Promoting Numerical Stability on Neural Surrogate Models of Turbulent Flows

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Accurate surrogate models of turbulent simulations can be used for tasks that require many function evaluations and fast inference such as design optimization and control. Recent advances on Deep Learning have opened the opportunity for learning data-driven surrogate models of turbulent flows with better accuracy and generality than other reduced-order modeling techniques [1]. However, one of the limitations of Deep Learning methods is on maintaining numerical stability over long-time horizons. In this work we propose a framework to enforce numerical stability, by adding regularization terms to the loss function based on the diffusion, advection and time-derivative of the Navier-Stokes equation. Also, we employ a method of adding perturbations to the inputs of our models, known as the push-forward method [2]. This results in a optimization objective (see eq. 1) with multiple terms where the weight of each term plays an important role.

$$L_{total} = \lambda_{data} L_{MSE} + \lambda_{diff} L_{diff} + \lambda_{adv} L_{adv} + \lambda_{D_t} L_{D_t} + \lambda_{pf} L_{pf} \tag{1}$$

In order to find the right balance of terms of the loss function, we employ a hyperparameter tuning strategy based on Bayesian optimization [3]. We tested our framework on different Neural Network architectures: Autoencoder - LSTM [4], U-NET [5] and Fourier Neural Operators [6], trained for regression of a 2D Kolmogorov Flow [7] (see a sample of results on fig. 1). We observe that this strategy improves the results of the aforementioned models, meaning this can be applied to other architectures developed in the future.

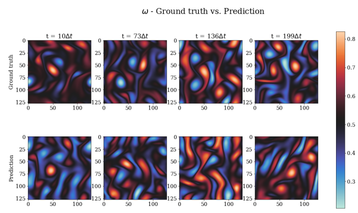

Figure 1: Predictions made by a Neural Operator model at different time-steps.

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