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Alice Pietri, Xavier Capet, Francesco d'Ovidio, Marina Lévy, Julien Le Sommer, et al.. Skills and Limitations of the Adiabatic Omega Equation: How Effective Is It to Retrieve Oceanic Vertical Circulation at Mesoscale and Submesoscale?. Journal of Physical Oceanography, 2021, 51 (3), pp.931-954. 10.1175/jpo-d-20-0052.1 . hal-03096579

HAL Id: hal-03096579

<https://hal.science/hal-03096579>

Submitted on 5 Jan 2021

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**Skills and limitations of the adiabatic omega equation: how effective is it to
retrieve oceanic vertical circulation at meso and submesoscale ?**

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ABSTRACT

13 The quasi-geostrophic and the generalized omega equations are the most
14 widely used methods to reconstruct vertical velocity (w) from *in-situ* data.
15 As observational networks with much higher spatial and temporal resolutions
16 are being designed, the question rises of identifying the approximations and
17 scales at which an accurate estimation of w through the omega equation can
18 be achieved and what are the critical scales and observables needed. In this
19 paper we test different adiabatic omega reconstructions of w over several re-
20 gions representative of main oceanic regimes of the global ocean in a fully
21 eddy-resolving numerical simulation with a $1/60^\circ$ horizontal resolution. We
22 find that the best reconstructions are observed in conditions characterized by
23 energetic turbulence and/or weak stratification where near-surface frontal pro-
24 cesses are felt deep into the ocean interior. The quasi-geostrophic omega
25 equation gives satisfactory results for scales larger than ~ 10 km horizon-
26 tally while the improvements using a generalized formulation are substantial
27 only in conditions where frontal turbulent processes are important (provid-
28 ing improvements with satisfactory reconstruction skill down to ~ 5 km in
29 scale). The main sources of uncertainties that could be identified are related
30 to processes responsible for ocean thermal wind imbalance (TWI), which is
31 particularly difficult to account for (especially in observation-based studies)
32 and to the deep flow which is generally improperly accounted for in omega
33 reconstructions through the bottom boundary condition. Nevertheless, the
34 reconstruction of mesoscale vertical velocities may be sufficient to estimate
35 vertical fluxes of oceanic properties in many cases of practical interest.

36 1. Introduction

37 In geophysical fluids, the combined effect of stratification and rotation strongly inhibits vertical
38 velocities over a broad range of horizontal scales (L_h), near and above the so-called deformation
39 radius (Rd), typically 30 km in the ocean. Vertical velocities remain small even for L_h much below
40 Rd (Pollard and Regier 1992; Giordani et al. 2006), typically a few meters to several tens of me-
41 ters per day for submesoscale motions, $L_h \sim O(1)$ km, although their intensity tends to increase
42 somewhat at finer scales. Much weaker than horizontal advection, vertical transport of oceanic
43 properties such as heat and biogeochemical tracers is nevertheless of crucial importance for the
44 overall functioning of the world ocean (Lévy et al. 2012a). In some regions, atmospheric forc-
45 ings are such that the large-scale flow (100 km and larger) has a vertical component, *e.g.*, under
46 the influence of coastal upwelling favourable winds or positive wind stress curl. At finer scale
47 (1-100km) intermittent vertical velocities are associated with the mesoscale and submesoscale tur-
48 bulence and can be generated by forced and unforced motions such as frontogenesis, baroclinic
49 instabilities or air-sea interactions, with possible coupling between them (*e.g.* Thomas and Lee
50 2005). They are responsible for vertical fluxes that have proved difficult to quantify but are widely
51 believed to play a major role in the heat (Ferrari 2011; Su et al. 2020; Siegelman et al. 2020) and
52 salt budgets (Lien et al. 2014), in the carbon and nutrient cycles (Ledwell et al. 2008; Balwada
53 et al. 2018), and in shaping oceanic biodiversity (Lévy et al. 2010, 2012b, 2014, 2018; Siegelman
54 et al. 2020). It should be noted that vertical velocities also vary at the scales smaller than the
55 submesoscale in particular vertical fluxes associated with 3D turbulence (Whitt et al. 2019). How-
56 ever the submesoscale-mesoscale (hereafter SMS) range on which this study focuses is important
57 because i) it presumably contains a large fraction of co-variance between w and many key tracer
58 fields (Ledwell et al. 2008; Chenillat et al. 2015; Balwada et al. 2018), ii) SMS vertical motions

59 can be coherent over relatively long/large time/space scales (including vertically) such that they
60 produce long range vertical displacements and fluxes, *e.g.*, , organic and inorganic carbon from the
61 euphotic layer into the dark ocean (Boyd et al. 2019).

62 Direct measurements of vertical velocities with SMS spatiotemporal resolution would thus be
63 highly desirable. However the magnitude of w at these scales is typically $O(1) \text{ mm s}^{-1}$ ($\sim 100 \text{ m}$
64 day^{-1}) or less (*e.g.*, up to $2\text{-}3 \text{ mm s}^{-1}$ in the highly turbulent Gulf Stream, Lindstrom and Watts
65 1994) which places them below the noise level of any existing current meter for the typical time
66 scales of a few days to weeks over which they vary. Different ingenious ways to circumvent this
67 difficulty have been developed over time. For instance, direct integrated measurements of vertical
68 displacements $\int w dt$ have been made using Lagrangian drifters (Bower and Rossby 1989; D’Asaro
69 et al. 2004; Steffen and D’Asaro 2002). Alternatively, indirect reconstruction methods have been
70 proposed based on the heat/density conservation equation (Strass 1994; Lindstrom et al. 1997; Yu
71 et al. 2019), the vorticity equation (Strass 1994; Giordani et al. 2005) or the 3D non-divergence of
72 the flow (Helber and Weisberg 2001; Horii et al. 2011). A different framework has also emerged
73 to infer vertical velocities from the theory of surface quasigeostrophy (SQG) (Held et al. 1995;
74 Lapeyre and Klein 2006a; LaCasce and Mahadevan 2006), where the 3D flow structure can be
75 essentially determined from the knowledge of the surface buoyancy field (Isern-Fontanet et al.
76 2006; Klein et al. 2009; Ponte and Klein 2013; Qiu et al. 2020). Overall, the most commonly used
77 method to infer w is based on frontogenetic theories and the so-called omega equation, which is
78 the subject of the present study.

79 Quasi-geostrophic and semi-geostrophic versions of the omega equation (Hoskins et al. 1978)
80 have been applied for decades (Leach 1987; Pollard and Regier 1992). The former and to a lesser
81 extent the latter are by nature suited to low Rossby number environments, *i.e.*, a priori away from
82 regions of intense vertical velocities. A generalized version of the omega equation was first intro-

83 duced in the atmospheric community (Davies-Jones 1991; Pauley and Nieman 1992; Giordani and
 84 Caniaux 2001) and subsequently applied to the ocean (Viúdez et al. 2002; Giordani et al. 2006).
 85 Vertical velocity forcing processes present in this generalized omega equation are kinetic defor-
 86 mation that arises in shear and confluence situations, mixing and momentum diffusion which can
 87 also disrupt the thermal wind balance and an additional prognostic term due to the rate of change
 88 of unbalanced motions. This latter term shall be zero under the quasi-geostrophic approximation
 89 and is systematically neglected in ocean applications, which makes the omega equation diagnos-
 90 tic for w (see Qiu et al. 2020 for the only evaluation of this term that we know of). Despite this
 91 simplification, the generalized formulations of the omega equation are expected to hold even in
 92 regions where the flow exhibits high Rossby number (Viúdez et al. 2002; Viúdez and Dritschel
 93 2004; Shearman et al. 2000). Since the omega equation is most frequently used to infer w from
 94 observations the chosen formulation usually depends on the data available. The adiabatic quasi-
 95 geostrophic version of the equation only requires density observations and a reference level to
 96 derive geostrophic currents from the thermal wind balance. Knowledge of the absolute horizontal
 97 velocity field allows to take into account the effect of the ageostrophic deformation and advection.
 98 Solving more elaborate forms of the omega equation require additional data, such as atmospheric
 99 forcing (Giordani et al. 2006). Statistical methods based on multivariate empirical orthogonal
 100 functions can be used to determine the SMS ocean state from surface satellite information and
 101 sparse in situ data (e.g. ARMOR3D high resolution operational product, Guinehut et al. 2012).
 102 Those methods have been used regularly to infer the forcing terms for omega inversions (Buon-
 103 giorno Nardelli and Santoleri 2005; Buongiorno Nardelli et al. 2012; Buongiorno Nardelli et al.
 104 2018; Barceló-Llull et al. 2018; Buongiorno Nardelli 2020).

105 Numerous investigations of oceanic vertical velocities based on the omega equation have been
 106 carried out since the 1980s, most frequently in the context of mesoscale-resolving observational

107 efforts. A few of them have used independent ways to estimate w and evaluate the skills of the
108 omega reconstructions. Conclusions are generally that the omega equation has reasonable skills
109 at the mesoscale. A few studies have also applied this equation to numerical model outputs to
110 test its reliability and degree of accuracy (Pinot et al. 1996; Allen et al. 2001; Rixen et al. 2003;
111 Uchida et al. 2019). The domain of validity and typical errors attached to an omega reconstruction
112 for realistic cases are however not clearly established. This is particularly true at submesoscale
113 where the omega equation has been increasingly applied (Pallàs-Sanz et al. 2010). The benefit
114 that one can expect from using more elaborate versions of the omega equation compared to the
115 quasigeostrophic formulation are also not clearly established. An overview of the literature on the
116 subject offers a great diversity of conclusions (from major to no benefits or even degradation of the
117 reconstruction). We provide a review of omega-reconstructions literature in the the bibliography
118 table (SI1). Overall, this literature appears to be mainly composed of an accumulation of test cases
119 (Pascual et al. 2017; Buongiorno Nardelli et al. 2012; Rixen et al. 2003; Allen et al. 2001), many
120 of which are in idealized settings (Viúdez and Dritschel 2004). These individual cases can be
121 difficult to compare against one another.

122 The main novelty of the present study is to apply the same analysis framework to assess the skills
123 of the adiabatic omega equation in several dynamical regimes representative of a broad diversity
124 of ocean conditions. The aim is to propose a more integrated and comprehensive understanding
125 of the skills and limitations of omega reconstructions. Given this ambition, we restrict the scope
126 somewhat by mainly focusing on vertical velocities outside mixed layers, typically at depths $\sim$
127 200 – 400 m. Submesoscale velocities in the mixed layer are important too (*e.g.*, Smith et al.
128 2016) but they more strongly compete and interact with 3D turbulent processes responsible with
129 intense mixing in ways that are just beginning to be clarified (Thomas and Lee 2005; Hamlington
130 et al. 2014; Suzuki et al. 2016; Sullivan and McWilliams 2018; Callies and Ferrari 2018). On

131 the other hand, we expect SMS vertical velocities obtained by means of omega reconstruction to
132 be more readily useful to estimate tracer fluxes below the mixed layer, typically upward fluxes of
133 nutrient into the euphotic layer (Pascual et al. 2015) or downward fluxes of oxygen into subsurface
134 hypoxic layers (Thomsen et al. 2016).

135 Exploring the ability of the adiabatic omega equation to reconstruct w in our realistic, eddy-
136 resolving, circulation model reveals that, in this depth range, reconstruction skills turn out to be
137 strongly sensitive to the dynamical regime under consideration, but also to the physical (length)
138 scale of interest. In particular, it is shown that omega reconstructions perform well for scales
139 down to ~ 10 km while rapid degradation occurs at smaller scales. Consequently, the best results
140 are obtained in conditions characterized by high vertical velocity variance which are found in
141 regions with intense *mesoscale* frontogenesis. On the other hand, relaxing the QG assumptions
142 with the generalized formulation is shown to have a modest impact on the reconstruction. Instead,
143 an analysis of the relative importance of the sources of errors reveals that a major impact can
144 be attributed to the choice of the bottom boundary conditions (BBC). The impact of neglecting
145 vertical mixing terms, though presently deemed limited to the upper layers, would also require
146 dedicated investigations.

147 The paper is organized as follows. Data and methods are presented in section 2. In section 4
148 vertical velocity reconstructions in the different dynamical regimes retained for this study are
149 evaluated. A series of sensitivities allows us to test the impact of the level of complexity of the
150 omega equation; the formulation of the discrete problem; and several possible choices related to
151 the boundary conditions. Some reflections on the sources of errors and the dynamical environment
152 are offered in the discussion.

2. Data and Methods

Mathematical symbols have their usual meaning. T , S , ρ and σ_t refer to (respectively) potential temperature, salinity, density and potential density anomaly. x (resp. y and z) and u (resp. v and w) refer to zonal (resp. meridional and vertical) directions and velocity. More precisely in the case of vertical velocities we will distinguish true velocities w from reconstructed velocities denoted ω with a subscript that refers to the precise omega equation formulation that is being used (see below Sec. 2b). N^2 is the buoyancy frequency.

a. The NATL model

The outputs from a submesoscale-permitting numerical simulation are used to reconstruct vertical velocity fields using different versions of the omega equation and compare them to the ground truth model vertical velocities w_{model} . The NATL60 MJM155 simulation is run using the NEMO v3.5 code. It has a horizontal resolution of $1/60^\circ$ (dx comprised between 0.8 and 1.6 km depending on the latitude), yielding an effective resolution of ~ 10 dx ($\sim 10 - 15$ km) (Soufflet et al. 2016). This means that a turbulent feature associated with a typical wavelength around $\sim 10 - 15$ km (typical scale $\sim 1.5 - 2$ km) are energetically subjected to a negligible influence of the dissipation operator. Below those scales numerical errors can arise that will affect the representation of physical processes although the misrepresented dynamics in the model solutions may still share important properties with the dynamics of the system obtained after resolution convergence (Le Sommer et al. 2018). On the vertical, the simulation has 300 levels (dz increases with depth and ranges from 1 to 30 m) and in the range of depths of analysis (200-400 m depth), the vertical resolution is ~ 10 m. The simulation is forced by realistic atmospheric forcings (DFS5.2) and boundary conditions (GLORYS2V3). It was integrated over a 5 years period (2004-2008) (Amores et al. 2018; Ducousso et al. 2017; Fresnay et al. 2018).

176 The model domain encompasses the whole North Atlantic. For this study, four contrasted sectors
177 were selected. For each region, eleven consecutive daily averaged outputs are analysed for two
178 opposite seasons of the year, in June and December. Near-inertial motions produced by the high-
179 frequency variability of the atmospheric forcings are partly filtered out and partly aliased in model
180 u, v , σ_t and w daily fields that are used in this study. A cleaner separation between balanced
181 and unbalanced motions would be useful to untangle their respective roles (e.g., see Qiu et al.
182 2020). Lacking the high-frequency model outputs needed to do better, we note that, in most
183 situations, omega estimations made using observations contain an unknown but presumably larger
184 inertia-gravity (IG) wave contribution. Our study can thus be considered as a favorable evaluation
185 in which this source of errors is minimized by the daily averaging. Absence of tidal forcing
186 in NATL60 will also tend to underestimate the energy level of unbalanced motion (Qiu et al.
187 2018) and thus has a similar consequence. The relevance of the study to the real ocean context
188 is however justified by the fact that model vertical velocities in the submesoscale-permitting class
189 of simulations are known to capture the patterns expected from the theory and observation based
190 studies.

191 The four regions we focus on are:

- 192 – the Gulf Stream/LatMix region (Shcherbina et al. 2013, LMX) centered around 38°N and
193 67°W. It encompasses the very energetic Gulf Stream current. It is characterized by intense
194 mesoscale activity composed of meanders and eddies. Vertical motions in the Gulf Stream
195 region have been the subject of many studies aimed at describing water exchanges between
196 the jet core and its vicinities (Bower and Rossby 1989; Lindstrom and Watts 1994; Joyce et al.
197 2013). This environment and the large amplitude meanders of the Gulf Stream in particular
198 are well known to produce intense vertical velocities (Fig. 1a).

- The region of the Azores current (AZO) centered at 33°N , 34°W which is characteristic of a subtropical regime with limited atmospheric forcing and modest mesoscale activity. It is the least energetic of the four regions in terms of vertical velocities (Fig. 1b). We relate this to the modest role played by surface density contrasts and upper ocean frontogenesis in the regional dynamics (Lapeyre 2009; Volkov and Fu 2010, 2011)
- An area of the subpolar gyre South West of Iceland encompassing part of the Rekjanes ridge (REK) and centered around 54°N , 31°W . The regional dynamics is characterized by weak mean flow and a moderately intense mesoscale activity made of deep reaching isolated structures (Fig. 1c).
- A sector of the Atlantic North-Eastern margin near 49°N and 15°W , where the Osmosis experiment took place (Buckingham et al. 2016, OSM). The regional dynamics is characterized by weak large scale circulation, weak mesoscale activity, and a marked seasonality of the submesoscale activity which is very intense in the wintertime (Fig. 1d; Thompson et al. 2016).

To limit the computational cost of inverting the omega equation a 3D sub-domain of each region is retained with dimensions ~ 360 by ~ 270 km on the horizontal and 1600 m in the vertical (reduced depth ranges will also be used in sensitivity tests section 4d). Horizontal (native) resolution is ~ 1.5 km while the data is linearly interpolated on a regular vertical grid with a 5 m resolution. For each region, a particular depth is selected to perform some of our analyses. As presented in the introduction the spirit of this investigation led us to choose depth levels 50 m below the deepest winter mixed layers encountered in that region so near-surface frontal processes are attenuated at this depth and our study is useful to make progress on biogeochemical fluxes between the mixed layer and the ocean interior. Specifically, selected depths of analysis (referred to as z_a) are 220 m for LMX, 250 m for AZO, and 380 m for REK and OSM.

223 *b. Formulations of the omega equation*

224 The underlying principles of the omega equation combine two lines of argument (Hoskins 1982)
225 – kinematical: a turbulent flow stirring an heterogeneous surface buoyancy field produces re-
226 gions of gradient intensification. Specifically, frontal intensification is promoted in the con-
227 fluence and shear situations that are frequently encountered in mesoscale turbulent conditions
228 (e.g. Fig. 2).

229 – dynamical: the thermal wind balance, which should approximately hold at
230 meso/submesoscale, is disrupted in situations of frontal intensification where density
231 gradients are enhanced while the vertical velocity shear is being reduced. This leads to the
232 development of ageostrophic secondary circulations (ASC) that attempt to thwart thermal
233 imbalance by restoring shear and slumping isopycnals. In the ocean interior this process is very
234 efficient at preventing frontal intensification which is a further justification for the weakness
235 of vertical velocities away from the surface. At the air-sea interface, the upper boundary
236 condition $w \approx 0$ limits the efficiency of ageostrophic circulations so frontal intensification
237 can generally proceed further and yield intense vertical velocities.

238 Mathematically, the frontogenesis process is captured by a relationship between the spatial
239 derivatives of w and a forcing term expressed as the divergence of a vector of forcings $\mathbf{Q}$

$$\mathcal{L}(w) = \nabla \cdot \mathbf{Q} \quad (1)$$

240 $\mathcal{L}$ is a second-order differential operator that can also take different forms depending on which
241 processes responsible for thermal wind disruptions are being considered in $\mathbf{Q}$.

242 A starting point to derive the omega equation for the general case is the set of equations govern-
 243 ing hydrostatic and Boussinesq flows:

$$\frac{du}{dt} - fv = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} + F_x \quad (2)$$

$$\frac{dv}{dt} + fu = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} + F_y \quad (3)$$

$$\frac{d\rho}{dt} = F_\rho \quad (4)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (5)$$

$$(6)$$

244 where (F_x, F_y) and F_ρ are source/sink of momentum and buoyancy caused by turbulent mixing.

The flow is then decomposed into a geostrophic ($\mathbf{v}_g$) and ageostrophic ($\mathbf{v}_{ag}$) component

$$\mathbf{v} = \mathbf{v}_g + \mathbf{v}_{ag}$$

245 where the geostrophic velocity satisfies the thermal wind balance:

$$\begin{cases} f \frac{\partial u_g}{\partial z} = \frac{g}{\rho} \frac{\partial \rho}{\partial y} \\ f \frac{\partial v_g}{\partial z} = -\frac{g}{\rho} \frac{\partial \rho}{\partial x} \end{cases} \quad (7)$$

246 and the residual ageostrophic flow component departing from this balance (the so-called thermal
 247 wind imbalance - TWI) satisfies:

$$\begin{cases} f \frac{\partial u_{ag}}{\partial z} = f \frac{\partial u}{\partial z} - \frac{g}{\rho} \frac{\partial \rho}{\partial y} \\ f \frac{\partial v_{ag}}{\partial z} = f \frac{\partial v}{\partial z} + \frac{g}{\rho} \frac{\partial \rho}{\partial x} \end{cases} \quad (8)$$

248 The generalized omega equation (1) is obtained by manipulating the time evolution equation for
 249 the TWI and yields (Giordani and Planton 2000):

$$f^2 \frac{\partial^2 w}{\partial z^2} + \nabla_h (N^2 \cdot \nabla_h w) = \nabla \cdot \mathbf{Q}, \quad (9)$$

where the $\mathbf{Q}$ vector involved in the right hand side (rhs) of the equation can be expressed as a sum of different forcings:

$$\mathbf{Q} = 2 \underbrace{(\mathbf{Q}_{\text{twg}} + \mathbf{Q}_{\text{twag}})}_{\mathbf{Q}_{\text{tw}}} + \mathbf{Q}_{\text{dag}} + \mathbf{Q}_{\text{dr}} + \mathbf{Q}_{\text{th}} + \mathbf{Q}_{\text{dm}} \quad (10)$$

following the notations of Giordani et al. (2006). $\mathbf{Q}_{\text{tw}}$ is the kinematic deformation and can be decomposed into a geostrophic $\mathbf{Q}_{\text{twg}}$ and an ageostrophic component $\mathbf{Q}_{\text{twag}}$. $\mathbf{Q}_{\text{dag}}$ is the deformation of the thermal wind imbalance and $\mathbf{Q}_{\text{dr}}$ its material rate of change. In all practical situations, $\mathbf{Q}_{\text{dr}}$ cannot be estimated and is therefore unaccounted for in the remainder of the study. $\mathbf{Q}_{\text{th}}$ and $\mathbf{Q}_{\text{dm}}$ refer respectively to the diabatic turbulent buoyancy and momentum forcings.

Being interested in the ability to determine vertical velocities through and below the thermocline we neglect the effects of diffusive momentum and buoyancy fluxes which are mainly active in or immediately below the mixed layer (Giordani et al. 2006; Yoshikawa et al. 2012; Thomas et al. 2010) but have a limited effect on subsurface velocities (Nagai et al. 2006; Yoshikawa et al. 2012). In fact, Xie et al. (2017), using microstructure shear measurements to infer the vertical diffusivity, derived the vertical mixing terms ($\mathbf{Q}_{\text{th}}$ and $\mathbf{Q}_{\text{dm}}$) and showed that below the thermocline the vertical velocity associated to those terms is one to two order of magnitude smaller than the one associated to the deformation of the flow. An exception is the study of (Qiu et al. 2020) in which vertical velocities arising from diffusive terms remain of magnitude comparable to those produced by ageostrophic deformation ($\mathbf{Q}_{\text{twag}}$) well below the mixed layer. We suspect that this is because vertical velocities due to mixing are not calculated explicitly in Qiu et al. (2020) but instead are obtained as a residual and thus also contain contributions from various sources such as imperfect boundary conditions and other numerical errors (see Sec. 4c and 4d).

We will limit ourselves to comparing the two ω reconstructions that are most commonly used with real ocean data: the QG version where ω_{QG} is solely forced by the curvature of the

geostrophic flow ($\mathbf{Q}_{QG} = 2\mathbf{Q}_{tw_g}$) as in Hoskins et al. (1978); and a more complete formulation (NG) in which the $\mathbf{Q}$ vector forcing ω_{NG} includes some contribution from the ageostrophic flow ($\mathbf{Q}_{NG} = 2\mathbf{Q}_{tw} + \mathbf{Q}_{dag}$).

The $\mathbf{Q}_{tw_g}$ vector in the QG formulation has the form:

$$\mathbf{Q}_{tw_g} = \frac{g}{\rho_0} \left(\frac{\partial u_g}{\partial x} \frac{\partial \rho}{\partial x} + \frac{\partial v_g}{\partial x} \frac{\partial \rho}{\partial y}, \frac{\partial v_g}{\partial y} \frac{\partial \rho}{\partial y} + \frac{\partial u_g}{\partial y} \frac{\partial \rho}{\partial x} \right) \quad (11)$$

where u_g and v_g are the horizontal components of the geostrophic velocity. In this study, these velocities are estimated by applying the thermal wind balance downward starting from the sea level with the reference velocities at that level being derived from the model sea level anomalies. This procedure mimics what can be optimally done with real oceanic data, assuming that sea level elevation is known with good accuracy.

The NG formulation takes into account the curvature of the total flow and the deformation of the ageostrophic flow,

$$\mathbf{Q}_{tw} = \frac{g}{\rho_0} \left(\frac{\partial u}{\partial x} \frac{\partial \rho}{\partial x} + \frac{\partial v}{\partial x} \frac{\partial \rho}{\partial y}, \frac{\partial v}{\partial y} \frac{\partial \rho}{\partial y} + \frac{\partial u}{\partial y} \frac{\partial \rho}{\partial x} \right) \quad (12)$$

$$\mathbf{Q}_{dag} = f \left(\frac{\partial v}{\partial x} \frac{\partial u_{ag}}{\partial z} - \frac{\partial u}{\partial x} \frac{\partial v_{ag}}{\partial z}, \frac{\partial v}{\partial y} \frac{\partial u_{ag}}{\partial z} - \frac{\partial u}{\partial y} \frac{\partial v_{ag}}{\partial z} \right) \quad (13)$$

where u_{ag} and v_{ag} are the ageostrophic horizontal velocities. In practice, u_{ag} and v_{ag} are obtained as the difference between model horizontal velocities and the calculated geostrophic velocities u_g and v_g .

Two baseline reconstructions ω_{QG} and ω_{NG} are thus computed from the adiabatic QG and NG formulations of the $\mathbf{Q}$ vector. For each of them the computation is made on the horizontal subdomains defined in section 2a. The domain extension in the vertical goes from the surface down to 1600 m. Dirichlet boundary conditions are used at all the frontiers. A tridimensional buoyancy frequency, N^2 , that varies both in the horizontal and in the vertical is used to solve all the inversions, although tests were run using a horizontally averaged profile and little differences were

observed (not shown). Specific reconstructions using different resolution, domain size or boundary conditions are made to explore sensitivities and described in the corresponding sections.

To investigate the relative importance of different sources of errors we will carry out two forms of omega reconstruction with either perfect right-hand side (ω will be denoted $\omega_{\dagger}$) or perfect boundary conditions (ω will be denoted ω^*). Perfect rhs omega inversions are computed using forcing terms that are derived from model vertical velocities and the lhs of (9):

$$\nabla \cdot \mathbf{Q}_{\dagger} = f^2 \frac{\partial^2 w_{model}}{\partial z^2} + \nabla_h (N^2 \cdot \nabla_h w_{model}). \quad (14)$$

Precisely, (14) is evaluated using second order centered differences, i.e. in a way that is consistent with how the MUDPACK elliptic solver (Adams 1989) that we use is being implemented. For instance, along the x direction we use:

$$\left. \frac{\partial^2 w}{\partial x^2} \right|_i = \frac{1}{\Delta x} \left[\frac{(w_{i+1} - w_i)}{\Delta x} - \frac{(w_i - w_{i-1})}{\Delta x} \right] \quad (15)$$

Alternatively perfect boundary conditions can be imposed by applying w_{model} at the edges of the inversion domain. Note that this is however not precisely possible to do at the ocean surface because it is a moving interface in NEMO while it must be held fixed in the solving of the omega equation.

c. Baroclinic mode decomposition

Under the assumptions of flat bottom and rigid lid at the ocean surface the linearized primitive (or quasi-geostrophic) equations governing the horizontal and vertical components of inviscid fluid motion can be separated (Cushman-Roisin and Beckers 2011). In the vertical, two sets of normal mode eigenfunctions F_n and G_n form complete bases onto which pressure/horizontal velocity and vertical velocities can respectively be projected (see annex A1).

311 Normal mode decomposition has proved useful even in situations where all above assumptions
312 are not satisfied and in particular when the bottom of the ocean is not flat (e.g. Rocha et al. 2013).
313 In order to gain insight into the sources of reconstruction errors normal modes decomposition will
314 be used to interpret the differences in reconstruction skills for the different regimes.

315 In practice the MODES program available at <http://www.d.umn.edu/~smkelly/software.html>
316 (Kelly 2016) is used to determine the mode structure at each model point. The modal amplitude
317 of the model vertical velocity is then determined locally.

318 **3. Description of the vertical velocity regimes**

319 The four regions and two seasons selected for this study exhibit contrasted dynamical regimes.
320 This will allow us to explore the sensitivity of the omega reconstruction behaviour and skills to the
321 nature of the meso/submesoscale turbulence that produces the vertical velocities. The diversity of
322 vertical flow behavior is visually illustrated by snapshots of model vertical velocities (Figs. 1, 2,
323 3, 4, 5) and confirmed by their spectral distribution of variance (Fig. 6a,b).

324 In the LMX region, the displayed vertical section was chosen so as to cross the Gulf Stream
325 (Fig. 2). In this region the EKE is about ten times higher than in the other regions (Fig. 7c,d),
326 the root-mean-square (rms) of w is 3 to 5 times higher (Fig. 7e,f) and intense density fronts are
327 observed both in June and December (Fig. 2). In the frontal region, the vertical velocity structures
328 extend down to 1500 m (Fig. 7e,f) depth or more, with peak $|w|$ in excess of 80 m day^{-1} . Overall,
329 this is the region with the largest vertical velocity variance at all scales and a dominant fraction of
330 this variance is found at the largest scales fitting in the study domain. Also note that LMX interior
331 vertical velocities are only weakly affected by the seasonal cycle of the near-surface submesoscale
332 activity (which is present but hardly visible in Fig. 1).

333 Compared to the LMX region, the AZO region is a lot less energetic (Fig. 7c,d); the isopycnals
 334 are flatter; and the horizontal velocities are slower. The vertical circulation is by far the weakest
 335 of all four regions (Fig. 7e, f and 6) and exhibits limited seasonal changes. Vertical velocities are
 336 organized into structures whose size is intermediate (smaller than in LMX but larger than in OSM
 337 and to a lesser extent REK) as readily apparent from the inspection of fields in the physical space
 338 and also from the spectral distribution of w variance (Fig. 6): in the range of scales larger than 10
 339 km the w spectrum is flatter (resp. steeper) than that for LMX (resp. REK and OSM). w patterns
 340 in Fig. 3 also tend to be tilted with respect to the vertical axis. This is a plausible indication that
 341 vertically propagating IG waves are involved in the generation of w (slanted phase lines associated
 342 with near-inertial waves are found in numerous studies, e.g., Furuichi et al. 2008).

343 In the REK region, the average vertical velocity magnitude is $O(10 \text{ m day}^{-1})$ with localized
 344 higher values near mesoscale structures that can reach of up to 100 m day^{-1} and tend to have a
 345 large vertical extension (Fig. 1 and 4). In the physical space, w structures are frequently tilted
 346 with respect to the vertical although less so than in AZO. Again this is presumably the signature
 347 of near-inertial wave activity. But contrary to the AZO case, the horizontal patterns visible in w
 348 fields are consistent with the structuring role of the (sub)mesoscale activity particularly during
 349 summer: presence of multipolar w patterns (Lapeyre and Klein 2006b; Viúdez 2018), that could
 350 be the signature of eddy-induced Ekman pumping and/or vortex Rossby waves (McWilliams et al.
 351 2003; Buongiorno Nardelli 2013; Barceló-Llull et al. 2017), as in the left corner of Fig. 1c; elon-
 352 gated filaments of elevated w (Capet et al. 2016). During winter the enhancement of mixed layer
 353 submesoscale turbulence is particularly marked (Fig. 1c). Most of the fine-scale w patterns appear
 354 to be confined into the mixed layer and the visual aspect of the w field differs noticeably on ei-
 355 ther side of the mixed layer base. On the other hand, w increases significantly in magnitude from
 356 summer to winter (Fig. 7e,f). In terms of spatial scales summer w have a clear mesoscale domi-

357 nance with a peak around 50-100 km wavelength. For winter w , the role of the mesoscale is less
358 prominent while the contribution associated with submesoscales is strongly reinforced (Fig. 6).

359 Vertical velocities in the OSM region share many similarities with those of REK: magnitude is
360 $O(10 \text{ m day}^{-1})$; flatness of the w power spectrum in the mesoscale range 50 – 100 km; importance
361 of the near-surface submesoscales particularly during the wintertime; modest indication of vertical
362 tilt. The main difference between the two regions is the greater degree of w continuity across the
363 mixed layer and upper thermocline in winter, presumably as a consequence of very low upper
364 ocean stratification in the OSM region (Fig. 7b).

365 **4. Omega reconstruction of the vertical velocity fields**

366 *a. Baseline skill assessment*

367 The skills of the omega reconstructions vary greatly depending on the region and season as illus-
368 trated qualitatively (resp. as quantified) in Figs. 2-5 (resp. in Fig. 8). Fig. 8 represents the spectral
369 coherence between the model w and reconstructed ω , i.e., the degree of co-variance between them
370 as a function of scale. The scales and wavelengths above which the spectral coherence is larger
371 than 0.6 for the QG and NG inversion are listed in table 1 along with the fraction of w variance
372 retained at scales larger than that threshold.

373 In general, omega reconstructions perform best at scales $\gtrsim 10 - 20$ km. The energetic mesoscale
374 structures are better reproduced and spectral coherence drops rapidly at scales $\lesssim 2 - 10$ km, i.e.,
375 the omega reconstruction are not well-suited in the submesoscale range. This is particularly well
376 illustrated by the LMX region where spectral coherence reaches levels close to 1 above 20 km scale
377 but drops below 0.6 around 7 – 8 km (Table 1). On the other hand, there is relatively limited w
378 variance at fine-scale. Thus, the overall quality of the reconstructions is manifest for the randomly

379 chosen situation shown in Fig. 2 where both the intensity and lateral/vertical extension of the w
380 poles are well reproduced. Overall, 80 – 90% of the w signal is captured with a coherence of 0.6
381 or higher in LMX.

382 Wintertime OSM is a notable exception where coherence levels remain elevated down to 3 km
383 scales, particularly when ageostrophic effects are accounted for (see below). As in LMX, upper
384 ocean turbulent stirring and ageostrophic secondary circulations reach down to depths of 300 – 500
385 m in this region but the deformation radius is much smaller than in LMX and the stratification is
386 particularly weak. The w field is thus organised in fine-scale structures that are frequently several
387 hundred meters thick in the vertical (Fig. 5), many of which are well captured by the omega
388 reconstruction.

389 In the REK region, the omega equation reproduces adequately some of the stronger and larger
390 vertical velocity structures organized in alternated bands of upward and downward velocity inten-
391 sity (Fig. 4). As for the finer slanted structures visible in both seasons but more intense in winter
392 they are almost completely missed. The spectral coherence peaks for scales of ~ 10 km with lower
393 coherence for smaller and also larger scales. This might arise because vertical velocities at large
394 scale are driven by other dynamical processes associated with the terms not retained in our omega
395 reconstructions such as Ekman and inertial pumping.

396 Finally, in agreement with the visual impression drawn from Fig. 3, omega reconstructions per-
397 form very poorly for wintertime AZO with spectral coherence systematically below 0.5. Includ-
398 ing ageostrophic effects has virtually no impact on the reconstruction skill for the AZO region as
399 clearly illustrated in Fig. 3.

400 More generally, including the ageostrophic terms makes a significant difference for the LMX
401 and wintertime OSM reconstruction only (the scale where the 0.6 coherence threshold is found
402 decreases by up to 20% for these cases). We relate this to the fact that high Rossby number

dynamics is prevalent in both regions albeit for different reasons. In the LMX sectors, the frontality of the Gulf Stream leads to intense turbulent stirring by the mesoscale field. In the OSM sector deep mixed layers in winter lead to intense submesoscale activity whose influence reaches to great depths owing to the reduced subsurface stratification. Conditions resembling those found for winter OSM also exist in the REK region in winter but, in this latter case, the modest stratification present around 200 m depth (Fig. 7b) seems sufficient to isolate the interior circulation from the influence of the near-surface dynamics and thwart ageostrophic effects, hence the limited increase in coherence between ω_{QG} and ω_{NG} in Fig. 8.

b. Sensitivity to temporal averaging

An important limitation of the omega reconstructions presented in the previous section may arise from the role played by IG waves. This role cannot be captured by the forcing terms we retained for the expression of $\mathbf{Q}$ in the QG and NG reconstructions which ignores the material rate of change of the thermal wind imbalance ($\mathbf{Q}_{dr}$ in 10). Using daily averages tends to reduce the effects of these processes, particularly where the inertial period is close to 24 h (at 30° latitude), but does not eliminate them. It is unclear whether the IG wave and subinertial quasi-balanced flow contributions to w should be separated (see discussion section) but the behavior of the omega reconstruction as a function of the temporal scale content of the forcing term $\nabla \cdot \mathbf{Q}$ is of practical as well as theoretical interest. This behavior is explored by increasing the degree of temporal averaging that is performed prior to the computation of the omega reconstruction right-hand side. All simulated fields are averaged similarly, including w_{model} . The expectation is that more temporal averaging will reduce the amount of variance associated with the w field to be reconstructed but improve the skill of the omega reconstruction for that low-passed w . The existence of such a trade-off is confirmed in Fig. 9 for most dynamical regimes. Fig. 9 presents the spectral coherence

between ω_{NG} and w_{model} for larger (10 – 25 km) and finer (3 – 10 km) scales as a function of the remaining variance ratio $Var(< w >_t)/Var(w)$, where $< \cdot >_t$ is the low-pass temporal averaging whose length is varied from 1 day (standard output for that study) and 10 days. Results are shown for ω_{NG} but only minor differences were found with ω_{QG} .

For all regions except LMX an optimum in spectral coherence is found for time-averaging longer than 1 day, both for the large scales (10 – 25 km) and the fine scales (3 – 10 km). The averaging period associated with this optimum is between 2 and 5 days. As anticipated, spectral coherence improvement comes at the expense of a loss of reconstructed w variance. In several cases the loss of w variance is less than 25%: REK, AZO and OSM for the large scales and REK for the fine scales during summer; OSM for the large scales during winter. Particularly for this latter case the spectral coherence improvement is substantial and 2-5 day averaging seems justified. Conversely, the most dramatic improvement in (ω_{NG}, w) spectral coherence seen in the AZO region (winter, 10 – 25 km scales, 5-day averaging) has a major effect on the retained ω_{NG} variance (only 37% of the original w variance) and may be of limited utility in practice.

c. Discretization errors

We also wish to draw the reader’s attention on the delicacies of the omega inversion and the implications these delicacies have on the estimation of vertical velocities. To do so we attempt to minimize reconstruction errors. In addition to imposing perfect boundary conditions by applying w_{model} at the edges of our domain, we also compute a “perfect” right-hand side $\nabla \cdot \mathbf{Q}_\dagger$ to be used in the elliptic inversion (see section 2b). The resulting vertical velocity estimate $\omega_\dagger^*$ found as a numerical solution is associated with minute errors, on average 3 % with the solving parameter choices we pass to MUDPACK. These errors result from 1) the imperfect convergence of the elliptic solver and 2) the imperfect boundary condition at the ocean surface.

449 To gain insight into the sensitivity of the elliptic inversion, variant $\omega_{\dagger}^*$ were also computed by
 450 employing a discretization scheme alternative to (15) to calculate $\nabla_h^2 w_{model}$ in (14):

$$\left. \frac{\partial^2 w}{\partial x^2} \right|_i = \frac{1}{2\Delta x} \left[\frac{(w_{i+2} - w_i)}{2\Delta x} - \frac{(w_i - w_{i-2})}{2\Delta x} \right] \quad (16)$$

451 Both schemes are consistent, centered, and second order in accuracy. They only differ by the
 452 length of their stencil (3 or 5 points).

453 We find that the discretization choice has a moderate but significant impact. In the LMX region
 454 in June for instance the use of the scheme (16) to compute the “perfect” rhs produces relative w er-
 455 rors in excess of 12 %, to be compared with the minimal convergence errors of ~ 3 % with scheme
 456 (15). The elevated error figure obtained with the second scheme helps place realistic limits to verti-
 457 cal velocity estimation attempts and draws the attention on the fact that minute errors/uncertainties
 458 on the rhs of the omega equation can have significant impacts on the reconstructed vertical veloc-
 459 ities.

460 *d. Sensitivity and errors due to boundary conditions*

461 Finally, an important source of error when solving the omega equation is the choice of the bottom
 462 boundary condition. As numerous studies have pointed out (Allen and Smeed 1996; Rudnick
 463 1996; Pascual et al. 2004) ω is not very dependant on the lateral boundary conditions but the
 464 form of the BBC and the depth where it is applied can have a strong impact on the solution of
 465 the equation (Pidcock et al. 2012; Rudnick 1996). Two types of BBCs are generally used, the
 466 Dirichlet condition $w = 0$ or the Neumann condition $\partial w / \partial z = 0$. A third one was proposed by
 467 Rudnick (1996): to limit the influence of the boundary condition on the solution, the vertical grid
 468 was extended below the depth where observations were available. Over the depth range with no
 469 observations $\nabla \cdot \mathbf{Q}$ was simply assumed to be zero. In practice, this led Rudnick (1996) to shift

the bottom boundary from 400 m (where the deepest observation was available) to 2524 m depth where a Dirichlet BBC ($w = 0$) was imposed.

To assess the impact of the BBC on the solution we compare the errors obtained for Dirichlet and Neumann conditions and for different domain extensions, with the bottom boundary depth z_{bottom} ranging from 150 m to 1600 m (Fig. 10). This is done in the four regions and for the two seasons. We also test the boundary condition proposed by Rudnick (1996) with two different depths (400 m and 800 m) below which $\nabla \cdot \mathbf{Q}$ is assumed to be zero down to 800 m and 1600 m respectively. In this section, the omega reconstruction is solved using $\nabla \cdot \mathbf{Q}_\dagger$ forcing computed as described in section 2b so relative errors exceeding a few percents can only be due to boundary conditions.

Figure 10 shows the relative errors of omega reconstructions made at the reference depths z_a when different boundary conditions are applied. The errors at depth z_a are horizontally and temporally averaged over the entire reconstruction domain on the horizontal and over the 11 consecutive daily model outputs. The relative error field can be quite large, generally in excess of 0.5 for domain depths shallower than 500 m, despite a good agreement in w and ω patterns. This is generally consistent with the findings of several past studies (Pinot et al. 1996; Allen et al. 2001; Rixen et al. 2003).

Relative errors varies with z_{bottom} in a relatively simple and intuitive way: deeper z_{bottom} systematically translates into weaker errors with Neumann or Dirichlet boundary condition. More precisely, errors tend to stabilize around 20% when z_{bottom} greater than 1000 – 1500 meters are used (Table 2), with the notable exception of REK for which relative errors are $\sim 0.3 - 0.4$ and still decreasing at $z_{bottom} = 1600$ m. The most evident manifestation of error saturation behavior is found for LMX and Neumann boundary conditions, with a threshold around $z_{bottom} = 700$ m beyond which little improvement is observed. More generally we note that: the quality of the reconstruction can vary from low to high depending on the choice being made for the depth of the

boundary condition; except in the LMX region the Neumann and Dirichlet boundary conditions give relatively similar results; the use of a buffer region to increase the domain depth following Rudnick (1996) can ameliorate the reconstruction skill and provide an optimum over all possible choices but the improvement is generally marginal. Estimating the relative error as a volume-average over the whole water volume above the depth where the boundary condition is applied paints a more complicated picture. For instance, in a number of situations, reconstruction errors are found to increase when the location of the boundary layer deepens beyond certain thresholds (not shown). We relate this to the fact that deep vertical velocities can be particularly intense owing to processes not properly resolved by our implementations of the omega reconstructions (IG wave activity, flow-topography interaction).

In an attempt to gain further insight, we use vertical mode decomposition to characterize the vertical structure of the w field. Consider a situation where w would project onto a single mode, for instance baroclinic mode 2. In that case, w systematically vanishes at the zero crossing of G_2 and a Dirichlet boundary condition at that depth would not introduce any error. A perfect Neumann boundary condition would similarly exist at the zero crossings of F_2 . There are several potential obstacles preventing this from happening. Most importantly, vertical velocity tends to be associated with fine horizontal scales and this tends to be also true in the vertical (Fig. 3-5). The vertical mode decomposition of w generally involves many modes, and in most cases, less than half of the w signal is explained by the sum of the first three vertical modes (Fig. 12, annex A1). It is therefore impossible to choose a fixed depth where the dominant F_n or G_n are zeros. The LMX regime is an exception where the w vertical structure projects to a large extent onto the first three baroclinic modes (Fig. 12). For LMX the smallest reconstruction errors (volume averaged) are obtained for a Neumann boundary condition placed at approximately 750 m depth (not shown), *i.e.*, the depth below which errors evaluated at a single depth ($z_a = 220$ m) tend to reach a plateau

around 0.2 – 0.25 (Fig. 10a,e). The 750 m value falls in the depth range where F_1 and F_3 are very close to zero (Fig. 11a). The link between the vertical mode's structure and the effect of z_{bottom} on the reconstruction skill is far less clear for the other three regions. We attribute these inconsistencies to the limited role played by the gravest baroclinic modes in AZO, REK and OSM (Fig 12).

To better characterize the reconstruction errors due to imperfect (bottom) boundary conditions, we compute an alternative omega reconstruction ω_{NG}^* using perfect w_{model} information at the boundaries (see section 2b). Differences between ω_{NG}^* and w_{model} , can only arise from the simplification made to $\mathbf{Q}$ in the NG inversion (that is, considering $\mathbf{Q}_{dr}$, $\mathbf{Q}_{th}$ and $\mathbf{Q}_{dm}$ as null). They range from ~ 1 to ~ 5 m day $^{-1}$ depending on the region and season. They are typically one to three times as high as errors associated with a Dirichlet boundary condition at 1600 m (Table 2) and generally lower than the ones associated with a Dirichlet boundary condition at 500 m (Fig. 10). Discrepancies in spectral distribution between ω_{NG}^* and w_{model} are much reduced compared to those for ω_{NG} . This is particularly true for the scales below 1 km (Fig. 6c and 6d). A similar skill improvement is noticeable for the spectral coherence (Fig. 8). A significant fraction of the fine-scale vertical motions in the upper ocean is thus directly linked to unidentified processes active below 1600 m. Consistent with previous studies (e.g. see Jouanno et al. 2016) flow-topography interactions is a likely candidate, which would pose serious difficulties if it were to be explicitly incorporated into the omega reconstruction approach (inversion would need to be performed for the whole ocean depth range with the knowledge of the vertical velocity at the ocean floor $w = -\mathbf{u}\nabla h$). We do not see any prospect for this but this source of errors should be kept in mind.

5. Discussion

Since the 1980s a large number of studies have focused on inferring oceanic vertical velocities through more or less elaborate forms of the omega equation. Most of them have been applied to local *in-situ* data, in which the sources of errors are difficult to identify and quantify (see the bibliography table SI1). In some instances the reconstructed vertical velocity field has been used to qualitatively interpret concomitant tracer distributions (Pollard and Regier 1992; Rudnick 1996; Martin and Richards 2001; Allen et al. 2005; Ruiz et al. 2009; Pallàs-Sanz et al. 2010; Rousselet et al. 2019). The uncertainty on reconstructed w is an important limitation when doing so (also note that the vertical tracer distribution at any given time reflects the past history of vertical advection - and mixing). w velocities are now increasingly being used quantitatively, e.g., as inputs to tracer models (Pascual et al. 2015; Barceló-Llull et al. 2016).

Model studies have addressed the various sources of errors involved and the ways to reduce their impact with a general focus on three main issues: i) the merits of more complete versions of the omega equation; ii) the sensitivity to particular choices of boundary conditions when solving the omega equation; iii) the errors induced by the lack of resolution, homogeneity, and synopticity of in situ sampling when the omega reconstruction is applied to real ocean observations (see SI1). These model-based assessments of ω reconstructions were typically performed in simplified flow conditions, composed of a single coherent eddy or front, with a marked preference for the early stages of destabilisation of baroclinic zones (Strass 1994; Pinot et al. 1996; Allen et al. 2001; Rixen et al. 2003; Viúdez 2018). More recently, the omega equation has been used to determine oceanic vertical velocity fields over larger domains and extended time periods from observation-based gridded reconstructions of temperature and salinity fields (Pascual et al. 2015; Barceló-Llull et al. 2016; Buongiorno Nardelli et al. 2018). The resulting ω fields can subsequently be used

562 to estimate vertical fluxes and this has been attempted for several biogeochemical tracers, over
563 different relevant time scales.

564 Overall, a general assessment of the skills and limitations of the omega reconstruction is lacking.
565 The present study is an effort in that direction that mainly pertains to i) and ii) and we deliberately
566 excluded errors of the type iii). Although they pose important and perhaps leading-order limi-
567 tations to w reconstructions from observations, this type of errors could be significantly reduced
568 by observing the ocean at higher resolution in specific regions of interest and combining these
569 observations with fine-scale remotely sensed information and model integrations. Optimal ways
570 to produce such combinations may involve relocation strategies as proposed in Rixen et al. (2001)
571 and Pascual et al. (2004). Errors i) and ii) pose different type of challenges that have not received
572 much attention. We have followed the steps of Strass (1994) whose analyses of the omega re-
573 construction skills included a scale-dependant coherence diagnostic. An originality of our study
574 is to estimate the fidelity of w reconstructions for fully turbulent realistic flows. Several findings
575 reported in the previous section deserve further discussion.

576 *On the limited skills of omega reconstructions at fine-scale*

577 First, the important limitations to the omega reconstructions found at relatively fine-scale, de-
578 spite the absence of type iii) errors may seem surprising. Some remarks are thus in order. An
579 important motivation for this work is the representation of vertical tracer fluxes between the sur-
580 face and interior of the ocean. Therefore we focused on vertical velocities tens of meters below
581 the mixed layer. At such depths, vertical velocity spectra are significantly more red than closer
582 to the surface where whiter spectra have been reported (Ponte and Klein 2013; Klein et al. 2008).
583 This means that modest levels of variance remain in the scale range where coherence has dropped

584 down. Conversely, a large fraction of w variance ($> 60\%$ for all regions and seasons) is found in
585 the scale range where coherence is above 0.6 (table 1).

586 This being said, the coherence drop off at scales below 10 km is interesting in itself and deserves
587 further discussion. The only regime for which significant skill is being obtained into submesoscale
588 range is winter OSM, which clearly stands out in terms of coherence (Fig. 8). This is also the
589 only regime for which the influence of surface intensified frontal turbulence is found to penetrate
590 down to the depth of analysis ($z_a = 380$ m), owing to extremely weak subsurface stratifications.
591 This regime is also the one for which the NG reconstruction provides the largest improvement
592 over the QG reconstruction. The lack of reconstruction skills generally found at submesoscale is
593 therefore not due to a particular difficulty at capturing vertical velocities associated with frontal
594 turbulence. Instead, we attribute reconstruction errors to the imperfection of the BBC used to
595 invert the elliptic omega equation and to the neglect of fluctuations in thermal wind imbalance due
596 to partly or fully unbalanced fast processes such as inertial gravity waves. The former source of
597 error is identified and quantified explicitly while the importance of the latter is inferred indirectly.
598 Further elaboration on these two error sources follow.

599 The boundary conditions impact omega reconstructions over the entire study domain owing to
600 the elliptic nature of the omega equation. It has been known for a long time that the solution can
601 be improved by properly choosing the type and location of the BBC. We explored the possibility
602 that the BBC strategies could be rationalised based on vertical mode decompositions. Although
603 one exception was found in the Gulf Stream region, vertical velocities tend to project onto a large
604 number of vertical modes (Fig. 12) and no ideal positioning of the BBC can be chosen a priori.
605 Pushing the BBC position z_{bottom} toward greater depths leads to reconstruction improvements even
606 beyond 1500 m. This is not feasible when observations are used to perform omega reconstructions
607 and the typical choices made in this situation ($z_{bottom} \sim 500$ m see review table SI1) fall in the range

608 where errors are most sensitive to z_{bottom} . In the Gulf stream region, vertical velocities associated
 609 with upper ocean frontal dynamics extend deep into the water column and tend to project mainly
 610 onto the first 3 vertical modes (Fig. 12). These properties are qualitatively consistent with the fact
 611 that, for the LMX domain, the Neumann BBC outperforms the Dirichlet BBC and that the relative
 612 error curve as a function of BBC depth levels off for z_{bottom} below ~ 700 m. Similar behaviors
 613 may presumably be observed in other western boundary regions and the Antarctic Circumpolar
 614 Current region. Finally, note that, given a depth down to which data is available to feed an omega
 615 reconstruction, the so-called telescopic method developed by Rudnick provides at best a marginal
 616 improvement over the classical Dirichlet or Neumann boundary conditions.

617 The presence of inertia-gravity waves near and beyond the drop-off scale is not accounted for
 618 as a source of w (in our case, neglecting the forcing term $\mathbf{Q}_{dr}$ was due to limitations on the model
 619 outputs at our disposal but including this term for real ocean situations would pose extremely strin-
 620 gent if not impractical requirements on sampling strategies). The AZO region is the one where
 621 inertia-gravity waves are suspected to play the largest role, if only because balanced turbulence is
 622 very weak there. There may be other more subtle consequences of the inertia-gravity wave activity
 623 on the omega reconstruction we have presented. For instance, REK has more w variance in winter
 624 but coherence between ω_{NG} and w_{model} is degraded at that season compared to summer. Although
 625 seasonal changes appear comparatively unimportant in the LMX region, a slight coherence degra-
 626 dation occurs in winter: winter coherence for the NG reconstruction is ~ 0.1 lower than in summer
 627 over the scale range 2 – 8 km (gaps are smaller at larger scale but the degradation is noticeable up
 628 to 20 km). Again, signs of enhanced NIW activity for the winter analysis period compared to the
 629 summer one suggest that near-inertial waves are responsible for this degradation.

630 For completeness, two other possible sources of omega reconstruction errors are listed here.
 631 Daily averaged variables are used to compute the forcing terms which are nonlinear combinations

of these variables. This means that Reynold-type forcing terms should formally be included due to rapid (intra-day) fluctuations in u , v and ρ . Kinetic energy corresponding to motions with temporal scales below 1 day is very low in simulations with $dx \sim 2$ km and we have assumed that this is a small effect. It would need to be verified that the same applies when *in-situ* observations are low-passed filtered prior to computing rhs terms for a real ocean omega reconstruction. Forcing terms associated with mixing of momentum and buoyancy have also been ignored. This is generally considered as a valid approximation sufficiently far from the mixed layer while this source of error is expected to increase at shallower depth (see below for more elaboration on this) in the context of ocean tracer dynamics. Although generally consistent with our findings the latest results of Qiu et al. (2020) cast some doubts on the smallness of w -forcing by buoyancy and momentum diffusion. In a western boundary context, this term is found to be comparable to w -forcing by ageostrophic kinematic deformation and stronger than w -forcing by thermal wind imbalance deformation or thermal wind imbalance tendency, even well into the ocean interior (see their figure 4). This issue would however need to be scrutinized based on an explicit computation of the mixed effect on w . Qiu et al. (2020) infer this term as a residual which therefore lumps together various contributions including that due to BBC errors. Model output limitations have not allowed us to undertake this.

On the consequences of limited reconstruction skills at fine-scales for tracer dynamics

Ultimately, what matters in most applications is not vertical velocity per se but the vertical transport of oceanic properties, for instance upward fluxes of dissolved iron enriching the euphotic layer in the Southern Ocean (Nicholson et al. 2019), or downward fluxes of organic material filling the ocean interior and having key implications on O₂ consumption and distribution (Boyd et al. 2019). Vertical tracer fluxes arise from vertical motions because upward and downward motions

are, on average, associated with distinct tracer values. We find it useful to discuss three types of limit cases in which this can occur and where the limitations of the omega reconstruction described above may be more or less problematic depending on the scenario. To this end, we consider a nutrient-like tracer τ whose concentration gradient is directed downward. The same reasoning would apply to tracer with an upward gradient (e.g., phytoplankton or dissolved oxygen).

An important distinction between two types of limit cases can be made depending whether baroclinic instability (BCI) plays an important role or not.

Case 1

When BCI is important, turbulent vertical motions are strongly constrained by the fact that $\langle w'b' \rangle > 0$, where b refers to buoyancy, $\langle \cdot \rangle$ is a low-pass averaging operator and the prime notation refers to deviations from this average. BCI can thus contribute to transport a tracer τ vertically provided that the distributions of τ and b are correlated. Far enough from the surface in the ocean interior available potential energy (APE) release is mainly achieved through mesoscale velocities (Lapeyre et al. 2006; Capet et al. 2016). Unless the correlations of τ and b were weak at mesoscale and strong at submesoscale, the proper description of mesoscale w would thus suffice to capture the dominant part of $\langle w'\tau' \rangle$. Typically, correlations between a tracer τ and buoyancy exist owing to processes acting at large-scale, although large decorrelation can ensue from biological reactions (e.g. for oxygen and nitrate). Correlations are then transferred down to smaller scales by turbulent cascades and decorrelation between buoyancy and τ is preferentially found at the finest scales (see discussion in Fox-Kemper et al. 2013, and references therein). Therefore, we expect omega reconstructions to be useful in this case despite the limitations we have described.

We now turn to the situation where vertical motions are not constrained by baroclinic instability and result instead from, e.g., fossil mesoscale/submesoscale turbulence and/or internal wave activity. In this situation, any water parcel has a well defined reference depth position z_{ref} (quite

independent of horizontal position) around which it may oscillate and an additional process must be invoked for these oscillations to produce τ vertical/diapycnal fluxes. We take a Lagrangian viewpoint and consider $\delta z = \int_t w dt$, the vertical displacement of a water parcel from its equilibrium position and we distinguish two limit cases illustrated in Fig. 13.

Case 2

Let us consider the situation in which a sink term for τ is located in the euphotic layer where photosynthesis draws τ levels down (Fig. 13 a and b). The τ anomalies are schematically represented for a mesoscale (panel a) and a submesoscale (panel b) upward oscillation where the amplitude of the oscillations have been chosen so as to reflect the distribution of w variance found in the ocean interior for all regimes ($\delta z^m > \delta z^s$). Because $\delta z^m > \delta z^s$ and also because the mesoscale excursions last on average longer the photosynthesis sink term for τ is more effective at mesoscale than it is at submesoscale. The tracer biogeochemistry acts as a low-pass filter and a representation of fine-scale vertical motions is unessential in the determination of tracer vertical fluxes. The deficiencies of the omega equation evidenced in this study should thus have limited consequences on the determination of tracer vertical fluxes, e.g., as performed in Barceló-Llull et al. (2016).

Note that the depth where the mean gradient of τ resides is a parameter that is potentially important to consider. If this mean gradient were located very close below the mixed layer base, the region where the photosynthesis sink term is active would be closer and the relative amplitude of submesoscale vertical motions (compared to that for the mesoscale) would be larger, hence a stronger influence of submesoscale processes.

Case 3

The last limit case is the one where the only possible modification of the tracer concentration attached to water parcels is through (vertical/diapycnal) mixing with surrounding water masses when and where the underlying flow structure produces local shear enhancement. Shear being

703 proportional to spatial derivatives of the velocities, fine-scale vertical motions can potentially have
704 a major contribution on τ vertical/diapycnal fluxes despite their lesser magnitude relative to those
705 at mesoscale. Reconstructed vertical velocities have a general bias toward overly weak variance
706 that is particularly pronounced at scales below 30 to 50 km, depending on the regime. This bias
707 and its impact on the determination of tracer fluxes may be amenable to statistical corrections
708 if omega reconstructions for case 3 type problems turn out to be of importance. The impact of
709 (very) fine-scale motions on tracer dynamics is presently accounted for by shear-driven mixing
710 parametrizations (Gregg 1989; Polzin et al. 1995 and references therein) which represent the ef-
711 fect of internal gravity wave. There are evidences that different forms of heterogeneities such as
712 submesoscale flows affect internal wave breaking (Whitt and Thomas 2013; Avicola et al. 2007)
713 but the utility of the omega equation to incorporate these effects in our ocean representations is
714 presently unclear.

715 **6. Conclusions**

716 The ever expanding coverage of observational networks supplemented by satellite observations
717 with increasing spatio-temporal resolution like the upcoming SWOT mission (d' Ovidio et al.
718 2019) was a strong motivation for this work. In the coming years we may be able to estimate
719 vertical fluxes more accurately and at finer scale than ever before. Today, the most common
720 tool to infer vertical velocity is the omega equation. In this paper we explored the ability of the
721 most common configurations adopted to solve this equation to provide information on the vertical
722 circulation at different horizontal length scales. The main novelty of our work is to have used a
723 broad variety of regimes which helped unravel the diversity of reasons underlying the errors in
724 omega reconstructions of w fields, depending on the regional dynamics.

725 Generally the adiabatic omega reconstruction gives good results for mesoscale vertical circula-
 726 tion, typically for structures with horizontal scales larger than 10 km. These structures tend to be
 727 associated with a large part of the w variance, although their relative importance and the precise
 728 skills of the omega reconstruction at such scales depend on the local dynamics. Omega reconstruc-
 729 tion skills degrade strongly in the submesoscale range. This degradation is manifest both in terms
 730 of reduced variance levels and lack of coherence when comparing reconstructed and true vertical
 731 velocities. There are two main reasons explaining these findings: the overall weakness of (true)
 732 w variance levels below the surface boundary layer in the submesoscale range; the coexistence in
 733 that range of several processes contributing to vertical motions, not just frontal turbulence but also
 734 inertia-gravity waves which force vertical velocities through terms that are generally not accessi-
 735 ble. Overall, the best reconstructions are thus observed in conditions characterised by energetic
 736 turbulence and/or weak stratification (such that near-surface frontal processes are felt well into
 737 the ocean interior). In particular we observed the best results in regimes for a western boundary
 738 (LMX with elevated EKE) and wintertime Porcupine Abyssal Plain (OMS, very weak water col-
 739 umn stratification). Conversely the weak vertical flow found in the AZO region where EKE is low
 740 and subsurface stratification is relatively strong is poorly captured by the omega approach.

741 Implications on the role of submesoscale vertical velocities and whether/how to integrate them
 742 into our representations of property exchanges in the ocean interior will require further elabora-
 743 tion. Numerous studies have highlighted the strong impact frontal submesoscale turbulence can
 744 have on physical and biogeochemical fluxes (Lapeyre et al. 2006; Klein et al. 2008; Thomas and
 745 Ferrari 2008; Capet et al. 2008). For a given tracer τ , this is only true to the extent that the mean
 746 distribution of τ exhibits vertical contrasts sufficiently close to the surface where frontal activity
 747 remains important. How close depends on the background environment and in particular on the

748 upper ocean stratification. The Surface Quasi-Geostrophic (SQG) theory is useful to qualitatively
749 apprehend this dependance (Lapeyre et al. 2006).

750 In most past studies dealing with vertical velocities a quasi geostrophic version of the omega
751 equation was used, but more recently, several authors have included higher order terms. For this
752 reason, we also evaluated the possible improvements obtained by using a more elaborate version of
753 the adiabatic equation compared to the simple quasi geostrophic formulation. NG reconstructions
754 that include ageostrophic forcing terms due to flow deformation leads to improved reconstructions.
755 The improvements are substantial only in conditions where near-surface frontal processes (i.e.,
756 submesoscales) are important. This finding has important implications in the context of efforts
757 aimed at estimating vertical velocities in the real ocean because the adiabatic QG reconstruction
758 only requires the knowledge of the density field and of the sea surface height (or a reference level
759 of no motion).

760 The consequences of various numerical choices on the reconstruction skills have been investi-
761 gated in this work. Choices made for the bottom boundary condition have a major impact. Pushing
762 the boundary condition as deep as possible is the only rule of thumb that can be provided. The
763 relative performance of the Dirichlet versus Neumann boundary conditions cannot be anticipated
764 a priori while the BBC tweak proposed by Rudnick (1996) offers at best marginal improvements.
765 Obviously, omega reconstruction skills will worsen when it is applied to real observations with
766 lesser spatial resolution (for the ocean interior data), synopticity issues and instrumental errors.

767 APPENDIX

768 **A1. Baroclinic mode decomposition**

769 To support the results in section 4d, we use a normal mode decomposition to establish possible
 770 relations between the depth of the vertical boundary condition and the error committed when
 771 estimated w with ω . The eigenfunctions are solution of the eigenvalues problem:

$$\frac{\partial^2 G_n}{\partial z^2} + \frac{N^2}{c_n^2} G_n = 0 \quad (A1)$$

772 or

$$\frac{\partial}{\partial z} \left(\frac{1}{N^2} \frac{\partial F_n}{\partial z} \right) + \frac{1}{c_n^2} F_n = 0 \quad (A2)$$

773 with the boundary conditions:

$$G_n = 0 \text{ at } z = 0 \text{ and } z = -H \quad (A3)$$

774

$$\frac{\partial F_n}{\partial z} = 0 \text{ at } z = 0 \text{ and } z = -H \quad (A4)$$

775 where the vertical velocity modes G_n and the pressure modes F_n are related through the relation,

$$F_n = \frac{\partial G_n}{\partial z}. \quad (A5)$$

776 Vertical variability can then be projected onto the vertical modes F_n and G_n so that,

$$p(x, y, z, t) = \sum_{n=0}^{\infty} \tilde{p}_n(x, y, t) F_n(z) \quad (A6)$$

777

$$w(x, y, z, t) = \sum_{n=0}^{\infty} \tilde{w}_n(x, y, t) G_n(z), \quad (A7)$$

778 with $\tilde{p}_n$ and $\tilde{w}_n$ the modal amplitudes of the pressure and vertical velocity respectively.

779 To investigate more thoroughly the contribution of the vertical modes to the vertical velocity
 780 signal, we expressed the vertical velocity by the projection on the three firsts vertical modes and a
 781 residue,

$$w(x, y, z, t) = \sum_{n=1}^N \tilde{w}_n(x, y, t) G_n(z) + \varepsilon. \quad (A8)$$

782 ε was estimated for $N = [1 : 3]$. The number of profiles where ε/w was lower than 0.5, that is to
783 say that more than half of the w dynamics is explained by the first one, two or three vertical modes,
784 was estimated (Fig. 12).

785 Note that in Figure 11, F_n and G_n are calculated for a mean stratification that is obtained using
786 spatial averaging over the entire region and time averaging over 11 daily model outputs. However
787 they do not differ substantially from the modes calculated on each point and used to infer modal
788 amplitudes (Sec. 2c).

789 *Acknowledgments.* This work has been partly supported by the NASA/CNES Tosca project
790 BIOSWOT. Alice Pietri was supported by a CNES postdoctoral grant. The authors wish to
791 thanks the SWOT cal/val team for providing an stimulating environment in the development
792 of our study. The NATL60 simulation can be accessed at [https://meom-group.github.io/swot-](https://meom-group.github.io/swot-natl60/access-data.html)
793 [natl60/access-data.html](https://meom-group.github.io/swot-natl60/access-data.html). The authors wish to thank two anonymous reviewers for their comments
794 and suggestions for improving the paper.

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TABLE 1. Statistics derived from the spectral coherence field (fig.8). Note that relating the horizontal scale $L_{0.6}$ to the deformation radius, R_d , which is ~ 15 km in the OSM and REK regions and ~ 30 km in the LMX and AZO regions, yields a performance threshold of $0.3R_d$ on average, with a minimum $0.17R_d$ in winter OSM and a maximum $0.49R_d$ in winter REK. In the AZO region in December the squared coherence never exceeds 0.6 thus leading to a fraction of variance null.

	Horizontal scale $L_{0.6}$ [km] (and wavelength [km]) below which the squared coherence between true and reconstructed vertical velocities is below 0.6. Values are provided for QG and NG reconstructions				fraction of vertical velocity variance retained by the reconstructed vertical velocity over the scale range $L > L_{0.6}$. Values are only provided for the NG reconstruction	
	Jun		Dec		Jun	Dec
	QG	NG	QG	NG		
LMX	9.2 (58)	6.7 (42)	9.5 (60)	7.8 (49)	0.90	0.84
AZO	6.4 (40)	6.3 (40)	-	-	0.74	0
REK	4.7 (30)	4.6 (29)	7.3 (46)	6.5 (41)	0.87	0.61
OSM	3.9 (25)	3.9 (25)	3.0 (19)	2.6 (16)	0.72	0.88

1134 TABLE 2. Averaged errors (in m day^{-1} and percentage of w_{model}), at depths z_a , for ω with perfect right hand
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	$\omega_{\dagger}^*$		$\omega_{\dagger}$		ω_{NG}^*	
LMX	Jun	Dec	Jun	Dec	Jun	Dec
	0.41 (3%)	0.54 (5%)	4.08 (28%)	2.85 (24%)	4.87 (34%)	5.21 (44%)
AZO	Jun	Dec	Jun	Dec	Jun	Dec
	0.04 (3%)	0.04 (3%)	0.25 (20%)	0.27 (23%)	0.80 (65%)	0.95 (79%)
REK	Jun	Dec	Jun	Dec	Jun	Dec
	0.13 (4%)	0.11 (3%)	0.96 (29%)	1.19 (29%)	1.47 (45%)	2.85 (69%)
OSM	Jun	Dec	Jun	Dec	Jun	Dec
	0.06 (2%)	0.20 (4%)	0.66 (19%)	0.90 (16 %)	2.06 (58%)	2.96 (52 %)

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- 1179 **Fig. 11.** First three baroclinic pressure modes for the a) LMX, b) AZO, c) REK, and d) OSM region
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