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On modeling turbulent exchange in buoyancy-driven fronts

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ABSTRACT

Our primary objective is to quantify the uncertainty in the solution space associated with mixing and stirring in ocean general circulation models (OGCMs) due to common modeling choices, namely the spatial resolution, tracer advection schemes, Reynolds number and turbulence closures. In many cases the assessment of errors is limited by the observational data set, therefore, large eddy simulations from a spectral element Boussinesq solver are taken as ground truth. First, the lock-exchange problem is used to quantify the temporal evolution of mixing from shear-driven stratified overturns. It is found that mixing in an OGCM is more sensitive to the choice of grid resolution than any other parameters tested here. The results do not monotonically converge towards the ground truth as the resolution is refined. Second, stirring of a passive tracer by submesoscale eddies generated by surface density fronts is considered. We find that using a second-order turbulence closure leads to an accurate representation of the restratification in the mixed layer.

1. Introduction

Ocean general circulation models (OGCMs) are the primary tools for predicting ocean currents and changes in the ocean's stratification. Many OGCMs integrate the hydrostatic primitive equations (PE) set using a variety of horizontal and vertical coordinates, mixing parameterizations and advection schemes (e.g., Griffies et al., 2000, 2004). OGCMs have experienced significant development over the past two decades (Chassignet et al., 2006; Capet et al., 2008; Martin et al., 2009; Fox-Kemper and Menemenlis, 2008; Lemarié et al., 2012). These models can be configured at the global and regional scale, or can have a nested structure to represent multi-scale interactions (Debreu et al., 2012). Modern OGCMs contain realistic forcing, domain geometry, and assimilate ocean data available from a wide range of instruments, including (but not limited to) satellite altimeter, sea surface temperature, current meters, drifters and other *in situ* data for temperature and salinity.

The progress in OGCM development has been facilitated by the operational needs of the Navy as well as those of the basic research community (Shchepetkin and McWilliams, 1998; Hurlburt et al., 2009). Ocean observing and assimilation techniques have matured to a level where one can claim that the dynamics, phase and strength of the ocean's mesoscale features are adequately represented in OGCMs. For instance, Thoppil et al. (2011) show that the energetics of the mesoscale field observed by drifters and satellite can be reproduced by both data-assimilative and non-assimilative models using a horizontal resolution of 1/12°–1/25°. Operational OGCMs can also exhibit a good predictive skill for the turn over time scales of mesoscale eddies (Hurlburt et al., 2008).

Nevertheless, OGCMs may encounter significant obstacles for reproducing accurate results for scales smaller and faster than the mesoscale (scales smaller than O(10) km and shorter than a few days) due primarily to three reasons. First, data at such scales may not be available from observing systems, or contain technical challenges within the context of present assimilation methods. For instance, sea-surface height data is usually converted to velocity under the assumption of geostrophy, while submesoscale flows are distinctly ageostrophic (Mahadevan and Tandon, 2006; Thomas et al., 2008).

Second, OGCMs may not resolve submesoscale features fully and must rely on subgrid-scale (SGS) parameterizations (Fox-Kemper et al., 2008; Fox-Kemper and Ferrari, 2008). Recent numerical studies showed that the SGS parameterization can have important consequences in the temporal and spatial evolution of submesoscale instabilities even when the grid spacing resolves the submesoscale (Ramachandran et al., 2013). OGCMs were originally designed to model large scales processes (i.e., on the order of the radius of deformation), where the flow is anisotropic with lateral processes being far more energetic than vertical processes. Therefore, these models sub-divide the SGS parameterizations for

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the transport of momentum and tracers to whether they occur in the horizontal or vertical directions. In both cases, the unresolved processes are represented through an eddy viscosity or diffusivity. The vertical SGS models commonly used in OGCMs were originally designed for situations where turbulent processes are not even partially resolved and, therefore, the model resolution does not appear explicitly. These models fall into two basic categories: algebraic models, like KPP (K-Profile Parameterization, Large et al. (1994)) and second order turbulence closures (Large, 1998; Canuto et al., 2001). While there have been criticisms of KPP for needing tuning of dimensional parameters for different flows (Chang et al., 2005), the KPP algorithm has appeal not only because of its simplicity, but also because it has been shown to work reasonably well in challenging flows involving fully 3D stratified mixing affected by the details of bottom topography (Chang et al., 2008) within the limitations of the observational data sets. Second order turbulence closures have a long history of development (Mellor and Yamada, 1982; Kantha and Clayson, 1994; Burchard and Baumert, 1995; Burchard and Bolding, 2001; Canuto et al., 2001; Baumert and Peters, 2004; Baumert et al., 2005; Warner et al., 2005b; Umlauf and Burchard, 2005; Canuto et al., 2007), and they have also been shown to work reasonably well in complex problems involving shear-driven stratified mixing (e.g., the correct representation of mixing between overflows and ambient water masses; Ilicak et al., 2008). These models have a higher computational cost than algebraic models, since they require integration of two additional prognostic equations (typically turbulent kinetic energy and dissipation rate), as well as include significant assumptions on the form of these equations (Wilcox, 1998). Both classes of SGS models are aimed to estimate a diffusivity coefficient, parameterizing only the downward energy cascade processes. Parameterizations that potentially address upward energy cascade, or dispersion (as opposed to dissipation) potentially exist (San et al., 2011; Berselli et al., 2011), but have not been extensively investigated yet.

Third, even if the OGCMs contain the spatial resolution to extend into the submesoscales and below, the PE start losing validity, being subject to the hydrostatic approximation (Kantha and Clayson, 2000). The hydrostatic approximation affects both dissipative and dispersive properties of fluid motion. Neither the overturning of density surfaces by Kelvin–Helmholtz (KH) instability, which is one of the primary mechanisms responsible for mixing in the ocean (McWilliams, 2008; Taylor and Ferrari, 2009), nor the correct dispersion relation for non-linear internal waves can be explicitly captured with hydrostatic models. Since the inclusion of a non-hydrostatic pressure solver in OGCMs requires a substantial change in these codes, recent efforts have focussed on the development of suitable solvers (Scotti and Mitran, 2008) and hybrid hydrostatic and non-hydrostatic models (Botelho et al., 2009; Duan et al., 2010; Campin et al., 2010). As both of these avenues will not only require significant code development, but also will generate substantially larger model output for post-analysis, there is still need for further investigations within the formalism of the existing OGCMs.

To conclude, there is a need for carefully evaluating the accuracy of the OGCMs (and their SGS models) below the mesoscale regime. The scales of interest include submesoscales, as well as fully 3D stratified mixing.

The submesoscale phenomena were first recognized by McWilliams (1985) and received considerable attention in recent years, with the identification of mixed-layer instability (Boccaletti et al., 2007; Fox-Kemper et al., 2008) and the importance of submesoscale motions in biogeochemical transport in the ocean (Lévy et al., 2001; Klein and Lapeyre, 2009; Calil and Richards, 2010). In addition, submesoscale motions are thought to form the bridge between long-lived quasi-geostrophic motions and rapidly-dissipating small scale turbulence (Müller et al., 2005; McWilliams, 2008; Capet et al., 2008). Stratified mixing is of interest in coastal phenomena (Warner et al., 2005a; MacCready et al., 2009), as well as during deep water formation (Legg et al., 2009). Therefore, it is critical that OGCMs represent stratified mixing accurately, or alternatively, the errors associated with their parametric representation are quantified.

Here, we present a direct comparison of results from two types of problems that are challenging for OGCMs:

(1) So-called lock-exchange (LE) problem, which is a simple computational setting to quantify the temporal evolution of mixing in a stratified fluid. This problem is discussed in some detail by Özgökmen et al. (2009a,b).
(2) Mixed-layer instability (MLI) for submesoscale motions. MLI is very similar to the LE problem in terms of the computational setting, but differs dynamically due to the presence of ambient rotation and a high-aspect domain ratio. MLI was studied using LES by Özgökmen et al. (2011, 2012) and Özgökmen and Fischer (2012). The metric of interest here is the lateral stirring carried out by the submesoscale MLI eddies. This is of relevance to the lateral dispersion of pollutants and biogeochemical tracers in the ocean.

While computations for both problems are carried out in idealized settings, they have the advantage that LES (large eddy simulation, Sagaut (2006)) solutions are feasible and serve as ground truth. LES refers to numerical solutions of the non-hydrostatic equations in which the large eddies, carrying most of the Reynolds stresses, are resolved through computation, while the effect of the smaller eddies on the flow is represented by SGS models that depend explicitly on the resolution of the model. The goal of these SGS models is to anticipate higher resolution results at any given resolution (hence simulations performed using LES will converge as resolution is increased). The LES approach lies in between the extremes of direct numerical simulation (DNS), where all turbulence is resolved, and Reynolds-averaged Navier–Stokes (RANS), in which only the mean flow is computed while the entire effect of turbulence is represented by SGS models (such as the second order turbulence closures). Since LES greatly reduces the SGS parameterization problem, many studies on ocean turbulence have relied on this approach to establish a ground truth for particular problems (Wang et al., 1998; Large, 1998; Chang et al., 2005; Xu et al., 2006). In addition, recent studies (Fox-Kemper and Menemenlis, 2008; Ramachandran et al., 2013) have shown that LES techniques can replace the traditional RANS methods and are a promising avenue for SGS parameterizations in high-resolution ocean models.

The paper is organized as follows. Section 2 gives a brief introduction on the numerical models used in this study. In Sections 3 and 4, models configuration, experimental description, metrics employed and results are presented for the LE and the MLI problems, respectively. The principal findings are summarized in Section 5.

2. The numerical models

2.1. LES model – Nek5000

Our reference model is Nek5000, which integrates the Boussinesq equations (BE) based on the spectral element method, a high order finite element method for partial differential equations (Patera, 1984; Fischer, 1997). Nek5000 has been previously used for oceanic applications relevant to mixing and stirring, such as LES of LE problem (Özgökmen et al., 2007, 2009a,b) as well as