# Towards physics-informed deep learning for turbulent flow prediction

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# Abstract

While deep learning has shown tremendous success in a wide range of domains, 1 it remains a grand challenge to incorporate physical principles in a systematic 2 manner to the design, training and inference of such models. In this paper, we 3 study the challenging task of turbulent flow prediction by learning the highly 4 5 nonlinear dynamics from spatiotemporal velocity field of large-scale fluid simulations. We marry Reynolds-Averaging (RA) and Large Eddie Simulation (LES), the 6 most promising turbulent flow simulation techniques, with a novel design of deep 7 neural networks. Our hybrid model, Turbulent-Flow Net (TF-Net) is grounded 8 in a principled mathematical model, and simultaneously offers the flexibility of 9 learned representation. We conduct comprehensive comparisons with state-of-the-10 art baselines and observe a significant reduction in prediction error by TF-Net for 11 60 frames ahead prediction. Most importantly, TF-Net is capable of generating 12 physically meaningful predictions that preserve desired physical quantities such as 13 Turbulence Kinetic Energy and Energy Spectrum of turbulent flow. 14

# 15 **1 Introduction**

16 Modeling the dynamics of physical processes that evolve over space and time and over multiple scales is a fundamental task in science. For example, turbulent flow modeling, is at the heart of climate 17 science and has direct implications for our understanding of climate change. However, the current 18 paradigm in atmospheric computational fluid dynamics (CFD) is *physics-driven*: known physical laws 19 encoded in systems of coupled partial differential equations (PDEs) are solved over space and time via 20 numerical differentiation and integration schemes. These methods are tremendously computationally-21 intensive, requiring significant computational resources and expertise. Recently, data-driven methods 22 including deep learning have demonstrated great promises to automate, accelerate, and streamline 23 24 highly compute-intensive and customized modeling workflows for scientific computing [1]. But existing deep learning methods are mainly statistically and are yet insufficient at capturing complex 25 natural phenomena in physical sciences. 26

Developing deep learning methods that can incorporate physics in a systematic manner is a key 27 element in advancing AI for physical sciences. Towards this goal, we investigate the challenging 28 problem of turbulent flow prediction from high-dimensional non-linear fluid mechanics equations. 29 Several others have studied incorporating prior knowledge about physical system into deep learning. 30 For example, [2] propose a warping scheme to predict sea surface temperature (SST) but are limited to 31 linearized advection equations. [3, 4] develop deep learning models in the context of fluid animation, 32 where being physically meaningful is less of a concern. The most relevant work to ours is [5], 33 which study turbulent flow modeling and propose to incorporating physical knowledge by explicitly 34

regularizing the divergence of the prediction. However, their study focuses on spatial modeling
 without temporal dynamics. Adding regularization is also ad-hoc and difficult to adjust the parameters.

In this work, we propose a hybrid learning paradigm that unifies turbulence simulation and represen-37 tation learning. We develop a novel deep learning model, Turbulent-Flow Net (TF-Net) that enhance 38 the capability of large-scale fluid simulation methods with deep neural networks. TF-Net exploits the 39 multi-scale behavior of turbulent flow and design explicit scale separation operators to model each 40 range of scales individually. Building upon the most promising turbulent flow simulation techniques 41 including Reynolds Averaging (RA) and Large Eddie Simulation (LES), our model replace the hand 42 designed spectral filters with learnable deep neural networks. We design a specialized U-net for 43 each filter to guarantee the invariance properties of the equations. To the best of our knowledge, 44 our work is the first to perform spatiotemporal future prediction of large-scale turbulent flow with 45 physics principles in mind. We provide exhaustive comparisons of TF-Net and baselines and observe 46 significant improve in both the prediction error and desired physical quantifies. 47

### **48 2 Turbulent-Flow Net**

<sup>49</sup> The physical system we investigate is two-dimensional Rayleigh-Bénard convection, which is an <sup>50</sup> idealized model for turbulent atmospheric convection. The system consists of a fluid bounded by two <sup>51</sup> horizontal planar surfaces, where the lower surface is at a higher temperature than the upper surface. <sup>52</sup> The sufficiently large temperature gradients causes an unstable vertical profile of density, which <sup>53</sup> results in convective motions. The governing equations for this physical system are Naiver-Stokes <sup>54</sup> Equations shown below, which are believed to model the physics of almost all fluid flows.

	$\nabla \cdot \boldsymbol{w} = 0$	Continuity Equation
ł	$\frac{\partial \boldsymbol{w}}{\partial t} + (\boldsymbol{w} \cdot \nabla) \boldsymbol{w} = -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 \boldsymbol{w} + f$	Momentum Equation
	$\frac{\partial T}{\partial t} + (\boldsymbol{w} \cdot \nabla)T = \kappa \nabla^2 T$	Temperature Equation,

where  $\mathbf{w} = (u, v)$ , p and T are velocity, pressure and temperature respectively, k is the coefficient of heat conductivity,  $\rho_0$  is density at temperature at the beginning,  $\alpha$  is the coefficient of thermal

s7 expansion,  $\nu$  is the kinematic viscosity, f the body force that is due to gravity. Figure 1 shows a

snapshot of the u and v velocities, the spatial resolution of which is 1792 by 256 pixels in our dataset.



Figure 1: A velocity field (u and v) in the dataset.

Scientific numerical simulation mostly rely on mathematical modeling of first principles, assisted 59 by high-performance computing. Dominant approaches typically involve approximations of the 60 underlying physical processes, followed by mathematical discretization including Direct Numerical 61 Simultion (DNS), Reynolds Averaged Navier Stokes (RANS) and Large Eddie Simulation [6]. 62 However, the simulation process is highly computational expensive not generalizable. It means that 63 when the system input has to be adjusted, even slightly, in most of the cases the time-consuming 64 procedure has to be repeated from scratch. The high-level design of TF-Net is inspired by the 65 multi-scale modeling of turbulent flows. Multi-scale methods use explicit scale separation operators 66 to split turbulent flows into into several parts in the wave number space, then use different specific 67 numerical treatments for each range of scales of the flow, and particularly treat the scales which 68 are associated to the largest computational costs with less accuracy than the other ones. Detailed 69 descriptions of Reynolds-Averaged Method and Large Eddy Simulation are in [7, 8]. 70

**Reynolds-Averaged Method** The hypothesis behind this Reynolds decomposition is that there are at least two widely-separated time scales, which means any turbulent quantity can be divided into a

time-averaged value  $\bar{w}$  and a fluctuating quantity w' as below, where  $\bar{w}$  is the weighted average.

$$\boldsymbol{w}(\boldsymbol{x},t) = \bar{\boldsymbol{w}}(\boldsymbol{x},t) + \boldsymbol{w'}(\boldsymbol{x},t),$$

$$\bar{\boldsymbol{w}}(\boldsymbol{x},t) = \frac{1}{T} \int_{t-T}^{t} G(s) \boldsymbol{w}(\boldsymbol{x},s) ds$$

**Large Eddy Simulation** Similar to Reynolds-Averaged Method, Large Eddy Simulation also decompose the flow variables into a large-scale part and a small-scale parts but the large-scale part purportedly defined by a filtering process. The filtered variable  $\tilde{u}$  is usually expressed as a convolution product by the filter kernel *G* that is often taken to be a Gaussian kernel.

$$oldsymbol{w}(oldsymbol{x},t) = ilde{oldsymbol{w}}(oldsymbol{x},t) + oldsymbol{w}'(oldsymbol{x},t), ext{where}$$
  
 $oldsymbol{ ilde{oldsymbol{w}}}(oldsymbol{x},t) = rac{1}{T}\int G(oldsymbol{x}|oldsymbol{\xi})oldsymbol{w}(oldsymbol{\xi},t)doldsymbol{\xi}$ 

71 **Hybrid LES/RA Method** The hybrid LES-72 RA Method is a three-level decomposition with 73 the spatial filtering operator  $G_1$  and the tempo-74 ral average operator  $G_2$  from the previous two 75 ratio and 10 methods for the previous two

75 methods. We can define:



Figure 2: Model architecture of TF-Net, three modules with shared decoder correspond to three scale separation. Each module consists of a U-net with encoder and decoder structure.

$$\boldsymbol{w}^{*}(\boldsymbol{x},\boldsymbol{t}) = G_{1}(\boldsymbol{w}) = \frac{1}{T} \sum_{\boldsymbol{\xi}} G_{1}(\boldsymbol{x}|\boldsymbol{\xi}) \boldsymbol{w}(\boldsymbol{\xi},t)$$
$$\bar{\boldsymbol{w}}(\boldsymbol{x},\boldsymbol{t}) = G_{2}(\boldsymbol{w}^{*}) = \frac{1}{T} \sum_{s=t-T}^{t} G_{2}(s) \boldsymbol{w}^{*}(\boldsymbol{x},s)$$
$$\tilde{\boldsymbol{w}} = \boldsymbol{w}^{*} - \bar{\boldsymbol{w}}, \quad \boldsymbol{w}' = \boldsymbol{w} - \boldsymbol{w}', \quad \boldsymbol{w} = \bar{\boldsymbol{w}} + \tilde{\boldsymbol{w}} + \boldsymbol{w}^{*}$$

Figure 2 shows the architecture of our model TF-Net. The general idea behind TF-Net is multi-level 76 spectral decomposition, which is to separate the velocity into three components of different scales 77 with two scale separation operators, the spatial filter  $G_1$  and the temporal filter  $G_2$ . In the traditional 78 numerical methods, these two filters are usually pre-defined, like the Gaussian spatial filter, but both 79 filters are set as learnable parameters in our model. The spatial filtering process can be realized by 80 applying one convolutional layer with single  $5 \times 5$  filter to each input images. The temporal filter is 81 implemented with a convolutional layer with single  $1 \times 1$  filter applied to every T images. 82 After scale separation, we use three identical encoders to encode and learn the transformations of 83

the three components respectively, and pass the hidden states to decoder which is supposed to learn the interactions among these three components and generate the final prediction of the next velocity fields. Each encoder and the decoder together can be viewed as a small U-net with skip connections. To produce multiple time-step forecasts, we train and use our model auto-regressively, which means the model always make one-step ahead prediction and the predicted image is fed back to the inputs.

# 89 3 Experiments

- 90 3.1 Setup
- <sup>91</sup> We compare our model with a series of strong baseline models.
- ResNet[9]: thirty-four layer ResNet with a convolutional output layer.
- ConvLSTM[10]: three layer Convolutional LSTM.
- U-net[11] : four layer encoder and four layer decoder.
- GAN[12]: U\_net trained with adversarial loss.
- U\_con: U\_net with the divergence  $||\nabla \cdot \mathbf{w}||^2$  as a regularizer

- PDE-CDNN[2]: linearized advection equations  $(\mathbf{w} \cdot \nabla)u$ .
- DHPM[13]: numerical solver where finite difference is approximated by auto-differentiation.

The dataset for our experiments is two dimensional turbulent flow velocity vector fields simulated with a Lattice Boltzmann Method [14]. The spatial resolution of each image is 1792 by 256. Each image has two channels, one is the turbulent flow velocity along x direction and the other one is the velocity along y direction. Figure 1 is a sample of velocity fields. For the control parameters during numerical simulation, Prandtl number is 0.71, Rayleigh number is  $2.5 \times 10^8$  and the maximum Mach number is 0.1. The dataset contains 23000 high-resolutions images.

We divided each image into 7 sub-regions of size 256 by 256 pixels, then downsample them into
64 by 64 pixels images. We used sliding window generating 9870 samples of sequences of velocity
fields, including 6000 training samples, 1700 validation samples and 2170 test samples. The hyperparameters are tuned using a validation set based on averages RMSEs of six steps ahead prediction.
We predicted velocity fields up to 60 steps ahead. All results are averaged over three runs.

#### 110 **3.2 Results**

<sup>111</sup> We compare the Root Mean Square Error (RMSE) of all predicted pixel values over both u and v

channels. Figure 3 shows the growth of RMSE with prediction horizon up to 60 time steps ahead. We

can see that TF-Net outperforms other methods, and constraining it with divergence free regularizer  $||\nabla \cdot \mathbf{w}||^2$  can further improve the performance. Figure 4 shows the divergence of the all the methods w.r.t the ground truth data (target). Again, TF-Net is the closest to the numerical simulation.



Figure 3: RMSE vs. Forecasting Horizon

Figure 4: Divergence vs. Forecasting Horizon



Figure 5: The Energy Spectrum of TF-Net and the best baseline U-net. The left one is the energy spectrum plot on small wavenumbers and the right one is the spectrum on large wavenumbers.

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We also compare the energy spectrum of turbulence, E(k), which is related to the mean turbulence 116 kinetic energy per unit mass as  $\int_0^\infty E(k)dk = (\overline{(u')^2} + \overline{(v')^2})/2$ . k is the wave number. The large eddies have low wave number and the small eddies have high wave numbers. The spectrum tells how 117 118 much kinetic energy is contained in eddies with wave number k. Figure 5 shows the energy spectrum 119 of our model and the best baseline. We can see that TF-Net predictions are in fact much closer to the 120 target on large wavenumbers and more stable on small wavenumbers compared with U-net. Extra 121 divergence free constraint does not affect the energy spectrum of predictions. We also provide videos 122 of predictions by TF-Net and several best baselines in https://www.youtube.com/watch?v= 123 sLuVGIuEE9A and https://www.youtube.com/watch?v=VMeYHID5LL8, respectively. 124

### 125 **4 Discussion**

We propose a novel physics-informed deep learning approach to predict the spatio-temporal evolution of a turbulent flow. Our method TF-Net unifies LSE/RA and deep neural networks. It exploits multi-scale modeling and design explicit scale separation operators to model each range of scales individually. When evaluated on a large turbulent flow dataset, TF-Net outperforms state-of-the-art baselines in terms of RMSE and can preserve desired physical quantities such as Turbulence Kinetic Energy and Energy Spectrum of turbulent flow. Future work involves incorporating other variables

<sup>132</sup> such as pressure and temperature as a joint prediction task.

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