Reservoir computing model of two-dimensional turbulent convection

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Reservoir computing is one efficient implementation of a recurrent neural network that can describe the evolution of a dynamical system by supervised machine learning without solving the underlying mathematical equations. In this work, reservoir computing is applied to model the large-scale evolution and the resulting low-order turbulence statistics of a two-dimensional turbulent Rayleigh-Bénard convection flow at a Rayleigh number $Ra = 10^7$ and a Prandtl number $Pr = 7$ in an extended domain with an aspect ratio of 6. Our data-driven approach which is based on a long-term direct numerical simulation of the convection flow comprises a two-step procedure. (1) Reduction of the original simulation data by a Proper Orthogonal Decomposition (POD) snapshot analysis and subsequent truncation to the first 150 POD modes which are associated with the largest total energy amplitudes. (2) Setup and optimization of a reservoir computing model to describe the dynamical evolution of these 150 degrees of freedom and thus the large-scale evolution of the convection flow. The quality of the prediction of the reservoir computing model is comprehensively tested by a direct comparison of the results of the original direct numerical simulations and the fields that are reconstructed by means of the POD modes. We find a good agreement of the vertical profiles of mean temperature, mean convective heat flux, and root mean square temperature fluctuations. In addition, we discuss temperature variance spectra and joint probability density functions of the turbulent vertical velocity component and temperature fluctuation the latter of which is essential for the turbulent heat transport across the layer. At the core of the model is the reservoir, a very large sparse random network characterized by the spectral radius of the corresponding adjacency matrix and a few further hyperparameters which are varied to investigate the quality of the prediction. Our work demonstrates that the reservoir computing model is capable to model the large-scale structure and low-order statistics of turbulent convection which can open new avenues for modeling mesoscale convection processes in larger circulation models.
I. INTRODUCTION

The application of machine learning (ML) methods, in particular of deep neural networks (DNN)\cite{1–5}, to fluid flows has transformed the way of processing and analyzing large amounts of data. ML methods are used to parametrize unresolved scales in Reynolds stresses and subgrid scale models for complex physical or geometrical flow configurations at high Reynolds numbers which still remain inaccessible to direct numerical simulations or even large eddy simulations\cite{6–10}. They are also used for the detailed segmentation of complex images\cite{11, 12}. DNNs converted here large-scale patterns in an extended three-dimensional turbulent convection flow\cite{13, 14} into a planar dynamical network where the edges are regions of locally enhanced convective heat flux. All supervised ML algorithms make use of the fact that it is often easier to train a DNN with a number of labeled training data of an intended input-output behavior, than to develop a specific numerical code to provide the correct answer for all possible input data. During the training, information propagates forward through the network while weights and biases are updated at each neuron in each hidden layer of the network backwards from the output to the input layer. This back-and-forth iteration (which is called epoch) has to be repeated multiple times until a minimum of the loss function is obtained.

Turbulence problems are inherently highly chaotic with stochastic temporal variation of the involved fields. For such data, a large number of data points from the past evolution has to be processed by the DNN to predict the future values; in some cases they fail completely as for example discussed in detail in refs. \cite{15, 16}. Therefore, they suffer from a large dimension of the input vector which leads to expensive training procedures of the model. Recurrent neural networks (RNN) are better suited: due to their “internal memory” and feedback mechanisms they are by construction more appropriate to learn the dynamics (and thus the resulting statistics of the flow). The long short-term memory (LSTM) network\cite{17} is a specific subclass of RNNs, which provides a “gated mechanism” for information flow in a feedback loop. The “internal memory” allows the usage of a small number of hidden layers and short time series from the past in comparison to other DNNs. LSTMs have been applied recently with success for a small Galerkin 9-mode model of a turbulent shear flow\cite{18} and compared with a standard DNN\cite{19}. In order to circumvent expensive training procedures, echo state networks (ESN) or reservoir computing models (RCM)\cite{20, 21} seem to be a further alternative which is considered here. RCM have received recently renewed attention as a method of equation-free modeling of nonlinear dynamical systems, such as the 9-mode model\cite{22}, the Lorenz96 model\cite{23} or the one-dimensional partial differential Kuramoto-Sivashinsky equation\cite{24, 25}. These applications still had a relatively small number of degrees of freedom in comparison to a typical model for a turbulent flow.

The present work derives a reservoir computing model for a two-dimensional, fully turbulent Rayleigh-Bénard convection flow at a relatively large Rayleigh number of $Ra = 10^7$ and a Prandtl number of $Pr = 7$\cite{26, 27} in a domain $\Omega = L \times H$ with an aspect ratio $\Gamma = L/H = 6$ by means of reservoir computing. Here $L$ is the horizontal length and $H$ the height of the simulation domain. We set up a (Boussinesq-) equation-free model to describe the large-scale dynamics of the flow and to reproduce low-order statistics, such as profiles of the temperature fluctuations and the convective heat flux across the layer as well as the joint statistics of velocity components and temperature. This requires the following subsequent steps: (1) Data-driven reduction of the fully resolved direct numerical simulation (DNS) record to the most energetic degrees of freedom by a standard Proper Orthogonal Decomposition (POD) based on the snapshot method\cite{28–31}. (2) Construction and training of a RCM that predicts the dynamical evolution of the most energetic degrees of freedom obtained in step (1) and thus of the large-scale flow and the resulting statistics. We thus substitute a Galerkin-truncated reduced-order model (ROM), which is obtainable by a projection of the Boussinesq equations of turbulent convection on the individual POD eigenspaces, by the simple dynamics on a reservoir (which will be explained further below).

The combination of POD analysis and RNN has been reported by Deng et al.\cite{32} for the reconstruction of time-resolved turbulent flow measurement from discrete data obtained from the experiments, or by Mohan and Gaitonde\cite{33} for turbulent flow control. Pawar et al.\cite{34} combined POD with a standard DNN for predictions in a heated cavity flow.

The outline of this paper is as follows. Section II describes the Boussinesq model of turbulent Rayleigh-Bénard convection along with numerical procedure and some basic results. Section III illustrates the POD snapshot method. Section IV presents the RCM employed in this work and the variation of hyperparameters of the reservoir. The section discusses also the results which are obtained for the present application and provides a comparison with the original DNS and POD based data. We conclude with a summary and an outlook.

II. DIRECT NUMERICAL SIMULATION

Direct numerical simulations are applied to solve the Boussinesq equations for the two-dimensional case. These equations are made dimensionless by the height of the layer $H$, the free-fall velocity $U_f = \sqrt{g \alpha \Delta T H}$, where $g$ is the acceleration due to gravity, $\alpha$ is the thermal expansion coefficient at constant pressure, and $\Delta T$ represents the
imposed temperature difference between the bottom and the top. Times are expressed in units of the free-fall time $T_f = H/U_f$. The Rayleigh number is given by $Ra = g \alpha \Delta T H^3/(\nu \kappa) = 10^7$, the Prandtl number by $Pr = \nu/\kappa = 7$, and the aspect ratio is $\Gamma = L/H = 6$. Here, $\nu$ is the kinematic viscosity, $\kappa$ is the thermal conductivity of the fluid. The equations of motion in dimensionless form, which couple the two-dimensional velocity field $\mathbf{u} = (u_x, u_y)$, the pressure field $p$, and the temperature field $T$, are given by

\begin{align}
\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} &= -\frac{\partial p}{\partial x} + \sqrt{\frac{Pr}{Ra}} \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right), \\
\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} &= -\frac{\partial p}{\partial y} + \sqrt{\frac{Pr}{Ra}} \left( \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right) + T, \\
\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} &= \frac{1}{\sqrt{PrRa}} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right).
\end{align}

No-slip boundary conditions are imposed at the bottom ($y = 0$) and top ($y = 1$) for the velocity field. The temperature field is constant, $T = 1$ at $y = 0$ and $T = 0$ at $y = 1$. The side walls obey periodic boundary conditions for all fields. Equations (1)–(4) are numerically solved by the Nek5000 spectral element method package [35]. We use $N_c = 48 \times 16$ spectral elements and apply Lagrangian interpolations polynomials of order $N = 11$ on each element and in each spatial direction. Further details pertaining to the numerical procedure can be found in refs. [14, 27]. We sampled the turbulent flow every $0.25T_f$ for the subsequent POD snapshot analysis.

We apply the standard Reynolds decomposition which is given by

\begin{align}
&u_x(x, y, t) = \langle u_x(y) \rangle_{x,t} + u_x'(x, y, t) = u_x'(x, y, t), \\
&u_y(x, y, t) = \langle u_y(y) \rangle_{x,t} + u_y'(x, y, t) = u_y'(x, y, t), \\
&T(x, y, t) = \langle T(y) \rangle_{x,t} + T'(x, y, t),
\end{align}

Mean profiles which have been obtained by a combined $x$-line and time average are displayed in Fig. 1. In panel (a)

![FIG. 1. Mean profiles of (a): Temperature and (b): Velocity components. The average quantities are obtained by averaging in time and in homogeneous direction $x$. The diffusive equilibrium temperature profile $T_{lin}(y)$ is added to panel (a).](image)

of this figure we show linear profile of diffusive heat transfer $T_{lin}(y) = 1 - y$ which exists for Rayleigh numbers below the instability threshold $Ra_c = 1708$ together with the mean temperature profile $\langle T(y) \rangle_{x,t}$ for $Ra \gg Ra_c$. As expected the magnitude of mean velocity is practically zero which is shown in Fig. 1(b). This means that $u_x = u_x'$ and $u_y = u_y'$ as indicated in Eqns. (5) and (6). The DNS start from the diffusive equilibrium state and relax into the statistically stationary turbulent convection state after an initial period of $t \approx 100T_f$. Any subsequent snapshot analysis starts for $t > 100T_f$. For the data analysis, we interpolate all DNS snapshots spectrally onto a uniform, somewhat coarser two-dimensional mesh of $N_x \times N_y = 160 \times 108$ points. Our data base consists of $N_s = 2000$ equidistant simulation snapshots spanning a time range of $500T_f$. Figure 2 displays the time series of the Nusselt number, the dimensionless measure of the turbulent heat transfer, which is taken at the bottom and top plates as an average of the diffusive heat
III. PROPER ORTHOGONAL DECOMPOSITION OF SIMULATION DATA

Rather than using slices of DNS data as a direct input into a ML algorithm as done for example by King et al. [15] in a semi-supervised algorithm, we introduce an intermediate data reduction step. We take a standard POD analysis for simplicity, a prominent method to extract a subset of the energetically dominant degrees of freedom from the fully resolved turbulent convection data [28–31, 36, 37]. In detail, we will apply the snapshot method [38] which was developed by Sirovich and Park [28, 29]. Input is the three-dimensional vector field \( \mathbf{v} = (u_x, u_y, T') \) with zero mean, \( \langle \mathbf{v} \rangle_{x,y,t} = 0 \) and a mean turbulent energy (which comprises turbulent kinetic energy and scalar variance). It is given by

\[
E = \left\langle \int_{\Omega} (u_x^2 + u_y^2 + (T')^2) \, d\Omega \right\rangle = \left\langle \int_{\Omega} v^2 \, d\Omega \right\rangle. \tag{8}
\]

We want to determine POD modes \( \Phi(x) \) that maximize the functional

\[
\frac{\langle \langle (\mathbf{v}, \Phi) \rangle \rangle_t}{\langle \Phi, \Phi \rangle} \to \text{max}, \tag{9}
\]

where \( \langle \cdot, \cdot \rangle \) denotes a scalar product on \( L_2(\Omega, \mathbb{R}^2) \oplus L_2(\Omega) \) with \( \mathbf{u} = (u_x, u_y) \in L_2(\Omega, \mathbb{R}^2) \) and \( T' \in L_2(\Omega) \). Variational calculus translates (9) into the following integral equation

\[
\int \hat{K}_{ij}(x', x) \Phi^{(m)}_j(x') \, dx' \, dy' = \int \langle v_i(x, t) v_j(x', t) \rangle_t \Phi^{(m)}_j(x') \, dx' \, dy' = \lambda_m \Phi^{(m)}_i(x) \tag{10}
\]

with the Hermitean, non-negative kernel operator \( \hat{K}_{ij} \). Indices \( i, j, k, l = 1, 2, 3 \) and the Einstein summation convention is used. Index \( m \) is for the POD modes. The operator is described by \( 3N_xN_y \times 3N_xN_y \) matrix with \( N_x \times N_y \) being the size of the uniform data mesh. In addition, we use a Fourier expansion in the homogeneous \( x \)-direction and thus (10) translates into

\[
\int_0^1 \langle F_k(n_x, y, t) F^*_l(n_x, y', t) \rangle_t \Phi^{(m)}_{l,n_x}(y') \, dy' = \lambda_{k,n_x} \Phi^{(m)}_{k,n_x}(y) \tag{11}
\]

with (see [31] for details)

\[
F_k(n_x, y, t) = \frac{1}{L} \int_{-L/2}^{L/2} v_k(x, y, t) \exp \left( -i \frac{2\pi n_x x}{L} \right) \, dx \quad \text{and} \quad \Phi^{(m)}_k(x, y) \to \Phi^{(m)}_{k,n_x}(y) \exp \left( i \frac{2\pi n_x x}{L} \right) \tag{12}
\]
FIG. 3. Eigenvalue spectrum of POD modes as obtained from the analysis of 2000 DNS snapshots. (a): Individual contribution of each mode, and (b): Cumulative contribution of modes. The shaded region shows the contribution of first 150 modes which capture the 83% of the total energy of the convection flow and thus provides a good approximation of the large-scale structure.

Thus the velocity components and temperature fluctuation are expanded in the following POD base

\[ v_k(x, y, t) = \sum_{m, n_x=-N_x/2}^{N_x/2} a_{m, n_x}(t) \Phi_{k, n_x}^{(m)}(y) \exp \left( i \frac{2 \pi n_x x}{L} \right), \]

with \( m = 1, \ldots, 3N_xN_y = 51840, k = 1, 2, 3, n_x = -N_x/2, \ldots, N_x/2, \) and the reality condition \( a_{m, n_x}(t) = a_{m, -n_x}(t) \).

The snapshot method converts the eigenvalue problem (10) for the kernel operator into one for a \( N_s \times N_s \) matrix with \( N_s \ll 3N_xN_y \). We therefore expand the POD modes in the following way

\[ \Phi_{k, n_x}^{(m)}(y) = \sum_{n_s=1}^{N_s} \beta_{n_x}^{(m)}(n_s) F_k(n_x, y, n_s), \]

which is inserted into (12) and completes the procedure [31]. Here, \( n_s \) is the index of the DNS snapshot, a discrete time.

Figure 3 displays the spectrum of the eigenvalue analysis. The eigenvalues are sorted with respect to their magnitude which stands for the energy contained in the corresponding POD mode. As typical for a turbulent flow, the spectrum falls off quickly, but shows a long tail. We will truncate the POD mode expansion to the \( N_{\text{POD}} = 150 \) most energetic POD modes which contain 83 % after the total energy \( E \) as given by (8). This is shown in Fig. 3b. Other truncation levels can be taken, but would not change the subsequent results qualitatively. Figure 4 illustrates the spatial structure of the three components of the modes \( \Phi^{(1)}(x, y) \) and \( \Phi^{(50)}(x, y) \). We obtain the time-dependence of the expansion coefficients \( a_m(t) \) of the most energetic POD modes \( \Phi^{(m)} \) by

\[ a_m(t) = \left\langle v, \Phi^{(m)} \right\rangle = \left( \sum_{n, n_x} a_{n, n_x} \Phi_{n_x}^{(n)} \exp \left( \frac{2 \pi n_x x}{L} \right), \sum_{n_x} \Phi_{n_x}^{(m)} \exp \left( i \frac{2 \pi n_x x}{L} \right) \right\rangle = L \sum_{n_x} a_{m, n_x}(t). \]

Orthogonality of the POD modes has been used to obtain the final relation. The time series \( a_m(t) \) are used to train the reservoir computing model which is discussed in the following section. The first step of the RCM setup is now completed.

IV. RESERVOIR COMPUTING MODEL

A. Architecture and training of reservoir computing model

In the following, we summarize briefly the basics of the RCM, a special type of RNNs [5]. The RCM architecture is inspired by the brain where many neurons are randomly, recurrently and sparsely connected. Figure 5 shows the
FIG. 4. Spatial structure of two modes. (a,b): Temperature, (c,d): Horizontal velocity component, and (e,f): Wallnormal velocity component. Panels (a,c,e) are obtained from the 1st mode $\Phi(1)(x,y)$, panels (b,d,f) from the 50th mode $\Phi(50)(x,y)$. These modes are shown in simulation domain and were obtained by the inverse Fourier transform.

The general structure of a RCM. In the present case, the input consists of $a_i(t)$ with $i = 1, \ldots, N_{POD}$ and is converted into a reservoir input vector $r_k(t) \in \mathbb{R}^N$ with $N \gg N_{POD}$ by means of the random input weight matrix $W^{(in)} \in \mathbb{R}^{N \times N_{POD}}$. Here $N$ is the number of nodes in the reservoir, the latter of which is a big sparse random network which is described by a (symmetric) adjacency matrix $A$. The initialization is again randomly and different strategies for this initialization have been suggested which can improve the results as shown by Strauss et al. [39]. Two important parameters of $A$ are the density $D$ of active nodes and the spectral radius $\rho(A)$, which is set by the largest (real) eigenvalue. Across the reservoir nodes, a simple nonlinear dynamical system evolves which comprises the short-term memory of the network,

$$r_j(t + \Delta t) = (1 - \alpha)r_j(t) + \alpha \tanh \left[ A_{jk}r_k(t) + W^{(in)}_{jk}r_k(t) \right].$$

(16)

The nonlinearity enters in form of a typical activation function, here a hyperbolic tangent. A further parameter – the leakage rate $\alpha$ – enters the model which blends linear and nonlinear contributions. Optimally, the reservoir should be operated close to an instability which implies a spectral radius $\rho(A) \lesssim 1$. The final element is the random output weight matrix $W^{(out)} \in \mathbb{R}^{N_{POD} \times N}$.

The big advantage of the RCM is that the training is performed with respect to the output layer only. Thus a back propagation procedure that is required in case of DNNs is avoided (see e.g. [24, 25] for more details). The optimized output weight matrix, $W^{(out)*}$, is obtained by a minimization of a regularized quadratic cost function. A regularization term is added in the cost function to tackle the over-fitting problem [5]. During this training process, the number of nodes $N$, the reservoir density $D$, the spectral radius $\rho(A)$, the leaking rate $\alpha$, and the prefactor $\gamma$ of the regularization term $\gamma \text{Tr}[W^{(out)}(W^{(out)})^T]$ of the cost function are hyper-parameters to tune additionally.

The prediction mode of the RCM after the training with given POD coefficient time series, $a_i(t)$, is given by

$$r_j(t + \Delta t) = (1 - \alpha)r_j(t) + \alpha \tanh \left[ A_{jk}r_k(t) + W^{(in)}_{jk}r_k(t) + W^{(out)*}_{jm}r_m(t) \right].$$

(17)

This dynamics is used as a ROM to examine the large-scale evolution and low-order statistics of a two-dimensional turbulent convection flow without using the underlying Boussinesq equations (1)–(3).

B. Implementation of reservoir computing model

Previous studies that apply reservoir computing were mostly performed for dynamical systems with a smaller number of degrees of freedom as we discussed in the introduction. Here, we want to take the RCM approach to a new level of complexity by an application to a fully turbulent flow in an extended domain. This will result in
FIG. 5. The basic architecture of a reservoir computing model RCM (or echo state network ESN) consisting of an input layer, a reservoir, and an output layer. Dotted arrows mark connections which remain fixed during the training. The reservoir consists of \(N\) nodes and, both, the input and output layer have \(i = 1, \ldots, N_{\text{POD}}\) units. The reservoir substitutes the stack of hidden layers in a deep neural network.

Additional challenges that start with the architecture and training. The data base consists of the last 1400 (out of the originally 2000) snapshots of the turbulent velocity and temperature fields as reconstructed from the 150 POD modes. We use a 50-50% split of this dataset for training and testing. The current problem is related to time-series forecasting; therefore a random splitting of the data is not considered. The first 700 snapshots are used for the training of our RCM and the remaining 700 snapshots are exclusively used for (blind) testing of our framework. As already mentioned earlier, there are few tunable configuration parameters, commonly known as hyperparameters. All these parameters represent the dynamics of the reservoir \(A\) and thus affect the RCM [20, 21]. These hyperparameters have to be tuned carefully. Bayesian optimization [40, 41] is one of the sophisticated methods to find out the optimized hyperparameters in any machine learning task. Here, we applied a simpler grid search as a favorable option.

We use two measures to determine the quality of the RCM output in relation to the ground truth (GT) the latter of which provided by the training data. Note again, that ground truth in our case comprises the reconstructions of the large-scale convection flow as obtained from the first 150 POD modes. Therefore, we monitor the following mean square error (MSE) which is given by

\[
\text{MSE} = \frac{1}{N_s} \sum_{n=1}^{N_s} \left| a_{GT}^n - a_{RCM}^n \right|^2. \tag{18}
\]

We are however also interested in the actual flow quantities, such as mean and fluctuation profiles across the convection layer, and thus take furthermore the normalized average relative error (NARE) to ground truth, following [19] in this respect. For example, this error is given for the mean temperature profile by

\[
E \left(\langle T(y) \rangle \right) = \frac{1}{2 \max_{y \in [0,1]}} \left\{ \int_0^1 \left| \langle T(y) \rangle_{\text{GT}} - \langle T(y) \rangle_{\text{RCM}} \right| dy \times 100\% \right. \tag{19}
\]

Table I summarizes the MSE for both, training and testing phase, for different numbers of nodes in the reservoir \(N\), different spectral radii \(\rho(A)\) and leaking rates \(\alpha\), while leaving the other parameters unchanged. It is observed that the reservoir dynamics depends sensitively on all these parameters. The MSE shows its lowest training value at \(\rho = 0.4\), but the reconstructed flow results in a high NARE. This indicates our earlier argument regarding the necessity of an additional NARE monitoring of flow quantities rather than solely relying on the MSE of the POD expansion coefficients.

Table II depicts the final optimal values from the grid search. These values are obtained by a cross-validation procedure. Since we model a dynamical system that comprises of 150 modes, we need a large number of nodes \(N\) in
the reservoir $A$. However, this does not imply an unnecessarily large number of reservoir nodes. Such a case can lead to an overfitting because irrelevant statistical fluctuations in the training data will be learnt by the model [42]. The leaking rate $\alpha$ is kept close to 1 which indicates that reservoir evolves slowly [21, 24]. The spectral radius of adjacency matrix of the reservoir is the central parameter to tune [42]. We obtained a relatively large value of spectral radius close to one which was expected since our task involved long-memory dataset in which first few POD modes have the slow dynamics. Also, a spectral radius close to one drives the reservoir dynamics close to an instability as discussed in [5]. The training phases are relatively short and inexpensive when compared to standard DNN or LSTM networks since RCMs do not require a back-propagation. With the present data size, it took less than a minute when performed on 24 CPUs.

$$\langle (T')^2 \rangle = 0.95, \text{ and a leakage parameter } \alpha = 0.95. \text{ MSE is the mean square error.}$$

| $N$  | MSE $\times 10^{-5}$ Training/Test | $\rho(A)$ | MSE $\times 10^{-5}$ Training/Test | $\alpha$ | MSE $\times 10^{-5}$ Training/Test |
|------|-----------------------------------|-----------|-----------------------------------|---------|-----------------------------------|
| 1000 | 1.5/130.0                         | 0.1       | 0.2/68.1                          | 0.1     | 44.6/68.1                         |
| 1500 | 1.3/83.7                          | 0.4       | 0.1/71.6                          | 0.4     | 9.0/64.3                          |
| 2100 | 1.2/90.7                          | 0.7       | 0.4/88.4                          | 0.7     | 2.4/75.4                          |
| 3000 | 1.3/78.9                          | 0.95      | 1.2/90.7                          | 0.95    | 1.2/90.7                          |
| 10000| 1.6/80.9                          | 1.0       | 1.9/97.8                          |         |                                   |

TABLE II. Optimized hyperparamters which result from the grid search study. This includes the number of reservoir nodes $N$, the spectral radius $\rho(A)$, the leakage parameter $\alpha$, the reservoir density $D$, the prefactor of the regularization term $\gamma$, and the number of history points in the time series $p$. Note that $p > 1$ would be required for the input data if another RNN would have been applied. Also displayed are the mean square error MSE, see Eq. (18), and the normalized average relative error to ground truth as given by Eq. (19) for temperature fluctuations, mean temperature, and convective heat flux.

V. PREDICTION OF TWO-DIMENSIONAL TURBULENT CONVECTION

Figure 6 shows the temporal variation of four selected POD modes together with their predicted time series from our RCM. The prediction is good for first few coefficients. However, the capabilities decrease as one move towards the low-energy modes (i.e., with growing index $m$) due to highly nonlinear chaotic nature of the flow. Nevertheless, the predicted time series follow the trends of the original data closely. Moreover, the amplitude of fluctuations along with their frequency are also well predicted by the RCM. For instance, the first mode, $a_1(t)$ varies on a much smaller frequency as the last mode, $a_{150}(t)$ as seen in Fig. 6.

Figure 7 depicts an instantaneous snapshot of all three fields from the original DNS and compares the data with reconstructed field from the 150 POD modes as well as with the prediction from our RCM. We present results only for blind test to show the generality of trained network for all three variables, i.e., the temperature and the two velocity components. It can be observed that POD model can capture all the large-scale features of the turbulent convection flow with a very good quality. This includes a reproduction of the large-scale motion as seen in Figs. 7(b,c). Thermal plumes, which are a result of thermal boundary layer instabilities [43], can also be captured by the RCM which is a challenging task at such high Rayleigh number (see Fig. 7a).

Next, we report mean and fluctuations profiles of the flow in Fig. 8. Again we show a comparison between the DNS, the ROM based on POD snapshot analysis and the prediction from RCM. In the Boussinesq case, the flow has an up-down-symmetry with respect to the midline at $y = 0.5$ such that we show the upper half only and mirror the data from the lower half. This symmetry which is in line with a transformation $(x,u_x,u_y,T') \rightarrow (x,1-y,u_x,-u_y,-T')$ could possibly be embedded as a physical constraint into the model, a task which we leave for the future work on the three-dimensional case (see also [44] for a Hamiltonian system).

Figure 8a compares the mean temperature profiles $\langle T(y) \rangle_{x,t}$ which is perfectly reproduced by the POD as well as the reservoir computing. Figure 8b displays the mean profiles of the turbulent convective heat flux, $\langle u_y T' \rangle_{x,t}$. It
FIG. 6. Temporal evolution of four POD modes coefficients. From top to bottom: (a) $a_1(t)$; (b) $a_{50}(t)$; (c) $a_{100}(t)$, and (d) $a_{150}(t)$. The green shaded range shows the training part while the other range depicts the blind validation. Here $n_s = 1, \ldots, N_s = 1400$ is the snapshot index which translates with $t = (n_s/4)T_f$ into a time instant.

FIG. 7. Comparison of the turbulence fields. (a,d,g): Original DNS snapshot. (b,e,h): POD model reconstruction with the 150 most energetic modes which serves as the ground truth for our machine learning problem. (c,f,i): Predicted field from the reservoir computing model. In panels (a,b,c), the instantaneous temperature field $T(x, y, t_0)$ is shown, in (d,e,f) the velocity component $u_x(x, y, t_0)$, and in (g,h,i) the wallnormal velocity component $u_y(x, y, t_0)$.

can be seen that the RCM result is in good agreement with the POD data, both close to the wall and the center of the layer. A deviation to the original DNS data base is caused by the truncation at 83 % of the total energy. Figure 8c shows the temperature fluctuations $\langle (T')^2 \rangle^{1/2}_{x,t}$. Again the agreement is very good. To summarize, the RCM successfully predicts first and second-order statistics as demonstrated by these mean profiles.

To have a thorough comparison, we add results obtained for the Fourier spectra. Figure 9 depicts the spectrum of the temperature variance at three different locations $y_0$ in the wall-normal direction. As expected, both POD and RCM spectra deviate from the DNS spectra, particularly in the high-wavenumber tail representing the small eddies. The reason is the truncation to 150 POD modes. Our prediction from the RCM follows however closely the trend of
FIG. 8. Comparison line- and time averaged mean profiles obtained from original DNS, truncated POD, and RCM. (a): Mean temperature, (b): Mean turbulent convective heat flux, and (c): Root mean square fluctuations of temperature. The profiles in case of the RCM were obtained from the test data set only and thus not used in the training phase.

the POD-based ROM.

Furthermore, we show a comparison of probability density functions (PDF) of local convective heat flux at three different vertical locations in our turbulent convection domain. Figure 10 displays the PDFs and we can again observe a very good agreement, even for most of the tails of the distribution. After having found such a good agreement of the PDFs of turbulent heat flux, we assess the joint probability density function (JPDF) of the two individual fluctuating fields of the turbulent heat flux. We have therefore sampled instantaneous fluctuations of the wall normal velocity component $u'_y$ and the temperature fluctuation $T'$ at the midline. With these data, we determined the JPDF and their contours are shown in figure 11. The RCM is capable to reproduce the plume ejections from the bottom and the top which correspond to the skewness of the contours in the first and third quadrants, respectively.

FIG. 9. Comparison of energy spectra for temperature variance at different distances from the wall (a): $y_0 = 0.07$, (b): $y_0 = 0.15$, and (c): $y_0 = 0.50$. The legend indicates the three data sets taken for the calculation. Line color is the same for all three panels.

VI. CONCLUSIONS AND OUTLOOK

In the present work, we have discussed a machine learning–based approach to convective turbulence that aimed at a simple modeling of the large-scale evolution and low-order statistics. We applied a specific recurrent neural network with an efficient design, the reservoir computing model also known as the echo state network. Since it is not possible to feed the direct numerical simulation data directly into such a model, in particular in view to future applications to three-dimensional cases, we had to add an intermediate data reduction procedure. In this work, we applied therefore a standard and well-established Proper Orthogonal Decomposition snapshot analysis which extracted the most energetic degrees of freedom in form of empirical orthogonal modes of the fully turbulent flow at hand. Turbulence fields which
FIG. 10. Comparison of probability density function (PDF) of the local convective heat flux \((u'_y T'_y)\) at (a): \(y = 0.07\), (b): \(y = 0.15\), and (c): \(y = 0.50\). The legend indicates the three data sets taken for the calculation. Line color is the same for all three panels.

FIG. 11. Comparison of joint probability density function (JPDF) of the turbulent vertical velocity component and the turbulent temperature fluctuation, \(P(u'_y, T'_y)\), at the midline at \(y = 0.50\) (a): DNS, (b): POD, and (c): RCM. The isocontour levels in the legend are logarithmically spaced and hold for all three panels.

are reconstructed from this finite number of POD modes are the ground truth and serve as training and testing data for the reservoir computing model. The quality of the prediction of the reservoir computing model is in the final part of the work comprehensively tested. This is done by a direct comparison of the RCM results with both, the original direct numerical simulations and fields reconstructed with the POD modes. In detail, we find a good agreement of the vertical profiles of mean temperature, mean convective heat flux, and root mean square temperature. In addition, we discuss temperature variance spectra and joint probability density functions of the turbulent vertical velocity component and temperature fluctuation, the latter of which is essential for the turbulent heat transport across the layer.

Our presented work should be considered as a first step and a proof-of-concept investigation which certainly can be extended into several directions which we want to discuss briefly now. (1) Although, we report a rather comprehensive analysis of the reservoir parameters, a full Bayesian hyperparameter optimization might improve the performance of the RCM even further. (2) For the present case, it was not necessary to augment the training data since we could generate a long-term DNS record for the two-dimensional case with a reasonable computational effort. In a three-dimensional application this will not be the case anymore as discussed for example in refs. [12, 14]. Data augmentation can be done for example by using symmetries of the corresponding turbulent flow, an idea that goes back to Sirovich and Park in their application of POD to convection [28, 29]. Similar aspects of physics-informed ML were recently discussed in another context by Mattheakis et al. [44] for the symplectic nature of Hamiltonian systems which were modeled by neural networks. (3) First efforts have been discussed to generalize the RCM or ESN to deep-ESN for which consists of multiple reservoirs for a possible direct simulation data processing [45]. The successful application of this network architecture to turbulence is yet open.

To summarize, our presented reservoir computing model could successfully capture essential properties of the
dynamics of the larger scales of a turbulent convection flow. It is a recurrent neural network that describes the turbulent convection flow without explicit knowledge of the Boussinesq equations which can lead to interesting applications, e.g., for global circulation models where mesoscale (moist) convection processes have to be parametrized [46]. Our presented efforts will be extended to the three-dimensional RBC case and to subsequent tests of the performance of the RCM with respect to variations of $Ra$ and $Pr$.

[1] G. Hinton, L. Deng, and D. et al. Yu, “Deep neural networks for acoustic modeling in speech recognition,” IEEE Signal Process. Mag. 29, 82–97 (2012).
[2] M. I. Jordan and T. M. Mitchell, “Machine learning: Trends, perspectives, and prospects,” Science 349, 255–260 (2015).
[3] Y. LeCun, Y. Bengio, and G. Hinton, “Deep learning,” Nature 521, 436–444 (2015).
[4] J. Schmidhuber, “Deep learning in neural networks: An overview,” Neural Netw. 61, 85–117 (2015).
[5] I. Goodfellow, Y. Bengio, and A. Courville, Deep learning (MIT press, 2016).
[6] J. Ling, A. Kurzawski, and J. Templeton, “Reynolds averaged turbulence modeling using deep neural networks with embedded invariance,” J. Fluid Mech. 807, 155–166 (2016).
[7] J. N. Kutz, “Deep learning in fluid dynamics,” J. Fluid Mech. 814, 1–4 (2017).
[8] K. Duraisamy, G. Iaccarino, and H. Xiao, “Turbulence modeling in the age of data,” Annu. Rev. Fluid Mech. 51, 357–377 (2019).
[9] R. Fang, D. Sondak, P. Protopena, and S. Succi, “Neural network models for the anisotropic Reynolds stress tensor in turbulent channel flow,” J. Turb., 1–19 (2019).
[10] S. Brunton, B. R. Noack, and P. Koumoutsakos, “Machine learning for fluid mechanics,” Annu. Rev. Fluid Mech. 52, 477–508 (2020).
[11] O. Ronneberger, P. Fischer, and T. Brox, “U-Net: Convolutional networks for biomedical image segmentation,” LNCS 9351, 234–241 (2015).
[12] E. Fonda, A. Pandey, J. Schumacher, and K. R. Sreenivasan, “Deep learning in turbulent convection networks,” Proc. Natl. Acad. Sci. USA 116, 8667–8676 (2019).
[13] M. S. Emran and J. Schumacher, “Large-scale mean patterns in turbulent convection,” J. Fluid Mech. 776, 96–108 (2015).
[14] A. Pandey, J. D. Scheel, and J. Schumacher, “Turbulent superstructures in Rayleigh-Bénard convection,” Nat. Commun. 9, 2118 (2018).
[15] R. King, O. Hennigh, A. T. Mohan, and M. Chertkov, “From deep to physics-informed learning of turbulence: Diagnostics,” arXiv:1810.07785 (2018).
[16] A. T. Mohan, D. Daniel, M. Chertkov, and D. Livescu, “Compressed convolutional LSTM: An efficient deep learning framework to model high fidelity 3d turbulence,” arXiv:1903.00033 (2019).
[17] S. Hochreiter and J. Schmidhuber, “Long short-term memory,” Neural Comput. 9, 1735–1780 (1997).
[18] J. Moehlis, H. Faisst, and B. Eckhardt, “A low-dimensional model for turbulent shear flows,” New J. Phys. 6, 56 (2004).
[19] P. A. Srinivasan, L. Guastoni, H. Azizpour, P. Schlatter, and R. Vinuesa, “Predictions of turbulent shear flows using deep neural networks,” Phys. Rev. Fluids 4, 054603 (2019).
[20] H. Jaeger and H. Haas, “Harnessing nonlinearity: Predicting chaotic systems and saving energy in wireless communication,” Science 304, 78–80 (2004).
[21] M. Lukoševičius and H. Jaeger, “Reservoir computing approaches to recurrent neural network training,” Comput. Sci. Rev. 3, 127–149 (2009).
[22] S. Pandey, J. Schumacher, and K. R. Sreenivasan, “A perspective on machine learning in turbulent flows,” J. Turb., submitted (2020).
[23] P. R. Vlachas, J. Pathak, B. R. Hunt, T. P. Sapsis, M. Girvan, E. Ott, and P. Koumoutsakos, “Forecasting of spatiotemporal chaotic dynamics with recurrent neural networks: a comparative study of reservoir computing and backpropagation algorithms,” arXiv:1910.05266 (2019).
[24] Z. Lu, J. Pathak, B. R. Hunt, M. Girvan, R. Brockett, and E. Ott, “Reservoir observers: Model-free inference of unmeasured variables in chaotic systems,” Chaos 27, 041102 (2017).
[25] J. Pathak, B. R. Hunt, M. Girvan, Z. Lu, and E. Ott, “Model-free prediction of large spatiotemporally chaotic systems from data: A reservoir computing approach,” Phys. Rev. Lett. 120, 024102 (2018).
[26] F. Chillà and J. Schumacher, “New perspectives in turbulent Rayleigh-Bénard convection,” Eur. Phys. J. E 35, 58 (2012).
[27] J. D. Scheel, M. S. Emran, and J. Schumacher, “Resolving the fine-scale structure in turbulent Rayleigh-Bénard convection,” New J. Phys. 15, 113063 (2013).
[28] L. Sirovich and H. Park, “Turbulent thermal convection in a finite domain: Part I. Theory,” Phys. Fluids A 2, 1649–1658 (1990).
[29] H. Park and L. Sirovich, “Turbulent thermal convection in a finite domain: Part II. Numerical results,” Phys. Fluids A 2, 1659–1668 (1990).
[30] J. Bailon-Cuba, M. S. Emran, and J. Schumacher, “Aspect ratio dependence of heat transfer and large-scale flow in turbulent convection,” J. Fluid Mech. 655, 152–173 (2010).
[31] J. Bailon-Cuba and J. Schumacher, “Low-dimensional model of turbulent Rayleigh-Bénard convection in a Cartesian cell with square domain,” Phys. Fluids 23, 077101 (2011).
[32] Z. Deng, Y. Chen, Y. Liu, and K. C. Kim, “Time-resolved turbulent velocity field reconstruction using a long short-term memory (LSTM)-based artificial intelligence framework,” Phys. Fluids 31, 075108 (2019).

[33] A. T. Mohan and D. V. Gaitonde, “A deep learning based approach to reduced order modeling for turbulent flow control using LSTM neural networks,” arXiv:1804.09269 (2018).

[34] S. Pawar, S. M. Rahman, H. Vaddireddy, O. San, A. Rasheed, and P. Vedula, “A deep learning enabler for nonintrusive reduced order modeling of fluid flows,” Phys. Fluids 31, 085101 (2019).

[35] P. F. Fischer, “An overlapping Schwarz method for spectral element solution of the incompressible Navier-Stokes equations,” J. Comput. Phys. 133, 84–101 (1997).

[36] B. Podvin and A. Sergent, “Proper orthogonal decomposition investigation of turbulent Rayleigh-Bénard convection in a rectangular cavity,” Phys. Fluids 24, 105106 (2012).

[37] B. Podvin and A. Sergent, “A large-scale investigation of wind reversal in a square Rayleigh-Bénard cell,” J. Fluid Mech. 766, 172–201 (2015).

[38] J. Weiss, “A tutorial on the Proper Orthogonal Decomposition,” in AIAA Aviation 2019 Forum (2019) p. 3333.

[39] T. Strauss, W. Wustlich, and R. Labahn, “Design strategies for weight matrices of echo state networks,” Neural Comput. 24, 3246–3276 (2012).

[40] J. S. Bergstra, R. Bardenet, Y. Bengio, and B. Kégl, “Algorithms for hyper-parameter optimization,” in Advances in Neural Information Processing Systems (2011) pp. 2546–2554.

[41] J. Snoek, H. Larochelle, and R. P. Adams, “Practical bayesian optimization of machine learning algorithms,” in Advances in Neural Information Processing Systems (2012) pp. 2951–2959.

[42] H. Jaeger, Tutorial on training recurrent neural networks, covering BPPT, RTRL, EKF and the “echo state network” approach, Vol. 5 (GMD-Forschungszentrum Informationstechnik Bonn, 2002).

[43] A. K. De, V. Eswaran, and P. K. Mishra, “Dynamics of plumes in turbulent Rayleigh-Bénard convection,” Eur. J. Mech. B/Fluids 72, 164–178 (2018).

[44] M. Mattheakis, P. Protopapas, D. Sondak, M. Di Giovanni, and E. Kaxiras, “Physical symmetries embedded in neural networks,” arXiv:1904.08991 (2019).

[45] C. Gallicchio and A. Micheli, “Richness of deep echo state networks,” LNCS 11506, in press (2019).

[46] P. Gentine, M. Pritchard, S. Rasp, G. Reinaudi, and G. Yacalis, “Could machine learning break the convection parametrization deadlock,” Geophys. Res. Lett. 45, 5742 (2018).