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ABSTRACT

In this paper, the surface quasi-geostrophic (SQG) turbulence with a spatially periodic initial condition is numerically simulated by means of two methods: one is the traditional direct numerical simulation (DNS) whose numerical noise quickly increases to the same order of magnitude as its physical solution, the other is the so-called clean numerical simulation (CNS) whose numerical noise is much smaller than the physical solution and thus is negligible in a finite but long enough interval of time. Influence of numerical noises is investigated in detail by comparing the two simulations of the SQG turbulence given, respectively, by the DNS and CNS. It is found that the artificial stochastic numerical noises would lead to huge derivations apart from CNS benchmark solution not only in the spatiotemporal trajectories but also in the spatial symmetry of turbulence and many statistical results. However, it is surprisingly found that, despite so many huge deviations mentioned earlier, the kinetic energy spectra given by the DNS agrees well with that given by the CNS benchmark solution: both of them satisfy the famous $-5/3$ law. It indicates that the kinetic energy spectra have stability, i.e., insensitive to stochastic disturbances. On one side, this is a good new. Unfortunately, on the contrast, it also provides us an evidence that correctly capturing the $-5/3$ law of kinetic energy spectra cannot guarantee the correction of statistical results of DNS. In other words, a correct kinetic energy spectra alone cannot serve as a reliable criterion for assessing the correctness of numerical solutions of turbulence.

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I. INTRODUCTION

The governing Navier–Stokes equations in turbulence are nonlinear and inherently exhibit characteristics of chaotic behavior. While both turbulence and chaos display sensitive dependence on initial conditions and a high degree of nonlinearity, their relationship is subtle and multifaceted. This connection can be explored through the framework of nonlinear dynamics. Early discussions on the generation of turbulence were presented by Landau¹ and Hopf,² who proposed that turbulence arises from a Hopf bifurcation mechanism. They noted that the system exhibits an infinite number of incommensurate frequencies, which eventually lead to turbulent motion. However, Ruelle and Takens³ demonstrated that only a finite number of bifurcations can give rise to a strange attractor, which is synonymous with turbulence. In contrast to these theoretical frameworks, experimental results by Maurer and Libchaber⁴ revealed that turbulence may initially emerge through the appearance of two incommensurate frequencies, which later lock to one of these frequencies and undergo period doubling. Understanding the intricate relationship between turbulence

and chaos has profound implications for fluid dynamics, statistical mechanics, and the study of nonlinear systems. Regardless of the specific mechanism behind turbulence generation, its sensitive dependence on initial conditions significantly impacts numerical predictions, particularly in the field of weather forecasting.⁵ The latter involves modeling fluid flows in the atmosphere and oceans, where small variations in initial conditions can lead to vastly different outcomes.⁶

In this paper, let us consider the unbounded surface quasi-geostrophic (SQG) turbulence, a classical phenomenological model that effectively describes synoptic-scale eddies in both the atmosphere and ocean.⁷ First introduced by Blumen,^{8,9} SQG turbulence serves as a bridge between two-dimensional and three-dimensional quasi-geostrophic dynamics, allowing for a deeper understanding of energy transfer processes characteristic of fully developed turbulence. The surface quasi-geostrophic model is particularly valuable for studying the energy spectrum and energy cascade phenomena, which are crucial in explaining how kinetic energy dissipates through various scales of motion in both atmospheric and oceanic contexts. Its unique

properties have led to its application in a range of studies, particularly those focusing on potential temperature anomalies in the atmosphere^{10,11} and the ocean.^{12–14} Moreover, the model has been instrumental in exploring the statistical properties of developed turbulence,^{7,15–17} revealing insights into the shape of kinetic energy spectra¹⁸ and the chaotic characteristics of turbulent flows.¹⁹

Geophysical turbulence exhibits a broad spectrum of spatial and temporal scales.^{20,21} Due to this multi-scale nature, it is chaotic and irregular in velocity and pressure field, thus some researchers tried to use “chaos theory” or “dynamical theory” to explain these characteristics.^{19,22} As a chaotic system, micro-level disturbances in turbulence increase exponentially to macro-scale. Numerical methods such as large eddy simulation (LES)²³ and direct numerical simulation (DNS)²⁴ are widely used to obtain numerical simulation of turbulence. Especially, results given by DNS are nowadays regarded as reliable benchmark solution, since DNS does not introduce any extra turbulence models. However, all numerical algorithms (including DNS) contain artificial numerical noises caused by round-off error and truncation error, which increases exponentially to macro-scale for a chaotic system or turbulence. Therefore, a numerical simulation of chaos or turbulence is quickly polluted badly by artificial numerical noise. Despite this, such kind of badly polluted numerical simulation is often used to calculate various statistics: it is widely “believed” that those statistics given by a badly polluted simulation $S = P + \delta'$ should be the same as the statistics given by the true physical solution P , i.e.,

$$\langle P + \delta' \rangle = \langle P \rangle, \quad \text{when } \delta' \sim P, \quad (1)$$

where $\langle \rangle$ represents a statistical operator, δ' denotes the artificial numerical noise that is mostly at the same order of magnitude as the true solution P . Unfortunately, this is only a *hypothesis*. In addition, the famous $-5/3$ law of kinetic energy spectra of turbulence is widely used as a criterion to check the correction of DNS for turbulence.

In the method of pseudo-spectral DNS, time discretization plays a critical role. Implicit time integration methods are stable and allow for larger time steps than explicit methods, but computationally expensive for pseudo-spectral DNS. Thus, explicit time integration methods are widely adopted due to their simplicity and parallel scalability. Despite the relatively average performance of the Runge–Kutta scheme in turbulence or chaotic dynamics simulations, the Fourier pseudo-spectral method, an established technique for spatial discretization, is frequently coupled with the fourth-order Runge–Kutta (RK4) scheme. This combination offers a balance between computational efficiency and temporal accuracy.^{25,26} While RK4 remains the most common choice, alternative approaches such as lower-order Runge–Kutta variants or multistep methods have also been used.²⁷ Naturally, these alternatives generally demand even smaller time steps to ensure that temporal errors remain consistent with the high spatial precision achieved by spectral methods. By employing a high-order explicit time integration method, the truncation error can be significantly reduced. However, the high-order Runge–Kutta scheme can be unstable and challenging to implement. In contrast, alternative methods such as the Taylor series method²⁸ or the Bulirsch–Stoer method²⁹ may offer improved performance.

In this paper, the surface SQG turbulence with a spatially periodic initial condition is numerically solved by means of the traditional DNS, whose numerical noises quickly increases to the same order of magnitude as its physical solution, and the so-called clean numerical

simulation (CNS).^{30–35} Unlike DNS, artificial numerical noise of CNS is much smaller than the physical solution and thus is negligible in a finite but long enough interval of time suitable for calculating statistics. Note that CNS has been successfully used to solve many chaotic systems, such as the Lorenz equation,³⁶ the famous three-body problem,³⁷ turbulent flows^{38–42} and so on. Influence of numerical noises is investigated in detail by comparing the two simulations of the SQG turbulence, respectively, given by the DNS and CNS. It is found that the artificial stochastic numerical noises of DNS would lead to huge derivations apart from CNS benchmark solution *not only* in the spatiotemporal trajectories *but also* even in the spatial symmetry of turbulence and several statistics, i.e., the hypothesis (1) does *not* hold for the SQG turbulence under consideration. However, it is very interesting that, despite so many huge deviations in statistics, the kinetic energy spectra given by the DNS agrees well with that given by CNS: both satisfy the famous $-5/3$ law, indicating that the kinetic energy spectra has instability. This is a good new. Unfortunately, it also provides an evidence that correctly capturing the $-5/3$ law of kinetic energy spectra *cannot* guarantee the correctness of statistical results of DNS, say, a correct kinetic energy spectra alone *cannot* serve as a reliable criteria to assess the correctness of numerical solutions of turbulence.

In Sec. II, we briefly introduce the mathematical model of the SQG turbulence and the basic ideas of the numerical algorithms. The detailed comparisons between CNS and DNS solutions, especially the statistics and kinetic energy spectra, are given in Sec. III. The conclusions and discussions are given in Sec. IV.

II. MATHEMATICAL MODEL

A. Governing equation

The model is introduced by a representation of Eady dynamics⁴³ as the Blumen model,⁸ which obeys the SQG dynamics in the horizontal plane $(x, y) \in [0, L] \times [0, L]$ on the two surfaces ($z = 0, H$), where L is the length of the square domain, H is the height of the upper boundary ($z = H$) from the low boundary ($z = 0$), independently. It describes the relation between two scalars: the potential temperature $\theta(x, y, z, t)$ and the stream-function $\psi(x, y, z, t)$, where (x, y, z) denotes the spatial position with either $z = 0$ or $z = H$ only, and t is the time, respectively, whose governing equations in the horizontal spectral space (k_x, k_y, z, t) are as follows:

$$\hat{\theta}_t + \hat{J}(\hat{\psi}, \hat{\theta}) = -\mathbf{i}k_x(U_z \hat{\theta} + \hat{\psi} \Theta_y), \quad z = 0, H, \quad (2)$$

where $\hat{\theta}(k_x, k_y, z, t)$ and $\hat{\psi}(k_x, k_y, z, t)$ are the potential temperature spectrum and the stream-function spectrum in the spectral space (k_x, k_y) of the horizontal surface (x, y) with the wave numbers k_x and k_y , respectively, U_z is the zonal wind velocity, Θ_y is the mean surface temperature gradients, the subscript denotes partial derivative if not mentioned, $\mathbf{i} = \sqrt{-1}$ is the imaginary unit, and $\hat{J}$ means the sum over the horizontal wave numbers of the Jacobian terms,

$$\hat{J}(\hat{\psi}, \hat{\theta}) = J(\hat{\psi}, \hat{\theta}) = \overline{\psi_x \theta_y - \psi_y \theta_x} \quad (3)$$

where $\hat{\cdot}$ denotes the transformation from (x, y) to the spectral space (k_x, k_y) . The relation between the potential temperature spectrum $\hat{\theta}$ and the stream-function spectrum $\hat{\psi}$ is given by

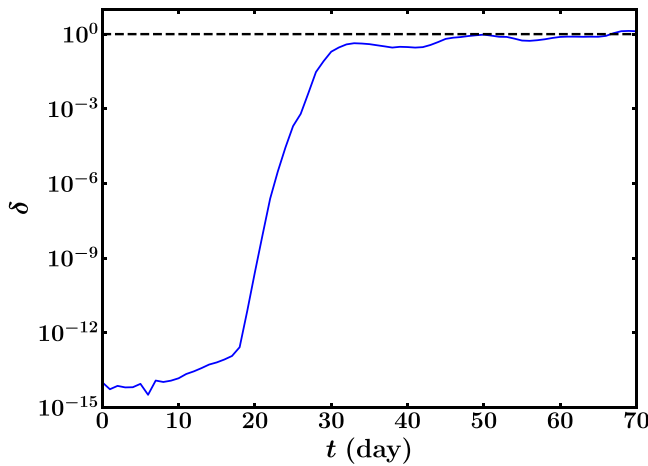


FIG. 1. Deviation of the potential temperature field θ from the results of the CNS and DNS. The black dashed line denotes $\delta = 1$.

$$\hat{\psi} = \frac{H}{\mu \sinh \mu} \left[\cosh \left(\mu \frac{z}{H} \right) \hat{\theta}(k_x, k_y, H, t) - \cosh \left(\mu \frac{z-H}{H} \right) \hat{\theta}(k_x, k_y, 0, t) \right], \quad (4)$$

where $\mu = \frac{|\mathbf{k}|NH}{f}$ is the non-dimensional wavenumber, f is the Coriolis frequency, N is the Brunt-Vaisala frequency, and $|\mathbf{k}| = \sqrt{k_x^2 + k_y^2}$ is the total horizontal wavenumber. Thus, according to (4), the governing Eq. (2) contains one unknown function $\hat{\theta}$ only.

Following Wang *et al.*,⁴⁴ we set $U_z = 0$ and $\Theta_y = 0$ in (2), but introduce a thermal relaxation term to bring the system back to equilibrium, with the jet acting as an external energy input, say,

$$\hat{\theta}_t + \hat{T}(\hat{\psi}, \hat{\theta}) = \frac{1}{T}(\hat{\theta}_b - \hat{\theta}), \quad z = 0, H, \quad (5)$$

where T is the thermal relaxation damping time, and the equilibrium jet spectrum $\hat{\theta}_b$ is given by

$$\hat{\theta}_b(k_x, k_y, z, t) = \frac{NU}{2f \tanh\left(\frac{\pi NH}{fL}\right)} \cos\left(\frac{2\pi y}{L}\right), \quad z = 0, H, \quad (6)$$

where L is the size of the square domain, and U is the flow velocity, respectively. Here, we choose the initial condition

$$\theta(x, y, z, 0) = \cos(2x) \cos(2y), \quad z = 0, H, \quad (7)$$

corresponding to a periodic boundary in space. Note that this initial condition (7) has a kind of spatial symmetry. Without loss of generality, we consider here the following physical parameters: $H = 10^3$ (m), $L = 2 \times 10^6$ (m), $U = 30$ (m/s), $T = 10$ days, $f = 10^{-4}$ (1/s), and $N = 10^{-2}$ (1/s).

B. Numerical algorithm

Equations (5) and (7) are solved by means of CNS. Note that every numerical algorithm contains artificial numerical noises, i.e.,

truncation error and round-off error, which increases exponentially for a chaotic system and turbulent flow. Unlike DNS that uses double-precision in general, CNS adopts multiple-precision⁴⁵ with sufficient significant digits to decrease greatly the round-off error, as well as sufficiently high-order Taylor expansion with a reasonably small time step and the pseudo-spectral method with small enough spacing to decrease greatly truncation errors in time and space, respectively, so that artificial numerical noise can be negligible over a finite but long enough time interval $t \in [0, T_c]$ suitable for calculating statistics, where T_c is called the critical predictable time. As pointed out by Liao,^{31,46} Hu and Liao,³² and Liao and Wang,³⁶ for two different order of Taylor expansion and numbers of significant digits numerical routines $\theta(t)$ and $\theta'(t)$, the $\theta'(t)$ has a higher-order Taylor expansion and a greater number of significant digits than the $\theta(t)$. The critical predictable time T_c of $\theta(t)$ and $\theta'(t)$ is defined by

$$\left| 1 - \frac{\theta(t)}{\theta'(t)} \right| < \delta, \quad (8)$$

where $\delta > 0$ is a small constant ($\delta = 5\%$ is adopted in this paper). It is important that each CNS result $\theta(t)$ is rigorously compared with another CNS result $\theta'(t)$, obtained using a higher-order Taylor expansion and a greater number of significant digits. This comparison ensures that the difference between the two results remains smaller than the required precision over the entire computation time, $t \in [0, T_c]$.

In this paper, the flow field is discretized into $N_x \times N_y = 256 \times 256$ uniform mesh, and the 3/2 rule is used to control the alias error. Here, we use the time step $\Delta t = 60$ (second), with the total simulation time of 365 days, i.e., one year. In the frame of CNS, it is found that T_c increases linearly with respect to the order M of Taylor expansion in time, say, $T_c = 19.15M - 25.8$, when we use a sufficiently large number of significant digits $N_s = 150$ (i.e., round-off error is small enough). In addition, using a sufficiently large order $M = 25$ of Taylor expansion, it is found that T_c also increases almost linearly with respect to the number N_s of significant digits, i.e., $T_c = 2.65N_s + 5.98$. Thus, to obtain a reliable/convergent numerical simulation of Eqs. (5) and (7) in one year, say, $T_c = 365$ days, we should use the 25th-order (i.e., $M = 25$) Taylor expansion in time and 145 number of significant digits (i.e., $N_s = 145$) by means of CNS. For the detailed algorithm of CNS, please refer to Appendix A.

On the other hand, a traditional DNS algorithm is applied on the same uniform mesh $N_x \times N_y = 256 \times 256$ using the fourth-order Runge-Kutta method with double precision. Obviously, its numerical noise of DNS increases exponentially, quickly reaching the same order of magnitude as the “true” physical solution. As a result, the result given by DNS becomes a mixture of the “true” physical solution and the “false” numerical noise, say, its spatiotemporal trajectory is badly polluted by artificial numerical noises. Comparing the traditional DNS solution with the CNS result, the influences of the artificial numerical noise on the surface quasi-geostrophic (SQG) turbulence can be investigated in detail.

III. INFLUENCES OF ARTIFICIAL NUMERICAL NOISES

As presented in the previous section, by comparing the DNS result, which is badly polluted by artificial numerical noises, with the CNS benchmark solution, whose numerical noise is negligible over a sufficiently long time interval, we can investigate the influences of

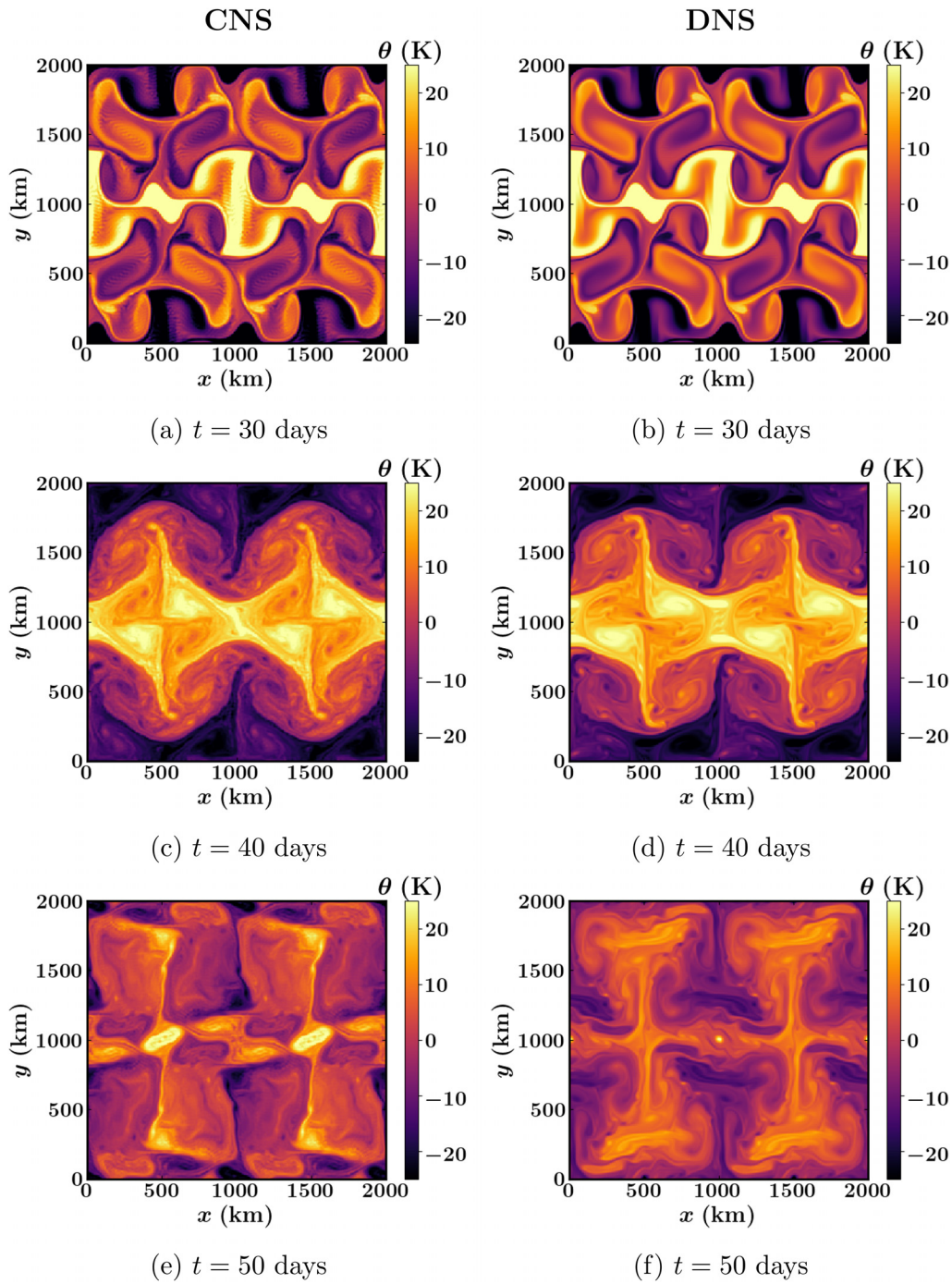


FIG. 2. Comparisons of the potential temperature field θ in Kelvin temperature (K) at $z = 0$ given by the CNS (left) and the DNS (right) at different times. (a)-(b) $t = 30$ days; (c)-(d) $t = 40$ days; (e)-(f) $t = 50$ days.

artificial numerical noise on the SQG turbulence, as mentioned below. Intuitively, the artificial numerical noise can be shown by the deviation of the potential vorticity θ from the results of the CNS and DNS, which is defined by

$$\delta = \frac{\int_0^{2L} \int_0^{2L} |\theta_{DNS} - \theta_{CNS}| dx dy}{\int_0^{2L} \int_0^{2L} |\theta_{CNS}| dx dy}, \quad (9)$$

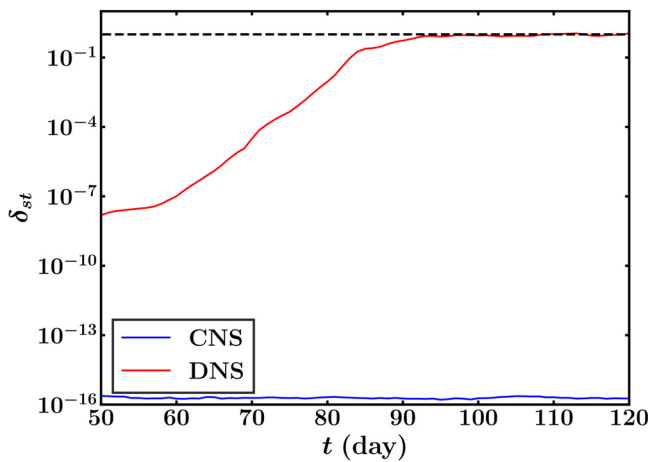


FIG. 3. Deviation of the potential temperature field θ and its space-symmetric transformation field θ_{st} from the results of the CNS (blue line) and DNS (red line). The black dashed line denotes $\delta_{st} = 1$.

where θ_{DNS} and θ_{CNS} denote the potential vorticity calculated by DNS and CNS, respectively.

As shown in Fig. 1, around 30 days, the magnitude of the deviation δ grows exponentially to $\delta = 10^{-1}$, marking the onset of solution divergence. The deviation then remains at $\delta = 10^{-1}$ for approximately 20 days, before reaching a value of 1 at around 50 days, at which point, the solutions from CNS and DNS begin to diverge significantly. This is an interesting result, as $\delta = 10^{-1}$ suggests that the majority of the flow field remains similar, while certain regions, such as small vortices, start to show noticeable differences. This indicates that numerical noise first disturbs the turbulence in localized regions or small vortices, and after accumulating over time, it eventually affects the entire flow field. Therefore, the potential temperature field θ is required to assess the impact of artificial numerical noise on the flow field.

Corresponding to Fig. 1, the potential temperature field θ in Kelvin temperature (K) at $z = 0$ given by the CNS and the DNS at time $t = 30, 40, 50$ days is illustrated in Fig. 2. It is found that the DNS result agrees well with the CNS benchmark solution until $t = 30$ days, mainly because the artificial numerical noise is small and thus negligible compared to the “true” physical solution. As illustrated in Figs. 2(c) and 2(d), small-scale vortices located near the coordinates $(x, y) = (500, 400)$ km, $(500, 1600)$ km, $(1500, 400)$ km, and $(1500, 1600)$ km begin to exhibit distinct differences between the two simulations. These differences align with earlier findings, demonstrating that numerical noise initially perturbs turbulence in localized regions or small vortices. Notably, the differences in these regions exhibit spatial symmetry. This symmetry implies that artificial numerical noise first manifests as divergences in the solutions rather than simultaneously causing divergences and disrupting the inherent symmetry of the flow. After 10 days, from day 40 to day 50, the potential temperature field θ becomes entirely different while maintaining its spatial symmetry, as shown in Figs. 2(e) and 2(f). This confirms the result presented in Fig. 1 and demonstrates that the solution divergence does not affect the spatial symmetry.

Now, we examine the spatial symmetry of the potential temperature field θ . As discussed previously, the initial condition (7) possesses a spatial symmetry, which should be preserved throughout the duration of the calculation. To quantify the spatial symmetry of the potential temperature field θ , we use Eq. (9) to calculate the deviation between θ and its space-symmetric transformation θ_{st} ,

$$\delta_{st} = \frac{\int_0^{2L} \int_0^{2L} |\theta - \theta_{st}| dx dy}{\int_0^{2L} \int_0^{2L} |\theta_t| dx dy}, \quad (10)$$

where $\theta_{st}(x, y, z, t) = \theta(L - y, L - x, z, t)$. Similar to Eq. (9), $\delta_{st} \sim 1$ indicates a complete loss of spatial symmetry.

As shown in Fig. 3, the deviation between the potential temperature field θ and its space-symmetric transformation field θ_{st} from the results of CNS and DNS is presented. Between 90 and 100 days, it is evident that δ_{st} for DNS rapidly increases to 1, indicating a complete loss of spatial symmetry. In contrast, δ_{st} for CNS remains at the level of 10^{-16} , indicating that spatial symmetry is preserved. It is important to note that a value of 10^{-16} corresponds to the round-off error in double precision calculations. Unlike the deviation of the potential vorticity θ from the CNS and DNS results in Fig. 1, θ_{st} quickly approaches the dashed line, suggesting that the accumulation of differences occurs more rapidly in this case than for δ . The result of Fig. 3 indicates that the influence of artificial numerical noise will disturb the spatial symmetry eventually. As the artificial numerical noise reaches the same order of magnitude as the physical solution, the DNS result has significant deviation from the CNS benchmark solution, as shown in Fig. 2. Note that the initial condition (7) has a kind of spatial symmetry. In theory, such kind of spatial symmetry should remain.

Corresponding to Fig. 3, the potential temperature field θ in Kelvin temperature (K) at $z = 0$ given by the CNS and the DNS at time $t = 90, 100, 365$ days is illustrated in Fig. 4. It is observed that the CNS benchmark solution consistently maintains the same spatial symmetry as the initial solution (7) throughout the time interval (i.e., one year). In contrast, the DNS result rapidly loses this spatial symmetry, as shown in Fig. 4. This serves as clear evidence that the DNS solution is significantly affected by artificial numerical noise. As indicated in Fig. 3, δ_{st} for DNS reaches 10^{-1} at 90 days. This is further illustrated in Fig. 4(b), where small-scale vortices near the coordinates $(x, y) = (900, 200)$ km, $(100, 1700)$ km, $(1200, 1700)$ km, and $(1900, 200)$ km begin to lose spatial symmetry due to the influence of artificial numerical noise. Subsequently, these vortices quickly disrupt the spatial symmetry, as shown in Figs. 4(d) and 4(f).

How about the influence of artificial numerical noises on the statistics of the SQG turbulence? First, let us consider the spatial average kinetic energy $\langle KE \rangle_a$, whose definition is given in Appendix B. As illustrated in Fig. 5, the spatial average kinetic energy $\langle KE \rangle_a$ given by DNS diverges from the CNS benchmark solution around 40 days. The spatial average kinetic energy $\langle KE \rangle_a$ of the DNS shows significant averaging effects, highlighting its considerable sensitivity to stochastic numerical noise. It also indicates that the spatial average kinetic energy $\langle KE \rangle_a$ is influenced by the solution divergence, which is also consistent with the results of a previous study.³³ In addition, unlike the mean kinetic energy $\langle KE \rangle_a$ from CNS, the mean kinetic energy $\langle KE \rangle_a$ from DNS loses its periodicity due to the external energy input with a thermal relaxation damping time of $T = 10$ days.

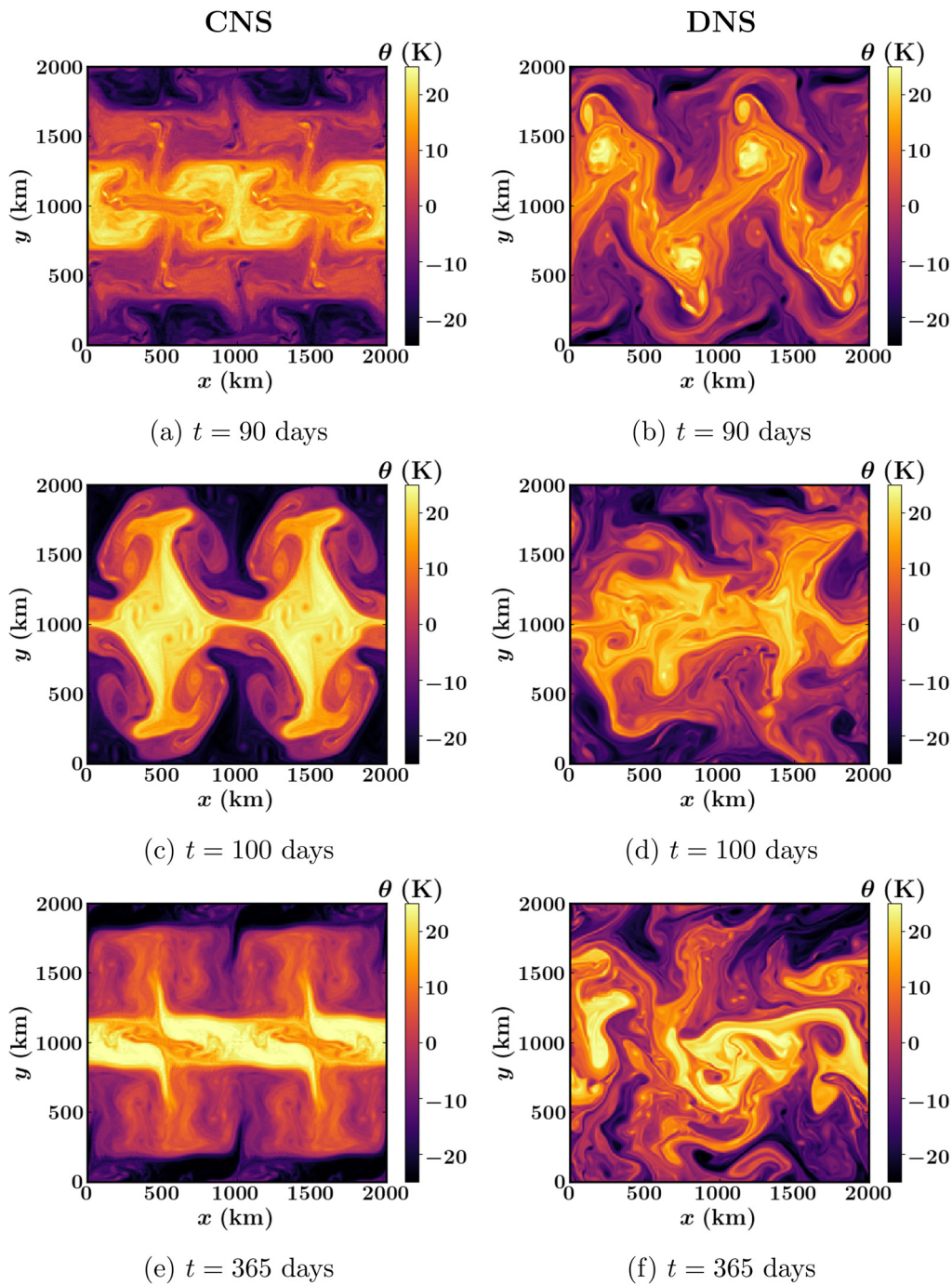


FIG. 4. Comparisons of the potential temperature field θ in Kelvin temperature (K) at $z = 0$ given by the CNS (left) and the DNS (right) at different times. (a)-(b) $t = 90$ days; (c)-(d) $t = 100$ days; (e)-(f) $t = 365$ days.

Then, let us consider the distribution of KE along the x and y directions. As shown in Fig. 6, the $\langle KE \rangle_{x,t}$ and $\langle KE \rangle_{y,t}$ given by DNS are completely different from those given by CNS. The CNS results exhibit symmetry in both directions, whereas those given by DNS have

no symmetry at all. As shown in Fig. 7, the probability density function (PDF) of kinetic energy KE given by DNS is quite different from that given by CNS. Note that the CNS benchmark solution retains the energy within a relatively high magnitude range, suggesting that

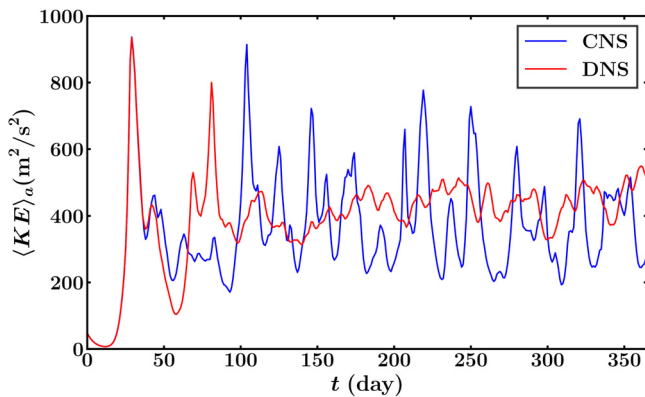


FIG. 5. Comparison of the spatial average kinetic energy $\langle KE \rangle_a$ averaged in $x \in [0, L]$, $y \in [0, L]$, and $z = 0, H$ given by CNS (blue line) and DNS (red line).

stochastic noise induces additional energy dissipation that results in the leftward shift of its PDF. Similarly, the PDF of potential temperature variance PTV is also affected by stochastic numerical noise, as shown in Fig. 8. Note that the above statistic results given by DNS using different time-steps are the same, indicating a kind of statistic stability under numerical noises.

Consider the autocorrelation

$$C(\mathbf{r}, \tau) = \langle \theta(\mathbf{R}, t) \cdot \theta(\mathbf{R} + \mathbf{r}, t + \tau) \rangle_t, \quad (11)$$

where $\mathbf{R}$ represents a point within the computational domain, τ is the temporal interval, $\mathbf{r}$ is the spatial interval, and $\langle \cdot \rangle_t$ denotes the time average. Specifically, $C(0, \tau)$ represents the temporal autocorrelation, while $C(\mathbf{r}, 0)$ represents the spatial autocorrelation. Without loss of generality, the reference point is selected here as $\mathbf{R} = (500, 1000)$ kilometer, and $\mathbf{r} = (r, r)$ is added to $\mathbf{R}$ identically in both directions. Figure 9 shows the comparison of the time autocorrelation $C(0, \tau)$ and the space autocorrelation $C(\mathbf{r}, 0)$ given by DNS and the CNS benchmark solution. Note that both the temporal and spatial autocorrelations are significantly influenced by stochastic numerical noises, as

evident from the discrepancies between the CNS and DNS results. This provides an evidence that stochastic numerical noise might sometimes disrupt key statistics of the SQG turbulence, particularly those associated with autocorrelation.

As shown in Fig. 10, the kinetic energy spectra given by DNS and the CNS benchmark solution agree well with the theoretical value of $-5/3$. This similarity suggests that the slope of the kinetic energy spectra is insensitive to stochastic numerical noise. Although the artificial numerical noises could lead to significant deviations in spatiotemporal trajectories and statistic results as mentioned earlier, the essential mechanism of energy transfer, i.e., the energy cascade, is fortunately correctly captured, indicating that the kinetic energy spectra of the SQG turbulence is robust against stochastic disturbances. This is a good new. Unfortunately, it also illustrates that correctly capturing the $-5/3$ law of the kinetic energy *cannot* guarantee the corrections of the spatial symmetry of flow and statistic results such as those mentioned earlier. This is indeed a bad new for us. Why do artificial numerical noises not affect the kinetic energy spectra? It can be interpreted that the DNS flow field, which contains artificial numerical noise, can be viewed as the combination of two distinct flow fields: one corresponding to the artificial numerical noise and the other representing the “true” physical flow. The flow field of artificial numerical noise can be considered as another “clean” numerical simulation, which calculates Eq. (5) using a random disturbance at the level of the 10^{-16} initial condition. So, the flow field associated with the artificial numerical noise exhibits some turbulence characteristics, including the $-5/3$ energy law. As a result, the kinetic energy spectra of the two flow fields share the same shape, and the combined energy spectra of both should still conform to the $-5/3$ law.

IV. CONCLUSION

In this paper, the surface quasi-geostrophic (SQG) turbulence with a spatially periodic initial condition is numerically simulated by means of two methods: one is the traditional direct numerical simulation (DNS) whose numerical noise quickly increases to the same order of magnitude as its physical solution, the other is the so-called clean numerical simulation (CNS) whose numerical noise is much smaller

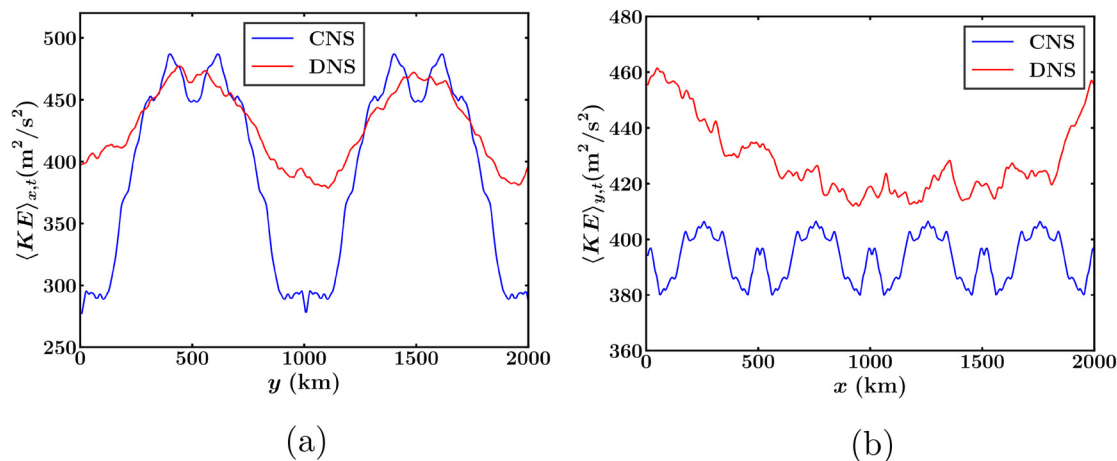


FIG. 6. Comparisons of the spatiotemporal averaged kinetic energy: (a) $\langle KE \rangle_{x,t}$ averaged in $z = 0, H$, $t \in [100, 365]$ days, and $x \in [0, L]$ (along x direction) and (b) $\langle KE \rangle_{y,t}$ that averaged in $z = 0, H$, $t \in [100, 365]$ days, and $y \in [0, L]$ (along y direction) given by CNS (blue line) and DNS (red line), respectively.

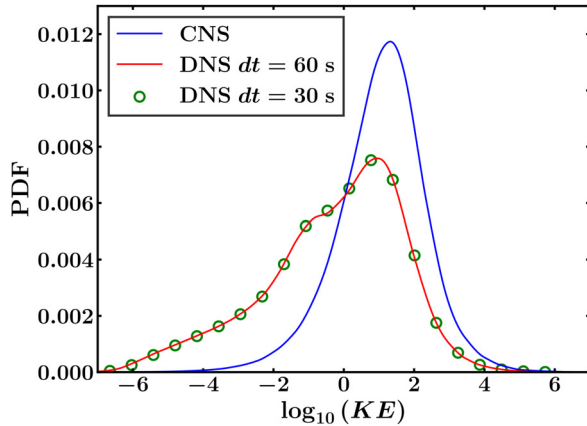


FIG. 7. Comparisons of the probability density function (PDF) of the kinetic energy KE . The PDFs are integrated in two-surface $z = 0, H$ with $x, y \in [0, L]$ and $t \in [100, 365]$ days, given by CNS (solid blue line), DNS with $dt = 60$ s (solid red line) and DNS with $dt = 30$ s (green symbol).

than the physical solution and thus is negligible in a finite but long enough interval of time. Influence of numerical noises is investigated in detail by comparing the two simulations of the SQG turbulence given, respectively, by the DNS and CNS. It is found that the artificial stochastic numerical noises would lead to huge derivations apart from CNS benchmark solution not only in the spatiotemporal trajectories but also in the spatial symmetry of turbulence and several statistics such as the spatiotemporal averaged kinetic energy, the probability density function (PDF) of the kinetic energy, the PDF of the potential temperature variance, the time autocorrelation, the space autocorrelation, and so on. However, it is surprisingly found that despite so many huge deviations mentioned earlier, the kinetic energy spectra given by the DNS agrees well with that given by the CNS benchmark solution: both of them satisfy the famous $-5/3$ law. It indicates that the kinetic energy spectra has stability, i.e., insensitive to stochastic disturbances. On one side, this is a good new. Unfortunately, on the contrast, it also

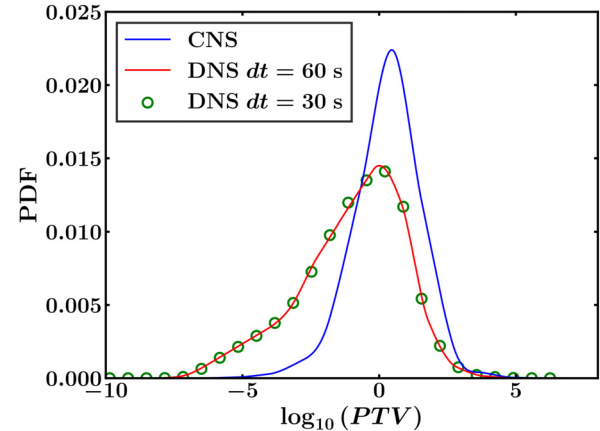


FIG. 8. Comparisons of the probability density function (PDF) of the potential temperature variance PTV . The PDFs are integrated in two-surface $z = 0, H$ with $x, y \in [0, L]$ and $t \in [100, 365]$ days, given by CNS (solid blue line), DNS with $dt = 60$ s (solid red line) and DNS with $dt = 30$ s (green symbol).

provides us an evidence that correctly capturing the $-5/3$ law of kinetic energy spectra cannot guarantee the correction of statistical results of DNS. In other words, a correct kinetic energy spectra alone cannot serve as a reliable criterion to assess the correctness of numerical solutions of turbulence.

Our findings have general and important meanings, especially for the reliability of numerical simulation of turbulence. Today, it has been widely believed by the turbulence community that a numerical simulation of turbulence should be correct as long as its kinetic energy spectra satisfy the famous $-5/3$ law (or a related law). However, using the 2D SQG turbulence as an example, we illustrated in this paper that this is *not* enough: other statistical results and even the spatial symmetry of flow might be wrong, even if the famous $-5/3$ law of kinetic energy spectra is satisfied. Thus, one should check the reliability of all statistics of DNS of turbulence very carefully.

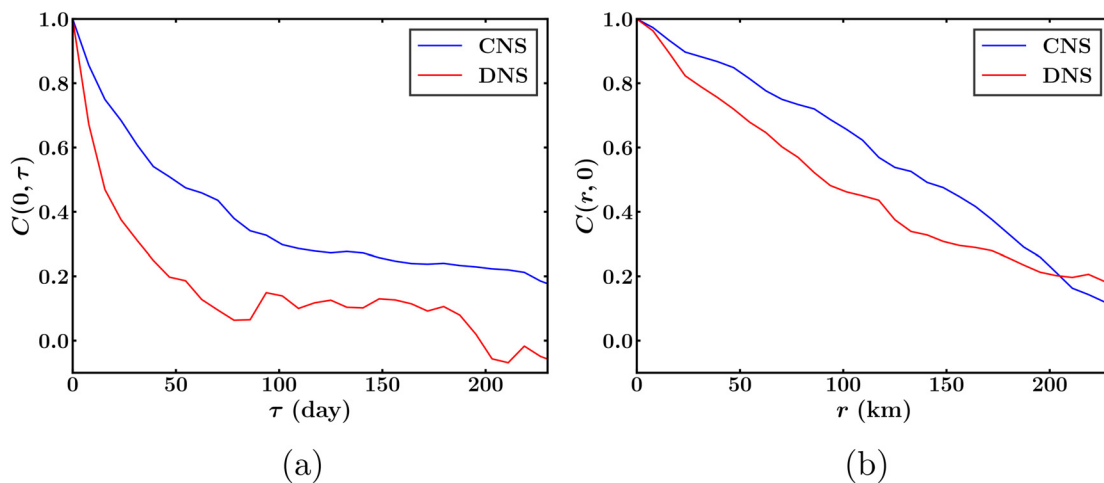


FIG. 9. Comparisons of (a) the time autocorrelation $C(0, \tau)$, (b) the space autocorrelation $C(r, 0)$, respectively, given by CNS (blue line) and DNS (red line), respectively.

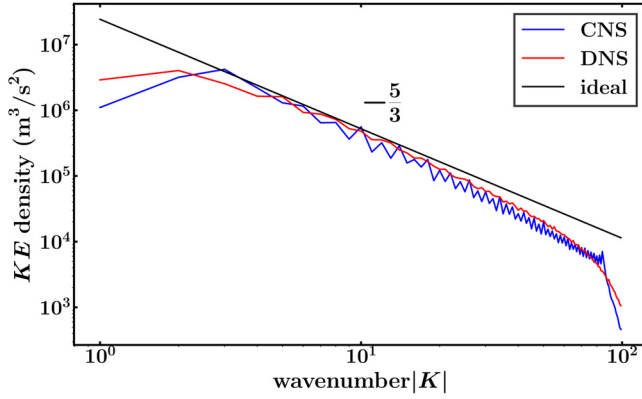


FIG. 10. Kinetic energy density vs horizontal wavenumber magnitude $|k|$ given by CNS (blue line) and DNS (red line). The black line is the ideal kinetic energy cascade with the $-5/3$ slope.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Bo Zhang: Data curation (lead); Methodology (lead); Validation (lead); Visualization (lead); Writing – original draft (lead). **Tianli Hu:** Methodology (supporting); Software (supporting). **Shijie Qin:** Methodology (supporting); Software (supporting). **Jing Li:** Methodology (equal); Writing – original draft (equal). **Shijun Liao:** Conceptualization (equal); Supervision (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

APPENDIX A: CNS ALGORITHM OF SQG TURBULENCE

The spatial domain $x, y \in [0, L]$ is discretized by means of $N_x \times N_y$ equidistant, i.e.,

$$x_j = \frac{jL}{N_x}, \quad y_k = \frac{kL}{N_y}, \quad j = 0, 1, \dots, N_x - 1 \text{ and } k = 0, 1, \dots, N_y - 1, \quad (\text{A1})$$

and the corresponding wavenumbers $k_x, k_y \in \mathbb{Z}$ (in the set of integers) are

$$k_x \in \left[-\frac{N_x}{2}, \frac{N_x}{2} - 1\right], \quad k_y \in \left[-\frac{N_y}{2}, \frac{N_y}{2} - 1\right]$$

for even N_x and N_y ,

$$k_x \in \left[-\frac{N_x - 1}{2}, \frac{N_x - 1}{2}\right], \quad k_y \in \left[-\frac{N_y - 1}{2}, \frac{N_y - 1}{2}\right]$$

for odd N_x and N_y .

By rewriting the governing Eq. (5) on $z = 0$ or $z = H$,

$$\hat{\theta}_t(k_x, k_y, z, t) + \hat{J}(k_x, k_y, z, t) = \frac{1}{T} [\hat{\theta}_b(k_x, k_y, z, t) - \hat{\theta}(k_x, k_y, z, t)], \quad (\text{A2})$$

where $\hat{J}$ is the shortening of the term $\hat{J}(\hat{\psi}(k_x, k_y, z, t), \hat{\theta}(k_x, k_y, z, t))$ in (5).

Consider the Taylor expansion in time,

$$\begin{cases} \hat{\theta}(k_x, k_y, z, t + \Delta t) \approx \sum_{m=0}^M \hat{\theta}^{[m]}(k_x, k_y, z, t) (\Delta t)^m, \\ \hat{\psi}(k_x, k_y, z, t + \Delta t) \approx \sum_{m=0}^M \hat{\psi}^{[m]}(k_x, k_y, z, t) (\Delta t)^m, \\ \hat{J}(k_x, k_y, z, t + \Delta t) \approx \sum_{m=0}^M \hat{J}^{[m]}(k_x, k_y, z, t) (\Delta t)^m, \end{cases} \quad (\text{A3})$$

where Δt is the time step, M is the order of Taylor expansion, with the definitions

$$\begin{cases} \hat{\theta}^{[m]}(k_x, k_y, z, t) = \frac{1}{m!} \frac{\partial^m \hat{\theta}(k_x, k_y, z, t)}{\partial t^m}, \\ \hat{\psi}^{[m]}(k_x, k_y, z, t) = \frac{1}{m!} \frac{\partial^m \hat{\psi}(k_x, k_y, z, t)}{\partial t^m}, \\ \hat{J}^{[m]}(k_x, k_y, z, t) = \frac{1}{m!} \frac{\partial^m \hat{J}(k_x, k_y, z, t)}{\partial t^m}. \end{cases} \quad (\text{A4})$$

Differentiating $(m - 1)$ times both sides of (13) with respect to t and dividing them by $m!$, we have $z = 0$ or $z = H$

$$\begin{aligned} \hat{\theta}^{[m]}(k_x, k_y, z, t) = \frac{1}{m} \left\{ -\hat{J}^{[m-1]}(k_x, k_y, z, t) \right. \\ \left. + \frac{1}{T} [\hat{\theta}_b^{[m-1]} - \hat{\theta}^{[m-1]}(k_x, k_y, z, t)] \right\}, \end{aligned} \quad (\text{A5})$$

where $m \geq 1$ and

$$\hat{\theta}_b^{[m-1]} = \begin{cases} \hat{\theta}_b, & m = 1, \\ 0, & m > 1. \end{cases} \quad (\text{A6})$$

Adopt the spatial Fourier series

$$\begin{aligned} \hat{J}^{[m-1]}(k_x, k_y, z, t) \\ = \frac{1}{N_x N_y} \sum_{j=0}^{N_x-1} \sum_{k=0}^{N_y-1} \hat{J}^{[m-1]}(x_j, y_k, z, t) \exp(-ik_x x_j) \exp(-ik_y y_k), \end{aligned} \quad (\text{A7})$$

where

$$J^{[m-1]}(x_j, y_k, z, t) = \sum_{r=0}^{m-1} [\psi_x^{[r]}(x_j, y_k, z, t) \theta_y^{[m-1-r]}(x_j, y_k, z, t) - \psi_y^{[r]}(x_j, y_k, z, t) \theta_x^{[m-1-r]}(x_j, y_k, z, t)] \quad (\text{A8})$$

and

$$\begin{aligned} \psi_x^{[r]}(x_j, y_k, z, t) &\approx \sum_{k_x=-[N_x/3]}^{[N_x/3]} \sum_{k_y=-[N_y/3]}^{[N_y/3]} \mathbf{i} k_x \hat{\psi}^{[r]} \\ &\times (k_x, k_y, z, t) \exp(\mathbf{i} k_x x_j) \exp(\mathbf{i} k_y y_k), \\ \psi_y^{[r]}(x_j, y_k, z, t) &\approx \sum_{k_x=-[N_x/3]}^{[N_x/3]} \sum_{k_y=-[N_y/3]}^{[N_y/3]} \mathbf{i} k_y \hat{\psi}^{[r]} \\ &\times (k_x, k_y, z, t) \exp(\mathbf{i} k_x x_j) \exp(\mathbf{i} k_y y_k), \\ \theta_x^{[r]}(x_j, y_k, z, t) &\approx \sum_{k_x=-[N_x/3]}^{[N_x/3]} \sum_{k_y=-[N_y/3]}^{[N_y/3]} \mathbf{i} k_x \hat{\theta}^{[r]} \\ &\times (k_x, k_y, z, t) \exp(\mathbf{i} k_x x_j) \exp(\mathbf{i} k_y y_k), \\ \theta_y^{[r]}(x_j, y_k, z, t) &\approx \sum_{k_x=-[N_x/3]}^{[N_x/3]} \sum_{k_y=-[N_y/3]}^{[N_y/3]} \mathbf{i} k_y \hat{\theta}^{[r]} \\ &\times (k_x, k_y, z, t) \exp(\mathbf{i} k_x x_j) \exp(\mathbf{i} k_y y_k), \end{aligned}$$

where $\lfloor \cdot \rfloor$ is the floor function, and the value is set to be zero for wavenumbers outside the above-mentioned domain $\sum$ and

$$\begin{aligned} \hat{\psi}^{[r]}(k_x, k_y, z, t) &= \frac{H}{\mu \sinh \mu} \left[\cosh \left(\mu \frac{z}{H} \right) \hat{\theta}^{[r]}(k_x, k_y, H, t) \right. \\ &\quad \left. - \cosh \left(\mu \frac{z-H}{H} \right) \hat{\theta}^{[r]}(k_x, k_y, 0, t) \right]. \end{aligned}$$

To increase the computational efficiency, the parallel fast Fourier transform (FFT) algorithm is adopted for the above-mentioned process. To decrease the round-off error, all variables in the above-mentioned process are presented in multiple precision (MP, called the MPFR library in the C language)⁴⁵ with N_s significant digits. To gain the reliable solution in a time duration $t \in [0, T_c]$, one should use large enough N_s and M to guarantee that numerical noise can be negligible.

APPENDIX B: MEASURES OF THE FLOW

For the sake of simplicity, the definitions of some important quantities are briefly described below. The definition of kinetic energy KE is

$$KE = \frac{1}{2} (u^2 + v^2) = \frac{1}{2} |\nabla \psi|^2, \quad (\text{B1})$$

where $(u, v) = (-\psi_y, \psi_x)$ are the velocities in the (x, y) directions, and $\nabla(\cdot) = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right)$ is the gradient operator. Another statistic is the potential temperature variance PTV , which is defined by

$$PTV = \theta^2. \quad (\text{B2})$$

We use KE as an example to define the statistics. The temporal average kinetic energy $\langle KE \rangle_t$ is defined by

$$\langle KE \rangle_t = \int KE dt. \quad (\text{B3})$$

For the horizontal domain average kinetic energy $\langle KE \rangle_h$ in one surface ($z = 0, H$),

$$\langle KE \rangle_h = \iint KE dx dy = \sum_{|\mathbf{K}|} \frac{1}{2} |\mathbf{K}|^2 |\hat{\psi}|^2 = \sum_{|\mathbf{K}|} \frac{1}{2} |\mathbf{K}|^2 \hat{\psi} \hat{\psi}^*, \quad (\text{B4})$$

and for spatial average kinetic energy $\langle KE \rangle_a$,

$$\langle KE \rangle_a = \frac{1}{2} (\langle KE \rangle_h|_{z=0} + \langle KE \rangle_h|_{z=H}). \quad (\text{B5})$$

In addition, the spatiotemporal average kinetic energy $\langle KE \rangle_{x,t}$ or $\langle KE \rangle_{y,t}$ (along x or y direction) is defined by

$$\langle KE \rangle_{x,t} = \iint KE dx dt, \quad \langle KE \rangle_{y,t} = \iint KE dy dt, \quad (\text{B6})$$

and for spatiotemporal average kinetic energy $\langle KE \rangle$ for the whole domain,

$$\langle KE \rangle = \int \langle KE \rangle_a dt. \quad (\text{B7})$$

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