Recurrent neural networks and Koopman-based frameworks for
temporal predictions in turbulence

Hamidreza Eivazi\textsuperscript{a}, Luca Guastoni\textsuperscript{b,c}, Philipp Schlatter\textsuperscript{b,c}, Hossein Azizpour\textsuperscript{d,c}, Ricardo Vinuesa\textsuperscript{b,c,}\textsuperscript{*}

\textsuperscript{a}Faculty of New Sciences and Technologies, University of Tehran, Tehran, Iran
\textsuperscript{b}SimEx/FLOW, Engineering Mechanics, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden
\textsuperscript{c}Swedish e-Science Research Centre (SeRC), Stockholm, Sweden
\textsuperscript{d}Division of Robotics, Perception, and Learning, School of EECS, KTH Royal Institute of Technology, Stockholm, Sweden

Abstract
The prediction capabilities of recurrent neural networks and Koopman-based frameworks are assessed in the low-order model of near-wall turbulence by Moehlis et al. (New J. Phys. 6, 56, 2004). Our results show that it is possible to obtain excellent predictions of the turbulence statistics and the dynamic behavior of the flow with properly trained long-short-term memory (LSTM) networks, leading to relative errors in the mean and the fluctuations below 1%. Besides, a newly developed Koopman-based framework, called Koopman with nonlinear forcing (KNF), leads to the same level of accuracy in the statistics at a significantly lower computational expense. Furthermore, the KNF framework outperforms the LSTM network when it comes to short-term predictions. We also observe that using a loss function based only on the instantaneous predictions of the flow can lead to suboptimal predictions in terms of turbulence statistics. Thus, we propose a stopping criterion based on the computed statistics which effectively avoids overfitting to instantaneous predictions at the cost of deteriorated statistics. This suggests that a new loss function, including the averaged behavior of the flow as well as the instantaneous predictions, may lead to an improved generalization ability of the network.

Keywords: Turbulent flows, Machine learning, Data-driven modeling, Recurrent neural networks, Koopman operator

1. Introduction
The potential of machine-learning methods in a wide range of areas (Jean et al., 2016; De Fauw et al., 2018; Norouzzadeh et al., 2018; Ham et al., 2019; Udrescu and Tegmark, 2020; Vinuesa et al., 2020) has motivated its recent use in the context of fluid mechanics, as discussed for instance by Jiménez (2018), Duraisamy et al. (2019) and Brunton et al. (2020). Neural networks (NNs), which are computational frameworks used to learn certain tasks from examples, are a widely used tool in machine learning. Their success in a number of applications,
mainly related to pattern recognition, can be attributed to the increase in available computational power (through graphics processing units, \textit{i.e.} GPUs) and training data which explains the increasing interest in their use for turbulence (Kutz, 2017). Several studies have explored the possibility of using neural networks to develop more accurate Reynolds-averaged Navier–Stokes (RANS) models (Ling et al., 2016; Wu et al., 2018), while other studies aim at developing subgrid-scale (SGS) models for large-eddy simulations (LESs) of turbulent flows (Lapeyre et al., 2019; Beck et al., 2019). On the other hand, NNs have been used for non-intrusive sensing of turbulent flows (Guastoni et al., 2019a; G"uemes et al., 2019), for the development of efficient flow-control strategies (Rabault et al., 2019), and to model the near-wall region of wall-bounded turbulence (Milano and Koumoutsakos, 2002). Other relevant applications of neural networks include the development of robust inflow conditions for high-Reynolds-number turbulence simulations (Fukami et al., 2019b), super-resolution reconstruction (Fukami et al., 2019a) and pattern identification in flow data (Raissi et al., 2020).

On the other hand, data-driven finite-dimensional approximations of the Koopman operator have also received attention in recent years, in particular, for problems dealing with complex spatiotemporal behavior such as turbulent flows (Arbabi and Mezić, 2017; Giannakis et al., 2018; Page and Kerswell, 2019). Koopman operator theory is an alternative operator-based perspective to dynamical systems theory, which provides a versatile framework for the data-driven study of nonlinear systems. The theory is grounded on the work by Koopman (1931) and Koopman and Neumann (1932). The so-called \textit{Koopman operator} is an infinite-dimensional linear operator acting on Hilbert space of observable functions of the state of the system, which describes the evolution of a dynamical system in time. The spectral decomposition of the Koopman operator provides useful insight into the underlying dynamics of the nonlinear system and allows to employ traditional techniques in numerical linear algebra for nonlinear systems. In particular, Koopman modes offer a set of coherent structures useful for studying the evolution of the system and to identify the dominant patterns in the data. Modal decomposition of the Koopman operator has been utilized for analysis of complex systems in various engineering fields, including fluid dynamics (Rowley et al., 2009), neuroscience (Brunton et al., 2016), robotic control (Berger et al., 2015), image processing (Kutz et al., 2016), and system identification (Mauroy and Goncalves, 2016).

The aims of the present work are to assess the potential of NNs and Koopman frameworks to predict the temporal dynamics of turbulent shear flows, and to test various strategies to improve such predictions. In order to easily obtain sufficient data for training and validation, we considered a low-order representation of near-wall turbulence, described by the model proposed by Moehlis et al. (2004). The mean profile, streamwise vortices, the streaks and their instabilities as well as their coupling are represented by nine spatial modes $u_j(x)$. The spatial coordinates are denoted by $x$ and $t$ represents time. The instantaneous velocity fields can be obtained by superimposing the nine modes as: $u_{\text{inst}}(x,t) = \sum_{j=1}^{9} a_j(t)u_j(x)$, where Galerkin projection can be used to obtain a system of nine ordinary differential equations (ODEs) for the nine mode amplitudes $a_j(t)$. A model Reynolds number $Re$ can be defined in terms of the channel full height $2h$ and the laminar velocity $U_0$ at a distance of $h/2$ from the top wall. Here we consider $Re = 400$ and employ $U_0$ and $h$ as velocity and length scales, respectively. The ODE model was used to produce over 10,000 time series of the nine amplitudes, each with a time span of 4,000 time units, for training and validation. The domain size is $L_x = 4\pi$, $L_y = 2$ and $L_z = 2\pi$, where $x$, $y$ and $z$ are the streamwise, wall-normal and spanwise coordinates respectively, and we consider only time series that are turbulent over the whole time span. In the next sections we will discuss the feasibility of using various data-driven approaches to predict the temporal dynamics
of this simplified turbulent flow. All the neural-network-based results discussed in this study were obtained using the machine-learning software framework developed by Google Research called TensorFlow (Abadi et al., 2016). The results from the Koopman-based frameworks were obtained through an in-house implementation of the methods.

This article is organized as follows: in §2 we provide an overview of the predictive capabilities of recurrent neural networks and we summarize some of our previous results; in §3 we discuss the theoretical background relevant to the Koopman-based frameworks under consideration in this work; the predictive capabilities of both data-driven approaches are compared in §4; possible ways of improving the performance of recurrent neural networks are discussed in §5; and finally, in §6 we provide a summary and the conclusions of the study.

2. Predictions with recurrent neural networks

The simplest type of neural network is the so-called multilayer perceptron (MLP) (Rumelhart et al., 1985), which consists of two or more layers of nodes (also denoted by the term neurons or units), where each node is connected to the ones in the preceding and succeeding layers. Although MLPs are used in practice, their major limitation is that they are designed for point prediction as opposed to time-series prediction, which might require a context-aware method. Nevertheless, MLPs provide a solid baseline in machine-learning applications and thereby help verifying the need for a more sophisticated network architecture. In a previous study (Srinivasan et al., 2019) we assessed the accuracy of MLP predictions of the nine-equation model by Moehlis et al. (2004), where the time evolution of the nine coefficients was predicted with several different architectures. The turbulence statistics were obtained by averaging over the periodic directions (i.e. $x$ and $z$) and in time over 500 complete time series, which was sufficient to ensure statistical convergence in this case. In order to quantify the accuracy of the predictions, we will consider the relative error between the model and the MLP prediction (denoted by the subindices ‘mod’ and ‘pred’, respectively) for the mean flow as:

$$E_u = \frac{1}{2 \max(\bar{u}_{\text{mod}})} \int_{-1}^{1} |\bar{u}_{\text{mod}} - \bar{u}_{\text{pred}}| \, dy,$$

where the normalization with the maximum of $\bar{u}$ is introduced to avoid spurious error estimates close to the centerline where the velocity is 0. This error is defined analogously for the streamwise velocity fluctuations $\bar{u}^2$. Note that the same approach will be used in this study to compute statistics and assess the accuracy of the statistics predictions. A number of MLP architectures were investigated (see additional details in the work by Srinivasan et al., 2019), and the best predictions were obtained when considering $l = 5, n = 90$ and $p = 500$, which denote respectively the number of hidden layers, the number of neurons per layer and the number of previous $a_j(t)$ values used to obtain a prediction. With this architecture, the errors in the mean and fluctuations are $E_u = 3.21\%$ and $E_{u^2} = 18.61\%$ respectively, indicating that although acceptable predictions of the mean flow can be obtained, the errors in the fluctuations are high. Furthermore, the size of the input was $d = 9p = 4,500$ (i.e. 9 coefficients over the past 500 time steps are used to predict the next 9 coefficients), which is quite large. Since the MLP performs point predictions, it does not exploit the sequential nature of the data, and it is therefore important to assess the feasibility of using other types of networks, i.e. the so-called recurrent neural networks (RNNs), which can benefit from the information contained by the temporal dynamics in the data.
In its simplest form, an RNN is a neural network containing a single hidden layer with a feedback loop. As opposed to MLPs, each node of the RNN layer has an internal state vector that is combined with the input vector to compute the output. The output of the hidden layer in the previous time instance is fed back into the hidden layer along with the current input. This allows information to persist, making the network capable of learning sequential dependencies. In practice, this simple recurrent network is not effective to learn long-term dependencies, hence a more sophisticated model is required, such as the long-short-term memory (LSTM) network proposed by Hochreiter and Schmidhuber (1997), or the gated recurrent unit (GRU) network developed by Cho et al. (2014). Both architectures use a gating mechanism to actively control the dynamics of the recurrent connections. Each unit in the LSTM layer performs four operations through three different gates. The forget gate uses the output in the previous time instance $\xi_{t-1}$ and the current input $\chi_t$ to determine which part of the cell state $C_{t-1}$ should be retained in the current evaluation. The input gate uses the same quantities to determine which values of the cell state should be updated and it also computes the candidate values for the update. Finally the output gate uses the newly-updated cell state to compute the output. Algorithm 1 illustrates how the output is computed and how the cell state is updated, where $\otimes$ indicates the Hadamard product and $\sigma$ denotes the logistic sigmoid function. A schematic representation of a multi-layer LSTM is shown in Figure 1. The model is defined by a set of parameters $\mathcal{P}$ which comprise the weight matrices $W$ and the biases $b$. During training, the values of the parameters are optimized to minimize a certain loss function.

Algorithm 1: Compute the output sequence of an LSTM network.

Input: Sequence $\chi_1, \chi_2, \ldots, \chi_p$
Output: Sequence $\xi_1, \xi_2, \ldots, \xi_p$

Set $h_0 \leftarrow 0$
Set $C_0 \leftarrow 0$

for $t \leftarrow 1$ to $p$ do
  \[ f_t \leftarrow \sigma(W_f[\chi_t, \xi_{t-1}] + b_f) \]
  \[ i_t \leftarrow \sigma(W_i[\chi_t, \xi_{t-1}] + b_i) \]
  \[ \tilde{C}_t \leftarrow \tanh(W_c[\chi_t, \xi_{t-1}] + b_c) \]
  \[ C_t \leftarrow f_t \otimes C_{t-1} + i_t \otimes \tilde{C}_t \]
  \[ o_t \leftarrow \sigma(W_o[\chi_t, \xi_{t-1}] + b_o) \]
  \[ \xi_t \leftarrow o_t \otimes \tanh(C_{t-1}) \]

In our previous work (Srinivasan et al., 2019) we analyzed the prediction capabilities of LSTM networks for this turbulent shear flow wall model by considering a network with a single layer of 90 LSTM units. We trained it with three different datasets, consisting respectively of 100, 1,000, and 10,000 time series spanning 4,000 time units each. We considered a validation loss defined as the sum over $p$ time steps of the squared error in the prediction of the instantaneous coefficients $a_j$, and observed that better flow predictions could be obtained when larger datasets were employed for training. Note that we considered 20% of the training data as a validation set, which is used to check the evolution of the loss on data which has not been seen by the network during training. Using 10,000 time series for training, we obtained accurate predictions of the turbulence statistics, with $E_u = 0.45\%$ and $E_{u^2} = 2.49\%$. This was obtained with $p = 10$, i.e. with an input size 50 times smaller than that used with the MLP. The agreement of all the
statistics with the reference data was compelling, and even higher-order moments exhibited low relative errors, i.e. 1.01% and 2.57% for skewness and flatness, respectively (Srinivasan et al., 2019). These results highlight the excellent predicting capabilities of the LSTM network, given that sufficient training data is provided, due to the ability of the network to exploit the sequential nature of the data.

3. Koopman-based frameworks

Predicting the spatiotemporal evolution of high-dimensional and nonlinear dynamical systems (such as turbulent flows) based on finite-dimensional approximations of the Koopman operator is of particular interest for fluid mechanics. Dynamic Mode Decomposition (DMD) (Schmid, 2010; Tu et al., 2014) is one of the most popular algorithms for modal decomposition based on the Koopman operator (Rowley et al., 2009). DMD, in its original formulation, implicitly utilizes linear observables of the state of the system. However, linear functions may not be rich enough to describe many nonlinear dynamical systems. The Extended DMD (EDMD) (Williams et al., 2015) is proposed to include a richer set of nonlinear observable functions (such a set is denoted as dictionary) for better approximations of the Koopman eigenfunctions. Through a careful choice of the dictionary, it is shown that the EDMD algorithm has better performance than DMD (Williams et al., 2015). However, a drawback of the EDMD algorithm is the fact that, without a-priori knowledge about the underlying dynamics, it is not clear how to choose a dictionary that is sufficiently rich to span a useful Koopman-invariant subspace. Recently, several studies have introduced fully data-driven approaches for learning Koopman embedding and autonomous dictionary learning using Deep Neural Networks (DNNs): Takeishi et al. (2017); Li et al. (2017); Lusch et al. (2018).

The necessity of choosing appropriate input data is critical for data-driven modeling and prediction of dynamical systems using Koopman-based frameworks. Instead of utilizing linear or nonlinear observable functions of the state variables, it may be possible to construct a rich feature space using delay-embedding of time series measurements. Time delay-embedding, also
known as delay-coordinate embedding, is based on Takens embedding theorem (Takens, 1981) and refers to the inclusion of previous data in dynamical system models. Time-delay embedding has been widely used for state space reconstruction and analysis of chaotic systems (Farmer and Sidorovich, 1987; Crutchfield and McNamara, 1987; Abarbanel et al., 1993; Sugihara et al., 2012). By combining delay embedding with DMD, Arbabi and Mezić (2017) introduced the Hankel-DMD method, which is a linear model that can provide a representation of the Koopman eigenvalues and eigenfunctions.

Brunton et al. (2017) presented a universal data-driven decomposition of chaos as an intermittently forced linear system. Their model, referred to as Hankel alternative view of Koopman (HAVOK), combines Takens’ delay embedding with modern Koopman-operator theory and sparse regression to obtain linear representations of strongly nonlinear dynamics. Brunton et al. (2017) applied this model to the canonical Lorenz system, as well as to real-world examples of chaos leading to accurate prediction of attractor switching and bursting phenomena in such cases. More recently, Khodkar et al. (2019) introduced a successful Koopman-based framework for data-driven spatiotemporal prediction of high-dimensional and highly chaotic systems. The main novelty of their approach is the fact that the nonlinearities are modeled through external forcing, where the observables are vector-valued and delay-embedded. The model has been shown capable of accurate prediction of well-known prototypes of chaos, such as the Kuramoto-Sivashinsky equation (Kuramoto and Tsuzuki, 1976; Sivashinsky, 1982) and the Lorenz-96 system (Lorenz, 2006), as well as high-Reynolds-number lid-driven cavity flows (Arbabi and Mezić, 2017) for several Lyapunov timescales.

In this work, we leverage the recent advances in the prediction of chaotic systems using Koopman-based frameworks for the prediction of turbulent shear flows. In particular, we utilize the method introduced by Khodkar et al. (2019) for time series prediction of the nine-equation model.

3.1. Koopman-operator theory

The Koopman operator theory is central to all that follows in this section, therefore we provide a brief overview of the mathematical aspects and definition of the properties relevant to our study. To this end, we focus on an autonomous discrete-time dynamical system:

$$x_{t+1} = F(x_t),$$

(2)

on the state space $\mathcal{M} \subseteq \mathbb{R}^n$, where $x$ is a coordinate vector of the state, and $F : \mathcal{M} \rightarrow \mathcal{M}$ is the evolution operator. The Koopman operator $\mathcal{K}$ is defined as an infinite-dimensional linear operator that acts on functions of state space (observables) $g : \mathcal{M} \rightarrow \mathbb{C}$ (unlike $F$, which acts on $x \in \mathcal{M}$). The action of the Koopman operator is:

$$\mathcal{K}g = g \circ F,$$

(3)

where $\circ$ indicates the composition of $g$ with $F$. In fact, the Koopman operator defines a new infinite-dimensional linear dynamical system that governs the evolution of the observables $g_t = g(x_t)$ in discrete time. Note that $\mathcal{K}$ is infinite-dimensional even if $F$ is finite-dimensional, and also it is linear even when $F$ is nonlinear. For a detailed discussion of the Koopman operator, the readers are referred to the available research articles (Mezic, 2005; Rowley et al., 2009) and reviews on the topic (Budišić et al., 2012; Mezić, 2013).
3.2. Koopman-based framework with nonlinearities modeled as exogenous forcing

Obtaining finite-dimensional approximations of the Koopman operator is the focus of intense research efforts due to its capabilities when it comes to linear representation of the nonlinear dynamical systems. This is also related to the wealth of methods available for estimation, prediction, and control of linear systems. The Hankel DMD algorithm (Arbabi and Mezić, 2017) provides a practical numerical framework for computation of the Koopman spectrum by applying DMD to the so-called Hankel matrix of data $\mathcal{H}$:

$$\mathcal{H} = \begin{bmatrix}
x_1 & x_2 & \cdots & x_{N-q+1} \\
x_2 & x_3 & \cdots & x_{N-q+2} \\
\vdots & \vdots & \ddots & \vdots \\
x_q & x_{q+1} & \cdots & x_N
\end{bmatrix},$$  \hspace{1cm} (4)

where $N$ is the number of the vector-valued observables $x^i$ sampled at $t = i\tau$, $\tau$ is the sampling interval and $q$ is the delay-embedding dimension. For the nine-equation model of Moehlis et al. (2004), $x^i$ is equal to $[a_1^i \ a_2^i \ \cdots \ a_9^i]^T$ in equation (4), where $T$ indicates transpose. Therefore, $\mathcal{H}$ is a matrix with the size of $(n \times q) \times (N - q + 1)$, where $n$ is the number of state variables.

Following the Exact DMD algorithm formulation (Tu et al., 2014; Arbabi and Mezić, 2017), we define:

$$X = [X^1 \ \cdots \ X^{N-q}], \quad Y = [X^2 \ \cdots \ X^{N-q+1}],$$  \hspace{1cm} (5)

where $X^i$ denotes the $i$th column of the Hankel matrix $\mathcal{H}$. The Singular Value Decomposition (SVD) of matrix $X$ is computed as:

$$X = U S V^*,$$  \hspace{1cm} (6)

where $^*$ denotes the conjugate transpose, $U \in \mathbb{C}^{(n \times q) \times r}$, $S \in \mathbb{C}^{r \times r}$, and $V \in \mathbb{C}^{(N-q) \times r}$. Here, $r$ is the rank of the reduced SVD approximation to $X$. The finite-dimensional approximation of the Koopman operator using Hankel-DMD (HDMD) is computed as:

$$\tilde{A}_{HDMD} = U^* Y V S^{-1},$$  \hspace{1cm} (7)

with size $r \times r$. Once the HDMD operator $\tilde{A}_{HDMD}$ is calculated using the training set, a future vector-valued observable $x^{m+1}$ can be predicted from:

$$X^{m+1,r} = \tilde{A}_{HDMD} X^{m,r},$$  \hspace{1cm} (8)

where $X^{i,r}$ (of size $r \times 1$) is the projection of $X^i = [x^{i-q} \ x^{i-q+1} \ \cdots \ x^i]^T$, which has size $(n \times q) \times 1$, onto the subspace of first $r$ singular vectors.

On the other hand, Khodkar et al. (2019) showed that the linear combination of a finite number of DMD modes may not be sufficient to obtain an accurate representation of the long-term nonlinear characteristics of a chaotic dynamical system such as the Kuramoto-Sivashinsky equation (Kuramoto and Tsuzuki, 1976; Sivashinsky, 1982). On the other hand, the HAVOK model introduced by Brunton et al. (2017) has been shown to provide excellent predictions of nonlinear dynamics by adding a forcing term to the linear model. Inspired by the HAVOK model, Khodkar et al. (2019) proposed a new Koopman-based framework, which incorporates nonlinear
effects through external forcing, so a dynamical system can be modeled as:

$$x^{m+1} = Ax^m + Bf^m,$$

where \(f\) denotes the forcing term. It is important to note that \(f\) contains possible forms of nonlinearity in the system, it is chosen in a physics-driven fashion and it is based on some knowledge or intuition of the governing equations. It also may be possible to utilize algorithms such as sparse identification of nonlinear dynamics (SINDy) to identify the forms of nonlinearity in a fully data-driven approach. Here, for the nine-equation model, we construct the forcing term as any possible two by two multiplication of the coefficients in a time instance:

$$f_i = [a_i^1 a_i^2 \cdots a_i^q a_i^{q+1} \cdots a_i^r]^T.$$  (10)

We define the time-delay-embedded form of equation (9) as:

$$X^{m+1} = AX^m + B\mathcal{F}^m,$$  (11)

where \(X^m\) is the same as above, and \(\mathcal{F}\) is the Hankel representation of the forcing vectors:

$$\mathcal{F} = \begin{bmatrix} f^1 & f^2 & \cdots & f^{N-q} \\ f^2 & f^3 & \cdots & f^{N-q+1} \\ \vdots & \vdots & \ddots & \vdots \\ f^q & f^{q+1} & \cdots & f^{N-1} \end{bmatrix}.$$  (12)

The size of \(\mathcal{F}\) is \((n' \times q) \times (N - q)\), where \(n'\) is the size of the forcing vector \(f\) and it depends on the form of the nonlinearities and the number of nonlinear processes in the dynamical system. Here, for the nine-equation model, \(n'\) is equal to 36.

The unknown maps of \(A\) and \(B\) can be found using the DMDc algorithm (where \(c\) stands for control) introduced by Proctor et al. (2016) as:

$$A = \hat{U}^\dagger \hat{Y} \hat{V} \hat{S}^{-1} \hat{U}_1 \hat{U},$$
$$B = \hat{U}^\dagger \hat{Y} \hat{V} \hat{S}^{-1} \hat{U}_2,$$  (13)

where \(Y = \hat{U} \hat{S} \hat{V}^\dagger\), the truncation rank is \(r\) and \(\hat{U} \in \mathbb{R}^{n \times r}, \hat{S} \in \mathbb{R}^{r \times r}, \text{ and } \hat{V} \in \mathbb{R}^{(N-q) \times r}.\)

Also, \(\begin{bmatrix} X & \mathcal{F} \end{bmatrix}^T = \hat{U} \hat{S} \hat{V}^\dagger\), where the truncation rank is \(k\) and \(\hat{U} \in \mathbb{R}^{(n'+q) \times k}, \hat{S} \in \mathbb{R}^{k \times k}, \text{ and } \hat{V} \in \mathbb{R}^{(N-q) \times k}.\) Moreover, \(\hat{U}_1 \in \mathbb{R}^{(n+q) \times k}\) and \(\hat{U}_2 \in \mathbb{R}^{(n'q) \times k}\) where \(\hat{U} = \begin{bmatrix} \hat{U}_1 & \hat{U}_2 \end{bmatrix}^T\). Here, \((\hat{\cdot})\) and \(\hat{\cdot}\) denote the rank-truncated forms of the SVD matrices from \(Y\) and \(\begin{bmatrix} X & \mathcal{F} \end{bmatrix}^T\), respectively. Note that \(A\) and \(B\) are represented in a reduced-order subspace and have sizes of \(r \times r\) and \(r \times (n \times q)\), respectively. Moreover, \(r\) and \(k\) can be chosen based on SVD rank-truncation methods such as the optimal hard threshold presented by (Gavish and Donoho, 2014). Hereafter, we refer to the Hankel-DMD method introduced by Arbabi and Mezić (2017) as HDMD and the Koopman-based framework proposed by Khodkar et al. (2019) as KNF, which stands for Koopman with nonlinear forcing.
4. Comparison between predictions from Koopman-based frameworks and LSTM network

4.1. Short-term predictions

In this section, the short-term prediction capabilities of the two Koopman-based frameworks, i.e. the KNF and HDMD methods, are compared with the performance of the LSTM network in the prediction of the temporal behavior of the nine-equation model. The testing set is the same for all the methods and contains 500 time series, each of them spanning 4,000 time units. The KNF and HDMD models are trained with one set of time series comprising 10,000 time units generated from the nine-equation model. The training time series are checked to be turbulent over the whole time span. The delay-embedding dimension \( q \) is considered equal to 5. Moreover, an LSTM network consisting of one hidden layer with 90 LSTM units and \( p = 10 \) is also used for the predictions (see Srinivasan et al. (2019) for additional details). The LSTM network is trained with 10,000 sets of time series, each with a time span of 4,000 time units.

Due to the chaotic nature of the nine-equation model, the performance of the methods depends on the initial condition from which the prediction is conducted. To provide comprehensive insight into the performance of these methods, examples of the predicted trajectories for the amplitude of the first mode \( a_1(t) \) versus the true trajectory for two specific initial conditions are presented in Figure 2. Here we show the cases where the KNF method provided the longest (Figure 2, top) and the shortest (Figure 2, bottom) intervals in very close agreement with the reference. It can be seen in Figure 2 (top) that the KNF method accurately predicts the time evolution of the \( a_1 \) amplitude for up to \( t \approx 730 \), and provides acceptable results for even up to \( t \approx 950 \). The LSTM network provides the next best performance, exhibiting accurate predictions of the time evolution for over \( t \approx 90 \). On the other hand, Figure 2 (bottom) shows the case of worst performance from the KNF method, still providing accurate predictions up to \( t \approx 80 \) (approximately as long as the LSTM network), and producing acceptable predictions up to \( t \approx 170 \). The HDMD method provides accurate predictions for up to \( t \approx 10 \) in both cases. Note that the
Figure 3: Relative Euclidean norm of errors $\epsilon(t)$ averaged over 500 randomly chosen initial conditions, as defined in equation (14). The dashed horizontal line shows the threshold value considered for accurate predictions, namely $\epsilon = 0.3$. The blue line denotes the error in predictions using an LSTM network with 1 layer and 90 neurons, trained with 10,000 datasets (Srinivasan et al., 2019), and the orange line indicates the error in predictions using the KNF model trained with one time series, with $N = 10,000$ and $q = 5$.

first 10 and 5 time steps are used to start the predictions for the LSTM network and the Koopman-based models, respectively. Moreover, we define an averaged relative Euclidean norm of errors in nine-dimensional space between the true and predicted trajectories to compare the results over all 500 randomly chosen initial conditions:

$$\epsilon(t) = \left( \frac{\sum_{i=1}^{9} (a_{i,\text{mod}}(t) - a_{i,\text{pred}}(t))^2}{\langle \sum_{i=1}^{9} (a_{i,\text{mod}}(t))^2 \rangle_t^{1/2}} \right)^{1/2}_{\text{ens}},$$

(14)

where $\langle \cdot \rangle_{\text{ens}}$ and $\langle \cdot \rangle_t$ indicate ensemble averaging over 500 sets of time series and over 4,000 time units, respectively. Figure 3 compares $\epsilon(t)$ for the KNF method and the LSTM network. It is evident that the KNF method outperforms the LSTM network for short-term predictions, while it provides the same level of accuracy for long-term predictions. In particular, considering a threshold of $\epsilon = 0.3$ to define very good agreement of the coefficient predictions, we observe that the KNF method provides accurate instantaneous predictions for around 280 time units, while the prediction horizon for the LSTM network is 130 time units.

4.2. Long-term predictions and statistics

We have shown the performance of three data-driven approaches in the short-term prediction of the temporal dynamics of the nine-equation model. Our results indicate that the predictions of all the methods discussed earlier eventually diverge from the true trajectory. However, it is still interesting to examine the performance of the models in the prediction of the long-term statistical properties of the actual model. Reproduction of the long-term behavior of a chaotic dynamical system using inexpensive data-driven methods can be significantly beneficial in the domain of data-driven turbulence modeling. Here, we compare the performance of the KNF method and the LSTM network in the reproduction of the long-term dynamics of the nine-equation model. To this end, we first examine the effect of the sizes of the training set $N$ and the delay dimension $q$ on the performance of the KNF method in the prediction of the turbulence statistics, i.e., the mean velocity profile $\langle u(y) \rangle$ and streamwise velocity fluctuations $\langle u^2(y) \rangle$. A time series spanning $N$ time units with a delay dimension of $q$ is used to train the KNF method, where $N$ and $q$ vary from 5,000 to 40,000 and from 5 to 20, respectively. The KNF models are trained once, and then
the resulting turbulence statistics are compared with four different reference test sets (not seen during the training and validation steps), each containing 500 sets of time series. The results are reported in Table 1.

Table 1: Error of turbulence statistics with respect to four different reference test sets. The best-performing model is shown in boldface.

| N     | q   | Test set 1 |         | Test set 2 |         | Test set 3 |         | Test set 4 |         |
|-------|-----|------------|---------|------------|---------|------------|---------|------------|---------|
|       |     | $E_u$ [%]  | $E_{u'^2}$ [%] | $E_u$ [%]  | $E_{u'^2}$ [%] | $E_u$ [%]  | $E_{u'^2}$ [%] | $E_u$ [%]  | $E_{u'^2}$ [%] |
| 5000  | 5   | 2.97       | 16.29   | 3.00       | 16.45   | 2.80       | 14.48   | 3.05       | 16.05   |
| 5,000 | 10  | 2.22       | 12.80   | 2.22       | 12.78   | 2.72       | 15.02   | 1.86       | 10.77   |
| 5,000 | 20  | 5.72       | 27.10   | 5.72       | 27.10   | 6.69       | 31.98   | 6.73       | 31.74   |
| 10,000| 5   | 0.44       | 0.67    | 0.38       | 0.58    | 0.04       | 0.39    | 0.33       | 0.88    |
| 10,000| 10  | 0.98       | 6.48    | 0.98       | 6.48    | 1.21       | 6.47    | 1.27       | 6.40    |
| 10,000| 20  | 2.45       | 11.78   | 2.45       | 11.83   | 1.95       | 11.05   | 2.13       | 10.65   |
| 20,000| 5   | 2.81       | 14.68   | 2.76       | 14.50   | 4.05       | 19.77   | 3.36       | 17.45   |
| 20,000| 10  | 0.72       | 2.32    | 0.72       | 2.35    | 0.89       | 4.45    | 1.90       | 6.89    |
| 20,000| 20  | 1.49       | 7.31    | 1.57       | 7.71    | 1.40       | 7.77    | 2.24       | 10.38   |
| 30,000| 5   | 2.01       | 10.75   | 2.03       | 10.79   | 3.25       | 16.12   | 3.00       | 15.08   |
| 30,000| 10  | 0.96       | 3.62    | 0.99       | 3.79    | 1.57       | 7.08    | 1.45       | 6.58    |
| 30,000| 20  | 1.43       | 6.77    | 1.42       | 6.76    | 1.13       | 6.35    | 1.59       | 7.05    |
| 40,000| 5   | 4.44       | 22.73   | 4.44       | 22.73   | 4.49       | 22.53   | 5.39       | 25.08   |
| 40,000| 10  | 4.77       | 23.07   | 4.81       | 23.22   | 4.28       | 20.57   | 4.37       | 21.12   |
| 40,000| 20  | 2.99       | 14.50   | 2.97       | 14.46   | 2.91       | 15.19   | 3.07       | 15.01   |

Our results show that the model trained using a time series spanning 10,000 time units, with a delay dimension of 5, yields the best predictions of turbulence statistics, with mean errors of $E_u = 0.30\%$ and $E_{u'^2} = 0.63\%$ over four test sets. It can be seen in Table 1 that the errors, as expected, are robust for the four different reference test sets. This indicates that it is possible to use a data set as the validation set and find the best set of hyper-parameters, which leads to similar error levels in the testing data set. It can also be observed that utilizing larger training data sets with higher values for delay embedding dimension may not lead to a more accurate prediction of the long-term statistics. In the next test, we train the KNF model with five different time series to build five different models and predict the turbulence statistics based on 500 time series to provide error bars of the prediction. Results are presented in Table 2, showing the mean errors of $E_u = 0.35\%$ and $E_{u'^2} = 1.20\%$, using as a reference the test set number 2 from Table 1. Very similar error levels are obtained using the other test sets as a reference.

In our previous study (Srinivasan et al., 2019), we showed that using 10,000 time series for training, it is possible to obtain excellent predictions of turbulence statistics from the LSTM network, with $E_u = 0.45\%$ and $E_{u'^2} = 2.49\%$. This was obtained with $p = 10$. In Figure 4 we show a comparison of the turbulence statistics obtained from the nine-equation model, the KNF method, and this LSTM network, including mean flow, the streamwise fluctuations and the Reynolds shear-stress profile $\overline{uv}$. The KNF results are obtained from the best KNF model, with
Table 2: Error of turbulence statistics for KNF models obtained with 5 different training sets. In all the cases we consider $N = 10,000$ and $q = 5$. The best-performing KNF model is highlighted in boldface.

| Training Set | $E_u$ [%] | $E_{u^2}$ [%] |
|--------------|-----------|---------------|
| 1            | 0.38      | 0.58          |
| 2            | **0.16**  | **0.18**      |
| 3            | 0.33      | 1.15          |
| 4            | 0.69      | 3.17          |
| 5            | 0.20      | 0.95          |
| Mean         | 0.35      | 1.20          |

$E_u = 0.16\%$ and $E_{u^2} = 0.18\%$ (see Table 2). These results highlight the excellent predicting capabilities of the LSTM network, given that sufficient training data is provided, and of the KNF method, due to the ability of the network and the Koopman-based framework to exploit the sequential nature of the data.

Figure 4: Turbulence statistics corresponding to (left) streamwise mean profile, (middle) streamwise velocity fluctuations and (right) Reynolds shear stress. Dashed black line is used for the reference nine-equation model (Moehlis et al., 2004), blue for the predictions using an LSTM network with 1 layer and 90 neurons, trained with 10,000 datasets (Srinivasan et al., 2019), and orange for the predictions using a KNF model trained using a time series with $N = 10,000$ and $q = 5$.

The quality of the predictions was further assessed in terms of the dynamic behavior of the system, first through the Poincaré map defined as the intersection of the flow state with the hyperplane $a_2 = 0$ on the $a_1 - a_3$ space (subjected to $da_2/dt < 0$). This map essentially shows the correlation between the amplitudes of the first and third modes, i.e. the modes representing the laminar profile and the streamwise vortices in the nine-equation model. In Figure 5 (top) we show the probability density function (pdf) of the Poincaré maps constructed from the 500 time series obtained from the LSTM and KNF predictions and the reference nine-equation model. In this figure, it can be observed that the LSTM network and the KNF method capture the correlation between the amplitudes of both modes, which indicates that their interaction is adequately represented by the NN and the Koopman-based framework. Moreover, the KNF results are in a closer agreement with those from the nine-equation model. We also studied the separation among trajectories obtained from the reference model, the LSTM network and the KNF method.
by means of Lyapunov exponents. For two time series 1 and 2, we define the separation of these trajectories as the Euclidean norm in nine-dimensional space:

\[
|\delta A(t)| = \left[ \sum_{i=1}^{9} (a_{i,1}(t) - a_{i,2}(t))^2 \right]^{1/2},
\]

and denote the separation at \( t = t_0 \) as \( |\delta A_0| \). The initial divergence of both trajectories can be assumed to behave as: \( |\delta A(t')| = \exp(\lambda t') |\delta A_0| \), where \( \lambda \) is the so-called Lyapunov exponent and \( t' = t - t_0 \). We introduced a perturbation with norm \( |\delta A_0| = 10^{-6} \) (which approximately corresponds to the accuracy of the current LSTM architecture (Srinivasan et al., 2019)) at \( t_0 = 500 \), where all the coefficients are perturbed, and then we analyzed its divergence with respect to the unperturbed trajectory. In Figure 5 (bottom) we show the evolution of \( |\delta A(t)| \) with time for the reference, as well as the LSTM and KNF predictions, after ensemble averaging 10 time series. All the three rates of divergence are very similar, with almost identical estimations of the Lyapunov exponents \( \lambda \): 0.0264 for the LSTM, 0.0275 for the KNF, and 0.0296 for the nine-equation model. Also note that after around approximately 500 time units of divergence, all the
curves saturate. This result provides additional evidence supporting the excellent predictions of the dynamic behavior from the original system when using the present LSTM architecture and the Koopman-based framework.

The excellent performance of the KNF method is interesting since it needs a much smaller data set, namely 0.025% of that from the LSTM, for the training of the model. Moreover, the mapping matrices of $A$ and $B$ are computed in one shot, thus the KNF algorithm is orders of magnitude faster than the backpropagation algorithm, which is used for training the LSTM network. Figure 6 depicts a comparison of the training time required by the LSTM network and the KNF method. Note that the KNF method is trained with one time series, and the size of the training data set for this method indicates the number of time units in the training time series. This term for the LSTM network represents the number of time series (each of 4,000 time units) used for training. Here, relative time is the training time of the models divided by the training time of the LSTM network with 100 time series (note that the LSTM curve is multiplied by $10^{-4}$). In this figure, it can be seen that the required training time for the LSTM network is around four orders of magnitude larger than that of the KNF method. Our results show that the training time of the KNF method is comparable to that of the echo state network (ESN) (Pandey et al., 2020), while both the KNF method and LSTM network outperform the ESN in the prediction of turbulence statistics. Also note that, although in Figure 6 we consider a constant number of epochs for the various LSTM cases, typically larger datasets require fewer epochs to reach similar levels of accuracy.

We have shown in Table 1 that increasing the amount of training data for the KNF method will not necessarily lead to improved predictions of the turbulence statistics. Such an increase of training data can be achieved either by increasing the number of time units of the training data set $N$ or increasing the dimension of the delay embedding $q$. It is also of interest to evaluate the
Figure 7: Validation loss and statistical errors versus the number of time units of the training time series for the KNF method with a delay dimension of 5.

Figure 7: Validation loss and statistical errors versus the number of time units of the training time series for the KNF method with a delay dimension of 5. Here, we considered a time series with 40,000 time units as the validation set for the KNF method. For $N < 11,000$, the error in the instantaneous predictions and the statistical quantities both decrease with an increasing size of the training data set. Moreover, it can be seen that the error in instantaneous predictions is reduced with a further increase of $N$, a fact that indicates an improvement of instantaneous predictions with increasing amount of training data. However, this figure shows that better instantaneous predictions do not necessarily lead to a better approximation of the turbulence statistics. For $N > 11,000$, utilizing more data for training leads to an increase of the error in the statistics while the instantaneous error still follows a decreasing trend. As discussed in §5, a similar behavior is observed for the LSTM, a fact that can be used to define a stopping criterion for training.

5. Towards improving neural-network predictions

The results in §4 showed that the LSTM network is able to accurately predict the temporal dynamics and statistics of a low-dimensional representation of near-wall turbulence. Next we explore different strategies to potentially improve the accuracy and efficiency of RNN predictions (Guastoni et al., 2019b).

5.1. Validation loss and training stopping criterion

As discussed above, the amplitudes of the modes in the model by Moehlis et al. (2004) exhibit fluctuations that are compatible with a chaotic turbulent state. Given the high sensitivity of the model to very small variations in the mode amplitudes, a loss function based on short-time
horizon predictions, namely one time step ahead, is required to obtain satisfactory predictions. On the other hand the trained model needs to correctly reproduce not only the instantaneous behavior but also the statistical features of the original shear flow model. The approach used in the work by Srinivasan et al. (2019) involves a loss function based only on the error in the instantaneous prediction. Neural networks having at least one hidden layer have been shown to be universal approximators (Cybenko, 1989), hence they are in principle able to represent any real function. A perfect reproduction of the temporal behavior of the model would also provide correct mean and turbulent fluctuations at no added cost, however there is no guarantee that such a model can be learned and, even in that case, the model would theoretically be available after an infinitely long training. In order to verify to which extent the loss function based on instantaneous predictions represents an effective solution, different neural-network configurations were tested to assess the correlation between the achieved validation loss and the error in the statistics of the flow. In Table 3 we summarize the various LSTM architectures under study, where we vary the number of layers, the number of time series used for training and the time step between samples. Let us consider the case LSTM2–1–100, consisting of 2 layers, with 90 units per layer, trained with 100 time series and a timestep of 1. Figure 8 shows the validation loss and the relative errors $E_u$ and $E_{u^2}$ for this network, as functions of the number of epochs trained (i.e. the number of complete passes through all the samples contained in the training set). In the initial stage of the training, starting from the randomized initialization of the weights and biases, the reduction of the error in the instantaneous behavior and in the statistical quantities show a similar trend. However, this figure also shows that (as in the case of the KNF method) lower validation loss values do not always lead to a better approximation of the turbulence statistics. In fact, as the training progresses, the optimization algorithm continues to improve the short-term predictions, whereas beyond around 240 epochs the error in the statistics does not follow a descending trend anymore. The observed behavior is explained by the fact that the loss function does not contain any term explicitly related to the statistics which could guide the optimization algorithm towards parameter sets with a better representation of the statistical quantities. Note that since the initialization of the parameters of the network is random, the performance in the prediction of mean and fluctuation may vary when the same model is trained multiple times. The achievable accuracy and the epoch at which this value will be reached are unknown a priori.

These results indicate that different strategies can be implemented in order to reduce the error on the statistics of the flow. One possible approach consists in including a new term in the loss function accounting for the error in the turbulence statistics. In this case the relative importance of the two terms needs to be adjusted, as prioritizing the accuracy of the statistics may lead to a model that learns only the average behavior of the system. Alternatively, it is possible to use the fact that the time horizon of the predictions influences which features of the problem are learnt by the neural network, as highlighted by Chiappa et al. (2017). In that work it was shown how improvements in the short-term accuracy (i.e. in the prediction of the instantaneous behavior) come at the expense of the accuracy of global dynamics. Using the results of the network to make predictions several time steps ahead would encourage the network to learn the long-term behavior of the system and thus its global dynamics. As stated by Chiappa et al. (2017), this approach has the added advantage of training the model in a way that is similar to its actual utilization. In fact, during the evaluation and usage, our networks rely only on the previous predictions after the first $p$ time steps. Note however that taking into account the error in the current prediction based on previous predicted values typically results in a much more complex loss function. Both approaches require additional hyper-parameters that need to be optimized in order to obtain a satisfactory performance. In this study we aim at keeping a simple loss function,
and we use the error in the statistics as criterion to halt the training when a minimum is reached for this value. Note that the error can vary significantly from one epoch to the other, hence it is advisable to consider multiple epochs to identify the general trend of the error curves. Doing so, we can achieve excellent predictions of the turbulence statistics while using a simple loss function based on the instantaneous predictions of the coefficients. As shown in Table 3, the improvement over the models reported in our previous work (Srinivasan et al., 2019) is particularly evident for the models trained on the small dataset, yielding an accuracy in the statistics comparable with that of the networks trained with bigger data sets. It is also important to note that the improved scheduled reduction of the learning rate employed for the results in Table 3 allowed to obtain much lower validation losses than in our previous work, using a similar training time. When reaching such low values of the loss function, the trade-off between the instantaneous and the average performance is more apparent.

5.2. Effect of the time step

The sequences provided to the neural network for training are evenly spaced in time, however the choice of the proper time step between data points $\Delta t$ depends on the problem at hand. The time step acts as a low-pass filter on the data, preventing the model from learning higher-frequency dynamics. On the other hand, for a fixed amount of samples, a larger $\Delta t$ allows to train the model over a longer time span. As shown in Table 3, we considered the LSTM network with 1 layer and 90 neurons, and trained it using the same time series with $\Delta t = 10$, 1 and 0.1 time units. Note that the input dimension is maintained constant by setting $p = 10$. The number of time series and epochs for training were chosen so that it could be possible to compare models that have been trained on a similar number of samples. The results in Table 3 show that increasing the time step from 1 to 10 leads to a validation loss three orders of magnitude larger, a fact that indicates the difficulty in learning the model dynamics when such a coarse sampling in time is considered. On the other hand, reducing the time step from 1 to 0.1 does not yield any additional improvement in the predictions. The loss function has a similar trend and the final values are comparable when using time steps equal to 1 and 0.1, showing that most of the characteristics of
the system have been properly captured. It may be possible to find a $\Delta t$ that further reduces the error based on the temporal characteristics of the signal.

Table 3: Summary of LSTM cases and their performance using different numbers of training data sets and time resolutions. Note that we employed 90 units and $p = 10$ in all the cases. The statistical errors for LSTM1–10–1000 are not reported because the predictions exhibited a clearly non-physical behavior during all stages of training.

| Case        | N. Layers | $\Delta t$ | Training data sets | $E_u [%]$ | $E_{u^2} [%]$ | Validation Loss   |
|-------------|-----------|------------|--------------------|-----------|---------------|-------------------|
| LSTM1–1–100 | 1         | 1          | 100                | 0.26      | 0.59          | $6.68 \times 10^{-9}$ |
| LSTM1–01–100| 1         | 0.1        | 100                | 1.81      | 6.03          | $9.13 \times 10^{-10}$ |
| LSTM1–10–1000| 1         | 10         | 1,000              | –         | –             | $3.65 \times 10^{-5}$ |
| LSTM1–1–1000| 1         | 1          | 1,000              | 0.57      | 0.58          | $8.36 \times 10^{-9}$ |
| LSTM1–01–1000| 1         | 0.1        | 1,000              | 1.18      | 1.39          | $6.46 \times 10^{-9}$ |
| LSTM1–1–10000| 1         | 1          | 10,000             | 0.31      | 0.48          | $9.85 \times 10^{-9}$ |
| LSTM2–1–100 | 2         | 1          | 100                | 0.80      | 1.13          | $8.39 \times 10^{-9}$ |
| LSTM2–1–1000| 2         | 1          | 1,000              | 0.54      | 0.62          | $8.84 \times 10^{-9}$ |
| LSTM2–1–10000| 2        | 1          | 1,000              | 0.69      | 1.37          | $2.72 \times 10^{-9}$ |

5.3. Use of gated recurrent units (GRUs)

The performance of an alternative type of RNN, the so-called gated recurrent unit (GRU), is also studied here. The structure of GRU layers is simpler than in the LSTM, consisting of a single update gate instead of the forget and input gates. Also, the cell state and the output are merged into a single vector. The network architecture considered here has 1 layer of 90 nodes and it is similar in every aspect to the corresponding LSTM case, except for the node definition. The number of parameters that need to be optimized is smaller than in the LSTM, and therefore GRUs should require less computational resources to be trained. In our experience however, when training the considered architecture on CPU, the LSTM network was approximately as fast as its GRU counterpart. Despite the fact that it is possible to obtain similar validation losses with GRUs and LSTM networks, the resulting errors in the statistics are significantly higher in the former. In particular, when training with only 100 time series the predicted results exhibited a non-physical behavior. Although the results in Table 4 suggest that the predictions may improve when using much larger training databases, the LSTM networks provide much more accurate predictions and they are therefore preferred for the present application.

Table 4: Summary of GRU cases and their performance using different numbers of training data sets. Note that in all the cases 1 layer of 90 units was employed, with $p = 10$. The statistical errors for GRU100 are not reported because the predictions exhibited a clearly non-physical behavior during all stages of training.

| Case   | Training data sets | $E_u [%]$ | $E_{u^2} [%]$ | Validation Loss   |
|--------|--------------------|-----------|---------------|-------------------|
| GRU100 | 100                | –         | –             | $1.33 \times 10^{-8}$ |
| GRU1000| 1,000              | 2.30      | 12.49         | $6.13 \times 10^{-9}$ |
| GRU10000| 10,000             | 3.05      | 2.61          | $5.61 \times 10^{-9}$ |
6. Summary and conclusions

In this study we assessed the feasibility of using RNNs and Koopman-based frameworks to predict the temporal dynamics of the low-order model of near-wall turbulence by Moehlis et al. (2004). Our previous results (Srinivasan et al., 2019) indicated that it is possible to obtain excellent predictions of the turbulence statistics using LSTM networks. Here we show that it is possible to obtain the same level of accuracy for long-term predictions by utilizing the Koopman framework with nonlinearities modeled through external forcing. Both approaches are able to reproduce the temporal dynamics of the system characterized through e.g. Poincaré maps and Lyapunov exponents. However, the KNF method requires much less data and time for training: a data set with the size of 0.025% of that from the LSTM is sufficient to train the KNF model. Moreover, the training time of the LSTM network is about four orders of magnitude longer than that of the KNF model. Our results also indicate that the KNF method provides a longer prediction horizon for short-term forecasting in comparison with the LSTM network, producing accurate predictions (averaging over 500 time series) for 280 time units against 130 time units from the LSTM network. Furthermore, we show that even using relatively small LSTM networks trained with low numbers of time series, e.g. the LSTM1–1–100 case, it is possible to obtain very low errors in the mean and the fluctuations, i.e. $E_u = 0.26\%$ and $E_{u^2} = 0.59\%$. It is important to highlight that a loss function based only on the instantaneous predictions of the mode amplitudes may not lead to the best predictions in terms of turbulence statistics, and it is necessary to define a stopping criterion based on the values of $E_u$ and $E_{u^2}$. Our results also suggest that using more sophisticated loss functions, including not only the instantaneous predictions but also the averaged behavior of the flow, may lead to much faster neural-network training. It is however remarkable that using a simple loss function based on instantaneous values we also obtained very good predictions of Poincaré maps and Lyapunov exponents. We also assessed the impact of the time step, where the best network performance was obtained with $\Delta t = 1$. Additionally, we compared the performance of LSTM networks and GRUs, and the former clearly provided much better predictions.

The methods described in this work can be extended for their use in non-intrusive sensing applications (Borée, 2003) or in advanced flow-control methods (Tang et al., 2020), among others. In particular, the excellent short-term prediction capabilities of the KNF method may help to increase the temporal resolution of experimental measurements (Discetti et al., 2019), which may aid in the assessment of the dynamics of coherent structures in turbulent flows.

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