averaged diagnostics for the 3 time instants. Overall, the test results present ample evidence to the fact that due to the physically-interpretable selection of the wavelet basis, the *Wavelet-CLSTM* is capable of modeling the large and inertial scale spatio-temporal dynamics of HIT well. We point out that it is straightforward to include small scale behavior by including relevant wavelet coefficients, obviously on the expense of increase in the computational cost.

6 Conclusion

We present here the first results for the novel *Wavelet-CLSTM*, which is an efficient, scalable, high dimensional deep NN framework for reduced modeling of turbulence, and similar or related multi-scale physical phenomena. The key strength of the framework is in the combination of a well-developed and mathematically justified wavelet decomposition with its highly desirable physical model reduction and interpretation power. Further investigation is desired into intelligent thresholding methods for non-stationary spatio-temporal phenomena.

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