Numerical Accuracy of Advection Scheme Necessary for Large-Eddy Simulation of Planetary Boundary Layer Turbulence

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ABSTRACT: Recently, large-eddy simulation (LES) has been increasingly employed in meteorological simulations because it is a promising method for turbulent parameterization. However, it is still difficult to affirm that the numerical accuracy required for a dynamical core is fully understood. In this study, we derived two theoretical criteria for the order of accuracy of the advection term in a typical situation of the atmospheric boundary layer, and demonstrate their validity by numerical experiments. In the targeted grid-spacing of $O(10)$ m, we determined the required order of accuracy as follows: Based on the criterion of the numerical diffusion error, the upwind scheme must have at least seventh-order accuracy. The fourth-order central scheme is barely acceptable with fourth-order explicit diffusion, provided that its coefficient is one or two orders of magnitude smaller than the implicit diffusion coefficient of the third-order upwind scheme. Based on the criterion of numerical dispersion error, at minimum, the seventh or eighth order is required. The dispersion error was indirect for the energy spectra, although we expect it may affect the local turbulence mechanism. We also investigated the effects of temporal discretization for compressible models, and found that relatively lower-order time schemes are available up to the $O(10)$ m grid spacing if the time step is sufficiently small due to sound wave limitations. The importance of the derived criteria is that the required order of accuracy increases as the grid spacing decreases. This suggests that considerable care should be taken regarding the numerical error problem for future high-resolution LES.

KEYWORDS: Large eddy simulations; Model evaluation/performance; Numerical analysis/modeling; Parameterization; Subgrid-scale processes

1. Introduction

The spatial resolution of atmospheric models has been recently increasing to explicitly treat cloud dynamics using microphysics schemes. In the Dynamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains (DYAMOND) project, Stevens et al. (2019) compared the results of various global high-resolution models with a several-kilometer mesh in the horizontal direction: the Non-hydrostatic ICosahedral Atmospheric Model (NICAM; Tomita and Satoh 2004; Satoh et al. 2014), the ICosahedral Non-hydrostatic model (ICON; Zängl et al. 2015), the Model for Prediction Across Scales (MPAS; Skamarock et al. 2012), and the Goddard Earth Observing System model version 5 (GEOS-5; Putman and Suarez 2011). As an extreme high-resolution case, Miyamoto et al. (2013) successfully conducted global cloud-resolving simulation with a subkilometer horizontal mesh. Considering atmospheric turbulence, the spatial resolutions of those global simulations with several- or subkilometer horizontal mesh are still insufficient for the explicit representation of boundary layer turbulent eddies.

Usually, the effect of turbulence in such simulations is often parameterized by Reynolds-averaged Navier–Stokes (RANS) models (e.g., Mellor and Yamada 1974).

In contrast, many studies (e.g., Wyngaard 2004; Honnert et al. 2020) have pointed out that the RANS model is inappropriate for $O(10\text{--}100)$ m resolutions; it doubly counts the turbulent eddy effect because large-scale eddies in the planetary boundary layer (PBL) begin to be resolved. Wyngaard (2004) named this resolution regime the “terra-incognita,” and the concept is well known as the “gray zone problem” of turbulence (Honnert et al. 2020). To avoid this problem, the turbulence scheme should be changed to that of large-eddy simulation (LES), whose main concept is that only unresolved small-scale eddies are parameterized. The Smagorinsky–Lilly turbulence scheme (Smagorinsky 1963; Lilly 1962) is one such model, although turbulent parameterizations similar to the Smagorinsky scheme are sometimes used in general circulation models (e.g., Becker and Burkhardt 2007). To determine the characteristics of shallow clouds, LES is employed for meteorological simulations using regional models (e.g., Sommeria 1976; Savic-Jovicic and Stevens 2008; Corbetta et al. 2015; Sato et al. 2015). Heinze et al. (2017) conducted LES over a wide domain covering Germany. Stevens et al. (2020) discussed the added value of LES for simulating clouds by performing LES over a wide domain. Although LES in the global domain is still challenging owing to the limitations of computational resources, these studies indicate a link of the global LES. Recent computer technology developments will enable us to perform these simulations with a horizontal resolution of $O(10\text{--}100)$ m in the near future (e.g., Satoh et al. 2019).

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As is well recognized, LES requires a high numerical accuracy for spatial discretization. Nevertheless, state-of-the-art global models employ relatively low-order of spatial accuracy, such as second-order accuracy (e.g., Tomita and Satoh 2004; Zängl et al. 2015). In contrast, higher spatial accuracy is often used in the regional models (e.g., Skamarock et al. 2008; Nishizawa et al. 2015), although such high-order accuracy is applied only to the advection terms and is guaranteed only for uniform flow. Historically, the numerical accuracy of dynamical cores has not always been the primary factor in the numerical performance of atmospheric models because of the uncertainties of physical processes. However, the low-order discretization becomes critical to precisely perform LES for the following reasons.

Consider a situation in which the numerical error due to low-order advection schemes is significant or explicitly added numerical filters clearly affect the flow field. Basically, such errors can contaminate the subgrid-scale (SGS) eddy viscosity terms (e.g., Rogallo and Moin 1984). Vreman et al. (1994) evaluated the numerical error terms and SGS terms, noting that if the filter length of LES is equal to the grid spacing, the spatial discretization errors are more significant than the SGS terms even for the fourth-order spatial scheme. Because the low-order scheme requires greater filter length and increases computational cost, they recommended higher-order schemes. Ghosal (1996) formulated the numerical error of the finite-difference method (FDM). He showed that even if higher-order FDM is employed for nonlinear terms, the aliasing error contaminates the solutions. In addition to the suggestion of Vreman et al. (1994) for the filter length, Ghosal (1996) argued that numerical filters should be adopted to selectively suppress flow structures smaller than the filter length. He also showed that, if eighth-order FDM is employed with a filter length of double grid spacing, the spatial error against SGS terms decreases by two orders of magnitude. In contrast, Brandt (2006) noted that if the filter length is too long, the SGS terms are underestimated because the structural information corresponding to the energy containing wavelength is lost. Brandt (2006) proposed that the spatial filtering only for advection terms improved the results.

In this manner, the problem of dominating the numerical error terms over the SGS terms has been of historical concern in the research field of computational fluid dynamics (CFD). We should consider a further complicated situation in meteorological simulations: e.g., the stratification, vertical shear, and a wide dynamic range of wind velocity. There is still room to theoretically reconsider this problem, and confirm it using actual numerical experiments. Therefore, it is important to extend the knowledge of the CFD area to meteorology, paying attention to the aforementioned complicated factors. In this study, one of the factors considered is the effect of stratification, as discussed in section 4a. At the same time, to obtain clearer requirements of the numerical accuracy for dynamical cores, we should also consider the temporal discretization error that previous works have not addressed.

In this study, we derived two criteria for the order of the numerical accuracy of advection terms, in which the numerical error terms do not dominate over the SGS terms, focusing on the LES of atmospheric boundary layer turbulence. Our work follows the theory of three-dimensional homogeneous

isotropic turbulence, paying attention to a situation peculiar to meteorology. In addition, our approach is based on a more intuitive idea than that used in previous studies. We split the SGS terms into the diffusive and advective contributions, and compared them with numerical diffusion and dispersion accompanied by the discretization of advection terms, respectively. We investigated whether the derived criteria are useful for actual simulations. Finally, including the influence of temporal discretization, we clarified how high the order of numerical accuracy must be in space and time.

In the next section, we derive two ratios associated with numerical diffusion and dispersion. They provide the criteria for which the numerical errors do not dominate over the SGS terms and explain the qualitative behavior for the order of accuracy. As a typical problem, in section 3, we perform ideal numerical experiments of PBL turbulence using advection schemes with various order accuracy, investigating the influence of numerical accuracy on statistical quantities of turbulence. In section 4, we discuss the total numerical error, including temporal discretization error and spatial discretization error with SGS terms. Section 5 provides our conclusion together with scope for future work.

2. Theoretical formulation of criteria for numerical accuracy

The governing equations of LES can be given as

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial \tilde{u}_i \bar{p}}{\partial x_j} = 0, \quad (1a)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \bar{\rho} \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} - g \bar{\rho} \delta_{i3} - \frac{\partial \bar{\rho} \tau_{ij}^*}{\partial x_j}, \quad (1b)$$

$$\frac{\partial \bar{\rho} \tilde{\theta}}{\partial t} + \frac{\partial \tilde{u}_i \bar{\rho} \tilde{\theta}}{\partial x_j} = Q - \frac{\partial \bar{\rho} \tau_j^*}{\partial x_j}, \quad (1c)$$

where ρ , u_i , θ , and p are the density, velocity, potential temperature, and pressure, respectively; τ_{ij} and τ_j^* are the SGS stress tensor and SGS heat flux, respectively; Q is the diabatic heating; and g is the gravitational constant. The indices $i, j \in \{1, 2, 3\}$, and δ_{ij} is the Kronecker delta. The spatially filtered variable is denoted as $\bar{\phi}$. Using it, Favre-filtering is defined as $\tilde{\phi} = \bar{\rho} \phi / \bar{\rho}$ (Favre 1983). According to the Smagorinsky-Lilly model, the eddy viscosity flux is parameterized as

$$\tau_{ij} - \frac{2}{3} K_{\text{SGS}} \delta_{ij} = -2\nu_{\text{SGS}} \left(S_{ij} - \frac{1}{3} S_{kk} \delta_{ij} \right), \quad (2)$$

where S_{ij} is the strain tensor defined as $S_{ij} = (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) / 2$, and K_{SGS} is the SGS kinetic energy. The eddy viscosity ν_{SGS} is calculated by

$$\nu_{\text{SGS}} = (C_s \Delta_{\text{SGS}})^2 |S| f(R_i), \quad (3)$$

where C_s and Δ_{SGS} are the Smagorinsky constant and the filter length, respectively; $|S|$ is defined as $|S| = \sqrt{2S_{ij}S_{ij}}$; and $f(R_i)$ is a coefficient that expresses the stratification effect and depends on the Richardson number R_i .

In this section, we directly compare the SGS term with the numerical error term. To simplify the discussion, two

TABLE 1. Numerical error terms for approximating the first derivative term using the finite-difference scheme. Here, $f_{x(n)} = \partial^n f / \partial x^n$.

Finite-difference scheme	Numerical error term
First-order upwind	$-\frac{f_{x(2)}\Delta x}{2} + \frac{f_{x(3)}\Delta x^2}{6} - \frac{f_{x(4)}\Delta x^3}{24} + \frac{f_{x(5)}\Delta x^4}{120} + \dots$
Second-order central	$+\frac{f_{x(3)}\Delta x^2}{6} + \frac{f_{x(5)}\Delta x^4}{120} + \frac{f_{x(7)}\Delta x^6}{5040} + \frac{f_{x(9)}\Delta x^8}{362880} + \dots$
Third-order upwind	$+\frac{f_{x(4)}\Delta x^3}{12} - \frac{f_{x(5)}\Delta x^4}{30} + \frac{f_{x(6)}\Delta x^5}{72} - \frac{f_{x(7)}\Delta x^6}{252} + \dots$
Fourth-order central	$-\frac{f_{x(5)}\Delta x^4}{30} - \frac{f_{x(7)}\Delta x^6}{252} - \frac{f_{x(9)}\Delta x^8}{4320} - \frac{17f_{x(11)}\Delta x^{10}}{1995840} + \dots$
Fifth-order upwind	$-\frac{f_{x(6)}\Delta x^5}{60} + \frac{f_{x(7)}\Delta x^6}{140} - \frac{f_{x(8)}\Delta x^7}{840} + \frac{f_{x(9)}\Delta x^8}{720} + \dots$
Sixth-order central	$+\frac{f_{x(7)}\Delta x^6}{140} + \frac{f_{x(9)}\Delta x^8}{720} + \frac{7f_{x(11)}\Delta x^{10}}{52800} + \frac{f_{x(13)}\Delta x^{12}}{122850} + \dots$
Seventh-order upwind	$+\frac{f_{x(8)}\Delta x^7}{280} - \frac{f_{x(9)}\Delta x^8}{630} + \frac{f_{x(10)}\Delta x^9}{840} - \frac{f_{x(11)}\Delta x^{10}}{2310} + \dots$
Eighth-order central	$-\frac{f_{x(9)}\Delta x^8}{630} - \frac{f_{x(11)}\Delta x^{10}}{2310} - \frac{19f_{x(13)}\Delta x^{12}}{327600} - \frac{f_{x(15)}\Delta x^{14}}{198450} + \dots$

assumptions are imposed. The first one is to consider the well mixing PBL so that $f(R_i) = 1$. We discuss the effect of $f(R_i)$ in detail in section 4a. The second is to apply the Boussinesq approximation to Eq. (1b), i.e., $\tau_{ij} \simeq -2\nu_{\text{SGS}}S_{ij}$ and the density in the SGS terms is replaced with constant ρ_{ref} . Under those assumptions, the SGS terms in Eq. (1b) can be expressed as

$$-\frac{\partial \bar{p}\tau_{ij}}{\partial x_j} \simeq \rho_{\text{ref}} \left(\nu_{\text{SGS}} \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} + \frac{\partial \nu_{\text{SGS}}}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \nu_{\text{SGS}}}{\partial x_j} \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial K_{\text{SGS}}}{\partial x_j} \delta_{ij} \right). \quad (4)$$

The first term of the rhs in Eq. (4) is the Laplacian term, which contributes to the diffusion. If we regard $\partial \nu_{\text{SGS}} / \partial x_j$ as a kind of phase speed, we can interpret the second term as the dispersion. Among the four terms in Eq. (4), the first and second terms are important because they can be directly compared with the numerical diffusion and dispersion errors of advection schemes, respectively. If the turbulence is isotropic, the third term is statistically comparable to the second one. The fourth term is often absorbed into the pressure gradient term. For flows with a low turbulent Mach number, this contribution with K_{SGS} is sufficiently small compared to the thermodynamic pressure (e.g., Erlebacher et al. 1992). Thus, we focus on only considering the first two terms in this paper.

a. Numerical error due to advection scheme

In this subsection, we discuss the numerical errors caused by the advection scheme. Although FDM is treated here, the following discussion is essentially the same as in other gridpoint methods such as the finite volume method, if the corresponding modified equation can be obtained. The first derivative is approximated by $2p_{\text{max}} + 1$ stencil values as

$$\frac{\partial \phi}{\partial x} \Big|_j = \sum_{p=-p_{\text{max}}}^{p_{\text{max}}} \frac{A_p \phi(x_{j+p})}{\Delta x} + (\text{numerical error terms}),$$

where Δx is the grid spacing. The coefficient A_p , depending on the order of accuracy, is derived in appendix A. The numerical

error terms are summarized in Table 1. We divide them into even and odd differential terms; the former dissipates the solution, while the latter disperses the wave.

As shown in Table 1, the dissipation error does not appear in the central difference schemes, but only dispersion error exists. To stabilize the computations, we often explicitly give the numerical diffusion terms in the following form of

$$\frac{\partial}{\partial x} \left(\bar{\rho} \nu_{\text{num},2n} \frac{\partial^{2n-1} \phi}{\partial x^{2n-1}} \right) \simeq \rho_{\text{ref}} \nu_{\text{num},2n} \frac{\partial^{2n} \phi}{\partial x^{2n}}, \quad (5)$$

where n is a positive integer, and $\nu_{\text{num},2n}$ is a coefficient associated with the intensity of the numerical diffusion. By introducing a nondimensional coefficient of numerical diffusion γ_{2n} , the dimensional coefficient is given by

$$\nu_{\text{num},2n} = (-1)^{n+1} \gamma_{2n} \frac{(\Delta x)^{2n}}{2^{2n} \Delta t}, \quad (6)$$

where Δt is the time step. For details, see appendix A4 in Nishizawa et al. (2015). For the $2n$ -order central scheme, the numerical diffusion term with the $2n$ -order differential operator is often added together with appropriate γ_{2n} . Note that we can adopt higher-order numerical diffusion that selectively affects small-scale waves, provided that numerical stability is ensured.

In contrast, Table 1 shows that the $(2n - 1)$ -order upwind scheme has an infinite series of numerical diffusion terms whose dominant order of differential operator is $2n$. If we follow the form of Eq. (6), the nondimensional coefficient of implicit numerical diffusion is determined automatically. The dominant error term has a coefficient of

$$\gamma_{2n} = f_{\text{UD},2n} \frac{|U| \Delta t}{\Delta x}, \quad (7)$$

where U is the local wind speed, and we introduce another nondimensional constant coefficient $f_{\text{UD},2n}$, derived as Eq. (A4)

in [appendix A](#). As confirmed by substituting Eq. (7) into Eq. (6), note that $\nu_{\text{num},2n}$ for upwind schemes is proportional to $|U|$, but does not depend on Δt .

The numerical dispersion errors of the $(2n - 1)$ -order upwind and $2n$ -order central schemes are the same (e.g., compare the odd-order scheme with the even-order scheme in [Table 1](#)). The term can be written as

$$\frac{\partial}{\partial x} \left(\sum_{k=n}^{\infty} \bar{p} a_{\text{num},2k+1} \frac{\partial^{2k} \phi}{\partial x^{2k}} \right) \simeq \rho_{\text{ref}} \sum_{k=n}^{\infty} a_{\text{num},2k+1} \frac{\partial^{2k+1} \phi}{\partial x^{2k+1}}, \quad (8)$$

where $a_{\text{num},2k+1} = U(\Delta x)^{2k} \tilde{a}_{\text{num},2k+1}$ and $\tilde{a}_{\text{num},2k+1} = [(2k + 1)!]^{-1} \sum_{p=-p_{\text{max}}}^{p_{\text{max}}} A_p p^{2k+1}$. The value of $\tilde{a}_{\text{num},2k+1}$ corresponds to the coefficient of each odd-order differential term in [Table 1](#).

Actually, the temporal discretization also produces the numerical diffusion and dispersion errors. Here, we consider that such temporal errors are ideally small if an appropriate high-order scheme is used in time. We discuss its validity in [section 4](#) in detail.

$$\beta_e(l, n) = \begin{cases} \left[\frac{(\pi/l)}{\sin(\pi/l)} \right]^{2n} \\ \left[1 + \sum_{p=n+1}^{\infty} \left(\frac{\pi}{l} \right)^{2(p-n)} \frac{\gamma_{2p}}{\gamma_{2n}} \right]^{-1} \end{cases}$$

$\beta_e(l, n)$ is the factor associated with the numerical discretization. See [appendix A](#) for the derivation. The ratio of Eq. (9) to Eq. (10) is derived as

$$R_{\text{diff}} \equiv \frac{T_{e,\text{SGS}}}{T_{e,\text{num}}} = \frac{1}{2^2} \left(\frac{\pi}{l} \right)^{2(n-1)} \left(\frac{\gamma_{2n}}{\Delta t} \right) \left(\frac{\Delta x}{C_s \Delta_{\text{SGS}}} \right)^2 [|\beta_e(l, n)|]^{-1}. \quad (11)$$

If we give a physical meaning to the Laplacian term in eddy viscosity terms, the numerical diffusion term does not dominate it, i.e., $R_{\text{diff}} \ll 1$ should be satisfied.

c. Criterion due to numerical dispersion

We also derive the ratio of the phase speed of numerical dispersion due to advection schemes to that of cross terms that arise from eddy viscosity terms. To directly compare the former numerical dispersion errors with the latter cross terms, we consider the derivative of ν_{SGS} as the phase speed in the second term on the rhs of Eq. (4). The phase speed associated with the SGS terms is given as

$$S_{p,\text{SGS}} = \frac{\partial \nu_{\text{SGS}}}{\partial x} = (C_s \Delta_{\text{SGS}})^2 \frac{\partial |S|}{\partial x}. \quad (12)$$

In contrast, the phase speed associated with the dispersion error due to advection schemes can be derived considering the dispersion equation:

$$\frac{\partial \phi}{\partial t} + \sum_{k=n}^{\infty} a_{\text{num},2k+1} \frac{\partial^{2k+1} \phi}{\partial x^{2k+1}} = 0.$$

b. Criterion due to numerical diffusion

We derive the ratio of the e -folding decay time of the eddy viscosity to that of the numerical diffusion. Henceforth, a wavelength is denoted by $l\Delta x$, where l is an index representing the number of grids of the wavelength. Considering the diffusion equation with the $2n$ -order differential operator, we generally can give the e -folding decay time as $(-1)^{n+1} [l\Delta x / (2\pi)]^{2n} \nu^{-1}$ where ν is the eddy or numerical viscosity. Thus, the e -folding decay time of the Laplacian term in Eq. (4) is given as

$$T_{e,\text{SGS}} = \frac{1}{2^2} \left(\frac{l}{\pi} \right)^2 \left(\frac{\Delta x}{C_s \Delta_{\text{SGS}}} \right)^2 \frac{1}{|S|}, \quad (9)$$

whereas that of the $2n$ -order differential numerical diffusion of Eq. (5) is given as

$$T_{e,\text{num}} = \left(\frac{l}{\pi} \right)^{2n} \frac{\Delta t}{\gamma_{2n}} \beta_e(l, n), \quad (10)$$

where

for the $2n$ -order central scheme,

for the $(2n - 1)$ -order upwind scheme;

From this equation, the corresponding phase speed for a wavelength ($l\Delta x$) can be obtained as

$$\begin{aligned} S_{p,\text{num}} &= \sum_{k=n}^{\infty} (-1)^k \left(\frac{2\pi}{l\Delta x} \right)^{2k} a_{\text{num},2k+1} \\ &= (-1)^n \left(\frac{2\pi}{l} \right)^{2n} U \tilde{a}_{\text{num},2n+1} \tilde{\beta}(l, n), \end{aligned} \quad (13)$$

where $\tilde{\beta}(l, n)$ is defined as

$$\tilde{\beta}(l, n) = 1 + \sum_{k=n+1}^{\infty} (-1)^{k-n} \left(\frac{2\pi}{l} \right)^{2(k-n)} \frac{\tilde{a}_{\text{num},2k+1}}{\tilde{a}_{\text{num},2n+1}}.$$

The ratio of Eq. (13) to Eq. (12) is derived as

$$R_{\text{disp}} \equiv \frac{|S_{p,\text{num}}|}{|S_{p,\text{SGS}}|} = 2^{2n} \left(\frac{\pi}{l} \right)^{2n} \frac{|U \tilde{a}_{\text{num},2n+1}|}{(C_s \Delta_{\text{SGS}})^2 |\partial |S| / \partial x|} \tilde{\beta}(l, n). \quad (14)$$

If we give a physical meaning to the cross term in eddy viscosity terms, the numerical dispersion term does not dominate it, i.e., $R_{\text{disp}} \ll 1$ should be satisfied.

d. Behavior of derived criteria

How do R_{diff} and R_{disp} behave with decreasing grid spacing? This can be considered one of the main objectives of this study. Both of the two ratios should be sufficiently smaller than unity for the SGS terms to be effective. Here, we theoretically discuss this issue, considering two ratios as functions of grid spacing and wavelength. For this purpose, three definitions are introduced as follows.

First, the filter length is expressed by the index m which represents the number of grids in Δ_{SGS} :

$$\Delta_{\text{SGS}} = m\Delta x. \quad (15)$$

Second, the factor $\gamma_{2n}/\Delta t$ in Eq. (11) is expressed as a function of Δx to convert Δt into Δx . By introducing a nondimensional diffusive coefficient with regards to the advective time scale γ_{adv} , this factor is replaced as

$$\frac{\gamma_{2n}}{\Delta t} = \frac{|U|\gamma_{\text{adv}}}{\Delta x}. \quad (16)$$

For the central schemes with explicit numerical diffusion, let us consider the use of fully explicit temporal schemes for simplicity. In this case, the time step is limited by the acoustic wave speed c_{sound} , so that $\gamma_{\text{adv}} = [c_{\text{sound}}/(c_r^{\text{sound}}|U|)]\gamma_{2n}$ where c_r^{sound} is the Courant number against c_{sound} . For the upwind schemes, $\gamma_{\text{adv}} = f_{\text{UD},2n}$ because of Eq. (7). Third, we relate the strain tensor to the filter length. According to the Kolmogorov theory, the typical magnitude of the strain tensor can be derived as

$$\langle |S| \rangle = \eta \left(\frac{\pi}{\Delta_{\text{SGS}}} \right)^{2/3}, \quad (17)$$

where η is a constant value. Here, it is treated as an unknown parameter depending on the atmospheric conditions. In section 3, we determine the actual value via a numerical experiment. Similarly, the typical magnitude of the gradient of the strain tensor can be derived as

$$\left\langle \left| \frac{\partial |S|}{\partial x} \right| \right\rangle = \eta' \left(\frac{\pi}{\Delta_{\text{SGS}}} \right)^{5/3}, \quad (18)$$

where $\eta' = \sqrt{2/15} \eta$. The derivation of Eqs. (17) and (18) is described in appendix B.

By substituting Eqs. (15), (16), and (17) into Eq. (11),

$$R_{\text{diff}} = \frac{1}{\eta} \left(\frac{\pi}{m} \right)^{4/3} \frac{|U|\gamma_{\text{adv}}}{(2\pi c_s)^2} \left(\frac{\pi}{l} \right)^{2(n-1)} (\Delta x)^{-1/3} [\beta_e(l, n)]^{-1}; \quad (19)$$

R_{diff} is proportional to $(\Delta x)^{-1/3}$. This means that, if the parameters except grid spacing are fixed, R_{diff} increases as the grid spacing decreases. This property implies that numerical diffusion dominates the Laplacian part of the eddy viscosity terms as the grid spacing decreases. For upwind schemes, this problem is inevitable because numerical diffusion is determined by the local wind speed. In contrast, for the central schemes with explicit numerical diffusion, we can control the problem by decreasing the numerical diffusion as long as numerical stability is ensured. For the second-order central scheme with second-order numerical diffusion, R_{diff} does not decrease with wavelength because $(\pi/l)^{2(n-1)}$ becomes unity. This behavior is independent of the grid spacing. It is remarkable that using conventional dynamical cores with the low-order schemes is risk for future high-resolution LES.

By substituting Eqs. (15) and (18) into Eq. (14),

$$R_{\text{disp}} = \frac{2^{2n}}{\eta'} \left(\frac{\pi}{m} \right)^{1/3} \frac{|U\tilde{a}_{\text{num},2n+1}|}{(\pi c_s)^2} \left(\frac{\pi}{l} \right)^{2n} (\Delta x)^{-1/3} \tilde{\beta}(l, n); \quad (20)$$

R_{disp} is also proportional to $(\Delta x)^{-1/3}$. Thus, as the grid spacing decreases, the numerical dispersion dominates the cross-term associated with eddy viscosity terms. $|U\tilde{a}_{\text{num},2n+1}|$ in Eq. (20) is caused by the leading error of numerical dispersion. Thus, unlike the case of R_{diff} , the central schemes also cannot escape this issue. In decreasing the grid spacing or in order to maintain a small value of R_{disp} for short wavelengths, this suggests that we must adopt sufficient high-order schemes.

3. Turbulence simulation in an idealized planetary boundary layer turbulence by LES

In this section, to verify the numerical criteria derived in the previous section, we performed a series of numerical experiments for atmospheric turbulence in an idealized PBL. Although the numerical criteria were formulated under the Boussinesq approximation, here we used an LES model based on compressible equations. Such equations are often adopted in modern meteorological models to avoid the difficulties associated with the approximation of compressibility (e.g., solving the pressure Poisson equation in massive parallel computational environments). In contrast, based on Erlebacher et al. (1992), the compressibility effect is considered to have negligible impact on the turbulent fields discussed in this study.

a. Model and experimental setup

The experimental setup is based on Nishizawa et al. (2015, hereafter N2015). The model used is SCALE-RM (N2015; Sato et al. 2015). The computational domain has a square area of $9.6 \text{ km} \times 9.6 \text{ km}$ with a double periodic boundary condition and an altitude of 3 km. In the dynamical process, the fully compressible nonhydrostatic equations are solved. The turbulent process is expressed by the Smagorinsky–Lilly model considering the stratification effect (Brown et al. 1994). The filter length is set to two times the grid spacing. To focus on the turbulent process, the radiation and moist processes are absent. For the initial atmospheric condition, we provide the potential temperature that increases with height at a rate of 4 K km^{-1} and add the random disturbance with an amplitude of 1 K. The initial wind in the x direction is 5 m s^{-1} . At the surface, a constant heat flux of 200 W m^{-2} is continuously injected.

The numerical method is summarized as follows. The governing equations were spatially discretized by a conservative FDM with the Arakawa–C type staggered grid (Arakawa and Lamb 1977). For the advection terms with flux form, the spatial discretization was selected among the second, fourth, sixth, and eighth-order central, and the third-, fifth-, and seventh-order upwind schemes. Hereinafter, the n -order central and upwind schemes are denoted as CD n and UD n , respectively. The pressure gradient and SGS terms are spatially discretized by CD2. When using CD schemes for the advection terms, numerical diffusion is explicitly added for the numerical stabilization. We prepared the second-, fourth-, sixth-, and eighth-order differential operators, denoted by ND n . To prevent the reflection of waves at the upper boundary, we placed a sponge layer above 2 km. The horizontal grid-spacing was 10 m and the vertical grid spacing was the same as that in the horizontal direction except the sponge layer. As for the temporal

TABLE 2. Summary of a series of the numerical experiments for atmospheric turbulence in an idealized PBL.

	Advection flux (order, type)	Explicit numerical diffusion	Implicit numerical diffusion	RK scheme (order, stage)	Spatial resolution (m)
CD2ND2	2, central	$2n = 2, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	3, 3	10
UD3	3, upwind	—	$2n = 4, \gamma_{\text{adv}} = 4/3$	4, 4	10
CD4ND4	4, central	$2n = 4, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	4, 4	10
CD4ND8	4, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	4, 4	10
UD5	5, upwind	—	$2n = 6, \gamma_{\text{adv}} = 16/15$	6, 7	10
CD6ND6	6, central	$2n = 6, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	6, 7	10
UD7	7, upwind	—	$2n = 8, \gamma_{\text{adv}} = 32/35$	8, 11	10
CD8ND8 (control)	8, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	8, 11	10
CD2ND2_40m	2, central	$2n = 2, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	3, 3	40
CD8ND8_40m	8, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	8, 11	40
CD2ND2_80m	2, central	$2n = 2, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	3, 3	80
CD8ND8_80m	8, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	8, 11	80
CD8ND8_RK3	8, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	3, 3	10
CD8ND8_RK4	8, central	$2n = 8, \gamma_{\text{adv}} \sim 3.3 \times 10^{-2}$	—	4, 4	10

discretization, a fully explicit scheme was applied to all terms. We chose an explicit Runge–Kutta (RK) scheme among the three-stage and third-order (Wicker and Skamarock 2002), the classical four-stage and fourth-order, the seven-stage and sixth-order (Lawson 1967), and the 11-stage and eighth-order (Cooper and Verner 1972) schemes. The n -order RK scheme is denoted by RK n . Although the straightforward choice for the verification of our criteria would be to adopt a temporal scheme whose order of accuracy is higher than that of the highest-order advection scheme, such a choice is too difficult in terms of computational costs. Thus, we required that the order of temporal accuracy be at least the same as that of each advection scheme to avoid the situation where the temporal errors significantly dominate the numerical errors due to advection. The time step for the dynamical process was 0.012 s, and the SGS terms were evaluated at every stage of the RK scheme. For the central schemes, the explicit numerical diffusion was evaluated in the final stage of the RK scheme.

Table 2 provides a summary of the experiments. We performed eight experiments with a spatial resolution of 10 m, changing the advection scheme among the various order accuracies. CD8ND8 has the highest numerical accuracy in space and time and is referred to as the “control experiment.” The differential order of explicit numerical diffusion is basically equal to the order of accuracy of the CD scheme. For comparison with N2015, we used higher-order numerical diffusion only in CD4ND8. The intensity of the explicit numerical diffusion was set to $\gamma_{2n} = 2.0 \times 10^{-4}$ in Eq. (6); the value is the same as N2015. In this setup, γ_{adv} is approximately 3.3×10^{-2} , which is less than the corresponding values for UD schemes. In CD2ND2 and CD8ND8, we also performed experiments with grid spacings of 40 or 80 m in which the time step increased such that the Courant number was fixed. Furthermore, to discuss the influence of temporal errors, we performed two additional experiments in which RK8 in CD8ND8 was replaced with RK3 and RK4. For the control experiment, the temporal integration was performed for 4 h. For the other cases with 10 m resolution, to reduce computational costs, it was performed for only 1 h by setting the output at 3 h from the control

experiment as the initial condition. The results for the last 30 min were analyzed.

In our computational configuration,¹ computational and communication costs due to the higher-order advection scheme were negligible, whereas the increase in the overall computational time was caused by the increase in the stage of the high-order RK scheme. Temporal integration for 4 h for the control experiment required approximately 12 days. The reason for the relatively low computational cost of the high-order advection scheme is a virtue of the structured grid, such as the continuous or striped access of the memory space and effective use of the cache memory. These benefits are not necessarily guaranteed for an unstructured grid used in several recent global nonhydrostatic models. In addition, if MPI processes are increased by $O(10^4)$ with a reduction in the number of grids per process, communication costs with an increase of halo in high-order schemes will become nonnegligible. Thus, it is possible to underestimate the computational costs of high-order advection schemes, although we have not focused on this issue in the present study.

b. Results of the control experiment

After 4 h, the top of the PBL reaches approximately 1200 m in altitude. Figure 1a shows the horizontal distribution of the vertical velocity at $z = 500$ m as a typical field in the middle of PBL. The convective cells have well-known hexagonal or quadrangular structures. The updraft within the narrow boundaries of the cells is stronger than the downdraft in the remaining region. These features of the flow fields are qualitatively the same as those shown in Fig. 3a of N2015.

From the control experiment that provides the highest accuracy, we attempted to estimate the unknown parameter η as follows. We generated a series of coarsened data using the

¹ A series of numerical experiments were conducted in the Oakbridge-CX system at the University of Tokyo. Each experiment used 576 MPI processes, and the number of OpenMP threads was set to six per MPI process.

FIG. 1. Horizontal distribution at $z = 500$ m for (a) vertical velocity w and (b) absolute value of strain tensor $|S|$ in the control experiment. The domain bounded by the dashed black line in Fig. 1a represents the area where we focus on the turbulent structure for various advection schemes in Fig. 7. In Fig. 1b, we plot $|S|$ calculated from the coarsened data for $D = 70$ m.

top-hat filter, whose window size D increased from 30 to 350 m. For each D , $|S|$ was evaluated using a tenth-order central difference on the original mesh, and $\nabla|S|$ was evaluated by subsequently differentiating $|S|$. Figure 1b shows the distribution of $|S|$ for $D = 70$ m, as an example. Figure 2 shows the dependence of the square root of horizontally averaged $|S|^2$ and $(\nabla|S|)^2$ on D , with Eqs. (17) and (18) for three values of η . These slopes are consistent with the values expected by the Kolmogorov theory: $-2/3$ and $-5/3$ for $|S|$ and $\nabla|S|$, respectively. From Fig. 2, we can estimate the value of η as 0.15, although it varied by approximately 20%. Ideally, η should be

considered a constant if the energy spectra precisely obey the $-5/3$ power law with the same energy dissipation rate, as derived in appendix B. This constancy of η is also indicated by coarsened data based on CD8ND8 experiments with grid spacings of 40 and 80 m (refer to the green and blue lines in Fig. 2). The reason for the 20% variation is that the actual energy spectra did not precisely obey the $-5/3$ power law over the entire wavelength range. In addition, the filter used to obtain the coarsened data is considered to affect this behavior.

The typical wind speed is also necessary to quantify our numerical criteria defined by Eqs. (19) and (20). Figure 3 shows

FIG. 2. Dependence of the square root of horizontally averaged (a) $|S|^2$ and (b) $(\nabla|S|)^2$ on spatial resolution. The red line represents the result based on the coarsened data obtained from the CD8ND8 experiment with grid spacing of 10 m. The green and blue lines represent the results based on the coarsened data obtained from CD8ND8_40m and CD8ND8_80m, respectively. In these panels, the dotted, dashed, and dash-dotted lines show Eqs. (17) and (18) for $\eta = 0.10, 0.15$, and 0.20 , respectively. When $|S|$ is calculated from coarsened data obtained from CD8ND8_40m and CD8ND8_80m, we adjust the order of accuracy of central difference in the vertical direction such that the stencil does not extend outside the computational domain.

FIG. 3. Histogram of wind velocity at $z = 500$ m. The components of velocity in directions x , y , and z are shown in green, blue, and red, respectively.

the histograms of wind velocity at $z = 500$ m. The maximum wind frequencies in the x and y directions are approximately 5 and 0 m s^{-1} , respectively. In contrast, the maximum frequency of the vertical wind is negative and at approximately -0.5 m s^{-1} .

The numerical diffusion and dispersion should be smaller than the first term (Laplacian term) and the second term (dispersion term) in Eq. (4), respectively. However, if the typical sizes of the two terms in Eq. (4) are considerably different, we should not consider that the importance of R_{diff} is comparable with that of R_{disp} . To examine the actual contributions, Fig. 4 shows the histogram of the ratios of the dispersion term to the Laplacian term at each grid point. Although the Laplacian terms usually dominate the dispersion terms, in 15% grid points, the dispersion terms are comparable to or larger than the Laplacian terms. Thus, we consider the importance of R_{diff} and R_{disp} to be equal.

c. Quantification of numerical criteria

We discuss here the analytical dependence of R_{diff} in Eq. (19) and R_{disp} in Eq. (20) on the grid spacing and the wavelength, using the determined parameters: $m = 2$ in Eq. (15), $\eta = 0.15$ in Eq. (17), $|U| = 5 \text{ m s}^{-1}$, and $\gamma_{\text{adv}} = 3.3 \times 10^{-2}$ for the CD schemes. The values of R_{diff} and R_{disp} at which the numerical errors are considered acceptable are arbitrary. Here, however, we set the criteria in which they should be below 10^{-1} for more than eight grids: the one-order small value may be appropriate for practical cases, and targeting flow structures longer than eight grids is appropriate in terms of effective resolution, according to Skamarock (2004) and Abdalla et al. (2013).

The left panel in Fig. 5 and Fig. 5b show the results for CD schemes. In CD2ND2, R_{diff} is no longer smaller than 10^{-1} at the grid spacing usually used in LES. For CD4ND4, R_{diff} is approximately 10^{-1} around $l \sim 10$ in the $O(10)$ m resolution. The order is the boundary of whether our criterion of numerical diffusion is satisfied. For higher-order numerical diffusion than CD4ND4, this criterion is satisfied. The constraint from

FIG. 4. Contributions of the Laplacian term and cross term in square brackets in (4). Here, the ratios of these terms are $(\partial \nu_{\text{SGS}} / \partial x_j \times \partial \tilde{u}_i / \partial x_j) / (\nu_{\text{SGS}} \partial^2 \tilde{u}_i / \partial x_j^2)$. The terms are calculated using the coarsened data by a factor of 7 in the same manner as for $|S|$ in Fig. 2.

the numerical dispersion is more severe. Tighter constraints are imposed on the order accuracy of numerical schemes. For example, even for CD8ND8, the criterion of $R_{\text{disp}} < 10^{-1}$ is not satisfied unless the structure is longer than eight grids.

The right panel in Fig. 5 (except for Fig. 5b) shows the results for UD schemes. R_{diff} for the $(2n - 1)$ -order UD scheme is two orders of magnitude larger than that for the $2n$ -order CD scheme. In the $O(10)$ m resolution, UD7 satisfy the criterion of numerical diffusion but UD3 and UD5 are not acceptable. The constraint of numerical dispersion with the $(2n - 1)$ -order UD scheme is the same as that with the $2n$ -order CD scheme. In UD3 and UD5 schemes, the constraint of numerical diffusion is more severe than that of numerical dispersion at the wavelength longer than eight grids.

Here, we provide a short summary of the spatial accuracy of advection terms with a focus on the flow structure longer than eight grids. In terms of numerical diffusion, at least a fourth-order accuracy is necessary for CD schemes, provided that the differential order of explicit numerical diffusion terms is the same or higher than the order of the used scheme. At that time, the intensity of explicit numerical diffusion needs to be one or two order less than that of the third-order upwind scheme. The UD scheme requires at least seventh-order accuracy to satisfy the criterion. In terms of numerical dispersion, at least a seventh-order scheme is necessary in both the CD and UD schemes.

d. Validation of numerical criteria

In this section, we will verify the criteria quantified in section 3c. From the viewpoint of energy spectra, we focus on the difference between the advection schemes in Table 2 while referring to Fig. 5.

Figure 6 shows the density-weighted energy spectra of the three-dimensional velocity at $z = 500$ m. Regardless of the schemes, the energy spectra obey the $-5/3$ power law in the wavelength range of 10^3 – 10^2 m, and they drop with a steeper

FIG. 5. Dependence of R_{diff} and R_{disp} on $(\Delta x, l)$ for the advection schemes with various orders of numerical accuracy. The solid red line and tone represent R_{diff} , which is the criterion associated with the numerical diffusion. The dashed black line represents R_{disp} , which is the criterion associated with numerical dispersion. Considering that the value should be smaller than 10^{-1} in order for the numerical error terms to not dominate the SGS terms, we thicken the corresponding lines. In this calculation, we set $m = 2$ and $|U| = 5 \text{ m s}^{-1}$, and for the central schemes $\gamma_{\text{adv}} = 3.3 \times 10^{-2}$.

FIG. 6. (a) Density-weighted energy spectra $E(k)$ of three-dimensional wind at $z = 500$ m for the CD and UD schemes with various orders of accuracy. The dash-dotted gray line in (a) represents $ak^{-5/3}$, where $a = 1.7 \times 10^{-5}$, (b) compensated spectra, $E(k)/(ak^{-5/3})$, and (c) partial expanded view of the energy spectra in the wavelength range of 100 and 20 m.

slope at wavelengths shorter than 10 grids. The energy spectra for CD4ND8 well reproduce those of the control experiment shown in Fig. 1 of N2015.

The implication of R_{diff} depicted by Fig. 5 is consistent with the energy spectra. The most diffusive one is CD2ND2 followed by UD3. When comparing the two results, R_{diff} for CD2ND2 is slightly smaller than that for UD3 at a shorter wavelength (less than approximately 30 grids); however, it is larger than that for UD3 at longer wavelengths. Figure 7 also indicates that the two schemes do not capture the smaller-scale structure of flow near the updraft region of convections well, compared to other schemes. Among the CD schemes, the energy spectra essentially depend on the order of the differential operator of the numerical diffusion, in particular, over short wavelengths. For the CD schemes with more than fourth-order numerical diffusion, the energy spectra obey the $-5/3$ power law more at wavelengths shorter than eight grids. For higher-order UD schemes, R_{diff} for UD5 is larger than for CD4ND4 for wavelengths shorter than approximately 10 grids; for UD7, it has an intermediate value between CD4ND4 and CD6ND6 for the wavelength between approximately 6 grids and 20 grids. As suggested in Fig. 5, the energy spectra for UD5 and UD7 schemes are actually more diffusive than those for CD4ND4 and CD6ND6, respectively.

Although it is difficult to directly estimate the influence of R_{disp} , it can be indirectly inferred from the above energy spectra. Here, we compare schemes that have the same numerical diffusion terms but different numerical dispersion

terms. We focus on the difference between CD4ND8 and CD8ND8 and that between UD7 and CD8ND8. Figure 6 shows that the former is smaller than the latter. This implies that the influence of numerical dispersion on the energy spectra tends to be smaller than that of numerical diffusion. Nevertheless, note that it is possible to underestimate the problems of the numerical dispersion error because the current experiment is based on an idealized setup. The problem may appear essentially under more realistic situations.

Figure 5 indicates that the influence of the numerical diffusion in comparison to the SGS term strengthens as the grid spacing decreases. To examine this behavior in numerical experiments, Fig. 8 shows the density-weighted energy spectra obtained from CD2ND2 and CD8ND8 with different grid spacings. Here, we focused on the wavelength at which the energy spectra of CD2ND2 begin to deviate from that of CD8ND8. This wavelength was approximately 10-grids for a grid spacing of 80 m, whereas it was approximately 30 grids for a grid spacing of 10 m. Thus, the range of wavelengths for which the numerical diffusion errors significantly affected the energy spectra became wider as the grid spacing decreased.

4. Discussion

a. Effect of stratification on eddy viscosity

In section 2, we assume $f(R_i) = 1$ in Eq. (3). However, in our numerical experiments in section 3, where we use the turbulent model based on Brown et al. (1994), $f(R_i)$ is modified by the

FIG. 7. Horizontal distributions of vertical wind at $z = 500$ m for various advection schemes. We focus on the partial domain, which corresponds to the domain bounded by the black dashed line in Fig. 1a.

FIG. 8. (a) Density-weighted energy spectra $[E(k)]$ of three-dimensional wind at $z = 500$ m for CD2ND2 and CD8ND8 with grid spacings of 10, 40, and 80 m and (b) compensated spectra, $E(k)/(ak^{-5/3})$.

nonneutral stratification effect as follows: $f(R_i) = \sqrt{1 - 16R_i}$ for unstable stratification ($R_i < 0$), $f(R_i) = (1 - R_i/0.25)^4$ for weakly stable stratification ($0 < R_i < 0.25$), and $f(R_i) = 0$ for strongly stable stratification ($R_i \geq 0.25$).

To discuss the influence of stratification on R_{diff} , Fig. 9a shows the histogram of the Richardson number R_i at $z = 500$ m and the dependence on the resolution. Here, using the results of the control experiment, we calculated R_i for the different

resolutions in same manner in which $|S|$ was obtained in section 3b. At almost all the grid points, the magnitude spreads in the range of $|R_i| < 10^{-1}$. As the resolution increases, the influence of stratification on R_i tends to decrease, because the peak value increases at $R_i \sim 0$. Figure 9b shows the histogram of $f(R_i)$ for various coarsened data. For the unstable case, $f(R_i)$ has a value between 1 and 2. Thus, unstable stratification only affects R_{diff} by a factor of 2 at most. For weakly stable stratification case, at approximately 10% grid points, $f(R_i)$ is less than 10^{-1} .

To investigate the influence of stratification on R_{disp} , Fig. 10 shows the histogram of the ratio $\partial f(R_i)|S|/\partial x$ to $\partial|S|/\partial x$; this ratio is between 10^{-1} and 10^1 at approximately 90% grid points.

These facts indicate that the criteria with numerical errors derived for neutral stratification in section 2 can be approximately adopted for most grid points in our numerical experiments. For stable stratification case, it is more probable that the SGS terms become significantly smaller than the numerical errors. Such a situation occurs at only 10% grid points where the required order of accuracy indicated by R_{diff} and R_{disp} for the neutral stratification is not sufficient.

b. Influence of temporal numerical errors on R_{diff} and R_{disp}

In section 2, the temporal discretization is not treated. To investigate the influence of the temporal error terms on the numerical criteria, let us consider the one-dimensional linear advection equation discretized by CD8ND8 in space and RK n schemes in time ($n = 8, 4, 3$).

If we consider the even-order and odd-order differential terms arising from the temporal discretization, we can rewrite the e -folding decay time of numerical diffusion $T_{e,\text{num}}$ and the phase speed of numerical dispersion $S_{p,\text{num}}$, respectively, as

$$T'_{e,\text{num}} = T_{e,\text{num}} \left\{ 1 + \beta_e(l, 4) \frac{r'_{n,2m}}{\gamma_8} (2c_r)^{2m} \left(\frac{\pi}{l} \right)^{2(m-4)} \times \left[1 + \sum_{\tilde{m}=m+1}^{\infty} \frac{r'_{n,2\tilde{m}}}{r'_{n,2m}} \left(c_r \frac{2\pi}{l} \right)^{2(\tilde{m}-m)} \right]^{-1} \right\}, \quad (21)$$

FIG. 9. Histograms of (a) Richardson number (R_i) and (b) effect of stratification on $\nu_{\text{SGS}}, f(R_i)$, at $z = 500$ m. In (a), we also represent the dependence of R_i on the spatial resolution by showing the results obtained using coarsened data. In these panels, we show the results from the coarsened data by a factor $(D/\Delta x)$ of 1, 5, 7, and 9.

FIG. 11. Dependence of the density-weighted energy spectra $[E(k)]$ for three-dimensional wind at $z = 500$ m on the accuracy of temporal schemes when CD8ND8 was used as the advection scheme. The green and red lines represent the results when the RK8 scheme is changed to RK4 and RK3, respectively. For comparison, we also plotted the energy spectra for CD6ND6 and CD2ND2 in section 3d.

(eddy viscosity plus numerical diffusion) decay intensity by less than $O(1\%)$ between the 8 and 16 grids. In contrast, if we introduce $T_{e,SGS}^{CD2} - T_{e,SGS}$, which indicates how much the CD2 discretization increases the e -folding decay time with SGS terms compared to the true one, the ratio of this amount to $T_{e,SGS}$ is estimated as $O(1\%)$ between the 8 and 16 grids. Thus, $T_{e,SGS}^{CD2} - T_{e,SGS}$ dominates the e -folding time with CD8ND8. In section 3c, we suggested that at least the seventh order was necessary for the advection scheme to satisfy our criteria. This implies that high-order numerical schemes must be applied to all terms containing SGS terms. Although high-order discretization for SGS terms is beyond the scope of this paper, the extent of the influence on the simulated turbulence is an interesting subject.

d. Design of numerical filters on high-order discretization

Even if we use higher-order schemes, the numerical error inevitably affects the structure of several grid scale. Furthermore, when they are adopted for nonlinear terms, we must consider aliasing errors, as argued in Ghosal (1996). These facts are important for the coupling between dynamical and physical processes because the physical parameterizations often assume that the numerical errors in the dynamical process are small.

A remedy for this problem is to properly coarsen the spatial distributions of variables treated in the dynamical process and give them to the physical processes. In this case, we should design an appropriate filter that effectively damps the structure between the two-grid scale and the effective resolution, in addition to the aliasing errors. Although this idea has already been verified in the context of LES (e.g., Vreman et al. 1994; Ghosal 1996), for other physical parameterizations in atmospheric models, the effect must be explored further.

5. Conclusions

In recent dynamical cores in state-of-the-art models, relatively low-order schemes are used for spatial discretization. However, as the resolution increases for LES, a problem arises in that the errors of such low-order schemes contaminate the SGS terms. In this study, we revealed the numerical accuracy of the advection schemes necessary for atmospheric LES. Two criteria were derived for this purpose, based on the theory of homogeneous isotropic three-dimensional turbulence. The first is the ratio of the e -folding time with the SGS terms to that with the numerical diffusion. The second is the ratio of the phase speed with the numerical dispersion to that with the SGS terms. We verified the criteria by performing an LES in a typical planetary boundary layer turbulence with various numerical orders of advection schemes.

In terms of numerical dissipation, the criterion suggests the following. For the third-order and fifth-order upwind schemes or second-order central scheme with second-order numerical diffusion, numerical diffusion significantly dominates the diffusion due to the eddy viscosity terms even at wavelengths longer than eight grids. Hence, a seventh-order accuracy is required for the upwind schemes in this case. In general, the upwind scheme has inevitably implicit diffusion. As it is determined by the local wind speed, we cannot control the degree of numerical diffusion explicitly. In contrast, for the central schemes, we can adjust the numerical diffusion under the condition of numerical stability. To rapidly remove grid-scale noisy structures and properly work the eddy viscosity at an effective resolution, a higher differential operator than the fourth-order should be used. If a fourth-order numerical diffusion is used nevertheless, the nondimensional intensity of the numerical diffusion associated with the advection time scale should be set to one or two orders of magnitude smaller than that for the third-order upwind schemes. We confirmed that the above implication is consistent with the energy spectra obtained from the actual LES.

To satisfy the criterion from the numerical dispersion in the range of more than eight grids, seventh-order accuracy at least is required in the present experiment. For the central schemes, this constraint is more severe than that of high-order explicit numerical diffusion. Despite this strong constraint, the effect of the numerical dispersion error on the energy spectra is limited in our experiment, although it is not difficult to imagine that the numerical dispersion may affect the local turbulence mechanism. We must more intensively examine it in realistic experiments for future work.

We also examined the influence of temporal discretization on the criteria. In the atmospheric model used in this study, the time step is restricted by the sound wave, and the Courant number with advection is sufficiently smaller than unity. Thus, the temporal accuracy is not as essential as the spatial accuracy. For example, when an eighth-order spatial scheme is applied, eighth-order accuracy for the temporal scheme is excessive, and even the fourth-order temporal scheme is acceptable.

We statistically discuss the effect of stratification on our derived criteria in our numerical experiment. The numerical criteria for neutral stratification can be approximately applied for most grid points, because of the nearly neutral stratification. However, we must take care of approximately 10% grid points with $R_i > 0.1$, where a much higher order of accuracy is required than that for the neutral stratification.

In this paper, we focused on the advection terms that directly affect the turbulence simulations. Future studies should investigate other terms (e.g., the pressure gradient term including the isotropic part of the SGS strain tensor), and evaluate the impact of the discretization accuracy for such terms. Furthermore, considering atmospheric calculations with topography, we must evaluate the numerical errors associated with the vertical coordinate transformation. When adopting conventional high-order finite-volume schemes, we will face some difficulty in particular for the global models. The method is complex because of the distinction between the cell-center point and cell-averaged values, and the computational locality deteriorates as the stencil is extended. One promising method to counter these problems is the discontinuous Galerkin method (DGM). The performance of the DGM for dynamical cores has been evaluated (e.g., [Giraldo and Restelli 2008](#); [Kelly and Giraldo 2012](#); [Marras et al. 2016](#)). However, the practical performance in actual atmospheric simulations with physical processes has not been widely investigated. In terms of the balance between the physical representation and computational performance, investigating the suitability of DGM through the framework of this study should also be a focus of future work.

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Data availability statement. Source codes and configuration files for SCALE-RM used in this study are available from the Zenodo repository (<https://doi.org/10.5281/zenodo.4915846>). There, supplementary material helpful for the derivation of some equations in this paper is included. All data obtained from the numerical experiments has been deposited in the local storage at RIKEN R-CCS.

APPENDIX A

Numerical Diffusion and the Associated e -Folding Decay Time

Let us consider the one-dimensional linear advection equation as

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0. \quad (\text{A1})$$

In this section, we derive the modified equation for FDM and the e -folding decay time with the numerical diffusion. Note that the temporal discretization is not considered here.

a. General form of the finite-difference approximation of the first derivative

The first derivative at the grid point x_j is approximated by $2p_{\max} + 1$ stencils as $(f_x)_{\text{scheme}}(x_j) = \sum_{p=-p_{\max}}^{p_{\max}} A_p \hat{f}_{j+p} / \Delta x$ where $f_x = \partial f / \partial x$, Δx denotes equal grid spacing, and $\hat{f}_j = f(x_j)$. Taking the Taylor series expansion of $\hat{f}_{j+p}$ around x_j , we obtain the modified equation as

$$\begin{aligned} (f_x)_{\text{scheme}}(x_j) &= \sum_{p=-p_{\max}}^{p_{\max}} \frac{A_p}{\Delta x} \sum_{n=0}^{\infty} f_{x(n)}(x_j) \frac{(p\Delta x)^n}{n!} \\ &= \sum_{n=0}^{\infty} c(p_{\max}, n) f_{x(n)}(x_j), \end{aligned} \quad (\text{A2})$$

where $f_{x(n)} = \partial^n f / \partial x^n$ and $c(p_{\max}, n) = [(\Delta x)^{n-1} / n!] \sum_{p=-p_{\max}}^{p_{\max}} A_p p^n$. To approximate f_x , $c(p_{\max}, 0) = 0$, and $c(p_{\max}, 1) = 1$ are required. To obtain a desired n' -order accuracy, we constrained $c(p_{\max}, n) = 0$ for $2 \leq n \leq n'$. The remaining terms multiplied by $c(p_{\max}, n)$ for $n > n'$ produce numerical errors. The CD scheme takes the same number of stencils on both sides, whereas the UD scheme takes more stencils on the upwind side. Here, we treat UD schemes in which only one more stencil is taken on the upwind side. The matrix of A_p under the constraint of $c(p_{\max}, n)$ gives A_p and the numerical errors in [Tables 1 and A1](#), respectively.

b. Derivation of e -folding decay time: For CD schemes

The numerical errors for the CD schemes are an infinite series of dispersion terms without dissipation errors. For the numerical stabilization, the numerical diffusion is explicitly added as $\partial f / \partial t = \nu_{\text{num}, 2n} f_{x(2n)}$ where $\nu_{\text{num}, 2n}$ is defined in Eq. (6). For a wavelength λ (see [section 2](#) for the normalization of λ by Δx), the e -folding decay time with the numerical diffusion is obtained as $T_{e, \text{num}(2n)}^{\text{continuous}} = (\Delta t / \gamma_{2n})(l/\pi)^{2n}$. We spatially discretize the numerical diffusion terms by repeatedly applying a second-order Laplacian discrete operator, and evaluate it explicitly in the final stage of the RK schemes. By this operation, the e -folding decay time is modified as

$$T_{e, \text{num}(2n)}^{\text{discrete}} = T_{e, \text{num}(2n)}^{\text{continuous}} \alpha_c(2n), \quad (\text{A3})$$

where $\alpha_c(2n) = 2^{2n} (\pi/l)^{2n} \times \{2[1 - \cos(2\pi\Delta x/\lambda)]\}^{-n} = [(\pi/l)/\sin(\pi/l)]^{2n}$. For the detailed derivation of $\alpha_c(2n)$, see [section 3.3.3](#) in [Durran \(2010\)](#).

c. Derivation of e -folding decay time: For UD schemes

The $(2n - 1)$ -order UD scheme intrinsically has an infinite series of numerical diffusion terms as $-|U| \sum_{m=n}^{\infty} c(p_{\max}, 2m) f_{x(2m)}$.

TABLE A1. For equal grid spacing, we show the coefficient A_p in the finite-difference approximation of the first derivative term. Here, we assume that $U > 0$ in the upwind schemes.

Scheme	A_{-4}	A_{-3}	A_{-2}	A_{-1}	A_0	A_1	A_2	A_3	A_4
First-order upwind	0	0	0	-1	1	0	0	0	0
Second-order central	0	0	0	-1/2	0	1/2	0	0	0
Third-order upwind	0	0	1/6	-1	1/2	1/3	0	0	0
Fourth-order central	0	0	1/12	-2/3	0	2/3	-1/12	0	0
Fifth-order upwind	0	-1/30	1/4	-1	1/3	1/2	-1/20	0	0
Sixth-order central	0	-1/60	3/20	-3/4	0	3/4	-3/20	1/60	0
Seventh-order upwind	1/140	-1/15	3/10	-1	1/4	3/5	-1/10	1/105	0
Eighth-order central	1/280	-4/105	1/5	-4/5	0	4/5	-1/5	4/105	-1/280

Thus, we can write the corresponding coefficient of diffusion as $\nu_{\text{num},2n} = -|U|c(p_{\text{max}}, 2m)$. Like the form of Eq. (6), we introduce γ_{2m} for UD schemes as $\gamma_{2m} = f_{\text{UD},2m}|U|\Delta t/\Delta x$ where $f_{\text{UD},2m}$ is defined as

$$f_{\text{UD},2m} = (-1)^m \frac{2^{2m}}{(2m)!} \left(\sum_{p=-p_{\text{max}}}^{p_{\text{max}}} A_p p^{2m} \right). \quad (\text{A4})$$

In the dominant error, $f_{\text{UD},4} = 4/3$, $f_{\text{UD},6} = 16/15$, and $f_{\text{UD},8} = 32/35$, for example.

When discussing the properties of schemes, we often focus only on the dominant error. However, higher-order error terms do not always behave in the same manner. For example, for UD3, the $2(2n' + 1)$ -order differential error terms (where n'

is a natural number) perform destabilization. Thus, precisely, we need to consider all the terms. Taking care of the “true” e -folding decay time by a continuous representation, we obtain the e -folding decay time for the $(2n - 1)$ -order UD scheme as

$$T_{e,\text{num}}^{\text{UD}(2n-1)} = T_{e,\text{num}(2n)}^{\text{continuous}} \alpha_u(2n), \quad (\text{A5})$$

where $\alpha_u(2n) = \left[1 + \sum_{p=n+1}^{\infty} (\pi/l)^{2(p-n)} \gamma_{2p}/\gamma_{2n} \right]^{-1}$.

Figures A1a and A1b shows that α_u^{-1} almost converges for any wavelength when considering up to 20 terms. The sign of the converged value is positive, which indicates that the scheme is stable. Figures A1c and A1d shows the dependence of α_u^{-1} on the wavelength. $T_{e,\text{num}}^{\text{UD}(2n-1)}$ is longer than that considered the dominant error only. The differences become small

FIG. A1. (top) Convergence of the infinite series α_u^{-1} for (a) UD3 and (b) UD5. (bottom) Dependence of α_u^{-1} (up to 32 terms) on the wavelength for (c) UD3 and (d) UD5.

as the wavelength increases; for more than eight grids, it is less than 10%.

APPENDIX B

Dependency of Typical Magnitude of Strain Tensor on the Resolution

In incompressible flow with a high Reynolds number, we consider homogeneous isotropic three-dimensional turbulence. The average of $|S|^2$ in volume V in the context of the LES is written as

$$\frac{1}{V} \int \frac{|S|^2}{2} d\mathbf{x} \simeq \frac{1}{V} \int \frac{(\nabla \times \mathbf{u})^2}{2} d\mathbf{x} = (2\pi)^3 \int_0^{\pi/\Delta_{\text{SGS}}} k^2 [(4\pi k^2/V) E'(\mathbf{k})] dk,$$

where $E'(\mathbf{k})$ is the energy spectral density, $\mathbf{k}$ is the three-dimensional wave vector, and $k = |\mathbf{k}|$. According to the $-5/3$ power law of energy spectra, $(4\pi k^2/V) E'(\mathbf{k}) = \alpha k^{-5/3}$, where α is the constant that contains the energy dissipation rate. Using this relation,

$$\frac{1}{V} \int \frac{|S|^2}{2} d\mathbf{x} = (2\pi)^3 \int_0^{\pi/\Delta_{\text{SGS}}} k^2 \times \alpha k^{-5/3} dk = (2\pi)^3 \frac{3\alpha}{4} \left(\frac{\pi}{\Delta_{\text{SGS}}} \right)^{4/3}. \quad (\text{B1})$$

This result leads to Eq. (17) as the typical magnitude of $|S|$ with $\eta = [2(2\pi)^3(3\alpha/4)]^{1/2}$.

The typical magnitude of $\nabla|S|$ is formulated as follows. The average of $(\nabla|S|)^2$ in V is written as

$$\begin{aligned} \frac{1}{V} \int \sum_{i=1}^3 \left(\frac{\partial |S|}{\partial x_i} \right)^2 d\mathbf{x} &= \frac{1}{V} \int \sum_{i=1}^3 \left(\frac{\partial S}{\partial x_i} \right)^2 d\mathbf{x} \\ &= (2\pi)^3 \int_0^{\pi/\Delta_{\text{SGS}}} k^2 \left[(4\pi k^2/V) |\tilde{S}(\mathbf{k})|^2 \right] dk. \end{aligned} \quad (\text{B2})$$

From Eq. (B1), we obtain the Fourier transform of $|S|^2$ as $(4\pi k^2/V) |\tilde{S}(\mathbf{k})|^2 = (2\pi)^{-3} (4/3) \eta^2 k^{1/3}$. Substituting it into Eq. (B2):

$$\frac{1}{V} \int \sum_{i=1}^3 \left(\frac{\partial |S|}{\partial x_i} \right)^2 d\mathbf{x} = \frac{2}{5} \eta^2 \left(\frac{\pi}{\Delta_{\text{SGS}}} \right)^{10/3}.$$

where the relationship $\{[\partial_{t(k)} - (-U)^k \delta_{x(k)}] f\}_j^m = O(\Delta t^{R_n})$ is used. Thus, we can focus on replacing $\partial_{t(2)} f$ with the spatial differential terms explicitly written up to $O(\Delta t^{R_n})$. To systematically show the derivation, we introduce a linear operator as $[L(f)]_j^m \equiv (\partial_t f)_j^m - U(\delta_x f)_j^m$. Acting the operator L on Eq. (C3) once and using the relation $L[\delta_{x(k)} f] = -2U[\delta_{x(k+1)} f]_j^m + O(\Delta t^{R_n})$ (where $k = 0, 1, 2, \dots$), we obtain the following equation:

Thus, we can estimate the typical magnitude of $\nabla|S|$ for each direction using Eq. (18) with $\eta' = \sqrt{2/15} \eta$.

APPENDIX C

Influence of Numerical Errors due to Temporal Discretization

In this section, we investigate the influence of temporal discretization errors using the one-dimensional linear advection equation of Eq. (A1).

a. Derivation of the modified equation

Without losing generality, consider the R_s stage and R_n -order RK scheme as the temporal discretization and the CD scheme as the spatial discretization. Based on section 2.1 in Baldauf (2008), the discretization of Eq. (A1) can be written as

$$\begin{aligned} \frac{f_j^{m+1} - f_j^m}{\Delta t} &= -U(\delta_x f)_j^m + \sum_{k=2}^{R_n} \frac{\Delta t^{k-1}}{k!} (-U)^k [\delta_{x(k)} f]_j^m \\ &\quad + \sum_{k=R_n+1}^{R_s} r_{R_n,k} \Delta t^{k-1} (-U)^k [\delta_{x(k)} f]_j^m, \end{aligned} \quad (\text{C1})$$

where $f_j^m = f(x_j, t_m)$, δ_x is a discrete operator with CD schemes, and $[\delta_{x(k)} f]_j^m = [(\delta_x)^k f]_j^m$. In the case of $R_s \leq R_n$, the third term in the rhs of Eq. (C1) vanishes. We can derive the modified equation as follows. By taking a Taylor series expansion of f_j^{m+1} around t_m to Eq. (C1):

$$\begin{aligned} (\partial_t f)_j^m + U(\delta_x f)_j^m &= - \sum_{k=2}^{R_n} \frac{\Delta t^{k-1}}{k!} \{[\partial_{t(k)} - (-U)^k \delta_{x(k)}] f\}_j^m \\ &\quad + \sum_{k=R_n+1}^{R_n+2} r_{R_n,k} \Delta t^{k-1} (-U)^k [\delta_{x(k)} f]_j^m \\ &\quad - \sum_{k=R_n+1}^{R_n+2} \frac{\Delta t^{k-1}}{k!} [\partial_{t(k)} f]_j^m + O(\Delta t^{R_n+2}), \end{aligned} \quad (\text{C2})$$

where we consider $r_{R_n,k} = 0$ for $k > R_s$. If we replace the temporal differential terms on the rhs with the spatial differential terms, we can obtain the modified equation. Note that this operation must be consistent with Eq. (C1). For the current discussion, it is enough to derive the equation up to $O(\Delta t^{R_n+1})$. Equation (C2) can be written as

$$(\partial_t f)_j^m + U(\delta_x f)_j^m = - \frac{\Delta t}{2!} \{[\partial_{t(2)} - U^2 \delta_{x(2)}] f\}_j^m + \sum_{k=R_n+1}^{R_n+2} r_{R_n,k} \Delta t^{k-1} (-U)^k [\delta_{x(2)} f]_j^m - \sum_{k=R_n+1}^{R_n+2} \frac{\Delta t^{k-1} (-U)^k}{k!} [\delta_{x(k)} f]_j^m + O(\Delta t^{R_n+2}), \quad (\text{C3})$$

$$\begin{aligned} [\partial_{t(2)} f]_j^m - U^2 [\delta_{x(2)} f]_j^m &= \Delta t^{R_n} \times 2 \left[r_{R_n, R_n+1} - \frac{1}{(R_n+1)!} \right] \\ &\quad \times (-U)^{R_n+2} [\delta_{x(R_n+2)} f]_j^m + O(\Delta t^{R_n+1}). \end{aligned} \quad (\text{C4})$$

Substituting Eq. (C4) into Eq. (C3) and arranging some terms, we obtain

$$(\partial_t f)_j^m + U(\delta_x f)_j^m = \sum_{k=R_n}^{R_n+1} \Delta t^k (-1)^{k+1} r'_{R_n, k+1} U^{k+1} \times [\delta_{x(k+1)} f]_j^m + O(\Delta t^{R_n+2}), \quad (C5)$$

where $r'_{R_n, R_n+1} = -[(R_n + 1)!]^{-1} + r_{R_n, R_n+1}$, $r'_{R_n, R_n+2} = -[(R_n + 2)!]^{-1} + r_{R_n, R_n+2} - r'_{R_n, R_n+1}$. For example, the modified equation for RK8CD8 is given as

$$\begin{aligned} \left(\frac{\partial f}{\partial t}\right)_j^m + U\left(\frac{\partial f}{\partial x}\right)_j^m &= \left[\frac{U\Delta x^8}{630} \left(\frac{\partial^9 f}{\partial x^9}\right)_j^m + O(\Delta x^{10})\right] + \Delta t^8 \left(\frac{1}{9!} - r_{8,9}\right) U^9 \left[\left(\frac{\partial^9 f}{\partial x^9}\right)_j^m + O(\Delta x^8)\right] \\ &+ \Delta t^9 \left(-\frac{1}{10!} + r_{8,10} + \frac{1}{9!} - r_{8,9}\right) U^{10} \left[\left(\frac{\partial^{10} f}{\partial x^{10}}\right)_j^m + O(\Delta x^8)\right] + O(\Delta t^{10}), \end{aligned} \quad (C6)$$

where $r_{8,9} = (-191 + 39\sqrt{21})/16934400$ and $r_{8,10} = (-91 + 19\sqrt{21})/59270400$.

In our experiments, where the Courant number with advection c_r is significantly less than 1, the effect of the higher-order temporal error terms is expected to be small. To verify it, we calculate the amplification factor from Eq. (C6). Figure C1a shows the factor assuming that the spatial error is much smaller than the temporal error. When $c_r \sim O(10^{-1})$, the effect of the higher-order temporal error terms than $O(\Delta t^{R_n+1})$ is extremely small. Figure C1b indicates that the spatial error in the $O(\Delta t^9)$ term is essential for less than four grids. However, it is sufficient to discuss the influence of temporal errors on the numerical criteria for more than four grids. Thus, we explicitly treat the temporal errors up to $O(\Delta t^{R_n+1})$, but do not consider the spatial errors in such temporal error terms.

b. Modification of the numerical criteria due to temporal errors

From Eq. (C5), the numerical errors due to temporal discretization can be written as

$$r'_{n,n+1} \Delta x^n c_r^n U \frac{\partial^{n+1} \phi}{\partial x^{n+1}} + r'_{n,n+2} \Delta x^{n+1} c_r^{n+1} U \frac{\partial^{n+2} \phi}{\partial x^{n+2}} + O(\Delta x^n c_r^n, c_r^{n+1}), \quad (C7)$$

where $r'_{8,9} \sim 3.5 \times 10^{-6}$ and $r'_{8,10} \sim 3.1 \times 10^{-6}$ for RK8, $r'_{4,5} = 1/5!$ and $r'_{4,6} = 5/6!$ for RK4, and $r'_{3,4} = -1/4!$ and $r'_{3,5} = -4/5!$ for RK3. When the even-order differential terms in Eq. (C7) are considered, the e -folding decay time with the explicit numerical diffusion for CD8ND8 was modified as shown in Eq. (21). In contrast, the phase speed associated with the numerical dispersion for CD8ND8 was modified as shown in Eq. (22), when the odd-order differential terms in Eq. (C7) are considered.

In section 4b, we discussed the influence of temporal errors on the numerical criteria when CD8ND8 was adopted as the advection scheme, but we can evaluate other cases similarly. For example, for CD4ND4, the modification of R_{diff} due to the temporal errors is obtained as follows: for RK4:

$$\begin{aligned} T'_{e,\text{num}} &= T_{e,\text{num}} \left\{ 1 + \beta_e(l, 2) \frac{r'_{4,2 \times 3}}{\gamma_4} (2c_r)^{2 \times 3} \left(\frac{\pi}{l}\right)^{2(3-2)} \right. \\ &\times \left. \left[1 + \sum_{\tilde{m}=3+1}^{\infty} \frac{r'_{4,2 \times \tilde{m}}}{r'_{4,2 \times 3}} \left(c_r \frac{2\pi}{l}\right)^{2(\tilde{m}-3)} \right] \right\}^{-1}, \end{aligned}$$

whereas for RK3:

$$\begin{aligned} T'_{e,\text{num}} &= T_{e,\text{num}} \left\{ 1 + \beta_e(l, 2) \frac{r'_{3,2 \times 2}}{\gamma_4} (2c_r)^{2 \times 2} \left(\frac{\pi}{l}\right)^{2(2-2)} \right. \\ &\times \left. \left[1 + \sum_{\tilde{m}=2+1}^{\infty} \frac{r'_{3,2 \times \tilde{m}}}{r'_{3,2 \times 2}} \left(c_r \frac{2\pi}{l}\right)^{2(\tilde{m}-2)} \right] \right\}^{-1}. \end{aligned}$$

In our consideration, RK2 is excluded because numerical stability is not typically ensured for the central advection schemes. Let us focus on the leading contribution of temporal discretization, which comes from the first term in the square bracket. For both RK4 and RK3, this contribution is sufficiently small for the following reasons. The typical magnitudes of $r'_{4,6}/\gamma_4$ and $(2c_r)^6$ for RK4 and $r'_{3,4}/\gamma_4$ and $(2c_r)^4$ for RK3 are given by the second and first rows in Table 3, respectively (here, $\gamma_4 = \gamma_8 = 2 \times 10^{-4}$ in our experimental setup). In addition, $\beta_e(l, 2) \sim O(1)$ for $l > 2\pi$. The leading numerical diffusion error term due to RK4 is the sixth-order differential, which is higher than that due to CD4ND4. This causes a positive index of factor π/l , which decreases with the wavelength. Thus, the leading contribution of the temporal discretization is significantly small than the effect of numerical diffusion in CD4ND4. For RK3, because the differential order of the leading numerical diffusion error term is the same as that of CD4ND4, the factor π/l become unity. However, because of $r'_{3,4}/\gamma_4 (2c_r)^4 \sim O(10^{-6})$, we expect that the leading contribution of temporal discretization for RK3 is not significant.

We could approximately consider the maximum Courant number associated with the advection such that the temporal errors are no longer acceptable. For example, let us consider where we adopt the RK4 scheme and CD8ND8 for advection terms and appropriately treat the terms associated with fast waves using a temporal strategy. Furthermore, we set the criteria with temporal errors in which the leading contributions of the temporal error terms in Eqs. (21) and (22) should be less than 10% at $l \sim 10^2$ for the $O(10)$ m resolution. The typical magnitudes of the factors, except for c_r , are still given by the values in Table 3. The criteria with temporal errors require that $c_r < 0.07$, and $c_r < 0.04$ for R_{diff} and R_{disp} , respectively. Thus, if we set the model time step as long as the numerical stability for advection is ensured, the criteria with temporal errors can possibly be violated. This indication is consistent with the discussion of large time step in section 4b.

Although we focus on some RK schemes in this study, in the same manner as that used here, we can evaluate the impact of temporal errors for other temporal schemes.

FIG. C1. For the RK8CD8 case, the dependence of the amplification factor G per a time step on the wavelength is as follows: (a) the case in which the temporal error terms are considered from $O(\Delta t^{10})$ to $O(\Delta t^{14})$ in Eq. (C6) without the spatial discretization error, and (b) the case in which the spatial error terms are considered from $O(\Delta x^8)$ to $O(\Delta x^{20})$ in the $O(\Delta t^9)$ temporal error term in Eq. (C6). We compared the results obtained from the modified equation of Eq. (C6) with that from the Von Neumann stability analysis. The latter is represented with black lines. In the panels, we fixed $c_r = 0.2$.

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