A DATA-DRIVEN SGS MODEL THAT PRESERVES INFORMATION BASED ON THE LOCAL EQUILIBRIUM HYPOTHESIS

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ABSTRACT

Large-eddy simulation plays a crucial role in engineering applications by offering a cost-effective simulation of turbulent flows. In this study, we propose a novel data-driven subgrid scale model that reinterprets the local equilibrium hypothesis in terms of information preservation across scales. Our model achieves accuracy comparable to existing models in both homogeneous isotropic turbulence and wall turbulence, without any pre-determined parameters. This study explores the potential of turbulence models based on the information-theoretic framework of turbulence.

INTRODUCTION

Achieving accurate and efficient simulation of turbulence in engineering applications remains a challenging problem. Direct numerical simulation (DNS) resolves all eddy scales by numerically solving the Navier–Stokes equation without any model. However, its extremely high computational cost makes industrial application practically impossible. To address this limitation, large-eddy simulation (LES) has been widely used as it reduces the computational cost by solving the coarse-grained equations and resolving only the large-scale eddy structures. In the LES framework, a subgrid scale (SGS) model is introduced to represent the effects of unresolved small-scale eddy structures. In recent years, data-driven SGS models, including machine learning aided ones, have been proposed (Brunton *et al.*, 2020). Typical problems with the data-driven models are twofold: extrapolation and the black-box nature. The former deteriorates the model performance for the flows not included in the training data. The latter makes physical interpretation of the model difficult.

In recent years, information-theoretic analysis of turbulence has emerged as a branch of data-driven science. One of the main objectives of such studies is to investigate the energy cascade in developed 3D turbulence, i.e., a mechanism of energy transfer from large to small scales. Recent studies revealed scale-local nature of information transfer associated with the energy cascade (Lozano-Durán & Arranz, 2022; Tanogami & Araki, 2024; Araki *et al.*, 2024). These findings provide the foundation for an information-theoretic picture of turbulence.

In this study, we propose an SGS model that explicitly incorporates this mechanism as information preservation rather than information transfer. To this end, we introduce another length scale in the LES formulation, called the test scale (TS). We formulate our SGS model based on the concept of "information preservation". We found that our model achieves generalizability and interpretability, both of which are difficult to obtain in conventional data-driven SGS models (Hashimoto *et al.*, 2026).

In this manuscript, we first introduce the information-theoretic framework. Then, we describe the formulation of our proposed SGS model, called the information-preserving coherent structure model (IP-CSM). The results section shows the performance of our model in the periodic box turbulence and the channel turbulence, followed by the conclusion section summarizing our work.

INFORMATION THEORY

Information theory is the theoretical framework for information communication proposed by Shannon (1948). This theory quantifies the amount of information, often used ambiguously in our daily life, based on uncertainty. We define the Shannon entropy (SE) of a continuous random variable X with a probability density function $p(x)$ as

$$H(X) = -\int_{-\infty}^{\infty} p(x)\log p(x)\,\mathrm{d}x. \tag{1}$$

For two variables X and Y, we have the joint entropy

$$H(X,Y) = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x,y)\log p(x,y)\,\mathrm{d}x\mathrm{d}y. \tag{2}$$

With these quantities, we define the mutual information

$$I(X:Y) = H(X)+H(Y)-H(X,Y), \tag{3}$$

representing the information shared by X and Y. It becomes zero when X and Y are independent, and attains maximum when $X=Y$. We use mutual information as it can capture nonlinear dependencies, unlike the correlation coefficient.

GOVERNING EQUATIONS AND MODELING ASSUMPTIONS

We consider the coarse-grained continuity equation

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{4}$$

and the Navier–Stokes equation

$$\frac{\partial \overline{u}_i}{\partial t}+\overline{u}_j\frac{\partial \overline{u}_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i}+\nu\frac{\partial^2\overline{u}_i}{\partial x_j\partial x_j}+\overline{f}_i-\frac{\partial \tau_{ij}}{\partial x_j}. \tag{5}$$

Here, u_i, p, f_i denote the velocity, pressure, and external force, respectively. The flow is parameterized by the density ρ and kinematic viscosity ν. Besides, $\overline{(\cdot)}$ represents coarse-graining by a low-pass filter. Throughout the study, we employ a Gaussian filter

$$\overline{\phi}=\iiint G(\boldsymbol{x}-\boldsymbol{x}';\Delta)\phi(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}', \tag{6}$$

$$G(\boldsymbol{x};\Delta)=\prod_{i=1}^{3}\sqrt{\frac{6}{\pi\Delta^2}}\exp\left(-\frac{6x_i^2}{\Delta^2}\right), \tag{7}$$

where Δ is the filter width of the grid scale (GS). The last term in the right-hand side of Eq. (5) represents the SGS stress

$$\tau_{ij}=\overline{u_iu_j}-\overline{u}_i\overline{u}_j, \tag{8}$$

which cannot be computed from the GS velocity field. Thus, we need to introduce an SGS model defined by the GS velocity field.

To this end, we assume that τ_{ij} to be written by the rate-of-strain tensor

$$S_{ij}=\frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j}+\frac{\partial \overline{u}_j}{\partial x_i}\right) \tag{9}$$

and the rate-of-rotation tensor

$$\Omega_{ij}=\frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j}-\frac{\partial \overline{u}_j}{\partial x_i}\right), \tag{10}$$

as proposed by Lund & Novikov (1993). From the Cayley–Hamilton theorem and stress symmetry, we can express τ_{ij} as a linear combination of the following five tensors:

$$\begin{aligned}\tau_{ij}^{\mathrm{mod}}=&\underbrace{C_1f_1\Delta^2|\boldsymbol{S}|S_{ij}}_{M_{ij}^{[1]}}+\underbrace{C_2f_2\Delta^2S_{ik}S_{kj}}_{M_{ij}^{[2]}}+\underbrace{C_3f_3\Delta^2\Omega_{ik}\Omega_{kj}}_{M_{ij}^{[3]}}\\&+\underbrace{C_4f_4\Delta^2(S_{ik}\Omega_{kj}-\Omega_{ik}S_{kj})}_{M_{ij}^{[4]}}\\&+\underbrace{C_5f_5\frac{\Delta^2}{|\boldsymbol{S}|}(S_{ik}S_{kl}\Omega_{lj}-\Omega_{ik}S_{kl}S_{lj})}_{M_{ij}^{[5]}}.\end{aligned} \tag{11}$$

Here, $f_i(\boldsymbol{x},t)$ is a function of the invariants of S_{ij} and Ω_{ij}, and $C_i(t)$ is a time-dependent model coefficient.

MODEL TERM SELECTION

For the simplicity of the mode, we construct a two-term model from Eq. (11) as

$$\tau_{ij}^{\mathrm{mod}}=M_{ij}^{[\alpha]}+M_{ij}^{[\beta]},\quad \alpha,\beta\in\{1,2,...,5\}. \tag{12}$$

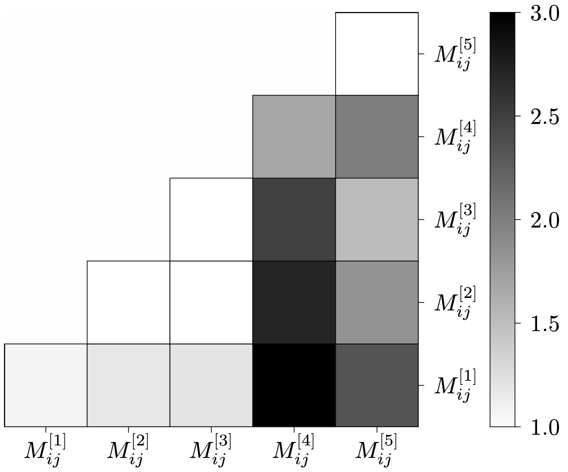


Figure 1: Mutual information of two energy fluxes and the force, Eq. (13), evaluated by the "true" SGS stress Eq. (8) and its model SGS Eq. (12). The row and column indicates the selected two terms from the right hand side of Eq. (11) in the model.

Here, the combination of (α,β) is chosen from Fig. 1, which shows the mutual information between the energy production $\tau_{ij}S_{ij}$ and the SGS stress divergence $\partial_j\tau_{ij}$,

$$I\left(\left[\tau_{ij}S_{ij},\frac{\partial\tau_{ij}}{\partial x_j}\right]:\left[\tau_{ij}^{\mathrm{mod}}S_{ij},\frac{\partial\tau_{ij}^{\mathrm{mod}}}{\partial x_j}\right]\right). \tag{13}$$

From this result, we choose $(\alpha,\beta)=(1,4)$ with the largest value of I. The resulting model reads

$$\tau_{ij}^{\mathrm{mod}}=C_1f_1\Delta^2|\boldsymbol{S}|S_{ij}+C_4f_4\Delta^2(S_{ik}\Omega_{kj}-\Omega_{ik}S_{kj}). \tag{14}$$

This combination is consistent with Lund & Novikov (1993) and has been adopted in many SGS models (Silvis, 2020; Lozano-Durán & Arranz, 2022).

DETERMINATION OF INVARIANT PARAMETERS

In this section, we determine the invariant parameters $f_1(\boldsymbol{x},t)$ and $f_4(\boldsymbol{x},t)$ in Eq. (14). To this end, we use the coherent structure function

$$F_{\mathrm{CS}}=\frac{\Omega_{ij}\Omega_{ij}-S_{ij}S_{ij}}{\Omega_{kl}\Omega_{kl}+S_{kl}S_{kl}}, \tag{15}$$

proposed by Kobayashi (2005). We define the invariant parameters as

$$f_1=|F_{\mathrm{CS}}|^{\frac{3}{2}},\quad f_4=|F_{\mathrm{CS}}|^2, \tag{16}$$

in order to satisfy the near-wall scaling of the SGS stress.

ESTIMATION OF MODEL PARAMETERS

In this section, we estimate the model parameters $C_1(t)$ and $C_4(t)$. For this purpose, we introduce the test scale (TS)

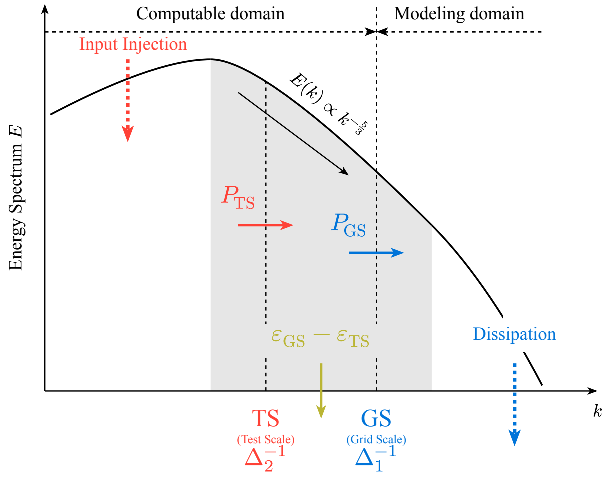


Figure 2: Schematic energy spectrum with energy balance. Energy production at the test and grid scales are denoted by P_{TS} and P_{GS}, respectively. Cumulative energy dissipation rates up to the test and grid scales are denoted by $\varepsilon_{\mathrm{GS}}$ and $\varepsilon_{\mathrm{TS}}$, respectively.

$\Delta_2 > \Delta_1$, as shown in Fig. 2. With the corresponding filter operation at the TS as $\widetilde{(\cdot)}$, we can define the kinetic energy of GS and TS as

$$k_{\mathrm{GS}} = \frac{1}{2}\bar{u}_i\bar{u}_i, \quad k_{\mathrm{TS}} = \frac{1}{2}\tilde{\bar{u}}_i\tilde{\bar{u}}_i, \tag{17}$$

respectively. To consider the energy balance between the GS and TS, we define the energy contained between TS and GS as

$$k_{\mathrm{TG}} = \widetilde{k_{\mathrm{GS}}} - k_{\mathrm{TS}}. \tag{18}$$

Its temporal evolution is described by

$$\frac{\partial k_{\mathrm{TG}}}{\partial t} + \tilde{\bar{u}}_j \frac{\partial k_{\mathrm{TG}}}{\partial x_j} = -\left(\widetilde{P_{\mathrm{GS}}} - P_{\mathrm{TS}}\right) - \left(\widetilde{\varepsilon_{\mathrm{GS}}} - \varepsilon_{\mathrm{TS}}\right). \tag{19}$$

Note that the energy production P and the energy dissipation ε are defined as

$$P_{\mathrm{GS}} = -\tau_{ij}S_{ij}, \qquad P_{\mathrm{TS}} = -(\widetilde{\bar{u}_i\bar{u}_j} - \tilde{\bar{u}}_i\tilde{\bar{u}}_j)\tilde{S}_{ij}, \tag{20}$$

$$\varepsilon_{\mathrm{GS}} = 2\nu S_{ij}S_{ij}, \qquad \varepsilon_{\mathrm{TS}} = 2\nu\tilde{S}_{ij}\tilde{S}_{ij}, \tag{21}$$

respectively. Spatial average of Eq. (19) reads

$$\left\langle \frac{\partial k_{\mathrm{TG}}}{\partial t} \right\rangle_V = \left\langle -(\widetilde{P_{\mathrm{GS}}} - P_{\mathrm{TS}}) - (\widetilde{\varepsilon_{\mathrm{GS}}} - \varepsilon_{\mathrm{TS}}) \right\rangle_V. \tag{22}$$

Here, $\langle\cdot\rangle_V$ denotes the spatial integral $\int_V \cdot\, \mathrm{d}V$ with appropriate boundary conditions.

Then, we assume that the temporal variation of k_{TG} is negligible compared to the energy production-dissipation balance. Upon this assumption, we arrive at the local equilibrium hypothesis

$$\langle P_{\mathrm{TS}} + \varepsilon_{\mathrm{TS}} \rangle_V = \left\langle \widetilde{P_{\mathrm{GS}}} + \widetilde{\varepsilon_{\mathrm{GS}}} \right\rangle_V. \tag{23}$$

Table 1: Parameters of the DNS and LES for the periodic box turbulence and the channel turbulence. The grid resolution N; the computational domain size L.

		$N_x \times N_y \times N_z$	$L_x \times L_y \times L_z$
Periodic	DNS	512^3	$(2\pi)^3$
	LES	64^3	
Channel	DNS	$2048 \times 480 \times 512$	$6.4 \times 2.0 \times 3.2$
	LES	$64 \times 64 \times 64$	

By assuming this relation to hold in a spatially local subdomain $v \in V$, we obtain

$$\langle P_{\mathrm{TS}} + \varepsilon_{\mathrm{TS}} \rangle_v = \left\langle \widetilde{P_{\mathrm{GS}}} + \widetilde{\varepsilon_{\mathrm{GS}}} \right\rangle_v. \tag{24}$$

By substituting the definition of τ_{ij}^{mod}, Eq. (14) into this relation, we obtain

$$\begin{aligned} \Gamma_1 &= \Gamma_2(C_1, C_4), \\ \Gamma_1 &= \left\langle \left(\widetilde{\bar{u}_i\bar{u}_j} - \tilde{\bar{u}}_i\tilde{\bar{u}}_j\right) + \varepsilon_{\mathrm{TS}} \right\rangle_v, \\ \Gamma_2(C_1, C_4) &= \left\langle \tilde{\tau}_{ij}^{\mathrm{mod}}\tilde{S}_{ij} - \widetilde{\tau_{ij}^{\mathrm{mod}}S_{ij}} + \widetilde{\varepsilon_{\mathrm{GS}}} \right\rangle_v. \end{aligned} \tag{25}$$

Note that Γ_1 is independent of the model parameters $C_i(t)$. We interpret this local equilibrium as 'information preservation' to evaluate $C_i(t)$ by maximizing the mutual information

$$C_1, C_4 = \arg\max_{C_1, C_4} I(\Gamma_1 : \Gamma_2). \tag{26}$$

IP-CSM SIMULATION PROCEDURE

Figure 3 summerizes the algorithm of our model, called the information-preserving coherent structure model (IP-CSM). This model follows the same conceptual framework as the information-preserving SGS (IP-SGS) model proposed by Lozano-Durán & Arranz (2022). The key difference lies in the model parameter estimation method: the IP-SGS utilizes scaling laws of probability distributions that involve an *a priori* parameter, while IP-CSM does not rely on any *a priori* scaling.

A POSTERIORI TEST

We conduct an *a posteriori* test to evaluate the performance of our IP-CSM in two flow configurations: periodic box turbulence and wall-bounded turbulence. For comparison, we also conducted LES with the Smagorinsky model (Smagorinsky, 1963)

$$\tau_{ij}^{\mathrm{mod}} = -2(C_S f_s \Delta)^2 |\boldsymbol{S}| S_{ij}, \tag{27}$$

and the coherent structure model (CSM) (Kobayashi, 2005)

$$\tau_{ij}^{\mathrm{mod}} = -0.1\Delta^2 |F_{\mathrm{CS}}|^{\frac{3}{2}} |\boldsymbol{S}| S_{ij}. \tag{28}$$

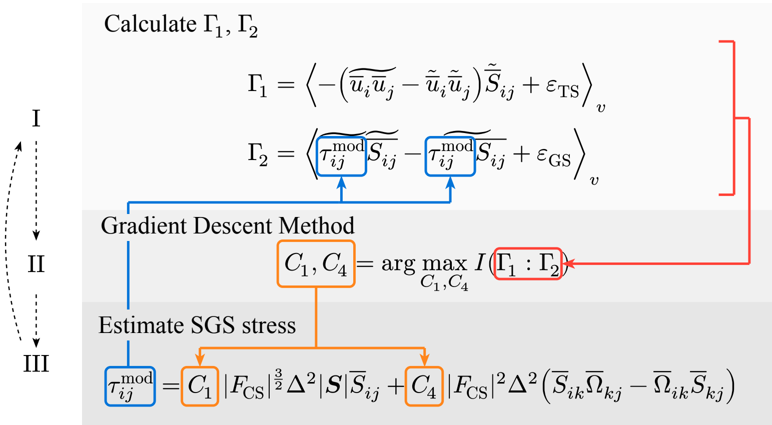


Figure 3: Flowchart for the IP-CSM. Step I–III are repeated with the gradient descent method until the mutual information $I(\Gamma_1 : \Gamma_2)$ reaches its maximum.

Here, the Smagorinsky constant C_S is set to 0.17 for the periodic box turbulence and 0.1 for the wall-bounded turbulence. Since the standard Smagorinsky model does not satisfy the near-wall scaling, we introduce the damping function f_s as

$$f_s = 1 - \exp\left(-\frac{y^+}{A^+}\right), \quad A^+ = 25, \tag{29}$$

only for the wall-bounded turbulence. The parameters of the DNS and LES are summarized in Table 1.

We first evaluate our model in the periodic box turbulence, as shown in Fig. 4. All three models and the coarse-grained DNS exhibit the characteristic $k^{-5/3}$ scaling of fully-developed turbulence. Similarly, different models reproduce the similar epectra of energy flux Π, indicating the energy cascade mechanism is captured by all the models. From these results, we confirm that our IP-CSM reproduces the low-order turbulent statistics without any pre-determined parameters.

We next evaluate our model in the channel turbulence, as shown in Fig. 5. IP-CSM reproduces the mean velocity profile in the three regions: linear, buffer, and log layers, along with the Smagorinsky model with the wall function and the CSM. The Reynolds shear stress profile is also well reproduced, owing to the invariant parameters $f_i(\boldsymbol{x},t)$ that satisfy the near-wall scaling. These results indicate that our model attains a similar performance compared to the existing models in the channel turbulence, without *a priori* parameters or wall function.

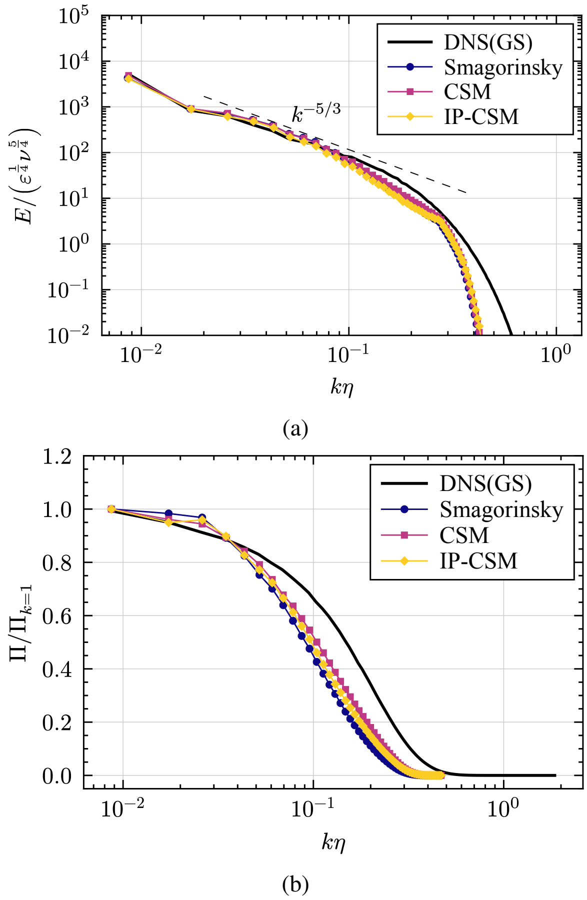


Figure 4: (a) Energy and (b) energy flux spectra in the periodic-box turbulence. In panel (a), the dashed line indicates the $k^{-5/3}$ scaling. Note that the DNS (GS) results are computed from the coarse-grained velocity field at scale Δ.

CONCLUSION

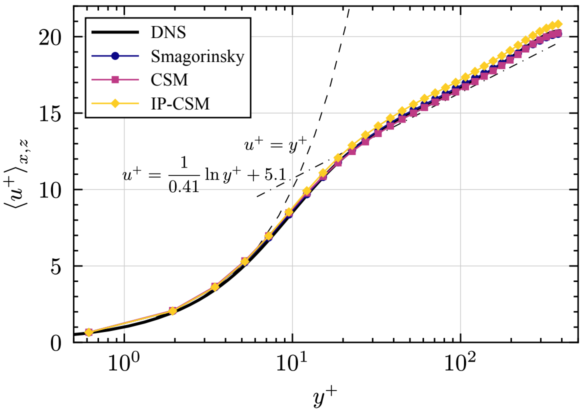
In this study, we proposed a data-driven SGS model called IP-CSM based on the information preservation between two adjacent scales, inspired by the local equilibrium hypothesis (Hashimoto *et al.*, 2026). Our new model is independent of *a priori* parameters and wall functions, yet it reproduces key turbulent statistics in both periodic box turbulence and wall-bounded turbulence. As future work, we aim to improve the accuracy of our model by extending the local equilibrium hypothesis and introducing information flow (Araki *et al.*, 2024; Tanogami & Araki, 2024), instead of information preservation.

REFERENCES

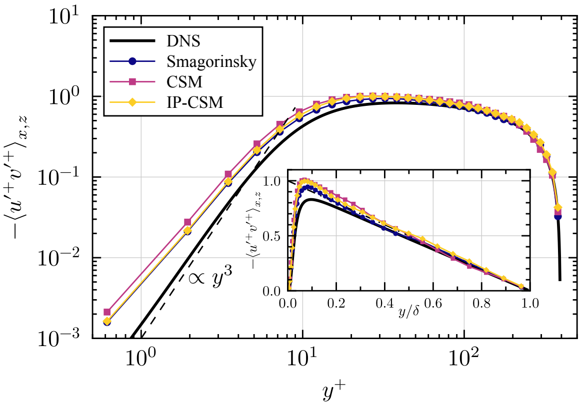
Araki, R., Vela-Martín, A. & Lozano-Durán, A. 2024 Forgetfulness of turbulent energy cascade associated with different mechanisms. *Journal of Physics: Conference Series* **2753** (1), 012001.

Brunton, S. L., Noack, B. R. & Koumoutsakos, P. 2020 Machine learning for fluid mechanics. *Annual Review of Fluid Mechanics* **52** (1), 477–508.

Hashimoto, T., Tsukahara, T. & Araki, R. 2026 Information-preserving SGS model based on the local inter-scale equi-



(a)



(b)

Figure 5: (a) Mean streamwise velocity profile and (b) Reynolds shear stress profile as a function of the wall-normal distance y^+ in wall units for the channel turbulence at a friction Reynolds number of 395. Note that $\langle\cdot\rangle_{x,z}$ denotes the spatial average in the streamwise and spanwise directions.

librium hypothesis. In prep.

Kobayashi, H. 2005 The subgrid-scale models based on coherent structures for rotating homogeneous turbulence and turbulent channel flow. *Physics of Fluids* **17** (4), 045104.

Lozano-Durán, A. & Arranz, G. 2022 Information-theoretic formulation of dynamical systems: Causality, modeling, and control. *Physical Review Research* **4**, 023195.

Lund, T. S. & Novikov, E. 1993 Parameterization of subgrid-scale stress by the velocity gradient tensor. In *Proceedings of NASA Annual Research Briefs*. 94N12286.

Shannon, C. E. 1948 A mathematical theory of communication. *Bell System Technical Journal* **27** (3), 379–423.

Silvis, M. H. 2020 Physics-based turbulence models for large-eddy simulation: Theory and application to rotating turbulent flows. PhD thesis, University of Groningen, The Netherlands.

Smagorinsky, J. 1963 General circulation experiments with the primitive equations: I. the basic experiment. *Monthly Weather Review* **91** (3), 99–164.

Tanogami, T. & Araki, R. 2024 Information-thermodynamic bound on information flow in turbulent cascade. *Physical Review Research* **6**, 013090.