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REDUCED-ORDER MODEL OF LARGE-SCALE STRUCTURES IN TURBULENCE IN A PERIODIC CUBE

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ABSTRACT
We propose a construction method of a closure model that reproduces the quasi-periodic dynamics of large-scale structures of turbulence driven by a steady force in a periodic cube. More concretely, using machine learning, we construct a model closed by variables that describe the dynamics of the largest eddies in the turbulence. Our novel model successfully reproduces the spatial structure and the quasi-periodic dynamics of the largest eddies. Furthermore, the fluctuation period is consistent with the results of direct numerical simulations.

INTRODUCTION
Turbulence is ubiquitous; therefore, its prediction is essential in many engineering applications. For this, we often employ large-eddy simulations (LES) to reduce computational cost by resolving only large-scale flow. To conduct LES, we need a turbulence model that characterizes how smaller-scale fluid motion impacts larger-scale one. Although LES with traditional turbulence models, such as the Smagorinsky model [Smagorinsky (1963)], has proven successful in real-world engineering applications [Meneveau & Katz (2000)], we must place the cut-off scale on a scale where the universality holds, i.e., within the inertial range. However, when considering transport phenomena, the relatively large-scale flows directly maintained by external force, mean flow, and boundary conditions are of utmost importance. If the cut-off scale exceeds an inertial-range scale, LES with conventional turbulence models often fails to be inaccurate, deviating greatly from the results of direct numerical simulations (DNS) [Fauconnier & Dick (2014)]. This significantly limits the ability to save computational costs.

The present study aims to construct an accurate closure model for turbulence motion larger than the inertial range. Here, we focus on turbulence driven by a steady force in a periodic cube. The dynamics of large-scale structures in the turbulence are quasi-periodic, and their fluctuation period is about twenty times the turnover time T_L of the largest eddies [Goto *et al.* (2017)]. When the cut-off scale is smaller than $L/4$, where L is the size of the largest eddies, LES with the Smagorinsky model can quantitatively reproduce the quasi-periodic dynamics [Yasuda *et al.* (2014)]. However, in our preliminary numerical experiments, LES with a cut-off scale larger than $L/4$ fails to reproduce such quasi-periodic dynamics. In this paper, we show that our novel model can correctly reproduce the quasi-periodic dynamics of the large-scale structures even when the cut-off scale is L, i.e., resolving only the largest eddies of the turbulence.

To model the turbulence motion larger than the inertial range, we employ a recurrent neural network called the echo state network (ESN) [Jaeger & Haas (2004)]. Machine learning (ML), such as ESN, has the potential to build appropriate models using only data without assuming the existence of the inertial range. Indeed, many previous studies have shown that ML is useful for turbulence modeling [Brunton *et al.* (2020)]. However, the required size, i.e., the number of nodes, of neural networks significantly increases with the dimensions of the input and output variables. Therefore, to construct the desired model, it is essential to appropriately reduce the dimensions of the input and output variables to ESN.

In the present study, we reduce the dimensions based on the physical properties of the turbulence in addition to using neural networks, and then model the dynamics of latent variables using ESN. Our approach differs from previous reduced-order modelings (ROM) [Hasegawa *et al.* (2020); Nakamura *et al.* (2021); Linot & Graham (2023)] because of the following two reasons. First, our modeling target is the three-dimensional turbulence with the hierarchical structures [Goto *et al.* (2017)]. In contrast, most previous ROM studies targeted turbulence without them, such as minimal wall turbulence [Jiménez & Moin (1991)]. Second, we model only the largest hierarchical structures, i.e., the largest eddies of the turbulence, which can be extracted by using a low-pass filter [Goto *et al.* (2017)]. Focusing on the hierarchical structures of turbulence, we study the ROM that is constructed in the following three steps: (i) extracting the largest eddies using the low-pass filter based on the recent knowledge of turbulence physics [Goto *et al.* (2017)], (ii) further reducing the dimensions of the low-pass filtered data using a convolutional neural network-based autoencoder (CNN-AE) [Hasegawa *et al.* (2020); Nakamura *et al.* (2021)], resulting in a few latent variables, and (iii) modeling the dynamics of the latent variables using ESN.

METHODS

Data Generation

We consider flow governed by the incompressible Navier–Stokes equations,

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u} = -\frac{\boldsymbol{\nabla} p}{\rho} + \nu\nabla^2\boldsymbol{u} + \boldsymbol{f}, \quad \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0, \qquad (1)$$

under periodic boundary conditions in the domain $[0,2\pi]^3$, where $\boldsymbol{u}(\boldsymbol{x},t)$, $p(\boldsymbol{x},t)$, ρ, and ν are the velocity field, pressure field, density, and kinematic viscosity, respectively, and $\boldsymbol{f}$ is the steady force described as,

$$\boldsymbol{f}(\boldsymbol{x}) = (-\sin x\cos y,\ \cos x\sin y,\ 0)^\top. \qquad (2)$$

Training and test datasets for neural networks are generated by DNS with a Fourier spectral method, which has been verified against the results from the study of Goto *et al.* (2017). The resolution N^3, density ρ, kinematic viscosity ν, and time steps Δt_{DNS} are chosen as $N^3 = 64^3$, $\rho = 1.0$, $\nu = 1.6\times10^{-2}$, and $\Delta t_{\mathrm{DNS}} = 3.0\times10^{-3}$, respectively.

As mentioned in the introduction, the primary purpose of the present study is to construct the closure model for turbulence motion larger than the inertial range. To this end, we use lowpass-filtered turbulence data for the modeling. More concretely, we extract flow fields for $|\boldsymbol{k}| \le 2$, where $\boldsymbol{k}$ is the wavenumber. These flow fields correspond to the largest eddies directly maintained by the steady force (2) and have a meandering structure in the z-direction (see the blue isosurfaces of figure 2).

Dimensionality Reduction

The following three steps achieve the dimensionality reduction of the input and output variables to ESN. First, we use only z-component of the lowpass-filtered vorticity $\omega_3^>(\boldsymbol{x},t)$ for the modeling. This variable selection reduces the dimension by a factor of $1/3$. This approach is appropriate because the flow field for $|\boldsymbol{k}| \le 2$ can be nearly perfectly captured by only $\omega_3^>$, as is evident from the definition (2) of $\boldsymbol{f}$ and the visualization results (figure 2). Next, we further reduce the dimension by a factor of $(1/4)^3$ by spatially sampling the grid points for every fourth point. Since the grid width for DNS is set to resolve the smallest eddies, the number (64^3) of original grid points is unnecessarily large for resolving only the largest-scale eddies. Therefore, we reduce the grid points as long as the fluctuations of the largest eddies are correctly captured. Finally, we reduce the dimension of $\omega_3^>(\bar{\boldsymbol{x}},t)$ by CNN-AE, where $\bar{x}$ is the sampled field. We describe the details of dimensionality reduction using CNN-AE below.

We show a schematic of the CNN-AE structure in figure 1. CNN-AE consists of an encoder, which maps input signals into a latent space, and a decoder, which expands the latent dimension and reconstructs the flow field. The encoder has alternating convolutional and pooling layers that reduce the input dimension by $(1/2)^3$. The decoder has alternating convolutional and upsampling layers that expand the latent dimension by a factor of 2^3 until it equals the input dimension. In the present study, we reduce the input dimension to 8. This value is chosen throughout the numerical experiments so that the reconstruction error of CNN-AE is small and ESN correctly reproduces the dynamics of largest eddies.

We use 5000 snapshots of the lowpass-filtered and sampled vorticity field $\omega_3^>(\bar{\boldsymbol{x}},t)$ to train CNN-AE. These snapshots are generated by DNS and sampled with a time interval $\Delta\tau = 4.5\times10^{-1}$, corresponding to $150\Delta t_{\mathrm{DNS}}$. The turnover time T_L of the largest eddies is about 0.56 in this case. Therefore, the training data length is about $4200T_L$. The weights of CNN-AE are optimized to minimize the squared error between the true vorticity field and the reconstructed one. The Adam algorithm proposed by Kingma & Ba (2014) is used as the optimizer for CNN-AE weights, and early stopping criteria proposed by Prechelt (1998) are applied to the training to avoid overfitting. We set the batch size and maximum epochs as 32 and 1000, respectively.

Modeling Dynamics of Latent Variables

For modeling the dynamics of the latent variables obtained by the dimensionality reduction, we use ESN proposed by Jaeger & Haas (2004). See Nakajima & Fischer (2021) for the details of ESN. The modeling of the latent variable dynamics consists of following three parts. Let $\boldsymbol{h}(t)$ denote the latent variables at time t. The first part is the one-step-ahead prediction of the sequence $\{\boldsymbol{h}(t)\}$; that is, we train ESN so that its output $\widetilde{\boldsymbol{h}}(t+\Delta\tau)$ is close to the true variables $\boldsymbol{h}(t+\Delta\tau)$, where the input to ESN is $\boldsymbol{h}(t)$. We use the time series $\{\boldsymbol{h}(t)\}$ of the latent variables corresponding to 3000 snapshots of $\omega_3^>(\bar{\boldsymbol{x}},t)$ for the training. Once the first part is completed, ESN can approximate the map from $\boldsymbol{h}(t)$ to $\boldsymbol{h}(t+\Delta\tau)$, i.e., $\boldsymbol{h}(t+\Delta\tau) \simeq \widetilde{\boldsymbol{h}}(t+\Delta\tau) = \boldsymbol{F}(\boldsymbol{h}(t),\boldsymbol{r}(t))$, where $\boldsymbol{F}$ is a map determined by the trained ESN, and $\boldsymbol{r}(t)$ is the state variable of ESN at t. In the second part of the modeling, the ESN dynamics is switched to the "self-feedback" mode; namely, the approximated latent states $\widetilde{\boldsymbol{h}}(t+\Delta\tau)$ are used for the input to ESN at the next step, and we obtain the future latent variables as $\widetilde{\boldsymbol{h}}(t+2\Delta\tau) = \boldsymbol{F}(\widetilde{\boldsymbol{h}}(t+\Delta\tau),\boldsymbol{r}(t+\Delta\tau))$. Repeating this procedure generates the time series $\{\widetilde{\boldsymbol{h}}(t)\}$. Finally, the decoder reconstructs the dynamics of the largest eddies from the time series $\{\widetilde{\boldsymbol{h}}(t)\}$.

RESULTS

First, we demonstrate the CNN-AE ability to reconstruct the lowpass-filtered vorticity fields when the latent dimension is 8. Figure 2 shows the visualization of the reconstructed $\omega_3^>(\bar{\boldsymbol{x}},t)$ by CNN-AE, using isosurfaces of the enstrophy $|\omega_3^>|^2$. CNN-AE appropriately reconstructs the vortex magnitudes and fluctuations in the z-direction. To quantify this result, we define the reconstruction error,

$$\mathscr{E}(t) = \frac{1}{\sigma^2 V}\int_V |\omega_3^>(\bar{\boldsymbol{x}},t) - \widetilde{\omega}_3^>(\bar{\boldsymbol{x}},t)|^2\,\mathrm{d}\bar{\boldsymbol{x}}, \qquad (3)$$

where $\omega_3^>$ and $\widetilde{\omega}_3^>$ are the true vorticity field and reconstructed one, respectively, and σ^2 is the variance of $\omega_3^>$ evaluated with the DNS result. Then, evaluating the time-averaged reconstruction error $\langle\mathscr{E}(t)\rangle_t$ of $\mathscr{E}(t)$, we obtain $\langle\mathscr{E}(t)\rangle_t \approx 4.4\times10^{-2}$. This result implies that CNN-AE accurately reconstructs the lowpass-filtered vorticity field and achieves the high dimensionality reduction ratio (about 1.0×10^{-5}).

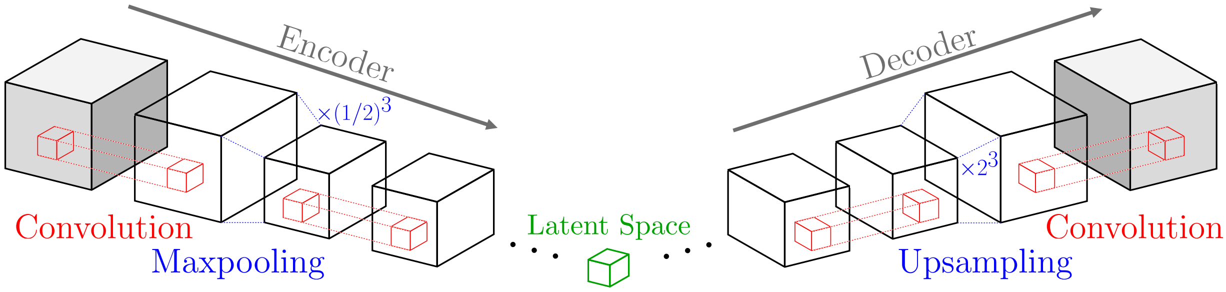


Figure 1. Schematic of CNN-AE structure. CNN-AE has two parts: an encoder and a decoder. The encoder consists of a convolution layer and a pooling layer connected alternately and reduces the input dimension. In the present study, we reduce the input dimension to 8. The decoder consists of a convolution layer and an upsampling layer connected alternately, which expands the latent dimension to the input dimension.

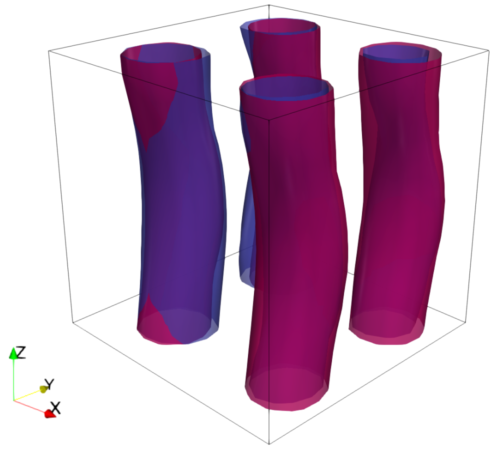
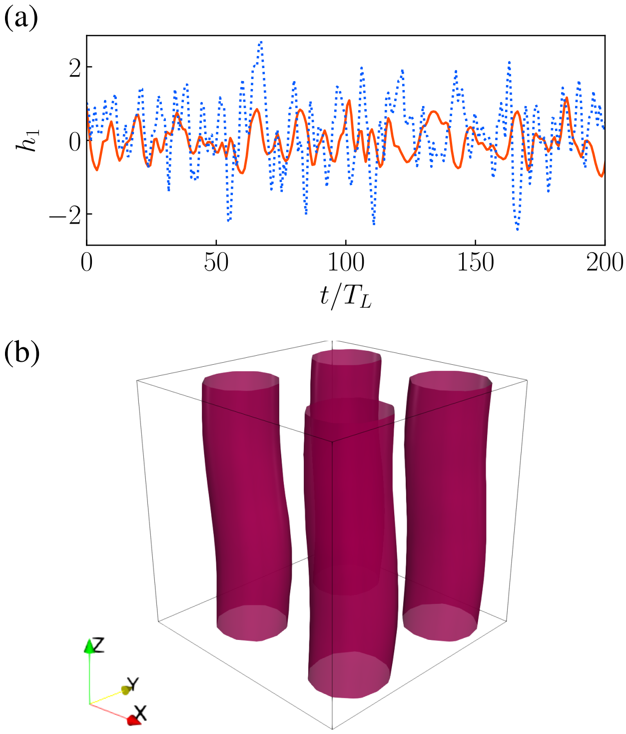


Figure 2. Visualization of the reconstructed vorticity field by CNN-AE (isosurfaces of $|\omega_3^>|^2$). The blue and red isosurfaces are the true and reconstructed vorticity fields, respectively. Here, the threshold is chosen as $m_q + 2\sigma_q$, where m_q and σ_q are the mean and standard deviation of $|\omega_3^>|^2$, respectively.

The remarkable success in the dimensionality reduction encourages us to construct the desired closure model. In fact, our model works well. Figure 3(a) shows the temporal evolution of the latent variable h_1 predicted by ESN. Although the time series of the model deviates from the true time series with time due to the chaotic nature of the sensitivity to initial conditions, and its magnitudes are smaller than the true ones, it shows irregular fluctuations similar to the true time series. We show in figure 3(b) the visualization result of the reconstructed flow. The model correctly reproduces the spatial structure of the largest eddies, such as the vortex magnitude and the winding in the z-direction. Figure 3(c) shows the time series of $\langle|\omega_3^>|^2\rangle_V$ evaluated from the reconstructed vorticity field. We can confirm the quasi-periodic fluctuation. Furthermore, its period is about $20T_L$, which is consistent with the DNS result by Goto *et al.* (2017). These results imply that it is possible to construct a model to describe the quasi-periodic dynamics of the largest eddies even when only they are resolved.



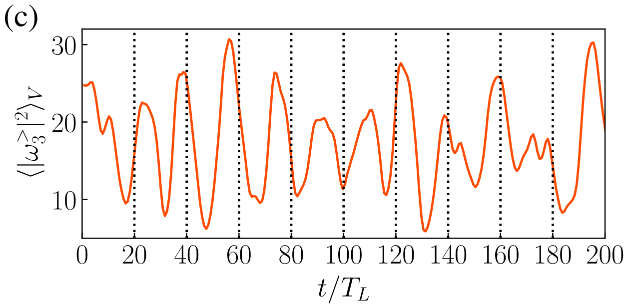


Figure 3. Modeling results. (a) Temporal evolution of the latent variable h_1. The blue dotted and red solid lines are the true and the modeled time series, respectively. (b) Visualization of the reconstructed vorticity field (isosurfaces of $|\omega_3^>|^2$). Here, the threshold is chosen the same as figure 2. (c) Time series of the volume-averaged enstrophy. To clarify the fluctuation period, we plot vertical lines every $20T_L$. Here, t is normalized by the turnover time T_L of the largest eddies.

CONCLUSIONS

We have constructed a closure model using ESN to describe the quasi-periodic dynamics of the largest eddies in turbulence driven by the steady force (2) in a periodic cube. The following two steps achieve this modeling. The first step is the dimensionality reduction of the input and output variables to ESN. In the present study, we have reduced the dimension of variables describing the dynamics of the largest eddies to 8 using a low-pass filter based on the recent knowledge of turbulence physics [Goto *et al.* (2017)], variable selection, spatial sampling, and CNN-AE (figure 1). Even with such a drastic dimensionality reduction, where the reduction rate is 1.0×10^{-5}, the reconstructed flow field is well consistent with the DNS results (figure 2). The second step is, using ESN, to build a model closed with the latent variables obtained in the first step. Although the instantaneous agreement of the temporal evolution is limited to finite time due to the sensitivity of initial conditions [figure 3(a)], our model reproduces the spatial structure [figure 3(b)] and the quasi-periodic dynamics [figure 3(c)] of the largest eddies directly generated by the steady force (2). Furthermore, the fluctuation period agrees well with the DNS result [Goto *et al.* (2017)]. These results support the feasibility of a model that describes the quasi-periodic dynamics of large structures in turbulence, even when resolving fluid motions larger than an inertial-range scale. At the same time, our results have opened the way to establish a new method that bridges the gap between Reynolds-averaged Navier–Stokes, which only captures the mean flow, and LES, which only cuts off the smaller scale than an inertial-range scale.

In the present study, we have investigated the generalization performance of the model for a single fixed Reynolds number. However, exploring its performance across various Reynolds numbers is crucial for real-world applications. Here, we recall the fact that the dynamics of large-scale structures in the turbulence are almost the same even when the Reynolds number increases [Goto *et al.* (2017)]. Since our approach focuses only on large-scale structures in turbulence, the model can be readily applied to cases with higher Reynolds numbers without the need for fine-tuning. Verifying this assertion is a target of our study in the near future.

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