# Energy cascades in surface semi-geostrophic turbulence

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# Abstract

Surface semi-geostrophic turbulence is examined in this study. In our simulations, the strength of the ageostrophic component of the flows is controlled by the Rossby number  $\varepsilon$ , varying from 0.01 to 0.2. The flows manifest a cyclone-anticyclone asymmetry with a cyclonic preference for cold vortices and an anticyclonic preference for warm filaments. This asymmetry becomes especially pronounced in the flows with large  $\varepsilon$ , where an abundance of warm filaments is observed. Strong vertical motions concentrate in the small-scale filaments and at the periphery of the vortices. There, the lateral divergence becomes significant. A negative correlation between the divergence and the relative vorticity is identified using joint probability density functions. Slopes of the kinetic and potential energy spectra vary between -2.2 and -1.7 at intermediate scales. Analyses of spectral fluxes demonstrate an inverse kinetic energy cascade and a forward cascade of potential energy. As  $\varepsilon$  increases, the filaments become more numerous in the flows. They wrap around cyclones, weakening their interactions and subsequent mergers, thus suppressing the inverse cascade of kinetic energy. We characterize lateral dispersion in the SSG flows using the finite-scale Lyapunov exponents (FSLEs). They are used to identify Lagrangian coherent structures, such as those created by the interaction of vortices. The FSLEs are also used to investigate the regimes of dispersion at different scales. The results show a smooth transition from hyper-ballistic diffusion at small scales to normal diffusion at large scales.

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# Key Points:

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7 8	•	An asymmetry between cyclonic cold vortices and anticyclonic warm filaments char- acterizes the surface semi-geostrophic turbulence.
9	•	The ageostrophic component strengthens the forward potential energy cascade by
10		exciting warm filaments but suppresses the inverse kinetic energy cascade by pre-
11		venting cyclone mergers.
12	•	Horizontal dispersion transforms from a hyper-ballistic regime at small scales to
13		a normal dispersion regime at large scales.

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### 14 Abstract

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# <sup>34</sup> Plain Language Summary

The generation of submesoscale structures by mesoscale currents is one of the im-35 portant pathways of energy dissipation in the ocean. It can be modeled with an ideal-36 ized surface semi-geostrophic (SSG) equations. The SSG model is able to reproduce ageostrophic 37 effects, including a cyclone-anticyclone asymmetry. In this study, we simulate a turbu-38 lent SSG flow and demonstrate that, as the ageostrophy increases, warm filaments be-39 come more numerous. The filaments contribute to transporting the potential energy to-40 wards smaller scales. Meanwhile, the cold cyclones shrink in size and become more iso-41 lated from each other due to the shielding by warm filaments wrapping around them. 42 As a result, cyclone interaction and the subsequent mergers are weakened, and the in-43 verse cascade of the kinetic energy towards larger scales is suppressed. 44

# 45 **1** Introduction

Oceanic turbulence comprises flows of different scales, including ocean-wide gyres, 46 mesoscale eddies, submesoscale eddies, fronts, and filaments. At the lowest end of the 47 scale, submesoscale flows become more familiar due to new evidence provided by field 48 measurements (Shcherbina et al., 2013; Mensa et al., 2018; Pearson et al., 2019; Balwada 49 et al., 2016) and high-resolution numerical simulations (Balwada et al., 2021; Jing et al., 50 2021). Submessical flows are characterized by an O(1) Rossby number and consequently 51 exhibit significant ageostrophy, including large vertical velocity and horizontal divergence 52 (McWilliams, 2016). Thus, they provide a pathway for energy transfer from almost two-53 dimensional (2D) quasi-geostrophic (QG) turbulence to three-dimensional (3D) turbu-54 lence. 55

Over the years, several theoretical models that go beyond QG but still retain cer-56 tain physical simplicity—referred to as "intermediate models" in the terminology of McWilliams 57 and Gent (1980)—have been developed. Some of these models exclusively address flows 58 generated by buoyancy perturbations at the surface of the ocean, such as the surface quasi-59 geostrophic (SQG) model (Blumen, 1978; Held et al., 1994) and the surface semi-geostrophic 60 (SSG) model (Ragone & Badin, 2016). The SQG model has been investigated by dif-61 ferent authors (Isern-Fontanet et al., 2006; Klein et al., 2008; Qiu et al., 2016) with re-62 spect to its capability to describe upper ocean currents using only surface data, such as 63

those obtained by satellite altimetry and thermal radiometry. It has been demonstrated 64 that SQG flows generate submesoscale structures (Capet et al., 2008; Carton et al., 2016). 65 Numerical simulations by (Capet et al., 2008) showed that these structures are due to 66 frontogenesis processes, which occur when forward-cascading surface potential energy 67 transfers into inversely-cascading kinetic energy. Spectra of kinetic energy exhibited an 68 approximately -5/3 slope. Similar spectral slopes were obtained from altimetry data by 69 (Traon et al., 2008) and in realistic numerical simulations by (Klein et al., 2008; Chas-70 signet & Xu, 2017). For a comprehensive review of SQG dynamics, readers are referred 71 to (Lapeyre, 2017). The SQG theory relies on the assumption of a small Rossby num-72 ber,  $\varepsilon = U/(f_0 L_D) < 1$ , where U is the characteristic velocity scale,  $L_D$  is the length 73 scale, and  $f_0$  is the Coriolis parameter. However, at submesoscales,  $\varepsilon$  can approach or 74 exceed unity (Thomas et al., 2008). Ageostrophic effects become significant at the sub-75 mesoscale; one example is that strong vortices in the upper ocean are predominantly cy-76 clonic (Shcherbina et al., 2013; Munk, 2000; Griffa et al., 2008). As  $\varepsilon$  approaches unity, 77 anticyclones become more vulnerable to frontal instability than cyclones (Hoskins & Brether-78 ton, 1972). Another manifestation of the ageostrophic effects is the vertical motion driven 79 by frontogenesis. It can release the available potential energy of the system, re-stratify 80 the upper ocean, and cause a warming trend at the surface. These features were real-81 ized in simulations based on the primitive equations (Roullet & Klein, 2010; Klein et al., 82 83 2008).

To include the ageostrophic effects, Hakim et al. (2002) extended the SQG model 84 to the next order of approximation. Their model, called SQG+1, exhibited ageostrophy, 85 including an asymmetry between cold and warm filaments and a preference for cyclonic 86 vortices. However, the SQG+1 model was still constrained by a requirement for a glob-87 ally small  $\varepsilon$ . To alleviate this constraint, Ragone and Badin (2016) reformulated the SQG 88 dynamics in a geostrophic coordinate system and proposed a surface semi-geostrophic 89 (SSG) model. The geostrophic coordinate system was previously introduced by Eliassen 90 (1948); Fjørtoft (1962). It is a moving coordinate system that follows the geostrophic 91 current. The total velocity in the advection term is retained rather than being approx-92 imated by the geostrophic velocity. SSG simulations by Ragone and Badin (2016) showed 93 features similar to those in the SQG+1 simulations, including a cyclone-anticyclone asym-94 metry and a surface warming trend. Besides, the SSG simulations demonstrated an im-95 proved ability to capture frontogenesis and showed an abundance of small-scale fronts/filaments 96 in the simulated flows due to the improved representation of the nonlinear advection term. 97

In what follows, we employ the SSG model to investigate the dynamics of surface-98 intensified flows generated by buoyancy forcing at the surface. The flows are ageostrophic 99 to a significant degree and exhibit frontogenesis and three-dimensional effects. We fo-100 cus on characterizing vertical velocity and lateral divergence, especially concerning their 101 relation to the relative vorticity and strain rate in filaments and eddies. Spectral char-102 acteristics of the flows are also investigated; we go beyond energy spectra and study an 103 energy cascade by computing energy fluxes across the scales. The last objective of this 104 work is a characterization of the Lagrangian dynamics. We compute the finite-size Lya-105 punov Exponents (FSLEs) to identify the regimes of lateral dispersion at different scales. 106

In Section 2, we briefly review the SQG and SSG models. Section 3 describes the numerical methods and control parameters employed in this study. The results of the simulations are reported in Section 4, and conclusions are given in Section 5.

# <sup>110</sup> 2 SQG and SSG models revisited

Buoyancy perturbation  $b(x, y, z, t) = -g\rho'/\rho_0$ , where g is the acceleration due to gravity and  $\rho'$  is the density perturbation with respect to the constant reference density  $\rho_0$ , it is a conserved quantity in both SQG and SSG models. b is related to the (pertur-

bation) geopotential,  $\phi = p/\rho_0$ , where p is the pressure, via hydrostaticity such that

$$b = \frac{\partial \phi}{\partial z}.$$
 (1)

The above equation combined with the geostrophic relation

$$f_0(v_g, -u_g) = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}\right),\tag{2}$$

where  $f_0$  is the Coriolis parameter, gives the thermal wind equation

$$\left(\frac{\partial b}{\partial x}, \frac{\partial b}{\partial y}\right) = f_0 \left(\frac{\partial v_g}{\partial z}, -\frac{\partial u_g}{\partial z}\right). \tag{3}$$

The ocean surface is subject to external heating or cooling. To model this effect, we specify the surface buoyancy perturbation  $b_s(x, y)$  at the initial moment t = 0 and then allow the flow to evolve freely. Here, the subscript s denotes a surface quantity. It is assumed that b vanishes in the ocean interior at depth z = -H, where H is the vertical scale of the motion driven by the buoyancy perturbation. Vertical boundary conditions for the geopotential can then be written as

$$\frac{\partial \phi}{\partial z} = b_s(x, y, t) \quad \text{at} \quad z = 0,$$
(4a)

$$\frac{\partial \phi}{\partial z} = 0$$
 at  $z = -H.$  (4b)

Note that the background stratification is taken to be linear such that the Brunt-Vaisalla frequency is N = const. The buoyancy perturbation is assumed to remain relatively small such that N remains approximately constant at all times (Hoskins & West, 1979; Ragone & Badin, 2016).

### 2.1 SQG model

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Quasi-geostrophic potential vorticity (q, PV) remains undisturbed in the interior of the fluid layer at all times such that

$$q = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{f_0^2}{N^2} \frac{\partial^2 \phi}{\partial z^2} = 0.$$
 (5)

The above equation takes the form of the Laplace's equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = 0, \tag{6}$$

when non-dimensionalized using the deformation radius  $L_D = NH/f_0$  as the horizontal scale, H as the vertical scale and U as the velocity scale. All quantities in Eq. (6) are dimensionless, but we keep the same notations. Vertical structure of the flow subject to the boundary conditions Eq. (4) can be obtained in the wavenumber space (Tulloch & Smith, 2006)

$$\tilde{\phi}(\boldsymbol{k}, z, t) = \frac{\cosh[(z+1)k]}{k\sinh(k)}\tilde{b}_s(\boldsymbol{k}, t)$$
(7)

where the tilde sign denotes the horizontal Fourier transform and  $\mathbf{k} = (k_x, k_y)$  is the horizontal wavenumber vector whose magnitude is  $k = \sqrt{k_x^2 + k_y^2}$ . On the surface,  $b_s$  is advected by the geostrophic current,

$$\frac{\partial b_s}{\partial t} + J_{xy}(\phi_s, b_s) = 0, \tag{8}$$

where  $J_{xy}(A, B) = A_x B_y - A_y B_x$  represents the nonlinear advection term in Jacobian form.

# 2.2 SSG model

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As we traverse the scales of the flows from mesoscale down to submesoscale, the Rossby number  $\varepsilon$  increases, and the ageostrophic component of velocity becomes significant. To study flows beyond the validity of the quasi-geostrophy, a coordinate system that follows the geostrophic component of the current was introduced (Hoskins & Bretherton, 1972; Hoskins, 1975). The relations between the physical coordinates (x, y, z) and geostrophic coordinates (X, Y, Z) are

$$x = X - \frac{1}{f_0} v_g = X - \frac{1}{f_0^2} \frac{\partial \phi_s}{\partial x},$$
(9a)

$$y = Y + \frac{1}{f_0}u_g = Y + \frac{1}{f_0^2}\frac{\partial\phi_s}{\partial y}$$
(9b)

$$z = Z. (9c)$$

In this system, the horizontal advection by the total velocity (u, v) which includes the ageostrophic component, can be expressed using the geostrophic velocity  $(u_g, v_g)$ 

$$\frac{D_g}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} = \frac{\partial}{\partial t} + u_g\frac{\partial}{\partial X} + v_g\frac{\partial}{\partial Y}.$$
(10)

In the geostrophic coordinate system, the Bernoulli function  $\Phi = \phi + (u_g^2 + v_g^2)/2$  assumes the role of the geopotential  $\phi$  such that

$$\left(\frac{\partial\Phi}{\partial X}, \frac{\partial\Phi}{\partial Y}, \frac{\partial\Phi}{\partial Z}\right) = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right) = (f_0 v_g, -f_0 u_g, b).$$
(11)

A full set of equations of the SSG model then includes the conservation of buoyancy b and the potential vorticity  $q_{sg}$ 

$$\left(\frac{D_g}{Dt} + w\frac{\partial}{\partial Z}\right) \begin{bmatrix} b\\ q_{sg} \end{bmatrix} = 0.$$
(12)

The potential vorticity is defined as:

$$q_{sg} = -\frac{g}{f_0\rho_0}\boldsymbol{\zeta}_{sg}\cdot\nabla\rho,\tag{13}$$

where the absolute vorticity

$$\boldsymbol{\zeta}_{sg} = \left(-\frac{\partial v_g}{\partial z}, \frac{\partial u_g}{\partial z}, f_0 + \frac{\partial v_g}{\partial x} - \frac{\partial u_g}{\partial y}\right) + \frac{1}{f_0} \left(J_{yz}(u_g, v_g), J_{zx}(u_g, v_g), J_{xy}(u_g, v_g)\right)$$
(14)

includes nonlinear terms in the second bracket (Hoskins & Draghici, 1977). In the ocean at rest,  $u_g = v_g = 0$ , the potential vorticity and the absolute vorticity reduce to their background values:

$$q_{sg} = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z} = N^2, \tag{15a}$$

$$\boldsymbol{\zeta}_{sg} = f_0 \boldsymbol{k},\tag{15b}$$

where k is the unit vector in the vertical direction. In the presence of the flow, the vertical component of the absolute vorticity,

$$\boldsymbol{\zeta}_{sg} = [f_0 + \frac{\partial v_g}{\partial x} - \frac{\partial u_g}{\partial y} + \frac{1}{f_0} J_{xy}(u_g, v_g)] \boldsymbol{k}.$$
(16)

remains dominant. The reciprocal of the Jacobian of a transformation from physical to geostrophic coordinates may be written as (Hoskins, 1976)

$$J_g^{-1} = \frac{f_0}{\zeta_{sg}} = 1 - \frac{1}{f_0^2} \left( \frac{\partial^2 \Phi}{\partial X^2} + \frac{\partial^2 \Phi}{\partial Y^2} \right) + \frac{1}{f_0^4} \left[ \frac{\partial^2 \Phi}{\partial X^2} \frac{\partial^2 \Phi}{\partial Y^2} + \left( \frac{\partial^2 \Phi}{\partial X \partial Y} \right)^2 \right].$$
(17)

and  $q_{sg} = \zeta_{sg}/f_0 \Phi_{zz}$ . An assumption of negligible potential vorticity in the fluid interior leads to a nonlinear Monge-Ampére equation:

$$\frac{1}{N^2}\frac{\partial^2\Phi}{\partial Z^2} + \frac{1}{f_0^2}\left(\frac{\partial^2\Phi}{\partial X^2} + \frac{\partial^2\Phi}{\partial Y^2}\right) - \frac{1}{f_0^4}\left[\frac{\partial^2\Phi}{\partial X^2}\frac{\partial^2\Phi}{\partial Y^2} + \left(\frac{\partial^2\Phi}{\partial X\partial Y}\right)^2\right] = 0.$$
(18)

<sup>119</sup> The above equation replaces the linear Laplace's equation Eq. (6) in the SQG model.

To solve Eq. (18) we follow a numerical technique developed by Ragone and Badin (2016). For further details, readers are referred to Appendix A.

### <sup>122</sup> 3 Numerical method

The model domain is discretized in the geostrophic space (X, Y, Z). The domain is periodic in both horizontal directions and contains  $N_x = 512$  grid points in each direction. The non-dimensional horizontal domain size is set to  $L/L_D = 6$ , where L is the dimensional horizontal domain size, and  $L_D$  is the deformation radius. This results in a non-dimensional horizontal grid size of approximately  $\Delta X \approx 0.01$ . In the vertical direction, the domain is bounded by rigid walls and contains  $N_z = 20$  levels which are spaced exponentially with the majority of grid points close to the top surface.

To initialize the simulation, an initial surface buoyancy perturbation  $b_s(X, Y, t = 0)$  is specified in wavenumber space

$$\tilde{b}_s(\mathbf{k}, t=0) = A \frac{k^{m/4}}{(k+k_0)^{m/2}}$$
(19)

Here, we follow (Hakim et al., 2002; Ragone & Badin, 2016) taking m = 20 and  $k_0 =$ 14 and assigning a random phase to each mode k such that the random initial field can have a prescribed spectrum structure. The amplitude A is tuned such that the initial RMS velocity is fixed at 1 m/s for all our simulations; this velocity magnitude is typical for oceanic fronts (Gula et al., 2016).

Eq. (A9) is integrated in time using the 4th-order Runge-Kutta scheme. The nonlinear Jacobian  $J_{XY}$  is discretized in the (X, Y) plane using (Arakawa, 1966)'s scheme, which conserves both the kinetic energy and enstrophy. Then, it is transformed into the  $(k_X, k_Y)$  space for the time integration. This semi-pseudo scheme was shown to be able to capture the development of sharp fronts (Constantin et al., 2012). To remove the aliasing errors introduced by the nonlinearity,  $\tilde{b}_s(\mathbf{k}, t)$  is multiplied by a low-pass filter (Hou & Li, 2007):

$$\exp\left[-\alpha\left(\left|\frac{k_X}{k_{nq}}\right|^\beta + \left|\frac{k_Y}{k_{nq}}\right|^\beta\right)\right] \tag{20}$$

where  $k_{nq} = \pi/\Delta X$  is the Nyquist wavenumber and  $\alpha = 512$  and  $\beta = 20$  as in (Ragone & Badin, 2016). Not unlike the Orszag 2/3 cutoff, this exponential filter suppresses the highest 1/3 wavenumbers. Moreover, it can capture extra 15% more effective wavenumbers than the Orszag 2/3 cutoff, thus providing a better representation for the small-scale structures.

Substituting the updated  $b_s(\mathbf{k}, t)$  into Eq. (A7) we obtain  $\Phi(\mathbf{k}, Z, t)$  at the next time step; its vertical derivative gives  $\tilde{b}(\mathbf{k}, Z)$ . To obtain  $b_s(X, Y, Z)$  and  $\Phi(X, Y, Z)$  in the geostrophic coordinates, an inverse Fourier transform in the horizontal plane at each depth is performed. The flow is then transformed into the physical space (x, y, z) using a fixed-point iteration method (Ragone & Badin, 2016).

Six simulations were performed where the characteristic Rossby number  $\varepsilon$  was varied between 0 and 0.2. Note that when  $\varepsilon = 0$ , the SSG solution Eq. (A7) reduces to the SQG solution Eq. (7). In that case, the geostrophic coordinate system becomes identical to the physical coordinate system, and no coordinate transformation is needed. Nondimensional surface buoyancy,  $b_s$ , and time, T, can be restored to their dimensional form using factors NU and  $(\varepsilon f_0)^{-1}$ , respectively.



Figure 1. (Colour online) Surface buoyancy  $b_s(x, y)$  in the simulations with  $\varepsilon = 0.05$  (a), 0.1 (b), 0.15 (c), and 0.2 (d) at T = 50.

### 151 4 Results

### 152 4.1 Flow evolution

We restrict our analyses to an early-time evolution of the SSG flows when there is an abundance of small-scale filaments and vortices with strong nonlinear interactions.

Figure 1 shows the buoyancy  $b_s$  at the surface captured at T = 50 in simulations 155 with different  $\varepsilon$ . Patches of cold (blue color) water induce cyclonic vortices, while warm 156 patches (yellow color) induce anticyclones. Numerous filaments fill the area between the 157 vortices. The filaments are embedded in strong shear and are unstable; they roll into smaller 158 vortices. When  $\varepsilon$  is relatively small, the cyclones and anticyclones populate the flow field 159 in approximately equal numbers (Fig. 1(a) and (b)). As  $\varepsilon$  increases, the cold cyclones 160 in Fig. 1(c) shrink in size while warm anticyclonic vortices expand. This effect is a man-161 ifestation of the pressure terms in the coordinate transform (second equality in Eq. (9)(a)162 and (b)) and is due to the lateral divergence and convergence of the velocity (Hoskins, 163 1975). The area between coherent vortices is now filled with predominantly warm fila-164 ments (Fig. 1(d)). Their accumulation at the surface results in a warming trend with 165 increasing  $\varepsilon$ . Similar scenarios have been shown previously in the simulations by (Ragone 166 & Badin, 2016; Hakim et al., 2002). They pointed out that the preference for cold cy-167 clones and the dominance of warm filaments are due to the inclusion of the ageostrophic 168 component. 169



Figure 2. (Colour online) The median values for surface buoyancy perturbation  $b_s^m(\mathbf{a})$ , relative vorticity  $\zeta^m(\mathbf{b})$ , strain rate  $\sigma^m(\mathbf{c})$ , and absolute horizontal divergence  $|\delta|^m(\mathbf{d})$  as functions of  $\varepsilon$  at different times.

The median value of  $b_s(x, y)$  versus  $\varepsilon$  at different times is shown in Fig. 2(a). When  $\varepsilon = 0.01$ , the high-order ageostrophic correction term in Eq. (A7) the SSG model is negligible, and the SSG flow becomes indistinguishable from the SQG flow. The distribution of cyclones and anticyclones becomes symmetric and the median value of the surface buoyancy perturbation,  $b_s^m$ , is close to zero. As  $\varepsilon$  increases,  $b_s^m$  shifts to positive values. It corresponds to the surface warming shown in Fig. 1(c,d). The warming effect decreases with time as the flows decay.

Accumulation of warm water at the surface leads to a general anticyclonic circulation, such that the median value of the relative vorticity becomes negative,  $\zeta^m < 0$ , Fig. 2(b). Here the (vertical component of) relative vorticity is  $\zeta = \partial v / \partial x - \partial u / \partial y$ . This mean anticyclonic circulation strengthens as  $\epsilon$  increases. The median value of the strain rate  $\sigma^m$  also increases with  $\epsilon$  because of the enhanced stirring created by the abundant small-scale filaments and vortices, Fig. 2(c). Here the strain rate is defined as:

$$\sigma = \left[ \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 \right]^{1/2}.$$
 (21)

<sup>177</sup> Since vertical motions concentrate in these small-scale structures (Fig. 3(b)) where the local convergence/divergence is large, the median value of the lateral divergence,  $|\delta|$ , also increases with  $\varepsilon$  (Fig. 2(d)).

Oceanic fronts are characterized by a relatively large vertical velocity of approx-180 imately 1 mm/s (Mahadevan & Tandon, 2006; McWilliams, 2016; Ruiz et al., 2019). In 181 the SSG model, vertical velocity can be diagnosed by solving the so-called " $\Omega$ -equation" 182 (Hoskins & West, 1979). An analytical solution of the " $\Omega$ -equation" in the wavenum-183 ber space is given in Appendix B. Vertical velocity fields right below the surface at z =184 -0.1 are shown in Fig. 3 for two simulations with different  $\varepsilon$ . In vortices, vertical veloc-185 ity appears as a quadrupolar structure Fig. 3(a). In filaments, positive and negative stripes 186 of w are created. At larger  $\varepsilon$ , the magnitude of w increases; the difference between Fig. 3(a) 187 and (b) is approximately one order of magnitude. Vertical motions become concentrated 188 at the periphery of vortices and the bands of upwelling (w > 0, yellow color) become 189 stronger than the bands of downwelling (w < 0, blue color). 190

Vertical profiles of w(x, y) (not shown here) show that the magnitude of w(x, y) is maximum in a subsurface layer at  $z_{max} \approx -0.1$ . Below this level, w(x, y) decays monotonically with depth. Vertical derivative of w is related to the lateral divergence of velocity,  $\delta$ , as:

$$\delta = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = -\frac{\partial w}{\partial z}.$$
(22)

Since w vanishes at the surface, the lateral divergence can be approximated as  $\delta \approx w(z_{max})/z_{max}$ .

Fronts/filaments are associated with strong buoyancy gradients in the cross-front direction and strain-dominated confluent flows which act to enhance the gradients. In an elongated front where the variation of velocity in the along-front direction is negligible,  $\delta$  is related to the relative vorticity,  $\zeta$ , and the rate-of-strain,  $\sigma$  as:

$$\delta^2 = \sigma^2 - \zeta^2. \tag{23}$$

The relation between these quantities was previously discussed for oceanic and numer-192 ical flows by (Shcherbina et al., 2013; Chavanne et al., 2010; Balwada et al., 2020; Maalouly 193 et al., 2023). Chavanne et al. (2010) reported a negative linear correlation between  $\delta$  and 194  $\zeta$  for an oceanic front during an active phase of its evolution. Their observation is in agree-195 ment with the prediction by (Hoskins & Bretherton, 1972) that  $\delta \propto -\bar{\sigma}\zeta$  where  $\bar{\sigma}$  is 196 the large-scale strain rate. Thus, cyclonic circulations in a strain field create lateral con-197 vergence while anticyclonic ones create lateral divergence. To obtain a  $\zeta - \delta$  relation for 198 our flows, we computed the joint probability density function (PDF) in the two-dimensional 199



Figure 3. (Colour online) Vertical velocity w(x, y) at z = -0.1 (a, b), normalized relative vorticity  $\zeta/f_0$  (c, d), and normalized strain rate  $\sigma/f_0$  (e, f) for the flows with  $\varepsilon = 0.01$  (left column) and  $\varepsilon = 0.2$  (right column) at T = 50.

<sup>200</sup> parameter space spanned by  $\zeta$  and  $\delta$ .  $\zeta$  and  $\delta$  were normalized by the Coriolis param-<sup>201</sup> eter  $f_0$ , they were then sorted according to their normalized values into bins of size 0.01 <sup>202</sup> by 0.01. After that, the joint PDF can be obtained by counting the number of occur-<sup>203</sup> rences when  $\zeta(x, y)$  and  $\delta(x, y)$  drop into each bin. Finally, the joint PDFs were tem-<sup>204</sup> porally averaged over a period from T = 45 to T = 55.

Figure 4(a) shows that the joint PDF of  $\zeta$  and  $\delta$  is aligned along a straight line with a negative slope. White dashed line in Fig. 4(a) is  $\delta = -\frac{1}{2}\bar{\sigma}\zeta$ , where  $\bar{\sigma} = 0.04$  is the spatial mean of  $\sigma$  averaged over the parameter region where PDF> 3;  $\bar{\sigma}$  represents a typical value of the large-scale strain rate. This relation was previously proposed in (Davies & Muller, 1988; Lapeyre & Klein, 2006b) for the surface-intensified currents decaying exponentially with depth, which is consistent with the SSG model employed here.

Fig. 4(b) shows the joint PDF in the  $\zeta - \sigma$  parameter space. The PDF is aligned along the lines  $\sigma = \pm \zeta$ , which indicates a pure shear relationship. This also suggests that a contribution of  $\delta$  in Eq. (23) is small.

To show the relation between  $\delta$ ,  $\sigma$ , and  $\zeta$  in a single diagram, we computed  $\delta$  av-214 eraged over each bin in the  $\zeta - \sigma$  parameter space. This procedure gives a conditional-215 mean lateral divergence shown in Fig. 4(c). Note that this diagram can also be interpreted 216 in terms of vertical velocity in the subsurface layer. Strong divergence/upwelling (vel-217 low color) is mainly associated with anticyclonic vorticity while convergence/downwelling 218 (blue color) is associated with the cyclonic vorticity in the strain-dominated areas located 219 above the line  $\sigma = |\zeta|$ . In the vorticity-dominated areas below the line  $\sigma = |\zeta|$ , the 220 divergence is generally of the same sign as vorticity, opposite to that in the strain-dominated 221 areas. However, the signal there is weaker and noisier than that in the strain-dominated 222 areas. Note that according to a frontogenesis model by Barkan et al. (2019) the three 223 quantities in Eq. (23) are of the same order of magnitude in a submesoscale front. In our 224 simulations, this can be locally satisfied in strong filaments. High levels of  $\delta$  create grain-225 iness in Fig. 4 (c). 226

#### 4.2 Spectral characteristics

227

Kinetic and potential energy spectra at depth Z are defined as

$$\mathcal{K}(\boldsymbol{k}, Z) = k^2 \tilde{\Phi}(\boldsymbol{k}, Z) \tilde{\Phi}^*(\boldsymbol{k}, Z), \qquad (24a)$$

$$\mathcal{P}(\boldsymbol{k}, Z) = \hat{b}_s(\boldsymbol{k}, Z) \hat{b}_s^*(\boldsymbol{k}, Z), \qquad (24b)$$

where  $\mathbf{k} = (k_x, k_y)$  and the superscript \* denotes the complex conjugate. One-dimensional 228 (1D) spectra K(k, Z) and P(k, Z) are computed by averaging the above equations over 229 the azimuthal angle  $\theta = \tan^{-1}(k_y/k_x)$  in the wavenumber space. Fig. 5 shows 1D ki-230 netic energy spectra  $\mathcal{K}_s(k)$  and  $P_s(k)$  for the flows at the surface at different  $\varepsilon$ . At larger 231  $\varepsilon$ , the fraction of total kinetic or potential energy at smaller scales (larger k) increases 232 while the fraction at larger scales (smaller k) decreases. This shift in the energy distri-233 bution across scales is a manifestation of abundant and energetic small-scale features in-234 cluding filaments at larger  $\varepsilon$ . As a result, the spectral slope becomes less steep at larger 235  $\varepsilon$ ; it varies between -2.2 and -1.7 for both  $\mathcal{K}_s$  and  $\mathcal{P}_s$  for  $\varepsilon$  varying between 0.01 and 0.2. 236 A middle point of this spectral seesaw is at approximately k = 20. 237

Previously, Ragone and Badin (2016) made an observation that energy accumu-238 lation at small scales strongly depends on  $\varepsilon$ . However, their -3 slope of  $\mathcal{K}_s$  was steeper 239 than the -2 slope in our flows. This difference might be due to the fact that their anal-240 yses were performed at a later time T = 100 when the flow is dominated by the long-241 lived coherent vortices rather than filaments. The presence of these vortices could steepen 242 the spectral slope. In our case, the nonlinear interactions are strong at T = 30 and fil-243 aments are abundant. A similar -2 slope was previously measured during an early stage 244 of the SQG flow simulation by (Capet et al., 2008). 245



Figure 4. (Colour online) Joint PDF in the  $\zeta$ - $\delta$  parameter space (a); that in the  $\zeta$ - $\sigma$  parameter space (b); and  $\delta/f_0$  conditioned in the  $\zeta$ - $\sigma$  parameter space (c) for the flow with  $\epsilon = 0.2$ . The color scales are logarithmic and areas with zero PDF are left blank. White dashed line in (a) corresponds to  $\delta = -\bar{\sigma}/2\zeta$ . Black dashed lines in (b) and (c) correspond to  $\sigma = \pm \zeta$ .



Figure 5. (Colour online) One-dimensional kinetic energy spectra  $\mathcal{K}_s(k)$  (a) and potential energy spectra  $\mathcal{P}_s(k)$  (b) for the flows with  $\varepsilon$  varying between 0.01 and 0.2 at T = 30. The solid, dotted, and dashed curves in panel (c) show the one-dimensional PDS for  $\tilde{\zeta}(k)$ ,  $\tilde{\delta}(k)$ , and  $\tilde{\sigma}(k)$ , respectively. Note that  $\tilde{\sigma}(k)$  is dominated by  $\tilde{\zeta}(k)$ , the dashed lines coincide with the solid ones. The insert shows the wavenumber  $k_{max}$  for the peak in  $\tilde{\delta}(k)$ , where a linear fit is shown by the straight line.

Boyd (1992) investigated spectral characteristics of a one-dimensional front using 246 the Burger's equation  $u_t + uu_x = 0$ . He showed that the kinetic energy spectrum of 247 the solution follows a  $k^{-2}$  scaling law shortly after the formation of the front. We be-248 lieve that the approximately -2 slope in Fig. 5 is due to the nonlinear advection term in 249 Eq. (A9). At later times, when filaments are getting destroyed in the strain field of co-250 herent vortices, a -3 or even steeper spectral slope emerges in all of our simulations (not 251 shown here). An approximately -5/3 slope is observed at larger  $\varepsilon = 0.15, 0.2$ . This re-252 sult is in agreement with that of the simulations by Ragone and Badin (2016) and with 253 the theoretical result by (Blumen, 1978) who predicted the -5/3 slope for an inertial range 254 of the potential energy. 255

Comparison of Fig. 5 (a) and (b) shows that the slopes of  $\mathcal{P}_s(k)$  are approximately equal to those of  $\mathcal{K}_s(k)$ . This feature was also observed in the SQG flows in an infinitely deep ocean (Lapeyre & Klein, 2006a). In that case, the SQG solution Eq. (7) becomes

$$\tilde{\phi}(\boldsymbol{k}, z, t) = \frac{1}{k} \tilde{b}_s(\boldsymbol{k}, z) \exp(-kz)$$
(25)

Substitution of the above equation into Eq. (24) shows that

$$\mathcal{P}_s(\boldsymbol{k}) = \mathcal{K}_s(\boldsymbol{k}) \tag{26}$$

is satisfied at the surface z = 0. Our computations suggest that this result is also valid for the SSG flows.

To assess the spectral characteristics of the small-scale filaments we computed the 258 power spectral density (PSD) for the gradient fields, namely the relative vorticity  $\zeta$ , lat-259 eral divergence  $\delta$  and strain rate  $\sigma$ , Fig. 5(c). An approximately flat ("white") spectrum 260 is observed in the wavenumber range where the kinetic energy slope is about -2. The 261 almost geostrophic flow ( $\varepsilon = 0.01$ ) is non-divergent such that  $\delta(k)$  is negligible (dot-262 ted blue curve) and the PSD of  $\zeta$  and  $\tilde{\sigma}$  (solid and dashed blue curves) are almost iden-263 tical. Although  $\tilde{\delta}$  increases significantly with  $\varepsilon$  it remains much smaller than  $\tilde{\zeta}$  or  $\tilde{\sigma}$ . At 264 larger  $\varepsilon$ , the flat spectrum extends to higher wavenumbers due to the growing contribu-265 tion of small-scale energetic filaments. An inset in Fig. 5(c) shows the wavenumber  $k_{max}$ 266 at which the maximum magnitude of  $\delta(k)$  is reached.  $k_{max}$  can be considered as a char-267 acteristic wavenumber of submesoscale filaments in our flows. It grows approximately 268

linearly with  $\varepsilon$  (thick-black line). This is a consequence of the linear dependence of the high-order correction term in Eq. (A7), which determines the lateral divergence, on  $\varepsilon$ .

Energy spectra are sustained by transfers of energy across the scales, an energy cascade. However, the spectra themselves do not allow us to determine the magnitude or the direction of the cascade. The investigation of the cascades requires a different approach. Here we employ the spatial filtering technique developed by (Germano, 1992; Chen et al., 2006; Aluie et al., 2018) and used in previous studies of rotating shallowwater and baroclinic turbulence (Afanasyev & Craig, 2013; Zhang & Afanasyev, 2016). Fluxes of the kinetic energy and the potential energy are defined as:

$$\Pi_u^l(x,y) = -[(v_i v_j)^l - v_i^l v_j^l] \frac{\partial v_i^l}{\partial x_j},$$
(27a)

$$\Pi_b^l(x,y) = -[(v_jb)^l - v_j^lb^l]\frac{\partial b^l}{\partial x_j},$$
(27b)

where  $v_i$  is the *i*th component of the horizontal velocity, and summation over repeated indices is implied. The superscript *l* denotes a spatial scale.  $\Pi_u^l$  and  $\Pi_b^l$  are computed using low-pass filtering which is performed by convolving the correspondent fields with a Gaussian kernel  $G(l) = 9/(2\pi l^2) \exp(-9r^2/2l^2)$ . Positive values of  $\Pi_u$  or  $\Pi_b$  indicate a forward cascade, i.e., energy transfers from larger to smaller scales while negative values indicate the cascade in the opposite direction, the inverse cascade. The cut-off scale *l* can be related to the non-dimensional wavenumber as  $k = 2\pi/l$ .

Figure 6 shows  $\Pi_{\mu}^{l}(x,y)$  and  $\Pi_{b}^{l}(x,y)$  computed for two wavenumbers k = 85 and 278 k = 18. At the larger wavenumber, both kinetic and potential energy fluxes are con-279 centrated predominantly along filaments and at the periphery of the vortices. Positive 280 and negative fluxes alternate; both forward and inverse energy transfers are present. Note 281 that  $\Pi_{u}^{l}$  is relatively small at k = 85 in Fig. 6 (a). The potential energy flux in Fig. 6 282 (b) is of a quadrupolar structure around vortices while in the filaments away from the 283 vortices, it is mainly positive. At the smaller wavenumber, the fluxes are mainly concen-284 trated within vortices and are quadrupolar Fig. 6 (c) and (d). Note that the quadrupo-285 lar structure of energy fluxes was observed in numerical simulations by Xiao et al. (2009) 286 as well as in laboratory experiments by Afanasyev and Craig (2013). The quadrupolar 287 structure appears to be due to vorticity gradient stretching by strain fields Kimura and 288 Herring (2001). Interestingly, the kinetic energy flux appears to be concentrated in in-289 tense cold cyclones (Fig. 6 (c)) while the potential energy flux reaches its largest mag-290 nitude in warm anticyclones (Fig. 6 (d)). 291

When both positive and negative fluxes are present in the flow, the overall direc-292 tion of the energy cascades can be revealed by spatial averaging over the flow domain. 293 Figure 7 shows mean fluxes  $\overline{\Pi}_u$  and  $\overline{\Pi}_b$  versus wavenumber k for simulations with vary-294 ing  $\varepsilon$ . The kinetic energy flux is negative across the entire range of wavenumbers which 295 indicates the energy transfers to larger scales, an inverse cascade. Maximum magnitudes 296 of the flux are achieved at  $k \approx 18$  Figure 7(a); the overall magnitude of the flux decreases 297 with increasing  $\epsilon$ . This decrease is most likely caused by the joint effect of the ageostrophic 298 correction term in Eq. (A8) and the coordinates transform Eq. (9). When  $\varepsilon$  increases 299 the cyclones become smaller and separated farther away from each other; their mergers 300 then become less likely. Potential energy cascades forward at all wavenumbers above  $k \approx$ 301 20 (Fig. 7(b)). Maximum values of  $\Pi_b$  are achieved at  $k \approx 85$  and the magnitude of the 302 flux increases with increasing  $\varepsilon$ . Since the potential energy flux mainly occurs at large 303 wavenumbers, it is clearly related to small-scale elements of the flows including cyclones 304 and filaments. These elements become more abundant and energetic with increasing  $\varepsilon$ . 305

To further explore the relation between the flux of potential energy with the velocity field we plotted the isolines of  $\Pi_b^l(x, y)$  computed at k = 85 together with the vertical velocity field, w, just below the surface (at z = -0.01) (Fig. 8(a)). w appears to be positively correlated with  $\Pi_b^l(x, y)$ ; filaments formed by upwelling water are associ-



**Figure 6.** (Colour online) Kinetic energy flux  $\Pi_{u}^{l}(x, y)$  (a, c) and potential energy flux  $\Pi_{b}^{l}(x, y)$  (b, d) for the surface flow with  $\varepsilon = 0.1$  at T = 30(contours). The fluxes are across the wavenumbers k = 85 (top row) and k = 18 (bottom row). Gray-scale background shows the surface buoyancy in the range between -1.2 and 1.2.



**Figure 7.** (Colour online) (a) Surface kinetic energy flux  $\bar{\Pi}_u^l$  and (b) potential energy flux  $\bar{\Pi}_b^l$  versus k in the flows with different  $\varepsilon$  at T = 30.

ated with the forward-cascading potential energy, while areas of downwelling exhibit an inverse cascade. This observation appears to be consistent with (Hakim et al., 2002)'s conclusion that the contraction of warm filaments develops faster than that of cold ones.

313

### 4.3 Finite-scale Lyapunov exponents

To study stirring in the SSG flows we compute trajectories of numerical particles in our flows. The trajectories can be used to obtain finite-scale Lyapunov exponents (FSLEs) which are a useful metric of stirring (d'Ovidio et al., 2004). FSLEs are inversely proportional to time  $\tau$  it takes a pair of particles initially separated by a distance  $\delta_i$  to reach a prescribed final separation  $\delta_f$ :

$$\lambda(x, y, t, \delta_i, \delta_f) = \frac{1}{\tau} \log \frac{\delta_f}{\delta_i}.$$
(28)

Trajectories of particles are computed by integrating velocity fields over time using the 314 fourth-order Runge-Kutta scheme. The velocity at particle locations is obtained by a bi-315 linear interpolation at each time step. Particles are initially seeded in between the nodes 316 of the computational grid such that their smallest initial separation is half of the grid 317 spacing,  $\delta_i = 0.5\Delta x$ . Each particle is surrounded by four neighboring particles in the 318 shape of a diamond. The separations between particles in the diamond in x- and y-directions 319 are calculated at each time step; when the maximum separation reaches  $\delta_f$ , the time  $\tau$ 320 is obtained. The velocity is integrated either forward or backward in time to obtain two 321 sets of the exponents  $\lambda_+$  and  $\lambda_-$ , respectively. High values of  $\lambda_+$  indicate areas where 322 particles separate from each other due to lateral divergence. High values of  $\lambda_{-}$ , on the 323 other hand, indicate areas of convergence where particles accumulate. 324

Spatial distributions of FSLEs can be used for detecting the so-called Lagrangian 325 structures, the structures formed by Lagrangian particles. High values of both exponents 326 often manifest themselves as filament-like structures in the ocean(d'Ovidio et al., 2004; 327 Calil & Richards, 2010; Siegelman et al., 2020). A typical spatial pattern of the expo-328 nents in our simulations is shown in Figure 8(b) where both  $\lambda_+$  (yellow color) and  $\lambda_-$ 329 (blue color) are plotted together. It is an illustration of stirring by strong vortices. Cy-330 clonic vortices created by cold patches (black color) create a fine structure of filaments 331 wrapped around their cores. Two pairs of cyclones located in the part of the computa-332 tional domain shown in Figure 8(b) create two figure-eight patterns where attracting lines 333 (blue color) intersect repelling lines (yellow color) at a hyperbolic point in the area be-334 tween the vortices. It is in this area the strain rate is as important as the relative vor-335 ticity. Two warm anticyclones (white color) do not seem to create distinct patterns of 336 filaments in their cores but contribute to strain in the areas between them and other vor-337 tices. 338

Domain-averaged FSLEs can be used to identify regimes of dispersion at different 339 scales. Here, we compute a spectrum of the mean exponent  $\bar{\lambda} = 0.5(\lambda_+ + \lambda_-)$  aver-340 aged over the surface area of the domain. In this computation, the initial separation be-341 tween the particles in diamond patterns was varied in a wide range between  $\delta_i = \Delta x$ 342 and  $\delta_i = 110\Delta x$ . The particles were followed until the separation between them reached 343 a prescribed final value  $\delta_f = \sqrt{2}\delta_i$  (Lacorata et al., 2001).  $\bar{\lambda}$  as a function of  $\delta_i$  is shown 344 in Fig. 9 for simulations with different  $\varepsilon$ . Note that the range of dimensionless  $\delta_i$  in Fig. 9 345 corresponds to the range of the dimensionless wavenumber,  $k = L/2\delta_i$ , from 256 down 346 to 3 for comparison with the energy spectra in Fig. 5. The slope of the  $\bar{\lambda}$  spectrum varies 347 continuously with  $\delta_i$  such that there is no extended interval where it remains constant. 348 At the smallest scales up to approximately  $\delta_i = 4\Delta x$  the spectrum is almost flat,  $\lambda \approx$ 349 constant. The flat spectrum indicates that the distance between particle trajectories in-350 creases exponentially in time. At larger scales, the slope varies from approximately -1/2351 to -2. 352



Figure 8. (Colour online) Typical patterns of the potential energy flux  $\Pi_b^l(x, y)$  (a) and the FSLEs  $\lambda_+$  and  $\lambda_-$  (b) in the flows  $\varepsilon = 0.1$ . Contours of  $\Pi_b^l(x, y)$  across wavenumber k = 85 are superposed over the vertical velocity field w(x, y) (gray-scale) in the range between  $-5 \times 10^{-3}$  and  $5 \times 10^{-3}$ . Contours of the FSLEs are superposed over the buoyancy field  $b_s(x, y)$  (gray-scale) in the range between -0.6 and 0.6. Black arrows indicate the direction of the velocity around one of the cyclone pairs.



Figure 9. (Colour online) FSLE spectra for five simulations with different  $\varepsilon$  at T = 30.

Scaling theory for turbulent flows where the kinetic energy spectrum is  $\mathcal{K}_s(k) \propto$ 353  $k^{-\alpha}$  predicts the power-law scale dependence of the FSLE,  $\bar{\lambda} \propto \delta_i^{-\beta}$ , and the power-law time dependence of the separation between particles,  $\delta^2(t) \propto t^{2/\beta}$  where  $\beta = (3 - 1)^{-\beta}$ 354 355  $\alpha$ /2 (Morel & Larceveque, 1974). These power-law equations are applicable when the 356 kinetic energy spectrum is not too steep,  $\alpha < 3$ . In this case, the dispersion regime is 357 local, the separation of particles at a certain scale is only determined by the velocity gra-358 dient components at the same scale. Otherwise, the dispersion regime is non-local; the 359 power-law is not applicable and the separation between particles grows exponentially in 360 time. 361

In our flows,  $\alpha \approx 2$  at intermediate values of the wavenumber (Fig. 5). In this in-362 terval, a local dispersion regime with  $\beta \approx 1/2$  is expected. The separation between par-363 ticles grows quite fast,  $\delta^2(t) \propto t^4$ , and the regime can be called hyper-ballistic.  $\beta$  then 364 keeps increasing with  $\delta_i$  up to  $\beta = 2$ . In this range, several distinct regimes of disper-365 sion can be pointed out. When  $\beta = 2/3$  the dispersion obeys the Richardson's law which 366 describes another case of the hyper-ballistic dispersion where  $\delta^2(t) \propto t^3$ ; in this case, 367 the energy spectrum has Kolmogorov's -5/3 slope. When  $\beta = 1$  and  $\delta^2(t) \propto t^2$  the 368 motion of particles is ballistic as if they move with constant speed away from one an-369 other. Finally, when  $\beta = 2$  the regime is a normal diffusion,  $\delta^2(t) \propto t$  is similar to that 370 of the Brownian motion. In our flows, the normal diffusion is due to the scattering of 371 particles by the energetic warm and cold eddies at large scales. 372

### **5** Conclusions

In this work, turbulent flows were simulated at different values of the Rossby number,  $\varepsilon$ , using the SSG model. The simulated flows exhibited typical ageostrophic effects, including a cyclone-anticyclone asymmetry with a cyclonic preference for vortices and an anticyclonic preference for filaments. The magnitude of the ageostrophic effects increased with  $\varepsilon$  due to the increasing higher-order ageostrophic term in the SSG solution (Equation A7). As  $\varepsilon$  increased from 0.01 to 0.2 between the simulations, the number of warm filaments on the surface increased, resulting in a surface warming trend.

The magnitude of the vertical velocity and, consequently, the lateral divergence also 381 increased with  $\varepsilon$ . Vertical motions occurred mostly in small-scale filaments and at the 382 periphery of vortices rather than in their cores. However, in all our simulations, the lat-383 eral divergence remained much smaller than the relative vorticity or the strain rate. This 384 contrasted with the results of (Balwada et al., 2021), where the authors used primitive 385 equations and obtained lateral divergence values comparable to those of relative vortic-386 ity and strain rate. We believe this difference is mainly due to the distinct forcing used 387 in their simulations compared to buoyancy-only initial forcing in ours. Our results demon-388 strated a negative correlation between lateral divergence and relative vorticity,  $\delta = -\bar{\sigma}/2\zeta$ (Figure 4). This indicates that cyclonic and anticyclonic motions are often associated 390 with local convergence and divergence, respectively. This effect is most pronounced in 391 strain-dominated areas where  $\sigma > |\zeta|$ . 392

Spectral analyses showed that the kinetic and potential energy spectra exhibited 303 similar slopes, varying between -2.2 and -1.7 as  $\varepsilon$  increased from 0.01 to 0.2. Notably, 394 the latter value of the slope is approximately equal to -5/3, in agreement with previous 395 SSG simulations by (Ragone & Badin, 2016) and SQG+1 simulations by (Capet et al., 396 2008). The similarity of the kinetic and potential energy spectra is a well-known feature 397 of SQG turbulence, where it is caused by the thermal-wind coupling between the veloc-398 ity field and the buoyancy field at the surface. In the SSG flow, this coupling seems largely 399 unaffected by the inclusion of the ageostrophic component. 400

<sup>401</sup> Spectra of gradient fields, including relative vorticity  $\zeta$  and strain rate  $\sigma$  (Figure 5(c)), were approximately flat in the wavenumber range where the kinetic energy slope

was approximately -2. The spectra of another gradient field, lateral divergence  $\delta$ , however, showed a maximum at a relatively large wavenumber  $k_{max}$ , which increased almost linearly with  $\varepsilon$ .

In addition to energy spectra, energy fluxes across different scales were computed. 406 The fluxes showed that kinetic energy is transferred towards larger scales, constituting 407 an inverse cascade. However, the cascade rate was not constant across scales; it reached 408 a peak at a scale  $l = 2\pi/k = 0.35$ , corresponding to wavenumber k = 18. This scale 409 roughly agreed with the typical distance between cold cyclones. Visual inspection of the 410 411 flux fields showed that kinetic energy flux concentrated in and around cold cyclones (Figure 6(c)). Interestingly, the magnitude of the flux decreased as  $\varepsilon$  increased, and the flows 412 became more ageostrophic and three-dimensional. One of the effects slowing down the 413 inverse cascade was warm filaments wrapping around cold cyclones, shielding them, and 414 preventing mergers. Potential energy, on the other hand, cascaded forward towards smaller 415 scales at all wavenumbers greater than  $k \approx 20$ . The potential energy flux was maxi-416 mum at  $k \approx 85$ . Comparison of the flux with the vertical velocity field (Figure 8(a)) 417 showed that the forward cascade was mainly associated with warm filaments created by 418 upwelling. The magnitude of the potential energy flux increased with  $\varepsilon$ , a consequence 419 of the growing number of filaments in ageostrophic flows. 420

To explore lateral stirring and dispersion of particles by eddies and filaments in our 421 flows, we computed the trajectories of numerical particles and obtained forward and back-422 ward FSLEs. Inspection of the FSLE fields showed that interacting cold cyclones cre-423 ated Lagrangian coherent structures in between them (Figure 8(b)). The relative dis-424 persion of particles was scale-dependent in our flows. To study the regimes of dispersion, 425 mean FSLEs were computed for different initial separations of particles  $\delta_i$ . The results 426 showed (Figure 9) that at the smallest scales, the relative dispersion of a pair of parti-427 cles was exponential in time and non-local. At larger scales, the dispersion regime was 428 local, and the mean FSLE,  $\bar{\lambda}$ , satisfied a power law,  $\bar{\lambda} \propto \delta_i^{-\beta}$ , where  $\beta$  varied smoothly 429 from approximately 1/2 to 2 with increasing  $\delta_i$ . The variation of  $\beta$  reflected a transition 430 from a hyper-ballistic dispersion regime ( $\beta \approx 1/2$ ) to Richardson's dispersion ( $\beta \approx 2/3$ ) 431 and then to a ballistic regime ( $\beta \approx 1$ ) and finally to normal diffusion ( $\beta \approx 2$ ). The 432 smooth transition of  $\beta$  from 1/2 to 2 was a robust feature in all our simulations for dif-433 ferent  $\varepsilon$ . A similar transition of the exponent  $\beta$  was previously found in SQG+1 turbu-434 lence (Maalouly et al., 2023, their figure 4) and observed for drifters in the Antarctic Cir-435 cumpolar Current (Balwada et al., 2021, their figure 9). 436

# 437 Appendix A Solution of the SSG equations

Eq. (18), can be written in non-dimensional form as:

$$\nabla^2 \Phi = \varepsilon D \Phi, \tag{A1}$$

where  $\nabla^2$  is the three-dimensional Laplacian operator in the geostrophic space and

$$D\Phi = \frac{\partial^2 \Phi}{\partial X^2} \frac{\partial^2 \Phi}{\partial Y^2} - \left(\frac{\partial^2 \Phi}{\partial X \partial Y}\right)^2 \tag{A2}$$

is the nonlinear differential operator. Horizontal Fourier transform can then be used to obtain a forced Helmholtz equation in the vertical direction which can be solved numerically by iteration:

$$\left(\frac{\partial}{\partial Z^2} - k^2\right)\tilde{\Phi}^{(n)} = \varepsilon \tilde{D}\Phi^{(n-1)}.$$
(A3)

The iteration is performed for each wavevector  $\mathbf{k} = (k_X, k_Y)$  in the (geostrophic) wavenumber space. Boundary conditions Eq. (4) can be written as:

$$\frac{\partial \Phi(\mathbf{k}, Z)}{\partial Z} = \tilde{b}_s \quad \text{at} \quad Z = 0,$$

$$\frac{\partial \tilde{\Phi}(\mathbf{k}, Z)}{\partial Z} = 0 \quad \text{at} \quad Z = -1.$$
(A4)

Equation (A3) with the boundary conditions Eq. (A4) has a solution in the form of the Green's function:

$$\tilde{\Phi}^{(n)}(\boldsymbol{k}, Z) = \tilde{b}_s(\boldsymbol{k}, t) G_k(Z, 0) + \varepsilon \int_{-1}^0 G_k(Z, Z') \tilde{D} \Phi^{(n-1)}(\boldsymbol{k}, Z') dZ'$$
(A5)

where

$$G_k(Z, Z') = \begin{cases} \cosh(kZ) \cosh[k(Z'+1)]/(k \cdot \sinh k), & Z \ge Z' \\ \cosh[k(Z+1)] \cosh(kZ')/(k \cdot \sinh k), & Z < Z'. \end{cases}$$
(A6)

The first-order approximation of the solution is given by

$$\tilde{\Phi}^{(1)}(\boldsymbol{k}, Z) = \tilde{\Phi}^{(0)}(\boldsymbol{k}, Z) + \varepsilon \int_{-1}^{0} G_{k}(Z, Z') \tilde{D} \Phi^{(0)}(\boldsymbol{k}, Z') dZ'$$
(A7)

where the zeroth-order approximation

$$\tilde{\Phi}^{(0)}(\boldsymbol{k}, Z) = \tilde{b}_s(\boldsymbol{k}, t) G_k(Z, 0) = \frac{\cosh[(Z+1)k]}{k \sinh(k)} \tilde{b}_s(\boldsymbol{k}, t)$$
(A8)

is the SQG solution Eq. (7). Following (Ragone & Badin, 2016) who showed that when  
$$\varepsilon$$
 is small, the first-order approximation provides reasonably accuracy we use Eq. (A7)  
for the numerical solution of the SSG problem.

Buoyancy,  $b_s$ , is a conserved quantity such that:

$$\frac{db_s}{dt} = \frac{\partial b_s}{\partial t} + u_g \frac{\partial b_s}{\partial X} + v_g \frac{\partial b_s}{\partial Y} = 0.$$
(A9)

Given an initial buoyancy perturbation field  $b_s(X,Y)$  in the geostrophic space, one can

calculate the Bernoulli function  $\Phi(X, Y)$  using Equation (A5). Geostrophic velocity,  $(u_q, v_q)$ ,

is then given by Eq. (11). Finally Eq. (A9) can be marched in time numerically.

# 444 Appendix B Vertical velocity

In the SSG model, a re-scaled vertical velocity  $w^* = J \cdot w$  can be obtained from the so-called " $\Omega$ -equation" (Hoskins & West, 1979; Ragone & Badin, 2016):

$$\frac{\partial^2 w^*}{\partial X^2} + \frac{\partial^2 w^*}{\partial Y^2} + \frac{\partial^2 w^*}{\partial Z^2} = -2\varepsilon \nabla \cdot \boldsymbol{Q},\tag{B1}$$

where

$$J = 1 - \varepsilon \left( \frac{\partial v_g}{\partial X} - \frac{\partial u_g}{\partial Y} \right) \tag{B2}$$

is the re-scaling factor and

$$\boldsymbol{Q} = (Q_1, Q_2) = \left(\frac{\partial u_g}{\partial X}\frac{\partial b}{\partial X} + \frac{\partial v_g}{\partial X}\frac{\partial b}{\partial Y}, \frac{\partial u_g}{\partial Y}\frac{\partial b}{\partial X} + \frac{\partial v_g}{\partial Y}\frac{\partial b}{\partial Y}\right)$$
(B3)

is the forcing vector. These two quantities can be calculated using Eqs. (11) and (A7). Applying Fourier transform in the horizontal direction, Eq. (B1) can be written as

$$-k^2 \tilde{w}^* + \frac{\partial^2 \tilde{w}^*}{\partial Z^2} = \tilde{Q}(k, Z), \tag{B4}$$

where  $\tilde{Q}(k, Z)$  is the Fourier transform of the RHS of Eq. (B1). For each geostrophic wavenumber  $k = \sqrt{k_X^2 + k_Y^2} \neq 0$ , Eq. (B4) subject to the boundary conditions  $\tilde{w}^* = 0$  at Z = 0 and Z = -1 has the following solution:

$$\tilde{w}^{*}(k,Z) = \exp(kZ) \int_{0}^{Z} \delta_{3}(k,z')dz' - \exp(-kZ) \int_{0}^{Z} \delta_{4}(k,z')dz' + 2\frac{\delta_{2}(k)}{\delta_{1}(k)}\sinh(kZ)$$
(B5)

where

$$\delta_1(k) = -2\sinh(k),\tag{B6a}$$

$$\delta_2(k) = \exp(k) \int_0^{-1} \delta_4 dz' - \exp(-k) \int_0^{-1} \delta_3 dz',$$
 (B6b)

$$\delta_3(k, z') = \exp(-kz') \frac{Q(k, z')}{2k},$$
 (B6c)

$$\delta_4(k, z') = \exp(kz') \frac{Q(k, z')}{2k}.$$
 (B6d)

<sup>445</sup> The above analytical solution is provided by the symbolic math toolbox in MATLAB.

Inverse Fourier transform of Eq. (B5) then gives the vertical velocity in the geostrophic coordinates, w(X, Y, Z).

### 448 **3** Availability Statement

The code for the SSG model is available at: github.com/zy-gdou/ The Matlab figures, the data and codes used for creating the figures are available from the ZENODO repository (https://doi.org/10.5281/zenodo.10431740).

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# **Energy cascades in surface semi-geostrophic turbulence**

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# Key Points:

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7 8	•	An asymmetry between cyclonic cold vortices and anticyclonic warm filaments char- acterizes the surface semi-geostrophic turbulence.
9	•	The ageostrophic component strengthens the forward potential energy cascade by
10		exciting warm filaments but suppresses the inverse kinetic energy cascade by pre-
11		venting cyclone mergers.
12	•	Horizontal dispersion transforms from a hyper-ballistic regime at small scales to
13		a normal dispersion regime at large scales.

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### 14 Abstract

Surface semi-geostrophic turbulence is examined in this study. In our simulations, the 15 strength of the ageostrophic component of the flows is controlled by the Rossby num-16 ber  $\varepsilon$ , varying from 0.01 to 0.2. The flows manifest a cyclone-anticyclone asymmetry with 17 a cyclonic preference for cold vortices and an anticyclonic preference for warm filaments. 18 This asymmetry becomes especially pronounced in the flows with large  $\varepsilon$ , where an abun-19 dance of warm filaments is observed. Strong vertical motions concentrate in the small-20 scale filaments and at the periphery of the vortices. There, the lateral divergence becomes 21 significant. A negative correlation between the divergence and the relative vorticity is 22 identified using joint probability density functions. Slopes of the kinetic and potential 23 energy spectra vary between -2.2 and -1.7 at intermediate scales. Analyses of spectral 24 fluxes demonstrate an inverse kinetic energy cascade and a forward cascade of potential 25 energy. As  $\varepsilon$  increases, the filaments become more numerous in the flows. They wrap around 26 cyclones, weakening their interactions and subsequent mergers, thus suppressing the in-27 verse cascade of kinetic energy. We characterize lateral dispersion in the SSG flows us-28 ing the finite-scale Lyapunov exponents (FSLEs). They are used to identify Lagrangian 29 coherent structures, such as those created by the interaction of vortices. The FSLEs are 30 also used to investigate the regimes of dispersion at different scales. The results show 31 a smooth transition from hyper-ballistic diffusion at small scales to normal diffusion at 32 33 large scales.

# <sup>34</sup> Plain Language Summary

The generation of submesoscale structures by mesoscale currents is one of the im-35 portant pathways of energy dissipation in the ocean. It can be modeled with an ideal-36 ized surface semi-geostrophic (SSG) equations. The SSG model is able to reproduce ageostrophic 37 effects, including a cyclone-anticyclone asymmetry. In this study, we simulate a turbu-38 lent SSG flow and demonstrate that, as the ageostrophy increases, warm filaments be-39 come more numerous. The filaments contribute to transporting the potential energy to-40 wards smaller scales. Meanwhile, the cold cyclones shrink in size and become more iso-41 lated from each other due to the shielding by warm filaments wrapping around them. 42 As a result, cyclone interaction and the subsequent mergers are weakened, and the in-43 verse cascade of the kinetic energy towards larger scales is suppressed. 44

# 45 **1** Introduction

Oceanic turbulence comprises flows of different scales, including ocean-wide gyres, 46 mesoscale eddies, submesoscale eddies, fronts, and filaments. At the lowest end of the 47 scale, submesoscale flows become more familiar due to new evidence provided by field 48 measurements (Shcherbina et al., 2013; Mensa et al., 2018; Pearson et al., 2019; Balwada 49 et al., 2016) and high-resolution numerical simulations (Balwada et al., 2021; Jing et al., 50 2021). Submessical flows are characterized by an O(1) Rossby number and consequently 51 exhibit significant ageostrophy, including large vertical velocity and horizontal divergence 52 (McWilliams, 2016). Thus, they provide a pathway for energy transfer from almost two-53 dimensional (2D) quasi-geostrophic (QG) turbulence to three-dimensional (3D) turbu-54 lence. 55

Over the years, several theoretical models that go beyond QG but still retain cer-56 tain physical simplicity—referred to as "intermediate models" in the terminology of McWilliams 57 and Gent (1980)—have been developed. Some of these models exclusively address flows 58 generated by buoyancy perturbations at the surface of the ocean, such as the surface quasi-59 geostrophic (SQG) model (Blumen, 1978; Held et al., 1994) and the surface semi-geostrophic 60 (SSG) model (Ragone & Badin, 2016). The SQG model has been investigated by dif-61 ferent authors (Isern-Fontanet et al., 2006; Klein et al., 2008; Qiu et al., 2016) with re-62 spect to its capability to describe upper ocean currents using only surface data, such as 63

those obtained by satellite altimetry and thermal radiometry. It has been demonstrated 64 that SQG flows generate submesoscale structures (Capet et al., 2008; Carton et al., 2016). 65 Numerical simulations by (Capet et al., 2008) showed that these structures are due to 66 frontogenesis processes, which occur when forward-cascading surface potential energy 67 transfers into inversely-cascading kinetic energy. Spectra of kinetic energy exhibited an 68 approximately -5/3 slope. Similar spectral slopes were obtained from altimetry data by 69 (Traon et al., 2008) and in realistic numerical simulations by (Klein et al., 2008; Chas-70 signet & Xu, 2017). For a comprehensive review of SQG dynamics, readers are referred 71 to (Lapeyre, 2017). The SQG theory relies on the assumption of a small Rossby num-72 ber,  $\varepsilon = U/(f_0 L_D) < 1$ , where U is the characteristic velocity scale,  $L_D$  is the length 73 scale, and  $f_0$  is the Coriolis parameter. However, at submesoscales,  $\varepsilon$  can approach or 74 exceed unity (Thomas et al., 2008). Ageostrophic effects become significant at the sub-75 mesoscale; one example is that strong vortices in the upper ocean are predominantly cy-76 clonic (Shcherbina et al., 2013; Munk, 2000; Griffa et al., 2008). As  $\varepsilon$  approaches unity, 77 anticyclones become more vulnerable to frontal instability than cyclones (Hoskins & Brether-78 ton, 1972). Another manifestation of the ageostrophic effects is the vertical motion driven 79 by frontogenesis. It can release the available potential energy of the system, re-stratify 80 the upper ocean, and cause a warming trend at the surface. These features were real-81 ized in simulations based on the primitive equations (Roullet & Klein, 2010; Klein et al., 82 83 2008).

To include the ageostrophic effects, Hakim et al. (2002) extended the SQG model 84 to the next order of approximation. Their model, called SQG+1, exhibited ageostrophy, 85 including an asymmetry between cold and warm filaments and a preference for cyclonic 86 vortices. However, the SQG+1 model was still constrained by a requirement for a glob-87 ally small  $\varepsilon$ . To alleviate this constraint, Ragone and Badin (2016) reformulated the SQG 88 dynamics in a geostrophic coordinate system and proposed a surface semi-geostrophic 89 (SSG) model. The geostrophic coordinate system was previously introduced by Eliassen 90 (1948); Fjørtoft (1962). It is a moving coordinate system that follows the geostrophic 91 current. The total velocity in the advection term is retained rather than being approx-92 imated by the geostrophic velocity. SSG simulations by Ragone and Badin (2016) showed 93 features similar to those in the SQG+1 simulations, including a cyclone-anticyclone asym-94 metry and a surface warming trend. Besides, the SSG simulations demonstrated an im-95 proved ability to capture frontogenesis and showed an abundance of small-scale fronts/filaments 96 in the simulated flows due to the improved representation of the nonlinear advection term. 97

In what follows, we employ the SSG model to investigate the dynamics of surface-98 intensified flows generated by buoyancy forcing at the surface. The flows are ageostrophic 99 to a significant degree and exhibit frontogenesis and three-dimensional effects. We fo-100 cus on characterizing vertical velocity and lateral divergence, especially concerning their 101 relation to the relative vorticity and strain rate in filaments and eddies. Spectral char-102 acteristics of the flows are also investigated; we go beyond energy spectra and study an 103 energy cascade by computing energy fluxes across the scales. The last objective of this 104 work is a characterization of the Lagrangian dynamics. We compute the finite-size Lya-105 punov Exponents (FSLEs) to identify the regimes of lateral dispersion at different scales. 106

In Section 2, we briefly review the SQG and SSG models. Section 3 describes the numerical methods and control parameters employed in this study. The results of the simulations are reported in Section 4, and conclusions are given in Section 5.

# <sup>110</sup> 2 SQG and SSG models revisited

Buoyancy perturbation  $b(x, y, z, t) = -g\rho'/\rho_0$ , where g is the acceleration due to gravity and  $\rho'$  is the density perturbation with respect to the constant reference density  $\rho_0$ , it is a conserved quantity in both SQG and SSG models. b is related to the (pertur-

bation) geopotential,  $\phi = p/\rho_0$ , where p is the pressure, via hydrostaticity such that

$$b = \frac{\partial \phi}{\partial z}.$$
 (1)

The above equation combined with the geostrophic relation

$$f_0(v_g, -u_g) = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}\right),\tag{2}$$

where  $f_0$  is the Coriolis parameter, gives the thermal wind equation

$$\left(\frac{\partial b}{\partial x}, \frac{\partial b}{\partial y}\right) = f_0 \left(\frac{\partial v_g}{\partial z}, -\frac{\partial u_g}{\partial z}\right). \tag{3}$$

The ocean surface is subject to external heating or cooling. To model this effect, we specify the surface buoyancy perturbation  $b_s(x, y)$  at the initial moment t = 0 and then allow the flow to evolve freely. Here, the subscript s denotes a surface quantity. It is assumed that b vanishes in the ocean interior at depth z = -H, where H is the vertical scale of the motion driven by the buoyancy perturbation. Vertical boundary conditions for the geopotential can then be written as

$$\frac{\partial \phi}{\partial z} = b_s(x, y, t) \quad \text{at} \quad z = 0,$$
(4a)

$$\frac{\partial \phi}{\partial z} = 0$$
 at  $z = -H.$  (4b)

Note that the background stratification is taken to be linear such that the Brunt-Vaisalla frequency is N = const. The buoyancy perturbation is assumed to remain relatively small such that N remains approximately constant at all times (Hoskins & West, 1979; Ragone & Badin, 2016).

### 2.1 SQG model

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Quasi-geostrophic potential vorticity (q, PV) remains undisturbed in the interior of the fluid layer at all times such that

$$q = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{f_0^2}{N^2} \frac{\partial^2 \phi}{\partial z^2} = 0.$$
 (5)

The above equation takes the form of the Laplace's equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = 0, \tag{6}$$

when non-dimensionalized using the deformation radius  $L_D = NH/f_0$  as the horizontal scale, H as the vertical scale and U as the velocity scale. All quantities in Eq. (6) are dimensionless, but we keep the same notations. Vertical structure of the flow subject to the boundary conditions Eq. (4) can be obtained in the wavenumber space (Tulloch & Smith, 2006)

$$\tilde{\phi}(\boldsymbol{k}, z, t) = \frac{\cosh[(z+1)k]}{k\sinh(k)}\tilde{b}_s(\boldsymbol{k}, t)$$
(7)

where the tilde sign denotes the horizontal Fourier transform and  $\mathbf{k} = (k_x, k_y)$  is the horizontal wavenumber vector whose magnitude is  $k = \sqrt{k_x^2 + k_y^2}$ . On the surface,  $b_s$  is advected by the geostrophic current,

$$\frac{\partial b_s}{\partial t} + J_{xy}(\phi_s, b_s) = 0, \tag{8}$$

where  $J_{xy}(A, B) = A_x B_y - A_y B_x$  represents the nonlinear advection term in Jacobian form.

# 2.2 SSG model

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As we traverse the scales of the flows from mesoscale down to submesoscale, the Rossby number  $\varepsilon$  increases, and the ageostrophic component of velocity becomes significant. To study flows beyond the validity of the quasi-geostrophy, a coordinate system that follows the geostrophic component of the current was introduced (Hoskins & Bretherton, 1972; Hoskins, 1975). The relations between the physical coordinates (x, y, z) and geostrophic coordinates (X, Y, Z) are

$$x = X - \frac{1}{f_0} v_g = X - \frac{1}{f_0^2} \frac{\partial \phi_s}{\partial x},$$
(9a)

$$y = Y + \frac{1}{f_0}u_g = Y + \frac{1}{f_0^2}\frac{\partial\phi_s}{\partial y}$$
(9b)

$$z = Z. (9c)$$

In this system, the horizontal advection by the total velocity (u, v) which includes the ageostrophic component, can be expressed using the geostrophic velocity  $(u_g, v_g)$ 

$$\frac{D_g}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} = \frac{\partial}{\partial t} + u_g\frac{\partial}{\partial X} + v_g\frac{\partial}{\partial Y}.$$
(10)

In the geostrophic coordinate system, the Bernoulli function  $\Phi = \phi + (u_g^2 + v_g^2)/2$  assumes the role of the geopotential  $\phi$  such that

$$\left(\frac{\partial\Phi}{\partial X}, \frac{\partial\Phi}{\partial Y}, \frac{\partial\Phi}{\partial Z}\right) = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right) = (f_0 v_g, -f_0 u_g, b).$$
(11)

A full set of equations of the SSG model then includes the conservation of buoyancy b and the potential vorticity  $q_{sg}$ 

$$\left(\frac{D_g}{Dt} + w\frac{\partial}{\partial Z}\right) \begin{bmatrix} b\\ q_{sg} \end{bmatrix} = 0.$$
(12)

The potential vorticity is defined as:

$$q_{sg} = -\frac{g}{f_0\rho_0}\boldsymbol{\zeta}_{sg}\cdot\nabla\rho,\tag{13}$$

where the absolute vorticity

$$\boldsymbol{\zeta}_{sg} = \left(-\frac{\partial v_g}{\partial z}, \frac{\partial u_g}{\partial z}, f_0 + \frac{\partial v_g}{\partial x} - \frac{\partial u_g}{\partial y}\right) + \frac{1}{f_0} \left(J_{yz}(u_g, v_g), J_{zx}(u_g, v_g), J_{xy}(u_g, v_g)\right)$$
(14)

includes nonlinear terms in the second bracket (Hoskins & Draghici, 1977). In the ocean at rest,  $u_g = v_g = 0$ , the potential vorticity and the absolute vorticity reduce to their background values:

$$q_{sg} = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z} = N^2, \tag{15a}$$

$$\boldsymbol{\zeta}_{sg} = f_0 \boldsymbol{k},\tag{15b}$$

where k is the unit vector in the vertical direction. In the presence of the flow, the vertical component of the absolute vorticity,

$$\boldsymbol{\zeta}_{sg} = [f_0 + \frac{\partial v_g}{\partial x} - \frac{\partial u_g}{\partial y} + \frac{1}{f_0} J_{xy}(u_g, v_g)] \boldsymbol{k}.$$
(16)

remains dominant. The reciprocal of the Jacobian of a transformation from physical to geostrophic coordinates may be written as (Hoskins, 1976)

$$J_g^{-1} = \frac{f_0}{\zeta_{sg}} = 1 - \frac{1}{f_0^2} \left( \frac{\partial^2 \Phi}{\partial X^2} + \frac{\partial^2 \Phi}{\partial Y^2} \right) + \frac{1}{f_0^4} \left[ \frac{\partial^2 \Phi}{\partial X^2} \frac{\partial^2 \Phi}{\partial Y^2} + \left( \frac{\partial^2 \Phi}{\partial X \partial Y} \right)^2 \right].$$
(17)

and  $q_{sg} = \zeta_{sg}/f_0 \Phi_{zz}$ . An assumption of negligible potential vorticity in the fluid interior leads to a nonlinear Monge-Ampére equation:

$$\frac{1}{N^2}\frac{\partial^2\Phi}{\partial Z^2} + \frac{1}{f_0^2}\left(\frac{\partial^2\Phi}{\partial X^2} + \frac{\partial^2\Phi}{\partial Y^2}\right) - \frac{1}{f_0^4}\left[\frac{\partial^2\Phi}{\partial X^2}\frac{\partial^2\Phi}{\partial Y^2} + \left(\frac{\partial^2\Phi}{\partial X\partial Y}\right)^2\right] = 0.$$
(18)

<sup>119</sup> The above equation replaces the linear Laplace's equation Eq. (6) in the SQG model.

To solve Eq. (18) we follow a numerical technique developed by Ragone and Badin (2016). For further details, readers are referred to Appendix A.

### <sup>122</sup> 3 Numerical method

The model domain is discretized in the geostrophic space (X, Y, Z). The domain is periodic in both horizontal directions and contains  $N_x = 512$  grid points in each direction. The non-dimensional horizontal domain size is set to  $L/L_D = 6$ , where L is the dimensional horizontal domain size, and  $L_D$  is the deformation radius. This results in a non-dimensional horizontal grid size of approximately  $\Delta X \approx 0.01$ . In the vertical direction, the domain is bounded by rigid walls and contains  $N_z = 20$  levels which are spaced exponentially with the majority of grid points close to the top surface.

To initialize the simulation, an initial surface buoyancy perturbation  $b_s(X, Y, t = 0)$  is specified in wavenumber space

$$\tilde{b}_s(\mathbf{k}, t=0) = A \frac{k^{m/4}}{(k+k_0)^{m/2}}$$
(19)

Here, we follow (Hakim et al., 2002; Ragone & Badin, 2016) taking m = 20 and  $k_0 =$ 14 and assigning a random phase to each mode k such that the random initial field can have a prescribed spectrum structure. The amplitude A is tuned such that the initial RMS velocity is fixed at 1 m/s for all our simulations; this velocity magnitude is typical for oceanic fronts (Gula et al., 2016).

Eq. (A9) is integrated in time using the 4th-order Runge-Kutta scheme. The nonlinear Jacobian  $J_{XY}$  is discretized in the (X, Y) plane using (Arakawa, 1966)'s scheme, which conserves both the kinetic energy and enstrophy. Then, it is transformed into the  $(k_X, k_Y)$  space for the time integration. This semi-pseudo scheme was shown to be able to capture the development of sharp fronts (Constantin et al., 2012). To remove the aliasing errors introduced by the nonlinearity,  $\tilde{b}_s(\mathbf{k}, t)$  is multiplied by a low-pass filter (Hou & Li, 2007):

$$\exp\left[-\alpha\left(\left|\frac{k_X}{k_{nq}}\right|^\beta + \left|\frac{k_Y}{k_{nq}}\right|^\beta\right)\right] \tag{20}$$

where  $k_{nq} = \pi/\Delta X$  is the Nyquist wavenumber and  $\alpha = 512$  and  $\beta = 20$  as in (Ragone & Badin, 2016). Not unlike the Orszag 2/3 cutoff, this exponential filter suppresses the highest 1/3 wavenumbers. Moreover, it can capture extra 15% more effective wavenumbers than the Orszag 2/3 cutoff, thus providing a better representation for the small-scale structures.

Substituting the updated  $b_s(\mathbf{k}, t)$  into Eq. (A7) we obtain  $\Phi(\mathbf{k}, Z, t)$  at the next time step; its vertical derivative gives  $\tilde{b}(\mathbf{k}, Z)$ . To obtain  $b_s(X, Y, Z)$  and  $\Phi(X, Y, Z)$  in the geostrophic coordinates, an inverse Fourier transform in the horizontal plane at each depth is performed. The flow is then transformed into the physical space (x, y, z) using a fixed-point iteration method (Ragone & Badin, 2016).

Six simulations were performed where the characteristic Rossby number  $\varepsilon$  was varied between 0 and 0.2. Note that when  $\varepsilon = 0$ , the SSG solution Eq. (A7) reduces to the SQG solution Eq. (7). In that case, the geostrophic coordinate system becomes identical to the physical coordinate system, and no coordinate transformation is needed. Nondimensional surface buoyancy,  $b_s$ , and time, T, can be restored to their dimensional form using factors NU and  $(\varepsilon f_0)^{-1}$ , respectively.



Figure 1. (Colour online) Surface buoyancy  $b_s(x, y)$  in the simulations with  $\varepsilon = 0.05$  (a), 0.1 (b), 0.15 (c), and 0.2 (d) at T = 50.

### 151 4 Results

### 152 4.1 Flow evolution

We restrict our analyses to an early-time evolution of the SSG flows when there is an abundance of small-scale filaments and vortices with strong nonlinear interactions.

Figure 1 shows the buoyancy  $b_s$  at the surface captured at T = 50 in simulations 155 with different  $\varepsilon$ . Patches of cold (blue color) water induce cyclonic vortices, while warm 156 patches (yellow color) induce anticyclones. Numerous filaments fill the area between the 157 vortices. The filaments are embedded in strong shear and are unstable; they roll into smaller 158 vortices. When  $\varepsilon$  is relatively small, the cyclones and anticyclones populate the flow field 159 in approximately equal numbers (Fig. 1(a) and (b)). As  $\varepsilon$  increases, the cold cyclones 160 in Fig. 1(c) shrink in size while warm anticyclonic vortices expand. This effect is a man-161 ifestation of the pressure terms in the coordinate transform (second equality in Eq. (9)(a)162 and (b)) and is due to the lateral divergence and convergence of the velocity (Hoskins, 163 1975). The area between coherent vortices is now filled with predominantly warm fila-164 ments (Fig. 1(d)). Their accumulation at the surface results in a warming trend with 165 increasing  $\varepsilon$ . Similar scenarios have been shown previously in the simulations by (Ragone 166 & Badin, 2016; Hakim et al., 2002). They pointed out that the preference for cold cy-167 clones and the dominance of warm filaments are due to the inclusion of the ageostrophic 168 component. 169



Figure 2. (Colour online) The median values for surface buoyancy perturbation  $b_s^m(\mathbf{a})$ , relative vorticity  $\zeta^m(\mathbf{b})$ , strain rate  $\sigma^m(\mathbf{c})$ , and absolute horizontal divergence  $|\delta|^m(\mathbf{d})$  as functions of  $\varepsilon$  at different times.

The median value of  $b_s(x, y)$  versus  $\varepsilon$  at different times is shown in Fig. 2(a). When  $\varepsilon = 0.01$ , the high-order ageostrophic correction term in Eq. (A7) the SSG model is negligible, and the SSG flow becomes indistinguishable from the SQG flow. The distribution of cyclones and anticyclones becomes symmetric and the median value of the surface buoyancy perturbation,  $b_s^m$ , is close to zero. As  $\varepsilon$  increases,  $b_s^m$  shifts to positive values. It corresponds to the surface warming shown in Fig. 1(c,d). The warming effect decreases with time as the flows decay.

Accumulation of warm water at the surface leads to a general anticyclonic circulation, such that the median value of the relative vorticity becomes negative,  $\zeta^m < 0$ , Fig. 2(b). Here the (vertical component of) relative vorticity is  $\zeta = \partial v / \partial x - \partial u / \partial y$ . This mean anticyclonic circulation strengthens as  $\epsilon$  increases. The median value of the strain rate  $\sigma^m$  also increases with  $\epsilon$  because of the enhanced stirring created by the abundant small-scale filaments and vortices, Fig. 2(c). Here the strain rate is defined as:

$$\sigma = \left[ \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 \right]^{1/2}.$$
 (21)

<sup>177</sup> Since vertical motions concentrate in these small-scale structures (Fig. 3(b)) where the local convergence/divergence is large, the median value of the lateral divergence,  $|\delta|$ , also increases with  $\varepsilon$  (Fig. 2(d)).

Oceanic fronts are characterized by a relatively large vertical velocity of approx-180 imately 1 mm/s (Mahadevan & Tandon, 2006; McWilliams, 2016; Ruiz et al., 2019). In 181 the SSG model, vertical velocity can be diagnosed by solving the so-called " $\Omega$ -equation" 182 (Hoskins & West, 1979). An analytical solution of the " $\Omega$ -equation" in the wavenum-183 ber space is given in Appendix B. Vertical velocity fields right below the surface at z =184 -0.1 are shown in Fig. 3 for two simulations with different  $\varepsilon$ . In vortices, vertical veloc-185 ity appears as a quadrupolar structure Fig. 3(a). In filaments, positive and negative stripes 186 of w are created. At larger  $\varepsilon$ , the magnitude of w increases; the difference between Fig. 3(a) 187 and (b) is approximately one order of magnitude. Vertical motions become concentrated 188 at the periphery of vortices and the bands of upwelling (w > 0, yellow color) become 189 stronger than the bands of downwelling (w < 0, blue color). 190

Vertical profiles of w(x, y) (not shown here) show that the magnitude of w(x, y) is maximum in a subsurface layer at  $z_{max} \approx -0.1$ . Below this level, w(x, y) decays monotonically with depth. Vertical derivative of w is related to the lateral divergence of velocity,  $\delta$ , as:

$$\delta = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = -\frac{\partial w}{\partial z}.$$
(22)

Since w vanishes at the surface, the lateral divergence can be approximated as  $\delta \approx w(z_{max})/z_{max}$ .

Fronts/filaments are associated with strong buoyancy gradients in the cross-front direction and strain-dominated confluent flows which act to enhance the gradients. In an elongated front where the variation of velocity in the along-front direction is negligible,  $\delta$  is related to the relative vorticity,  $\zeta$ , and the rate-of-strain,  $\sigma$  as:

$$\delta^2 = \sigma^2 - \zeta^2. \tag{23}$$

The relation between these quantities was previously discussed for oceanic and numer-192 ical flows by (Shcherbina et al., 2013; Chavanne et al., 2010; Balwada et al., 2020; Maalouly 193 et al., 2023). Chavanne et al. (2010) reported a negative linear correlation between  $\delta$  and 194  $\zeta$  for an oceanic front during an active phase of its evolution. Their observation is in agree-195 ment with the prediction by (Hoskins & Bretherton, 1972) that  $\delta \propto -\bar{\sigma}\zeta$  where  $\bar{\sigma}$  is 196 the large-scale strain rate. Thus, cyclonic circulations in a strain field create lateral con-197 vergence while anticyclonic ones create lateral divergence. To obtain a  $\zeta - \delta$  relation for 198 our flows, we computed the joint probability density function (PDF) in the two-dimensional 199



Figure 3. (Colour online) Vertical velocity w(x, y) at z = -0.1 (a, b), normalized relative vorticity  $\zeta/f_0$  (c, d), and normalized strain rate  $\sigma/f_0$  (e, f) for the flows with  $\varepsilon = 0.01$  (left column) and  $\varepsilon = 0.2$  (right column) at T = 50.

<sup>200</sup> parameter space spanned by  $\zeta$  and  $\delta$ .  $\zeta$  and  $\delta$  were normalized by the Coriolis param-<sup>201</sup> eter  $f_0$ , they were then sorted according to their normalized values into bins of size 0.01 <sup>202</sup> by 0.01. After that, the joint PDF can be obtained by counting the number of occur-<sup>203</sup> rences when  $\zeta(x, y)$  and  $\delta(x, y)$  drop into each bin. Finally, the joint PDFs were tem-<sup>204</sup> porally averaged over a period from T = 45 to T = 55.

Figure 4(a) shows that the joint PDF of  $\zeta$  and  $\delta$  is aligned along a straight line with a negative slope. White dashed line in Fig. 4(a) is  $\delta = -\frac{1}{2}\bar{\sigma}\zeta$ , where  $\bar{\sigma} = 0.04$  is the spatial mean of  $\sigma$  averaged over the parameter region where PDF> 3;  $\bar{\sigma}$  represents a typical value of the large-scale strain rate. This relation was previously proposed in (Davies & Muller, 1988; Lapeyre & Klein, 2006b) for the surface-intensified currents decaying exponentially with depth, which is consistent with the SSG model employed here.

Fig. 4(b) shows the joint PDF in the  $\zeta - \sigma$  parameter space. The PDF is aligned along the lines  $\sigma = \pm \zeta$ , which indicates a pure shear relationship. This also suggests that a contribution of  $\delta$  in Eq. (23) is small.

To show the relation between  $\delta$ ,  $\sigma$ , and  $\zeta$  in a single diagram, we computed  $\delta$  av-214 eraged over each bin in the  $\zeta - \sigma$  parameter space. This procedure gives a conditional-215 mean lateral divergence shown in Fig. 4(c). Note that this diagram can also be interpreted 216 in terms of vertical velocity in the subsurface layer. Strong divergence/upwelling (vel-217 low color) is mainly associated with anticyclonic vorticity while convergence/downwelling 218 (blue color) is associated with the cyclonic vorticity in the strain-dominated areas located 219 above the line  $\sigma = |\zeta|$ . In the vorticity-dominated areas below the line  $\sigma = |\zeta|$ , the 220 divergence is generally of the same sign as vorticity, opposite to that in the strain-dominated 221 areas. However, the signal there is weaker and noisier than that in the strain-dominated 222 areas. Note that according to a frontogenesis model by Barkan et al. (2019) the three 223 quantities in Eq. (23) are of the same order of magnitude in a submesoscale front. In our 224 simulations, this can be locally satisfied in strong filaments. High levels of  $\delta$  create grain-225 iness in Fig. 4 (c). 226

#### 4.2 Spectral characteristics

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Kinetic and potential energy spectra at depth Z are defined as

$$\mathcal{K}(\boldsymbol{k}, Z) = k^2 \tilde{\Phi}(\boldsymbol{k}, Z) \tilde{\Phi}^*(\boldsymbol{k}, Z), \qquad (24a)$$

$$\mathcal{P}(\boldsymbol{k}, Z) = \hat{b}_s(\boldsymbol{k}, Z) \hat{b}_s^*(\boldsymbol{k}, Z), \qquad (24b)$$

where  $\mathbf{k} = (k_x, k_y)$  and the superscript \* denotes the complex conjugate. One-dimensional 228 (1D) spectra K(k, Z) and P(k, Z) are computed by averaging the above equations over 229 the azimuthal angle  $\theta = \tan^{-1}(k_y/k_x)$  in the wavenumber space. Fig. 5 shows 1D ki-230 netic energy spectra  $\mathcal{K}_s(k)$  and  $P_s(k)$  for the flows at the surface at different  $\varepsilon$ . At larger 231  $\varepsilon$ , the fraction of total kinetic or potential energy at smaller scales (larger k) increases 232 while the fraction at larger scales (smaller k) decreases. This shift in the energy distri-233 bution across scales is a manifestation of abundant and energetic small-scale features in-234 cluding filaments at larger  $\varepsilon$ . As a result, the spectral slope becomes less steep at larger 235  $\varepsilon$ ; it varies between -2.2 and -1.7 for both  $\mathcal{K}_s$  and  $\mathcal{P}_s$  for  $\varepsilon$  varying between 0.01 and 0.2. 236 A middle point of this spectral seesaw is at approximately k = 20. 237

Previously, Ragone and Badin (2016) made an observation that energy accumu-238 lation at small scales strongly depends on  $\varepsilon$ . However, their -3 slope of  $\mathcal{K}_s$  was steeper 239 than the -2 slope in our flows. This difference might be due to the fact that their anal-240 yses were performed at a later time T = 100 when the flow is dominated by the long-241 lived coherent vortices rather than filaments. The presence of these vortices could steepen 242 the spectral slope. In our case, the nonlinear interactions are strong at T = 30 and fil-243 aments are abundant. A similar -2 slope was previously measured during an early stage 244 of the SQG flow simulation by (Capet et al., 2008). 245



Figure 4. (Colour online) Joint PDF in the  $\zeta$ - $\delta$  parameter space (a); that in the  $\zeta$ - $\sigma$  parameter space (b); and  $\delta/f_0$  conditioned in the  $\zeta$ - $\sigma$  parameter space (c) for the flow with  $\epsilon = 0.2$ . The color scales are logarithmic and areas with zero PDF are left blank. White dashed line in (a) corresponds to  $\delta = -\bar{\sigma}/2\zeta$ . Black dashed lines in (b) and (c) correspond to  $\sigma = \pm \zeta$ .



Figure 5. (Colour online) One-dimensional kinetic energy spectra  $\mathcal{K}_s(k)$  (a) and potential energy spectra  $\mathcal{P}_s(k)$  (b) for the flows with  $\varepsilon$  varying between 0.01 and 0.2 at T = 30. The solid, dotted, and dashed curves in panel (c) show the one-dimensional PDS for  $\tilde{\zeta}(k)$ ,  $\tilde{\delta}(k)$ , and  $\tilde{\sigma}(k)$ , respectively. Note that  $\tilde{\sigma}(k)$  is dominated by  $\tilde{\zeta}(k)$ , the dashed lines coincide with the solid ones. The insert shows the wavenumber  $k_{max}$  for the peak in  $\tilde{\delta}(k)$ , where a linear fit is shown by the straight line.

Boyd (1992) investigated spectral characteristics of a one-dimensional front using 246 the Burger's equation  $u_t + uu_x = 0$ . He showed that the kinetic energy spectrum of 247 the solution follows a  $k^{-2}$  scaling law shortly after the formation of the front. We be-248 lieve that the approximately -2 slope in Fig. 5 is due to the nonlinear advection term in 249 Eq. (A9). At later times, when filaments are getting destroyed in the strain field of co-250 herent vortices, a -3 or even steeper spectral slope emerges in all of our simulations (not 251 shown here). An approximately -5/3 slope is observed at larger  $\varepsilon = 0.15, 0.2$ . This re-252 sult is in agreement with that of the simulations by Ragone and Badin (2016) and with 253 the theoretical result by (Blumen, 1978) who predicted the -5/3 slope for an inertial range 254 of the potential energy. 255

Comparison of Fig. 5 (a) and (b) shows that the slopes of  $\mathcal{P}_s(k)$  are approximately equal to those of  $\mathcal{K}_s(k)$ . This feature was also observed in the SQG flows in an infinitely deep ocean (Lapeyre & Klein, 2006a). In that case, the SQG solution Eq. (7) becomes

$$\tilde{\phi}(\boldsymbol{k}, z, t) = \frac{1}{k} \tilde{b}_s(\boldsymbol{k}, z) \exp(-kz)$$
(25)

Substitution of the above equation into Eq. (24) shows that

$$\mathcal{P}_s(\boldsymbol{k}) = \mathcal{K}_s(\boldsymbol{k}) \tag{26}$$

is satisfied at the surface z = 0. Our computations suggest that this result is also valid for the SSG flows.

To assess the spectral characteristics of the small-scale filaments we computed the 258 power spectral density (PSD) for the gradient fields, namely the relative vorticity  $\zeta$ , lat-259 eral divergence  $\delta$  and strain rate  $\sigma$ , Fig. 5(c). An approximately flat ("white") spectrum 260 is observed in the wavenumber range where the kinetic energy slope is about -2. The 261 almost geostrophic flow ( $\varepsilon = 0.01$ ) is non-divergent such that  $\delta(k)$  is negligible (dot-262 ted blue curve) and the PSD of  $\zeta$  and  $\tilde{\sigma}$  (solid and dashed blue curves) are almost iden-263 tical. Although  $\tilde{\delta}$  increases significantly with  $\varepsilon$  it remains much smaller than  $\tilde{\zeta}$  or  $\tilde{\sigma}$ . At 264 larger  $\varepsilon$ , the flat spectrum extends to higher wavenumbers due to the growing contribu-265 tion of small-scale energetic filaments. An inset in Fig. 5(c) shows the wavenumber  $k_{max}$ 266 at which the maximum magnitude of  $\delta(k)$  is reached.  $k_{max}$  can be considered as a char-267 acteristic wavenumber of submesoscale filaments in our flows. It grows approximately 268

linearly with  $\varepsilon$  (thick-black line). This is a consequence of the linear dependence of the high-order correction term in Eq. (A7), which determines the lateral divergence, on  $\varepsilon$ .

Energy spectra are sustained by transfers of energy across the scales, an energy cascade. However, the spectra themselves do not allow us to determine the magnitude or the direction of the cascade. The investigation of the cascades requires a different approach. Here we employ the spatial filtering technique developed by (Germano, 1992; Chen et al., 2006; Aluie et al., 2018) and used in previous studies of rotating shallowwater and baroclinic turbulence (Afanasyev & Craig, 2013; Zhang & Afanasyev, 2016). Fluxes of the kinetic energy and the potential energy are defined as:

$$\Pi_u^l(x,y) = -[(v_i v_j)^l - v_i^l v_j^l] \frac{\partial v_i^l}{\partial x_j},$$
(27a)

$$\Pi_b^l(x,y) = -[(v_jb)^l - v_j^lb^l]\frac{\partial b^l}{\partial x_j},$$
(27b)

where  $v_i$  is the *i*th component of the horizontal velocity, and summation over repeated indices is implied. The superscript *l* denotes a spatial scale.  $\Pi_u^l$  and  $\Pi_b^l$  are computed using low-pass filtering which is performed by convolving the correspondent fields with a Gaussian kernel  $G(l) = 9/(2\pi l^2) \exp(-9r^2/2l^2)$ . Positive values of  $\Pi_u$  or  $\Pi_b$  indicate a forward cascade, i.e., energy transfers from larger to smaller scales while negative values indicate the cascade in the opposite direction, the inverse cascade. The cut-off scale *l* can be related to the non-dimensional wavenumber as  $k = 2\pi/l$ .

Figure 6 shows  $\Pi_{\mu}^{l}(x,y)$  and  $\Pi_{b}^{l}(x,y)$  computed for two wavenumbers k = 85 and 278 k = 18. At the larger wavenumber, both kinetic and potential energy fluxes are con-279 centrated predominantly along filaments and at the periphery of the vortices. Positive 280 and negative fluxes alternate; both forward and inverse energy transfers are present. Note 281 that  $\Pi_{u}^{l}$  is relatively small at k = 85 in Fig. 6 (a). The potential energy flux in Fig. 6 282 (b) is of a quadrupolar structure around vortices while in the filaments away from the 283 vortices, it is mainly positive. At the smaller wavenumber, the fluxes are mainly concen-284 trated within vortices and are quadrupolar Fig. 6 (c) and (d). Note that the quadrupo-285 lar structure of energy fluxes was observed in numerical simulations by Xiao et al. (2009) 286 as well as in laboratory experiments by Afanasyev and Craig (2013). The quadrupolar 287 structure appears to be due to vorticity gradient stretching by strain fields Kimura and 288 Herring (2001). Interestingly, the kinetic energy flux appears to be concentrated in in-289 tense cold cyclones (Fig. 6 (c)) while the potential energy flux reaches its largest mag-290 nitude in warm anticyclones (Fig. 6 (d)). 291

When both positive and negative fluxes are present in the flow, the overall direc-292 tion of the energy cascades can be revealed by spatial averaging over the flow domain. 293 Figure 7 shows mean fluxes  $\overline{\Pi}_u$  and  $\overline{\Pi}_b$  versus wavenumber k for simulations with vary-294 ing  $\varepsilon$ . The kinetic energy flux is negative across the entire range of wavenumbers which 295 indicates the energy transfers to larger scales, an inverse cascade. Maximum magnitudes 296 of the flux are achieved at  $k \approx 18$  Figure 7(a); the overall magnitude of the flux decreases 297 with increasing  $\epsilon$ . This decrease is most likely caused by the joint effect of the ageostrophic 298 correction term in Eq. (A8) and the coordinates transform Eq. (9). When  $\varepsilon$  increases 299 the cyclones become smaller and separated farther away from each other; their mergers 300 then become less likely. Potential energy cascades forward at all wavenumbers above  $k \approx$ 301 20 (Fig. 7(b)). Maximum values of  $\Pi_b$  are achieved at  $k \approx 85$  and the magnitude of the 302 flux increases with increasing  $\varepsilon$ . Since the potential energy flux mainly occurs at large 303 wavenumbers, it is clearly related to small-scale elements of the flows including cyclones 304 and filaments. These elements become more abundant and energetic with increasing  $\varepsilon$ . 305

To further explore the relation between the flux of potential energy with the velocity field we plotted the isolines of  $\Pi_b^l(x, y)$  computed at k = 85 together with the vertical velocity field, w, just below the surface (at z = -0.01) (Fig. 8(a)). w appears to be positively correlated with  $\Pi_b^l(x, y)$ ; filaments formed by upwelling water are associ-



**Figure 6.** (Colour online) Kinetic energy flux  $\Pi_{u}^{l}(x, y)$  (a, c) and potential energy flux  $\Pi_{b}^{l}(x, y)$  (b, d) for the surface flow with  $\varepsilon = 0.1$  at T = 30(contours). The fluxes are across the wavenumbers k = 85 (top row) and k = 18 (bottom row). Gray-scale background shows the surface buoyancy in the range between -1.2 and 1.2.



**Figure 7.** (Colour online) (a) Surface kinetic energy flux  $\bar{\Pi}_u^l$  and (b) potential energy flux  $\bar{\Pi}_b^l$  versus k in the flows with different  $\varepsilon$  at T = 30.

ated with the forward-cascading potential energy, while areas of downwelling exhibit an inverse cascade. This observation appears to be consistent with (Hakim et al., 2002)'s conclusion that the contraction of warm filaments develops faster than that of cold ones.

313

### 4.3 Finite-scale Lyapunov exponents

To study stirring in the SSG flows we compute trajectories of numerical particles in our flows. The trajectories can be used to obtain finite-scale Lyapunov exponents (FSLEs) which are a useful metric of stirring (d'Ovidio et al., 2004). FSLEs are inversely proportional to time  $\tau$  it takes a pair of particles initially separated by a distance  $\delta_i$  to reach a prescribed final separation  $\delta_f$ :

$$\lambda(x, y, t, \delta_i, \delta_f) = \frac{1}{\tau} \log \frac{\delta_f}{\delta_i}.$$
(28)

Trajectories of particles are computed by integrating velocity fields over time using the 314 fourth-order Runge-Kutta scheme. The velocity at particle locations is obtained by a bi-315 linear interpolation at each time step. Particles are initially seeded in between the nodes 316 of the computational grid such that their smallest initial separation is half of the grid 317 spacing,  $\delta_i = 0.5\Delta x$ . Each particle is surrounded by four neighboring particles in the 318 shape of a diamond. The separations between particles in the diamond in x- and y-directions 319 are calculated at each time step; when the maximum separation reaches  $\delta_f$ , the time  $\tau$ 320 is obtained. The velocity is integrated either forward or backward in time to obtain two 321 sets of the exponents  $\lambda_+$  and  $\lambda_-$ , respectively. High values of  $\lambda_+$  indicate areas where 322 particles separate from each other due to lateral divergence. High values of  $\lambda_{-}$ , on the 323 other hand, indicate areas of convergence where particles accumulate. 324

Spatial distributions of FSLEs can be used for detecting the so-called Lagrangian 325 structures, the structures formed by Lagrangian particles. High values of both exponents 326 often manifest themselves as filament-like structures in the ocean(d'Ovidio et al., 2004; 327 Calil & Richards, 2010; Siegelman et al., 2020). A typical spatial pattern of the expo-328 nents in our simulations is shown in Figure 8(b) where both  $\lambda_+$  (yellow color) and  $\lambda_-$ 329 (blue color) are plotted together. It is an illustration of stirring by strong vortices. Cy-330 clonic vortices created by cold patches (black color) create a fine structure of filaments 331 wrapped around their cores. Two pairs of cyclones located in the part of the computa-332 tional domain shown in Figure 8(b) create two figure-eight patterns where attracting lines 333 (blue color) intersect repelling lines (yellow color) at a hyperbolic point in the area be-334 tween the vortices. It is in this area the strain rate is as important as the relative vor-335 ticity. Two warm anticyclones (white color) do not seem to create distinct patterns of 336 filaments in their cores but contribute to strain in the areas between them and other vor-337 tices. 338

Domain-averaged FSLEs can be used to identify regimes of dispersion at different 339 scales. Here, we compute a spectrum of the mean exponent  $\bar{\lambda} = 0.5(\lambda_+ + \lambda_-)$  aver-340 aged over the surface area of the domain. In this computation, the initial separation be-341 tween the particles in diamond patterns was varied in a wide range between  $\delta_i = \Delta x$ 342 and  $\delta_i = 110\Delta x$ . The particles were followed until the separation between them reached 343 a prescribed final value  $\delta_f = \sqrt{2}\delta_i$  (Lacorata et al., 2001).  $\bar{\lambda}$  as a function of  $\delta_i$  is shown 344 in Fig. 9 for simulations with different  $\varepsilon$ . Note that the range of dimensionless  $\delta_i$  in Fig. 9 345 corresponds to the range of the dimensionless wavenumber,  $k = L/2\delta_i$ , from 256 down 346 to 3 for comparison with the energy spectra in Fig. 5. The slope of the  $\bar{\lambda}$  spectrum varies 347 continuously with  $\delta_i$  such that there is no extended interval where it remains constant. 348 At the smallest scales up to approximately  $\delta_i = 4\Delta x$  the spectrum is almost flat,  $\lambda \approx$ 349 constant. The flat spectrum indicates that the distance between particle trajectories in-350 creases exponentially in time. At larger scales, the slope varies from approximately -1/2351 to -2. 352



Figure 8. (Colour online) Typical patterns of the potential energy flux  $\Pi_b^l(x, y)$  (a) and the FSLEs  $\lambda_+$  and  $\lambda_-$  (b) in the flows  $\varepsilon = 0.1$ . Contours of  $\Pi_b^l(x, y)$  across wavenumber k = 85 are superposed over the vertical velocity field w(x, y) (gray-scale) in the range between  $-5 \times 10^{-3}$  and  $5 \times 10^{-3}$ . Contours of the FSLEs are superposed over the buoyancy field  $b_s(x, y)$  (gray-scale) in the range between -0.6 and 0.6. Black arrows indicate the direction of the velocity around one of the cyclone pairs.



Figure 9. (Colour online) FSLE spectra for five simulations with different  $\varepsilon$  at T = 30.

Scaling theory for turbulent flows where the kinetic energy spectrum is  $\mathcal{K}_s(k) \propto$ 353  $k^{-\alpha}$  predicts the power-law scale dependence of the FSLE,  $\bar{\lambda} \propto \delta_i^{-\beta}$ , and the power-law time dependence of the separation between particles,  $\delta^2(t) \propto t^{2/\beta}$  where  $\beta = (3 - 1)^{-\beta}$ 354 355  $\alpha$ /2 (Morel & Larceveque, 1974). These power-law equations are applicable when the 356 kinetic energy spectrum is not too steep,  $\alpha < 3$ . In this case, the dispersion regime is 357 local, the separation of particles at a certain scale is only determined by the velocity gra-358 dient components at the same scale. Otherwise, the dispersion regime is non-local; the 359 power-law is not applicable and the separation between particles grows exponentially in 360 time. 361

In our flows,  $\alpha \approx 2$  at intermediate values of the wavenumber (Fig. 5). In this in-362 terval, a local dispersion regime with  $\beta \approx 1/2$  is expected. The separation between par-363 ticles grows quite fast,  $\delta^2(t) \propto t^4$ , and the regime can be called hyper-ballistic.  $\beta$  then 364 keeps increasing with  $\delta_i$  up to  $\beta = 2$ . In this range, several distinct regimes of disper-365 sion can be pointed out. When  $\beta = 2/3$  the dispersion obeys the Richardson's law which 366 describes another case of the hyper-ballistic dispersion where  $\delta^2(t) \propto t^3$ ; in this case, 367 the energy spectrum has Kolmogorov's -5/3 slope. When  $\beta = 1$  and  $\delta^2(t) \propto t^2$  the 368 motion of particles is ballistic as if they move with constant speed away from one an-369 other. Finally, when  $\beta = 2$  the regime is a normal diffusion,  $\delta^2(t) \propto t$  is similar to that 370 of the Brownian motion. In our flows, the normal diffusion is due to the scattering of 371 particles by the energetic warm and cold eddies at large scales. 372

### **5** Conclusions

In this work, turbulent flows were simulated at different values of the Rossby number,  $\varepsilon$ , using the SSG model. The simulated flows exhibited typical ageostrophic effects, including a cyclone-anticyclone asymmetry with a cyclonic preference for vortices and an anticyclonic preference for filaments. The magnitude of the ageostrophic effects increased with  $\varepsilon$  due to the increasing higher-order ageostrophic term in the SSG solution (Equation A7). As  $\varepsilon$  increased from 0.01 to 0.2 between the simulations, the number of warm filaments on the surface increased, resulting in a surface warming trend.

The magnitude of the vertical velocity and, consequently, the lateral divergence also 381 increased with  $\varepsilon$ . Vertical motions occurred mostly in small-scale filaments and at the 382 periphery of vortices rather than in their cores. However, in all our simulations, the lat-383 eral divergence remained much smaller than the relative vorticity or the strain rate. This 384 contrasted with the results of (Balwada et al., 2021), where the authors used primitive 385 equations and obtained lateral divergence values comparable to those of relative vortic-386 ity and strain rate. We believe this difference is mainly due to the distinct forcing used 387 in their simulations compared to buoyancy-only initial forcing in ours. Our results demon-388 strated a negative correlation between lateral divergence and relative vorticity,  $\delta = -\bar{\sigma}/2\zeta$ (Figure 4). This indicates that cyclonic and anticyclonic motions are often associated 390 with local convergence and divergence, respectively. This effect is most pronounced in 391 strain-dominated areas where  $\sigma > |\zeta|$ . 392

Spectral analyses showed that the kinetic and potential energy spectra exhibited 303 similar slopes, varying between -2.2 and -1.7 as  $\varepsilon$  increased from 0.01 to 0.2. Notably, 394 the latter value of the slope is approximately equal to -5/3, in agreement with previous 395 SSG simulations by (Ragone & Badin, 2016) and SQG+1 simulations by (Capet et al., 396 2008). The similarity of the kinetic and potential energy spectra is a well-known feature 397 of SQG turbulence, where it is caused by the thermal-wind coupling between the veloc-398 ity field and the buoyancy field at the surface. In the SSG flow, this coupling seems largely 399 unaffected by the inclusion of the ageostrophic component. 400

<sup>401</sup> Spectra of gradient fields, including relative vorticity  $\zeta$  and strain rate  $\sigma$  (Figure 5(c)), were approximately flat in the wavenumber range where the kinetic energy slope

was approximately -2. The spectra of another gradient field, lateral divergence  $\delta$ , however, showed a maximum at a relatively large wavenumber  $k_{max}$ , which increased almost linearly with  $\varepsilon$ .

In addition to energy spectra, energy fluxes across different scales were computed. 406 The fluxes showed that kinetic energy is transferred towards larger scales, constituting 407 an inverse cascade. However, the cascade rate was not constant across scales; it reached 408 a peak at a scale  $l = 2\pi/k = 0.35$ , corresponding to wavenumber k = 18. This scale 409 roughly agreed with the typical distance between cold cyclones. Visual inspection of the 410 411 flux fields showed that kinetic energy flux concentrated in and around cold cyclones (Figure 6(c)). Interestingly, the magnitude of the flux decreased as  $\varepsilon$  increased, and the flows 412 became more ageostrophic and three-dimensional. One of the effects slowing down the 413 inverse cascade was warm filaments wrapping around cold cyclones, shielding them, and 414 preventing mergers. Potential energy, on the other hand, cascaded forward towards smaller 415 scales at all wavenumbers greater than  $k \approx 20$ . The potential energy flux was maxi-416 mum at  $k \approx 85$ . Comparison of the flux with the vertical velocity field (Figure 8(a)) 417 showed that the forward cascade was mainly associated with warm filaments created by 418 upwelling. The magnitude of the potential energy flux increased with  $\varepsilon$ , a consequence 419 of the growing number of filaments in ageostrophic flows. 420

To explore lateral stirring and dispersion of particles by eddies and filaments in our 421 flows, we computed the trajectories of numerical particles and obtained forward and back-422 ward FSLEs. Inspection of the FSLE fields showed that interacting cold cyclones cre-423 ated Lagrangian coherent structures in between them (Figure 8(b)). The relative dis-424 persion of particles was scale-dependent in our flows. To study the regimes of dispersion, 425 mean FSLEs were computed for different initial separations of particles  $\delta_i$ . The results 426 showed (Figure 9) that at the smallest scales, the relative dispersion of a pair of parti-427 cles was exponential in time and non-local. At larger scales, the dispersion regime was 428 local, and the mean FSLE,  $\bar{\lambda}$ , satisfied a power law,  $\bar{\lambda} \propto \delta_i^{-\beta}$ , where  $\beta$  varied smoothly 429 from approximately 1/2 to 2 with increasing  $\delta_i$ . The variation of  $\beta$  reflected a transition 430 from a hyper-ballistic dispersion regime ( $\beta \approx 1/2$ ) to Richardson's dispersion ( $\beta \approx 2/3$ ) 431 and then to a ballistic regime ( $\beta \approx 1$ ) and finally to normal diffusion ( $\beta \approx 2$ ). The 432 smooth transition of  $\beta$  from 1/2 to 2 was a robust feature in all our simulations for dif-433 ferent  $\varepsilon$ . A similar transition of the exponent  $\beta$  was previously found in SQG+1 turbu-434 lence (Maalouly et al., 2023, their figure 4) and observed for drifters in the Antarctic Cir-435 cumpolar Current (Balwada et al., 2021, their figure 9). 436

# 437 Appendix A Solution of the SSG equations

Eq. (18), can be written in non-dimensional form as:

$$\nabla^2 \Phi = \varepsilon D \Phi, \tag{A1}$$

where  $\nabla^2$  is the three-dimensional Laplacian operator in the geostrophic space and

$$D\Phi = \frac{\partial^2 \Phi}{\partial X^2} \frac{\partial^2 \Phi}{\partial Y^2} - \left(\frac{\partial^2 \Phi}{\partial X \partial Y}\right)^2 \tag{A2}$$

is the nonlinear differential operator. Horizontal Fourier transform can then be used to obtain a forced Helmholtz equation in the vertical direction which can be solved numerically by iteration:

$$\left(\frac{\partial}{\partial Z^2} - k^2\right)\tilde{\Phi}^{(n)} = \varepsilon \tilde{D}\Phi^{(n-1)}.$$
(A3)

The iteration is performed for each wavevector  $\mathbf{k} = (k_X, k_Y)$  in the (geostrophic) wavenumber space. Boundary conditions Eq. (4) can be written as:

$$\frac{\partial \Phi(\mathbf{k}, Z)}{\partial Z} = \tilde{b}_s \quad \text{at} \quad Z = 0,$$

$$\frac{\partial \tilde{\Phi}(\mathbf{k}, Z)}{\partial Z} = 0 \quad \text{at} \quad Z = -1.$$
(A4)

Equation (A3) with the boundary conditions Eq. (A4) has a solution in the form of the Green's function:

$$\tilde{\Phi}^{(n)}(\boldsymbol{k}, Z) = \tilde{b}_s(\boldsymbol{k}, t) G_k(Z, 0) + \varepsilon \int_{-1}^0 G_k(Z, Z') \tilde{D} \Phi^{(n-1)}(\boldsymbol{k}, Z') dZ'$$
(A5)

where

$$G_k(Z, Z') = \begin{cases} \cosh(kZ) \cosh[k(Z'+1)]/(k \cdot \sinh k), & Z \ge Z' \\ \cosh[k(Z+1)] \cosh(kZ')/(k \cdot \sinh k), & Z < Z'. \end{cases}$$
(A6)

The first-order approximation of the solution is given by

$$\tilde{\Phi}^{(1)}(\boldsymbol{k}, Z) = \tilde{\Phi}^{(0)}(\boldsymbol{k}, Z) + \varepsilon \int_{-1}^{0} G_{k}(Z, Z') \tilde{D} \Phi^{(0)}(\boldsymbol{k}, Z') dZ'$$
(A7)

where the zeroth-order approximation

$$\tilde{\Phi}^{(0)}(\boldsymbol{k}, Z) = \tilde{b}_s(\boldsymbol{k}, t) G_k(Z, 0) = \frac{\cosh[(Z+1)k]}{k \sinh(k)} \tilde{b}_s(\boldsymbol{k}, t)$$
(A8)

is the SQG solution Eq. (7). Following (Ragone & Badin, 2016) who showed that when  
$$\varepsilon$$
 is small, the first-order approximation provides reasonably accuracy we use Eq. (A7)  
for the numerical solution of the SSG problem.

Buoyancy,  $b_s$ , is a conserved quantity such that:

$$\frac{db_s}{dt} = \frac{\partial b_s}{\partial t} + u_g \frac{\partial b_s}{\partial X} + v_g \frac{\partial b_s}{\partial Y} = 0.$$
(A9)

Given an initial buoyancy perturbation field  $b_s(X,Y)$  in the geostrophic space, one can

calculate the Bernoulli function  $\Phi(X, Y)$  using Equation (A5). Geostrophic velocity,  $(u_q, v_q)$ ,

is then given by Eq. (11). Finally Eq. (A9) can be marched in time numerically.

# 444 Appendix B Vertical velocity

In the SSG model, a re-scaled vertical velocity  $w^* = J \cdot w$  can be obtained from the so-called " $\Omega$ -equation" (Hoskins & West, 1979; Ragone & Badin, 2016):

$$\frac{\partial^2 w^*}{\partial X^2} + \frac{\partial^2 w^*}{\partial Y^2} + \frac{\partial^2 w^*}{\partial Z^2} = -2\varepsilon \nabla \cdot \boldsymbol{Q},\tag{B1}$$

where

$$J = 1 - \varepsilon \left( \frac{\partial v_g}{\partial X} - \frac{\partial u_g}{\partial Y} \right) \tag{B2}$$

is the re-scaling factor and

$$\boldsymbol{Q} = (Q_1, Q_2) = \left(\frac{\partial u_g}{\partial X}\frac{\partial b}{\partial X} + \frac{\partial v_g}{\partial X}\frac{\partial b}{\partial Y}, \frac{\partial u_g}{\partial Y}\frac{\partial b}{\partial X} + \frac{\partial v_g}{\partial Y}\frac{\partial b}{\partial Y}\right)$$
(B3)

is the forcing vector. These two quantities can be calculated using Eqs. (11) and (A7). Applying Fourier transform in the horizontal direction, Eq. (B1) can be written as

$$-k^2 \tilde{w}^* + \frac{\partial^2 \tilde{w}^*}{\partial Z^2} = \tilde{Q}(k, Z), \tag{B4}$$

where  $\tilde{Q}(k, Z)$  is the Fourier transform of the RHS of Eq. (B1). For each geostrophic wavenumber  $k = \sqrt{k_X^2 + k_Y^2} \neq 0$ , Eq. (B4) subject to the boundary conditions  $\tilde{w}^* = 0$  at Z = 0 and Z = -1 has the following solution:

$$\tilde{w}^{*}(k,Z) = \exp(kZ) \int_{0}^{Z} \delta_{3}(k,z')dz' - \exp(-kZ) \int_{0}^{Z} \delta_{4}(k,z')dz' + 2\frac{\delta_{2}(k)}{\delta_{1}(k)}\sinh(kZ)$$
(B5)

where

$$\delta_1(k) = -2\sinh(k),\tag{B6a}$$

$$\delta_2(k) = \exp(k) \int_0^{-1} \delta_4 dz' - \exp(-k) \int_0^{-1} \delta_3 dz',$$
 (B6b)

$$\delta_3(k, z') = \exp(-kz') \frac{Q(k, z')}{2k},$$
 (B6c)

$$\delta_4(k, z') = \exp(kz') \frac{Q(k, z')}{2k}.$$
 (B6d)

<sup>445</sup> The above analytical solution is provided by the symbolic math toolbox in MATLAB.

Inverse Fourier transform of Eq. (B5) then gives the vertical velocity in the geostrophic coordinates, w(X, Y, Z).

### 448 **3** Availability Statement

The code for the SSG model is available at: github.com/zy-gdou/ The Matlab figures, the data and codes used for creating the figures are available from the ZENODO repository (https://doi.org/10.5281/zenodo.10431740).

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