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Eulerian Dynamics and Lagrangian Transport at the Submesoscale and Below

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UNIVERSITY OF MIAMI

EULERIAN DYNAMICS AND LAGRANGIAN TRANSPORT
AT THE SUBMESOSCALE AND BELOW

By
Jean A. Mensa

A DISSERTATION

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EULERIAN DYNAMICS AND LAGRANGIAN TRANSPORT
AT THE SUBMESOSCALE AND BELOW

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The goal of this work is to study the Lagrangian and Eulerian properties of the scales below the mesoscale. In the last few years, developments in the observations and numerical modeling capabilities allowed to venture in the domain of the submesoscale (SM) opening a broad range of questions on the dynamics of these scales and their role in the ocean circulation. In the first part of this dissertation we investigate some of the properties of these scales while in the last part we enter the domain of the fully 3D dynamics with a study of dynamics of the convective mixed layer.

The formation mechanism of SM is investigated in Chapter 2. In particular, we focus on the seasonality of SM. In order to approach this problem, a realistic simulation of the Gulf Stream (GS) region with the Hybrid Coordinate Ocean Model is integrated for 18 months at two horizontal resolutions: a high-resolution (1/48°) simulation able to resolve part of the submesoscale regime and the full range of mesoscale dynamics, and a coarser resolution (1/12°) case, in which submesoscales are not resolved. Results provide an insight into submesoscale dynamics highlighting a clear seasonal cycle, with submesoscale features mostly
present during winter. The limiting and controlling factor in the occurrence of submesoscales appears to be the depth of the mixed layer, which controls the reservoir of available potential energy available at the mesoscale fronts that are present most of the year. Atmospheric forcings are the main energy source behind submesoscale formation, but mostly indirectly through mixed layer deepening. This result represented the first evidence of seasonality of SM features and was successively confirmed by Shcherbina et al. (2013) via direct observations.

SM features have been found to play an important role on ocean material transport, governing horizontal dispersion at the small scales Poje et al. (2014). Similarly, it is thought that SM features, given their large vertical velocities, might play an important role in the transport of biogeochemical nutrients in the upper ocean. In particular, vertical transport of nutrients is thought to be located mostly in ocean eddies. Motivated by the lack of a clear understanding of these processes in Chapter 3 we perform a set of numerical simulations in order to study some of the proposed vertical transport mechanisms. The MITgcm is integrated in four different configurations: two summer configurations with shallow mixed layer, one with wind and one without, and two winter simulations with deep mixed layer, one with wind and one without. The goal is to simulate the effect of Eddy-Ekman pumping and SM pumping. Results show that wind forced simulations present strong internal wave activity in the near-inertial band. Also, large vertical velocities are found in the mixed layer of the winter simulations. No clear sign of Eddy-Ekman pumping is observed in the vertical velocity field. In order to investigate the associated vertical transport, synthetic particles are released in all
simulations. Results show that wind forced summer simulation can provide only weak vertical transport and that including a mixed layer and SM features, strong vertical transport is observed within the mixed layer and across the mixed layer and the water column.

Motivated by the importance that SM plays on the dynamics of the upper ocean in Chapter 4 we venture into smaller scales trying to bridge the gap between the SM and the fully 3D dynamics of the upper ocean. Here we present results from two non-hydrostatic simulations of a weakly wind and buoyancy forced mixed layer with semi-realistic diurnal cycling. Both purely buoyancy-forced and wind- and buoyancy-forced flows are sampled using passive tracers, as well as 2D and 3D particles to investigate characteristics of horizontal and vertical dispersion. It is found through tracer releases that the surface patterns of the tracer were determined by the convergence zones created by buoyancy-driven convection within a time scale of a few hours. For pure convections the results display the classic signature of Rayleigh-Benard cells. When combined with a wind stress the convective cells become organized such that the along-wind length scale becomes much larger than the cross-wind scale of the convective cells. Relative dispersion computed by sampling the flow fields using both 2D and 3D particles shows Richardson regimes meaning that particle separation is driven by processes at the scale of the particle separation. Relative dispersion is found to be much higher in wind driven mixed layer and 2D surface-releases transitioned to Richardson regime faster in the wind forced simulation. We also show that the buoyancy-forced case results in significantly lower amplitudes of scale-dependent relative diffusivity,
than those reported by Okubo (1970), but the wind- and buoyancy-forced case was in good agreement with Okubo’s diffusivity amplitude, and scaling was consistent with the Richardson law, $k_D \sim \ell^{4/3}$. These results represent a first investigation of the Lagrangian properties of the ~3D flows of the upper ocean and suggest that transport is governed by local processes.

The ultimate goal of this dissertation is to shed some light on the properties of the fine structure of the oceans in the belief that a complete understanding of the ocean dynamics cannot prescind from the understanding of its smaller scales.
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Contents

List of Figures viii

List of Tables xix

1 Introduction 1

1.1 Scales of motion in the ocean 3

1.1.1 Submesoscale and below 7

1.2 Material transport 11

1.2.1 Vertical material transport 14

1.3 Scientific motivation 18

1.4 Open questions 20

2 Seasonality of the Submesoscale Dynamics 24

2.1 Methods 26

2.1.1 Flow decomposition 31

2.2 Mechanisms of submesoscale generation: frontogenesis and mixed layer instabilities 35
2.2.1 Frontogenesis in the mixed layer ........................................ 35
2.2.2 Mixed Layer Instabilities .................................................... 40

2.3 Diagnosing the characteristics of submesoscale features .......... 44
2.3.1 Horizontal Length Scale .................................................... 45
2.3.2 Deviation from gradient wind balance .................................. 46
2.3.3 Relative vorticity and Rossby number .................................. 47
2.3.4 Okubo Weiss parameter ..................................................... 51

2.4 Role of stratification and mixed layer depth on submesoscale seasonality .......................................................... 56
2.4.1 Seasonality of surface stratification and MLD ................... 58
2.4.2 Dependence of MLIs on MLD ............................................. 64

2.5 Concluding remarks ............................................................. 67
2.5.1 Surface fluxes parametrization ............................................. 70

3 Material Transport in Ocean Eddies ................................. 74
3.1 Methods ................................................................................. 76
3.1.1 Model equations ................................................................. 77
3.1.2 Initial conditions and spin-up ............................................ 81

3.2 Results .................................................................................... 83
3.2.1 Eulerian Dynamics ............................................................... 84
3.2.2 Material Transport ............................................................... 106

3.3 Concluding remarks ............................................................. 119

4 Material Transport in the Mixed Layer ................................ 121
4.1 Methods .................................................. 123
   4.1.1 Numerical model and configuration ................. 124
   4.1.2 Forcing ........................................... 126
4.2 Dynamics ................................................. 130
   4.2.1 Buoyancy-driven mixing ............................ 130
   4.2.2 Buoyancy and wind driven mixing .................. 131
4.3 Material Transport ...................................... 136
   4.3.1 Passive scalar transport ........................... 136
   4.3.2 Lagrangian transport .............................. 143
4.4 Concluding remarks ...................................... 164

5 Conclusions .............................................. 169
   5.1 Mechanisms and Implications of the SM Dynamics .... 170
   5.2 Role of SM on vertical transport of nutrients in mesoscale eddies. 171

References .................................................. 174
# List of Figures

1.1 True color image of a phytoplankton bloom in the North Atlantic Ocean west of Ireland - http://oceancolor.gsfc.nasa.gov .......................... 3

1.2 Representation of the processes involved in the forward and backward energy cascade. In the box are represented the processes associated to the transition towards dissipative scales in the SM regime. ................................................................. 8

1.3 Chlorophyll concentration in ocean eddies from satellite observations McGillicuddy and Robinson (1998). ................................. 15

2.1 The domain of the LR simulation of the Atlantic Ocean at 1/12° horizontal resolution where the box represents the extent of the nested HR simulation at 1/48° horizontal resolution. The gray color represents the bathymetry of the region. ......................... 28

2.2 SST [°C] snapshot during the winter season from the HR simulation. The boxes represent the regions over which diagnostics are computed. ................................................................. 30
2.3 Values of $D$ (equation (2.1)) for $u,v$ and density $\rho$ as function of $\lambda$ computed over region A during the winter season of the all domain of the HR simulation. . . . . . . . . . . . . . . . . . . . . . . . . . 33

2.4 (a) Total ($c$), (b) filtered ($\bar{c}$) and (c) residual speed ($c' [m s^{-1}]$) at 60m depth during winter season for the HR simulation. . . . . . . 34

2.5 Vertical velocity $\omega [m s^{-1}]$ computed for HR (a) during winter at 60 m depth and (b) during summer at 5 m depth and (c) for LR during winter at 60 m depth. Depths are chosen in order to represent the mixed layer. . . . . . . . . . . . . . . . . . . . . . . . . . 38

2.6 Time series of the module of vertical velocity $|\omega| [m s^{-1}]$ computed as average values over region A at 4 m depth for the HR simulation. 39

2.7 $w'b' [m^2 s^{-3}]$ for (a) winter at 60 m, (b) summer season at 5 m in HR and (c) for winter LR at 60 m. . . . . . . . . . . . . . . . . . 41

2.8 Vertical dependence of $w'b'$ ($[m^2 s^{-3}]$, equation (2.5)) averaged over region A for HR during winter season. The dots represent the mixed layer depth (and corresponding value of PK) for HR ($\sim 171 m$, red dot) and LR ($\sim 226 m$, blue dot). . . . . . . . . . . . . 42

2.9 Time series of the conversion rate of available potential energy into eddy kinetic energy, PK $[m^2 s^{-3}]$, as computed in equation (2.5). PK is integrated over region A at 5 m depth for HR (solid line) and LR (dashed line). . . . . . . . . . . . . . . . . . . . . . . . . . 44
2.10 Kinetic energy (KE, \([m^2 \ s^{-2}]\)) integrated over the submesoscale wave numbers computed from equations (2.6), for both HR (black line) and LR (blue line). .................................................. 46

2.11 Unbalanced regions computed in region S for (a) winter at 60 \(m\) depth and (b) summer season at 5 \(m\) depth. ................................. 48

2.12 (a) Vertical dependence of the Rossby number averaged over region A for summer (dashed lines), winter (solid lines), HR (black lines) and LR (blue lines). The red dots on the curves represent the mixed layer depth. (b) Seasonal trend of the frequency of instances of \(Ro > 0.5\) over region A for both resolutions at 5 \(m\) and 500 \(m\) depth. ................................................................. 50

2.13 PDF of relative vorticity for winter season, HR (left panel) and LR (right panel), normalized over \(f_0\). The solid lines are for PDFs at 10 \(m\) depth and the dashed line for PDFs computed at 500 \(m\) depth. The red lines represent the pdf of the normal distribution computed with the same standard deviation as the 10 \(m\) depth PDF and with zero mean. ................................. 51

2.14 Okubo-Weiss parameter (\(OW\)) normalized by \(f_0^2\) computed at the surface (5 \(m\)) for winter (left column), summer (right column), HR (top row) and LR (bottom row). ................................. 53
2.15 Temporal evolution of the components of the Okubo-Weiss parameter \([s^{-2}]\), from equation (2.9)) integrated over region A at 5 \(m\) depth for (a) HR and (b) LR: \(OW\) (Okubo-Weiss parameter, red line), \(S^2\) (strain rate, black line), \(\zeta^2\) (relative vorticity squared, gray line) and \(\delta^2\) (divergence squared, blue line).

2.16 Density \((\sigma_2)\) sections showing the vertical stratification for the winter (left panels) and summer (right panels) season in the HR simulation. In the top panels daily snapshots are shown, while averages for the same sections over one month are shown in the lower panels (dashed lines are the mean values plus or minus the standard deviation). Mixed layer depth is represented by a white line in the top panels and black line in the lower panels.

2.17 (a) Temporal variability of the mixed layer depth \([m]\) averaged over region A (black line, HR and blue line LR). (b) The correlation in time between surface forcings \((f_T\) dashed line, \(f_S\) dashed-dotted line and \(u^*\) dotted line) and mixed layer depth is shown for the last 365 days of the simulation. Red line in (b) represents the mixed layer autocorrelation function. The gray line in (a) represents the begin of the portion of the time series that has been used to compute \(r[t]\).
2.18 Time series of the terms in equation \((2.13)\) for HR. \(\langle w' b' \rangle_{xyz}\) in red, \(\langle |\nabla b| \rangle_{xyz} \cdot \langle MLD \rangle_{xy}^2\) in blue, \(|\nabla b|\) in solid gray and \(\langle MLD \rangle_{xy}\) in dashed gray. All curves are normalized over the maximum value of each time series. ........................................... 64

2.19 Autocorrelation between the timeseries of \(\langle w' b' \rangle_{xyz}\) and \(\langle MLD \rangle_{xy}^2\) solid line, \(\langle w' b' \rangle_{xyz}\) and \(|\nabla b|\) dashed line and \(\langle w' b' \rangle_{xyz}\) and \(|\nabla b| \rangle_{xyz} \cdot \langle MLD \rangle_{xy}^2\) dotted line. ......................... 66

2.20 (a) Temporal variability of the bulk fluxes of (a) heat \([W m^{-2}]\), (b) salinity \([10^{-3} kg m^{-2} s^{-1}]\) and (c) wind speed \([m s^{-1}]\) averaged over region A. The gray line represents the first point of the time series considered. .............................................. 72

3.1 Daily cycle of the neat surface heat flux \(Q_0\). .................. 80

3.2 Potential density section of the warm core eddy extracted from HYCOM. The black lines represent the slice used to initialize the model in the Summer configuration. ................. 83

3.3 Temperature section \(\degree C\) for the (a) summer and (b) winter configurations after spin-up. ................................. 84

3.4 Temperature sections \(\degree C\) at 50 m depth for all four experiments at 30 days into the simulation. ................................. 86

3.5 Difference between temperature \(\degree C\) at 500 m depth for all four experiments at 30 days into the simulation. ................................. 88
3.6 Vertical sections of averaged horizontal velocity magnitude and anomalies respect to $S |\bar{u}|^{\theta,t} [ms^{-1}]$. (a) Exp. S (b) Exp. SW-S, (c) Exp. W-S and (d) Exp. WW-S after 30 days after spin-up. Contours represent the isothermal surfaces. .......................... 90

3.7 Vertical sections of the averaged vertical velocity magnitude $|\bar{w}|^{\theta,t} [ms^{-1}]$ for (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW after 30 days after spin-up. Contours represent the isothermal surfaces. .......................... 91

3.8 Sections of instantaneous vertical velocity $[ms^{-1}]$ at 50 m depth for (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW 30 days after spin-up. The dot represents the probe location used to compute frequency spectra. .......................... 93

3.9 Sections of instantaneous vertical velocity $[ms^{-1}]$ at 500 m depth for (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW 30 days after spin-up. The dot represents the probe location used to compute frequency spectra. .......................... 94

3.10 Q-vector divergence $g\rho_0^{-1}\nabla h \cdot \mathbf{Q} [m^{-1}s^{-3}]$ for the (a) summer and (b) winter configurations after 30 days. .......................... 98

3.11 Wind induced time average vertical velocity $w_e [ms^{-1}]$ at the surface for (a) Exp. SW and (b) Exp. WW after 30 days of spin-up. 100

3.12 Hovmöller diagram of vertical velocity $w [ms^{-1}]$ for the probes $p_0$, $p_1$ and $p_2$ for all simulations. Time is in inertial periods $IP \approx 17.5hrs$. All diagrams are computed starting 30 days after spin-up. 102
3.13 Vertical velocity power spectra for all experiments and all probes.

The vertical lines represent the inertial period (dashed line), the forcing period of 3 days (solid thin line) and two harmonics (solid thin lines). .......................................................... 104

3.14 Time series of the net surface stress magnitude $|\tau|$ for SW at different probe locations. .......................................................... 106

3.15 Final vertical position of particles released after 30 days and advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. .......................................................... 109

3.16 Final vertical displacement respect to 50 m release depth after 30 days and advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. Positive values mean upward displacement. .......................................................... 111

3.17 Final vertical displacement respect to 50 m release depth after 30 days and advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. Positive values mean upward displacement. .......................................................... 112

3.18 Total particle flux $|P|^2$ for each release depth for particles advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW .......................................................... 115

xiv
3.19 Net particle transport trajectories computed from equation 3.13 and 3.14 for each release depth for particles advected for 50 days in (a) Exp. \( S \), (b) Exp. \( SW \), (c) Exp. \( W \) and (d) Exp. \( WW \). Colors stand for temperature. 

4.1 (a) The initial condition for temperature (blue) and the corresponding Brunt-Väisälä frequency \( N \) (red). (b) Daily cycle of penetrating short wave radiation \( Q_s \). Cooling at the surface is constant in time and balances the short wave radiation. (c) Daily cycle of short wave radiation at the surface \( Q_0 \) (solid) and long wave radiation \( Q_L \) (dashed). 

4.2 Temperature field for the simulation Exp. \( B \) during the first two convective cycles: at the beginning of the surface heating ((a) at 12 hours and (c) at 36 hours) and at the end of the cycle ((b) at 24 hours and (d) at 48 hours). The animation is available from: \( http://youtu.be/QtOrKF2zgw \).

4.3 Temperature field in Exp. \( BW \) (a) after 12 hours, during the first cooling event, (b) after 24 hours, at the end the first day, (c) at 36 hours during the second cooling event and (d) at 48 hours at the end of the second day. The animation is available from: \( http://youtu.be/TTYI6VvB3Y \).

4.4 (a) Speed \([ m \, s^{-1}]\) and (b) vertical velocity \([ m \, s^{-1}]\) at the end of the second convective event (at 36 hours) in Exp. \( BW \).
4.5 Time evolutions of domain averaged (a) horizontal speed \([m s^{-1}]\) and (b) vertical speed \([m s^{-1}]\) for the entire integration time for both Exps. \(B\) (red) and \(BW\) (blue). The dashed lines mark the spin-up period.

4.6 (a) Divergence \([s^{-1}]\) of the horizontal velocity field at 1\(m\) depth and (b) passive tracer concentration 3.1 hours after the release in Exp. \(B\).

4.7 (a) Divergence \([s^{-1}]\) of the horizontal velocity field at 1\(m\) depth and (b) passive scalar concentration 1.5 hours after the release in Exp. \(BW\).

4.8 Time dependence of the spatial correlation between the horizontal velocity divergence and tracer concentration for Exp. \(B\) (solid) and Exp. \(BW\) (dashed).

4.9 Time dependence of tracer concentration normalized variance for Exp. \(B\) (solid) and Exp. \(BW\) (dashed).

4.10 Horizontal location of a subset of particles released in a 1\(km\) by 1\(km\) box in the center of the domain in Exp. \(B\) (a) using 2D advection, and (b) using 3D advection of particles released at 5\(m\) (blue) and 15\(m\) (red) depth after 144 hours of integration. Same for Exp. \(BW\) in the case of (c) for 2D and (d) 3D particles after 14 hours of advection.

4.11 Temporal and vertical variability of the horizontally-averaged kinetic energy dissipation rate \(log(\epsilon) [W Kg^{-1}]\) for (a) Exp. \(B\) and (b) Exp. \(BW\) over three days after the spin-up.
4.12 Horizontally averaged vertical shear after 72 hours for Exps. $B$ and $BW$.

4.13 Relative vertical dispersion $\sigma_{D_z}^2(t)$ computed from 3D particle released at 5 m depth. The black line has slope $t^3$ characteristic of Richardson regime and the inset shows normalized dispersion.

4.14 Diffusivity versus length scale for particles released at $t = 72 \, \text{hr}$ in both experiments. The canonical Richardson slope $\ell^{4/3}$ is shown for comparison. The symbol X represents the value of eddy viscosity computed from inverse Ekman theory ($K_z \approx 6 \times 10^{-4} \, m^2 s^{-1}$) against the mixed layer depth of 50 m.

4.15 (Upper panel) Vertical diffusivity $K_z(t)$ in Exps. $B$ (red line) and $BW$ (blue line). The circles indicate the instances when particles were released in the flow field. (Lower panel) Time series of surface buoyancy forcing.

4.16 Relative dispersion $\sigma_D^2(t)$ for (a) 2D particles (released at 5 m solid, 10 m dashed, 15 m dashed-dotted) and (b) 3D particles in Exp. $B$. The slope $t^3$ shows the Richardson regime for reference. The insets show relative dispersion normalized by the Richardson regime.

4.17 Relative dispersion $\sigma_D^2(t)$ for (a) 2D particles (released at 5 m solid, 10 m dashed, 15 m dashed-dotted) and (b) 3D particles in Exp. $BW$. The slope $t^3$ shows the Richardson regime for reference. The insets show relative dispersion normalized by the Richardson regime.
4.18 Scale-dependent relative diffusivity $k_D(\ell)$ for Exp. $B$ (upper panels (a), (b) 3D)) and Exp. $BW$ (lower panels, (c), (d) 3D) using 2D sampling (left panels) and 3D sampling (right panels). Diffusivity is computed from particles released at $5\, m$ (red), $10\, m$ (green) and $15\, m$ (blue) depths. Okubo’s (1970) curve is plotted for reference in solid line. The dashed line marks Richardson’s scaling of $k_D \sim \ell^{4/3}$. . . . 163
3.1 Characteristics of the four experiments conducted. Two experiments are wind forced (SW,WW) and two experiments have a deep winter mixed layer (W, WW) . . . . . . . . . . . . . . . . . . . 79

4.1 Domain and mesh sizes in the numerical experiments. $L_x$, $L_y$ and $H$ are the horizontal and vertical domain sizes, $\Delta x$ and $\Delta z$ are the horizontal and vertical mesh sizes. . . . . . . . . . . . . . . . . . . . 125
Chapter 1

Introduction

Oceans encompass scales ranging from entire continents to the scale of the eddies around a pier. The oceans fascinated mariners and sailors since the early times of civilization and with them the exploration and description of the physical processes in oceanography began thousands of years ago. As in many fields of human developments, the knowledge of the ocean physics grew exponentially with time. The study of Physical Oceanography can be dated as far as the Greeks that with Archimedes famously defined the key concept of buoyancy. After them generations of mariners roamed to oceans trying to understand its movements but it was only few hundred years ago, with the rapid improvement of the naval technologies that a systematic description of the ocean currents began. Its of 300 years ago the identification of the Gulf Stream by Benjamin Franklin.
While these years represent the first modern attempt to a physical description of the oceans, it is only with the Scandinavian school, about hundred years ago, that a true understanding of the underlying physics driving the ocean dynamics became the focus of the investigation. From the observation of the ice pack drifting in the Arctic Ocean, Nansen and his student Ekman developed the theory that describes wind-driven circulation of the oceans. It is of these years the development of the hydrografic method which allows to derive ocean currents given the density profiles; the so called geostrophic velocities. The use of the hydrografic method to study the currents of the world imposed the development of a universal equation of state for sea water. These years represent the first rigorous description of the physics of the large scales ocean currents and represent the beginning of the modern oceanography. The Meteor expedition in the Atlantic from 1925 and 1927 allowed to discover the overturning circulation. And 20 years later most of the modern understanding of the upper ocean global circulation was completed with the theories on the general ocean surface circulation by Sverdrup, Stommel and Munk who were finally able to explain the original observations of the western boundary currents of almost 200 years before. The past few generations brought the discovery of mesoscale eddies with the Polygon 70 expedition and, in this generation, the first observations of the dynamic below the mesoscale. In this race
to explore smaller and smaller scales, a crucial role has been played by satellite measurements of altimetry and sea surface temperature which firstly allowed the observation of mesoscale eddies and sub-mesoscale dynamics. The present work fits in this scheme trying to push the boundary towards even smaller scales.

1.1 Scales of motion in the ocean

While the vastity of the oceans has been source of inspiration for the journeys of the first explorers it also represents most of the conceptual and technical chal-
lenge of the scientific investigation. The ocean dynamic extends form the ocean basins to the Kolmogorov scale in a range of scales which represents an enormous challenge for observations, modelers and theoreticians. Ocean basins are wide enough that it takes weeks to cross them and cruises sampling along these distances, even with today’s technologies, are extremely expensive and challenging. To large length scales also correspond slow time scales and the observation of basin wide phenomena can require up to years. On the other side, the ocean is also populated by small scale processes such as surface waves and coastal processes with time scales of few seconds and length scales of few centimeters. Sampling and describing this huge variety of scales is the ultimate challenge in physical oceanography.

At the upper end, i.e. the basin scale, the ocean dynamics can be described by the balance between pressure gradient and Coriolis force. This relationship, the geostrophic balance, allows describe most of large scale ocean dynamics. Fluids evolving in accordance to these prognostic equation are stationary and no vertical motion is allowed. The range of validity of the geostrophic balance is limited to large and slowly evolving scales. For slowly evolving large scales, Coriolis force dominates over the inertial term a relation described by the Rossby number,

\[ Ro = \frac{U}{fL} \] (1.1)
where $U$ and $L$ are the characteristic scales for horizontal velocity and length and $f$ is the Coriolis parameter. For flows in geostrophic balance, $Ro \ll 1$.

Allowing some degree of time dependence and vertical motion leads to the Quasi-Geostrophic (QG) equations, which can describe the time evolution of density fronts and their instability. The scales of the processes governed by the QG-equations, i.e. the mesoscale, is of the order of the Rossby deformation radius, i.e. the scale of the maximum growth rate of the instability of the thermocline. This is of the order of $\mathcal{O}(10) \text{ km} - \mathcal{O}(100) \text{ km}$ but varies in the oceans as it depends by the Coriolis parameter and stratification.

Both geostrophic and QG-equations are characterized by a backward energy cascade. The energy injected in the system by atmospheric forcing cascades towards larger scales and dissipation in the system is ultimately provided by some large scale mechanism such as friction with the ocean boundaries (McWilliams, 2008; Molemaker et al., 2010).

The range of scales right below the mesoscale, the so called submesoscales (SM), are an active field of research and the topic of Chapter 2 and Chapter 3. These are the smallest scales that can be described with the *primitive equations*, a simplification of the Boussinesq equations for small vertical velocities. The SM in many ways represent the gate before the fully 3D dynamics. These scales are
characterized by $Ro \sim 1$ which implies a weakening of the geostrophic constrain with weak Coriolis and buoyancy force which allows the flow to be more inertial and to develop large vertical velocities. These scales are thought to be responsible for the strong vertical velocities observed in the ocean mixed layer, that in theory are responsible for a large part of the biological production (Klein and Lapeyre, 2009). Also, the loss of geostrophy could lead to a more three-dimensional turbulent cascade, with energy flowing towards smaller scales as it would in isotropic turbulence (Muller et al., 2005; McWilliams, 2008; Molemaker et al., 2010). This would ultimately suggest a new mechanism for kinetic energy dissipation which would not involve large scale friction and would be solely associated to viscous dissipation.

Most of the human experience of the ocean develops nevertheless at scales well below the SM. Most human activities related to the ocean take place at the scales of the features that can be observed from a boat or a pier. These are the scales of the rip currents, surface gravity waves and Langmuir turbulence. These scales are fully three-dimensional. Compared to the large scale ocean circulation, at the small scales, the effect of planetary rotation is negligible ($Ro \gg 1$), and flows have the characteristics of the extensively studied non-rotating regime where the dynamics is dominated by advection and diffusion. As a consequence of such
small scales, energy is dissipated at the small scales by viscosity in the forward energy cascade described by Kolmogorov (1941).

1.1.1 Submesoscale and below

The present work focuses in particular on the SM and below. The SM length scale ranges from $O(100)\, m$ to $O(10)\, km$ and develop in a regime of weak stratification such as the mixed layer (Thomas et al., 2008). These are features that have been difficult to observe in nature because of their rapid evolution and the small length scale. Satellite observations of SST or ocean colors (Figure 1.1) allowed to have a visual cue on what these features look like. In particular, it is obvious from satellite imagery that the ocean is in fact extremely active at scales below the mesoscale. Recent studies allowed to measure the physical properties of the SM regime via Eulerian statistics (Shcherbina et al., 2013) and via Lagrangian observations (Poje et al., 2014). Nevertheless SM features have been observed in numerical models since many years and their dynamics is in the most part well understood (Fox-Kemper et al., 2008; Fox-Kemper and Ferrari, 2008).

The general mechanism of formation of SM features is illustrated in Figure 1.2 where the available potential energy stored in the highly energetic mesoscale features is transferred to the small scale by frontogenesis (Hoskins, 1982; Pedlosky,
1987; Giordani and Caniaux, 2001; Thomas and Lee, 2005; Lapeyre et al., 2006) and then released in form of eddy kinetic energy by instabilities of various type (Stone, 1966, 1970; Haine and Marshall, 1998; Boccaletti et al., 2007).

Frontogenesis develops mostly near the ocean surface, where the absence of vertical velocities allows straining from mesoscale eddies to increase density gradients, therefore leading to an effective sharpening of the existing density fronts (Bishop, 1993; McWilliams et al., 2009a,b). Surface horizontal density gradients $\mathbf{k} \cdot \nabla \rho$ spontaneously generate horizontal velocities in thermal wind balance with the density stratification increasing vorticity at the flanks of the front, and generating regions with strong horizontal strain.

Once fronts intensify instabilities can occur (Haine and Marshall, 1998). In particular, given the presence of a density gradient, baroclinic mixed layer in-
stabilities (MLI, Boccaletti et al. (2007); Stone (1966, 1970)) can develop. This is a class of instabilities that share the same mechanism of the classic mesoscale baroclinic instability but that generates features which have large $Ro$ and are thus ageostrophic. The idea, is that features generating in this ageostrophic realm are then unstable and will eventually decay towards smaller features instead of backward as in geostrophic turbulence (Molemaker et al., 2005; Muller et al., 2005; McWilliams, 2008; Molemaker et al., 2010).

This mechanism of formation of SM features is susceptible to the properties of the mixed layer, in which strong stratification can inhibit the formation of frontogenesis and MLIs. This condition is common in some regions during the summer season which could explain why SM features have been so hard to observe in the real ocean (Capet et al., 2008a; Mensa et al., 2013; Sasaki et al., 2014). Seasonality and formation mechanism of MLIs is described in Chapter 2.

The other major class of instabilities is represented by a shear instability, the Kelvin-Helmholtz instability. This is an instabilities which is fully ageostrophic and generates features fully 3D. Nevertheless observations of shear instabilities in the ocean are rare and numerical models resolving these processes in the context of a realistic ocean are still missing.
At higher wavenumbers than the submesoscales, e.g., at scales from 100 m to few meters, mixed layer processes get even richer. These are scales ranging from the lower limit of the SM regime, where Coriolis force and stratification are still important, to processes that are fully isotropic. One example of these processes is the Langmuir turbulence (Langmuir, 1938; Craik and Leibovich, 1976; Skyllingstad and Denbo, 1995; McWilliams et al., 1997; Thorpe, 2004; D’Asaro, 2014). This type of turbulence dominates the flow field in presence of strong winds (> 10 ms⁻¹) and fully developed surface gravity waves (Belcher et al., 2012).

The mixed layer circulation is also driven by convection due to surface buoyancy forcing. Convection is studied using laboratory experiments (Sharp, 1984; Bodenschatz et al., 2000), numerical simulations (Nagai et al., 2005) and ocean observations (Brainerd and Gregg, 1993a, 1995). It is still not entirely clear how convection affects vertical or horizontal material transport in the mixed layer (Klein and Lapeyre, 2009).

As we go towards even finer scales, we encounter other phenomena, e.g., so-called ramps, namely abrupt jumps in the SST which seem to develop in the regime of weak winds and strong buoyancy forcing at scales spanning from few meters to several hundred meters (Thorpe, 1985; Soloviev, 1990; Soloviev and Lukas, 1997; Thorpe and Osborn, 2003; Wijesekera et al., 2004). These type of
features have been observed in numerical simulations as well as in the ocean, but there is very little knowledge on how they all coexists and influence each other. This is because none of the ocean processes exists in isolation, and smaller scale processes typically last for brief periods. Therefore it is quite difficult to assess their individual roles in the presence of multi-scale interactions spanning a wide range.

In Chapter 4, we address some of the properties of this small scale regime focusing in particular on material transport. These are the scales of most of the human activities and are potentially important in the study of pollutant and biogeochemical tracers dispersion.

1.2 Material transport

An important part of this work is the study of the transport associated to the SM features and below. The study of material transport in the oceans is of interest due to its importance in the dynamics of passive and active tracers, such as heat (Chelton et al., 2007), biogeochemical tracers (McGillicuddy and Robinson, 1998; Klein and Lapeyre, 2009; Mahadevan et al., 2012; Lévy et al., 2011) and pollutants (Jernelöv and Lindén, 1981; Crone and Tolstoy, 2010; Poje et al., 2014). Most of these processes take place in the upper-ocean mixed layer. For example, primary
production occurs in the upper ocean as it requires sunlight, and it is sustained by the vertical provision of nutrients from underneath the euphotic zone (Lévy et al., 2001; McGillicuddy et al., 2007; Mahadevan et al., 2012). Similarly, hydrocarbons released during oil spills tend to accumulate on the ocean’s surface and interact with winds and ocean currents in ways that are often very hard to model and predict (Reed et al., 1999; James, 2002; Tkalich, 2006).

In general, problems involving material transport require an accurate characterization of the underlying currents, which is an extremely challenging problem due to the wide scale separation of the phenomena involved (Sanford et al., 2011). Given the impossibility to sample all scales of motion in an Eulerian sense, several Lagrangian techniques have been developed to measure transport associated with a flow field though the release in the flow field of Lagrangian particles (Rossby, 2007; Davis et al., 2008). Originally single-particle techniques (Taylor, 1921) have been used to quantify diffusion in models and observations. These techniques are effective in determining the asymptotic behavior of dispersion at time scales that are often too long for practical applications of the transport problem. Two-particle statistics (Babiano et al., 1990; LaCasce, 2008), or relative dispersion, is more closely related to the synoptic turbulent nature of the underlying Eulerian dynamics (Batchelor, 1952; Bennett, 1984).
While most of the Lagrangian instruments and theoretical frameworks to analyze these observations have been developed to study large-scale material transport (Fratantoni, 2001; Bauer et al., 2002), there is a growing interest to study smaller-scale processes within the mixed layer. At the SM with motions evolving on times scales of days to hours, the fluid motion is only partially constrained by rotation (McWilliams, 2008) and this is where 3D motions start becoming important. Submesoscales are found to be mainly constrained to the upper ocean mixed layer through numerical studies (Thomas et al., 2008; Capet et al., 2008b; Fox-Kemper et al., 2008; Klein and Lapeyre, 2009; Taylor and Ferrari, 2010; Mensa et al., 2013) and this has led to their exploration through observational programs (D’Asaro et al., 2011; Shcherbina et al., 2013). Since submesoscales are smaller and faster evolving than mesoscales, one of the main questions is whether they carry any importance for material transport in the multi-scale setting of the ocean. This question was at first studied using numerical models (Haza et al., 2008; Poje et al., 2010; Ö zgökmen et al., 2011; Ö zgökmen and Fischer, 2012), but the transport of surface oil during an important spill event stimulated a large experimental study confirming that submesoscales can indeed influence material transport (Poje et al., 2014).
1.2.1 Vertical material transport

Large part of the vertical material transport in the open ocean is thought to take place in ocean eddies. Ocean eddies are ubiquitous and persistent features of the oceans which play an important role in the horizontal transport of nutrients and tracers (Jenkins, 1988; McGillicuddy and Robinson, 1998; Siegel et al., 1999; Martin and Richards, 2001; Chelton et al., 2007; Siegel et al., 2011; Gaube et al., 2013). Eddies are generated from baroclinic instabilities of main the thermocline and as such develop at scales in the order of the first Rossby baroclinic deformation radius. In the Gulf Stream (GS) mesoscale eddies develop with scales from 50 km to 200 km radius and can be cyclonic, trapping cold waters from north of the GS or anticyclonic, in which case they have a core of warm waters trapped from south of the GS. GS eddies are persistent features that can last for up to several months (Olson, 1991). The role of mesoscale eddies on the ocean biological has been extensively documented as they have been found to host biological communities Olson (1986); Jenkins (1988). In particular it has been suggested that ocean eddies could be responsible for a significant part of the ocean primary production (McGillicuddy Jr. et al., 2003; Klein et al., 2008) (Figure 1.3). Phytoplankton, in order to be productive, requires a combination of nutrients and sunlight where nutrients are normally stored in the water column while sunlight can penetrate
only in relatively shallow waters, the euphotic zone. It has been suggested that ocean eddies, extending from the water column to the upper open, could provide a mechanism for the vertical transport of nutrients from the deep ocean to the euphotic zone. Evidence of such processes have been found by Mizobata et al. (2002) and McGillicuddy and Robinson (1998) (Figure 1.3). The details of this mechanism are not clear, and are investigated in Chapter 3.

A variety of mechanisms have been suggested that could explain the observed primary production in ocean eddies but the topic is still largely debated (McGillicuddy et al., 2008; Mahadevan et al., 2008; McGillicuddy et al., 2007).

The main processes have been schematically described by Siegel et al. (2011) but in the present dissertation we focus on those processes than act on the stable and steady eddy: Submesoscale Pumping and Eddy-Ekman pumping. On top of
these two processes we consider the effect on vertical mixing of near-inertial waves. In the oceans, internal waves, represents a strong signal in the vertical velocity and although substantially linear, near-inertial waves could play a significant role in the mixing between deep ocean and mixed layer.

Submesoscale pumping is the vertical transport associated to the submesoscale features in the mixed layer. Large mesoscale eddies are often characterized by smaller scale features developing at the eddy boundaries (Martin and Richards, 2001; Klein and Lapeyre, 2009; Siegel et al., 2011; Lévy et al., 2011). These are generated by the density gradients of the mesoscale eddy outcropping in a regime of weak stratification such as the mixed layer. From these, driven by shear and surface jets, frontogenesis and mixed layer instabilities can develop resulting in strong vertical velocities at the boundaries of the eddy (Mizobata et al., 2002). The resulting vertical fluxes can potentially explain the discrepancy between the primary production observed in the oceans and the primary production observed in the numerical simulations with mesoscale features alone (McGillicuddy Jr. et al., 2003; Lévy et al., 2011, 2001; McGillicuddy et al., 2007). It is known that increasing resolution in numerical simulations produces stronger vertical velocities Capet et al. (2008b); Mensa et al. (2013) nevertheless it is not clear: i) how vertical
velocities developing in the mixed layer could affect vertical transport at depth and ii) whether larger vertical velocities will result in stronger vertical transport.

SM pumping is often compared against the vertical transport due to Eddy-Ekman pumping (McGillicuddy et al., 2007; Mahadevan et al., 2008; Klein and Lapeyre, 2009; Siegel et al., 2011). Vertical transport in case of Ekman pumping would be generated by surface divergence due to the wind interacting with surface velocity and generating an Ekman current. In this case upwelling would be generated at the core of an anticyclonic eddy and downwelling in the core a cyclonic eddy. The main difference between the two processes in the case of an anticyclonic eddy is that in the case of SM pumping upwelling would be at the boundaries of the eddy while for Ekman-eddy pumping it would be at eddy core. While this process has been observed to produce substantially weaker vertical velocities than SM pumping Martin and Richards (2001), the pumping provided by Ekman-eddy interaction is constant in time and potentially more effective than the transient SM pumping where vertical velocities, although strong, could potentially cancel out in the time averaging. Precisely for this type of reasoning we approach the problem with Lagrangian methods.

To conclude, we compare the transport associated to the previous processes to the transport of near-inertial waves. In anticyclonic eddies, an important fraction
of the observed vertical velocities is due to the trapping of near-inertial waves in the proximity of the eddy core (Jaimes and Shay, 2010; Jaimes et al., 2011). Despite the fact that near-inertial waves are substantially linear, and thus presumably weak in transport, they are known to generate substantial dyapical mixing when breaking, a mechanism that could lead to significant vertical transport at the eddy core (Cardona and Bracco, 2012).

Lastly, some work has been done in idealized configurations of vortices and ocean eddies to understand the pathways and the structure of their vertical circulation (Fountain et al., 2000; Branicki and Kirwan Jr., 2010; Betencourt et al., 2012; Cardona and Bracco, 2012; Wang and Özgökmen, 2015). Nevertheless we think that a clear schematic of the vertical pathways of a semi-realistic ocean eddy such as the one we present here, is still missing.

### 1.3 Scientific motivation

The main goal of the present dissertation is to shed some light on the properties of the flows developing below the mesoscale. These are scales which present qualitative differences with the large mesoscale potentially affecting the ocean dynamics. The general idea that ocean motion can be safely approximated by its mesoscale structure collides for example with the observation of the produc-
tivity levels in the mixed layer. Productivity is sustained by fluxes of nutrients from below the euphotic zone that can be provided by near coast upwelling or baroclinic instabilities in regions far from the boundaries. In these regions the observed productivity due to mesoscale eddies has been found (McGillicuddy Jr. et al., 2003; McGillicuddy et al., 2007) to account for only 20-30\% of the annual amount of nutrients and the observed spatial scale of surface nutrients is too fine for being produced by mesoscale dynamics, thereby suggesting the presence of a SM regime. Klein and Lapeyre (2009) reviewed recent developments in this direction showing that submesoscale dynamics could indeed account for the high productivity observed near the surface.

Similarly, it is not clear what the properties of mixed layer transport is below the SM regime. These are scales with obvious relevance for the human activities but represent a domain almost inaccessible with the present technologies. The transport of the mesoscale has been studied in terms of Eulerian and Lagrangian dynamics, where the quasi-2D nature of the flow field allowed development of techniques to describe material transport. The concept of Lagrangian Coherent Structures (LCSs, Haller (2015)) were developed based on the notion that the temporal variability of 2D non-divergent coherent structures is an important consideration for stirring (Mezić and Wiggins, 1994; Haller and Poje, 1998; Haller and
Nevertheless, within the multi-scale setting of oceanic flows, it is not clear what the properties of a nearly-3D regime such as that below the SM can be investigated with the classical Lagrangian techniques. In particular, for scales below the submesoscales, phenomena such as Langmuir turbulence is well investigated through modeling, but these emerge only under wind speeds larger than $10 \text{ms}^{-1}$. Upper ocean transport under conditions of weak winds ($<10 \text{ms}^{-1}$) and regular diurnal buoyancy forcing is relatively less investigated, even though they prevail through much of the oceanic spatio-temporal scales.

### 1.4 Open questions

The study of SM flows and below is relatively new and presents a number of open questions.

The first studies on SM dynamics assumed that an ageostrophic flow would have signified a forward energy cascade. This idea has been partially addressed in numerical simulations but as of today there is no clear evidence of it (Molemaker et al., 2010; Muller et al., 2005; Molemaker et al., 2005; McWilliams, 2008). If a transition to an inertial range has to happen somewhere in the ocean spectrum, it is yet to be found.
The Lagrangian framework has been proven far more accessible than the Eulerian counterpart. Observations from Lagrangian drifters allowed to successfully sample many scales at once answering some important questions. In particular it has been found that transport at the small scales is in fact dominated by the small scales and not by the mesoscale dynamics. This is a crucial finding as it implies that the SM cannot simply be discard in the study of the ocean material transport. This finding opens a number of important questions. In particular it is unknown what is the lower limit of the scale dependency and where small scales will be come unimportant. Parallel to this question, it is not clear whether the tools and concepts developed to study 2D flows will hold in 3D flows.

Pushing towards smaller scales will very soon highlight the importance of non-hydrostatic processes. Currently primitive equation models are pushed to resolve scales of few hundred meters which are well in the limit of convective, non-hydrostatic processes. As of today it is not clear whether or where in the scale spectrum these processes will become of primary importance.

Very little is also known also about the ocean vertical transport. Observations will most likely never be able to study these processes extensively and numerical simulations, although more probable to succeed, will require a transition towards more accurate, and computationally expensive, discretizations. Vertical velocities
in numerical simulations seems to increase linearly with model resolution (Klein and Lapeyre, 2009) and it is not clear whether this is due to newly resolved physics or numerical issues in the primitive equations models. What is known is that the observed primary production is, as of today, far from being explained by the current modeling efforts.

From a more fundamental prospective, it is not clear whether the scale dependence of dispersion and eddy diffusivity described by Richardson (1926) will in fact hold throughout all the scales of the ocean. Evidence suggesting that this might not be the case have already been shown by Okubo (1971) but as of today there is no real alternative to the Richardson model nor any conclusive evidence that this is not the case.

In the push towards smaller scales, new processes will potentially be discovered. There is still little observational evidence of the processes at scales below the SM. Langmuir turbulence is a known process but not fully understood in terms of Lagrangian transport nor in terms of formation mechanism and dynamical properties. There is evidence of ramps like features but these are rare and they seem to include features with very broad characteristics and properties sometimes approaching the scales of Langmuir turbulence. Also, we know that at some point convective processes, Ekman transport and 3D turbulence will become important
but it is not at all clear at what scales and how these processes will interact with the larger scale features.

In the following we will try to address some of these questions. In particular the present dissertation will try to,

1. Investigate the mechanism governing the formation of SM features in the ML (Chapter 2);

2. Study the role of SM in the transport of nutrients in ocean eddies (Chapter 3);

3. Investigate the material transport and dynamics of the flows below the SM (Chapter 4);

4. Study the effectiveness of Lagrangian techniques in studying the sub-SM regime (Chapter 4).
Chapter 2
Seasonality of the Submesoscale Dynamics

The uncertainty coming from real ocean observations underlines the importance of understanding the mechanisms determining the presence of SM features. In the past years high resolution numerical simulations greatly enhanced our understanding of the mechanisms behind the formation of SM features with studies in idealized or semi-idealized configurations (Mahadevan and Tandon, 2006; Mahadevan, 2006; Boccaletti et al., 2007; Thomas and Ferrari, 2008; Thomas et al., 2008; Molemaker et al., 2010; Özgökmen et al., 2011, 2012). Nevertheless realistic simulations of these processes are still rare.

Basin wide simulations have been successfully implemented to study these processes in areas with strong SM activity such as upwelling regions (Capet et al., 2008c,b,d) and continental shelf (Capet et al., 2008a) and confirmed that SM
features are affected by the characteristics of the mixed layer and the strength of the horizontal density gradients (Fox-Kemper et al., 2008; Capet et al., 2008a; Lévy et al., 2011; Badin et al., 2011).

The goal of this chapter is to describe the mechanisms responsible for the presence of SM features in the mixed layer through the study of its seasonality. Here we consider a realistic high resolution model of the recirculating region of the Gulf Stream (here on GS). This region, that is of primary importance for relevant ecological and climate related processes, has been intensively studied in the literature in terms of mesoscale dynamics, ring formation and transport (Auer, 1987; Clarke et al., 1980; Johns et al., 1995; Sato and Rossby, 1995; Hogg, 1992), but SM have not been explored yet. Here we provide an analysis of the SM dynamics in this area, in terms of generation mechanisms, statistical properties and dependence on environmental parameters and seasonality.

The analysis is carried out with HYCOM which has been extensively and successfully tested in this region (Halliwell, 2004; Chassignet et al., 2003; Smith et al., 2000; Chassignet et al., 2009). The model is integrated for 18 months in a realistic configuration at two horizontal resolutions: a high resolution simulation (HR) 1/48° horizontal resolution (∼ 2 Km) that is at least partially SM resolving, and a low resolution simulation (LR) at 1/12° horizontal resolution (∼ 8 Km) that
does not explicitly resolve the submesoscale dynamics but can resolve mesoscale features. The comparison between the two simulations allows to isolate processes that are directly linked to submesoscale. Details of the model configuration are described in Section 2. Results are presented in Section 3.

2.1 Methods

The HYbrid Coordinate Ocean Model (HYCOM, Bleck (2002); Halliwell (2004); Chassignet et al. (2006)) is used to simulate the Gulf Stream at two different resolutions. The high resolution simulation (HR) is done in a Mercator horizontal grid at $1/48^\circ$ grid size, and has 30 vertical hybrid (z-sigma-isopycnal) layers, of which the top six layers are allowed to be in z coordinates and the ocean interior is generally in potential density coordinates, referred to $20MPa$, $\sigma_2$ (the equation of state is written in $\sigma_2$ with thermobaricity). The lateral boundary conditions are of a one-way nesting, with the external solution coming from a coarser resolution ($1/12^\circ$) simulation (LR) covering the Atlantic Ocean and the Mediterranean Sea in the latitudinal range between $28^\circ$S and $80^\circ$N (Fig. 2.1, Chang et al. (2009)). The lateral boundary conditions for the LR simulation are closed but with relaxation to climatology, for the thermodinamic variables, in the northern and southern boundaries.
The nested simulation (HR) covers the region from 81.44°W 28.78°N to 50°W 45.72°N. It is initialized from the low resolution solution on January 1st after 8 years of spin up, and ends at day 135 of the following year (May 15th) spanning a total of 501 days. A period of approximately one month is needed for the HR simulation to adjust from the LR simulation. In order to avoid the possible influence of the spin up, in the following we will focus on one model year, going from May 15th (day 135 from initialization) through the end of the simulation. In the paper we show typical snapshots of winter (February 1st) and summer season (July 19th).
The one-way nesting method employed here is available in the standard HYCOM source. For the barotropic flow, boundary conditions following the method of characteristics are applied to the normal velocities and pressure, while parallel velocities are imposed. For the baroclinic flow, normal velocities and total mass fluxes are prescribed, while tangential velocities are nudged at the boundary; interface pressures are nudged within a finite width zone.
An example of the HR simulation is shown in Fig. 2.2 where a snapshot of SST is displayed for the winter season. The configuration of the HR simulation has been used by Haza et al. (2012) to study the Lagrangian properties of the Gulf Stream. The model near surface circulation shows a defined Gulf Stream extension, Gulf Stream velocities and eddy kinetic energy consistent in magnitude and location of the current with drifter data analysis (Garraffo et al., 2001; Lumpkin and Johnson, 2013). The model sea surface height variability (not shown) is 20 – 40 cm in the Gulf Stream extension, consistent with altimeter data analysis (Ducet et al., 2000).

The present study focuses on a portion of the recirculation zone of the GS, region A (from 72.02°W 30.162°N to 55.86°W 33.442°N), characterized by the recirculating part of the subtropical gyre. This region is chosen because it allows us to study the dynamics of SM features in the presence of strong mesoscale features such as those generated in proximity of the GS. In order to visualize SM features, diagnostics are also computed for a smaller region (region S) located inside region A. Diagnostics are obtained at different depths after interpolation of the original hybrid vertical grid to a fixed depth grid.
Figure 2.2: SST [$^\circ$C] snapshot during the winter season from the HR simulation. The boxes represent the regions over which diagnostics are computed.

The LR and HR simulations are based on the same depth data set and forcing. The model topography was obtained from the Digital Bathymetric Data Base (DBDB2). The thermodynamic atmospheric forcing is based on monthly values from the ECMWF 40-year reanalysis (ERA40, Uppala et al. (2005)) for years 1978-2002. The mechanical forcing is based on the same data set plus 6-hourly perpetual year wind stress and wind speed anomalies (derived from Navy Operational Global Atmospheric Prediction System Model, NOGAPS, for Jan 2003-Jan 2004). Atmospheric forcing values are extrapolated from the ocean onto land to avoid discrepancies between atmospheric and ocean model land-sea masks (Kara et al., 2007), and several bias corrections are applied that are in use at Naval Re-
search Laboratory, some of them described for the ERA40 simulation by Metzger et al. (2010) (wind speed corrected through correlations with satellite observations (Wallcraft et al., 2009), limiting maximum wind velocity to non-hurricane winds).

The vertical mixing scheme is based on the KPP parametrization of Large et al. (1994). Horizontal mixing is parametrized as a linear combination of Laplacian and biharmonic mixing scaled with the grid size (Chassignet and Garraffo, 2001).

2.1.1 Flow decomposition

For a number of diagnostics presented in the following it is useful to separate the mesoscale and large fraction from the SM fraction of the flow field. This is done by filtering in space the variables of interest and removing the filtered fraction from the total field to obtain the SM residuals. The filter used here is a one lobe sine function with equation \( f(x) = \frac{\sin(x \cdot 2\pi/\lambda)}{x \cdot 2\pi/\lambda} \cdot \frac{\sin(x \cdot 4\pi/\lambda^2)}{x \cdot 4\pi/\lambda^2} \)

where the parameter \( \lambda \) is selected by minimizing the difference between the filtered fields in the mixed layer, where SM features are expected to be abundant (60 m depths, winter HR), and the same unfiltered fields below the mixed layer (500 m), where SM features are expected to be in first approximation absent. The fields considered are the two components of horizontal velocity \( u \) and \( v \) and density \( \rho \).
In Fig. 2.3 the rms difference between each filtered variable at 60 m depth ($V_F(\lambda)_{60\,m}$) and the original field at 500 m ($V_O_{500\,m}$) is computed as function of $\lambda$,  

$$D = \sqrt{(V_F(\lambda)_{60\,m} - V_O_{500\,m})^2},$$

where $D$ is normalized between 0 and 1 to facilitate the comparison. Results for the two velocity components are similar, showing a minimum around $\lambda \approx 100 \, km$, while for density the minimum is around $\lambda \approx 50 \, km$. In the following we choose a reference value of $\lambda = 70 \, km$ for filtering. Obviously, the partition between mesoscale and SM is not expected to be perfect, given the complexity of the flow and its multiscale nature. For this reason, in the following we also perform additional sensitivity tests for selected diagnostics. Notice that $\lambda = 70 \, km$ approximately corresponds to filtering scales smaller than the first baroclinic Rossby deformation radius, that is expected to be of the order of $30 \, km$ in this area (Chelton et al., 2010).

As an example, results of the filtering with $\lambda = 70 \, km$ are shown in Fig. 2.4 for speed ($c = |\mathbf{u}| = \sqrt{u^2 + v^2}$) over the whole domain, where filtered quantities and anomalies are displayed next to the original field (Fig. 2.4a). Here and in the following the mesoscale fraction is represented by the over-bar while submesoscale anomalies by the prime ($c = \bar{c} + c'$). The filtered fields show large scale mesoscale
eddies (Fig. 2.4b), while SM features (Fig. 2.4c) are ubiquitous in the residual fraction. SM features are especially developed around the edges of mesoscale structures such as rings, eddies and jets, as can be expected in a strain dominated region such as the GS (Bishop, 1993; McWilliams et al., 2009a,b).

![Figure 2.3](image)

**Figure 2.3:** Values of $D$ (equation (2.1)) for $u,v$ and density $\rho$ as function of $\lambda$ computed over region A during the winter season of the all domain of the HR simulation.
Figure 2.4: (a) Total \(c\), (b) filtered \(\bar{c}\) and (c) residual speed \(c' [m\,s^{-1}]\) at 60m depth during winter season for the HR simulation.
2.2 Mechanisms of submesoscale generation: frontogenesis and mixed layer instabilities

The SM regime is characterized by the ability to transfer energy from available potential energy (APE) and kinetic energy (KE) of the mesoscale to smaller scales, opening the road toward the dissipative scales (McWilliams, 2008; Molemaker et al., 2010). In particular APE, stored in the highly energetic mesoscale features of the Gulf Stream, can be transferred to the smaller scales by frontogenesis (Hoskins, 1982; Pedlosky, 1987; Giordani and Caniaux, 2001; Thomas and Lee, 2005; Lapeyre et al., 2006) and then released in form of eddy kinetic energy (EKE) by mixed layer instabilities (MLI) (Stone, 1966, 1970; Boccaletti et al., 2007).

Here we investigate the mechanisms of frontogenesis and MLI in the GS simulations, considering first specific examples occurring in winter and summer snapshots, and then quantifying their overall time dependence in terms of integral quantities.

2.2.1 Frontogenesis in the mixed layer

Frontogenesis develops mostly near the ocean surface, where the absence of vertical velocities allows straining from mesoscale eddies to increase density variance, therefore leading to a very effective sharpening of existing density fronts (Bishop, 1993; Lapeyre et al., 2006; McWilliams et al., 2009a,b). Surface horizontal density
gradients $\nabla_h \rho$ are in thermal wind balance with a surface jet that generates, as byproduct of frontal intensification, increased vorticity at the flanks of the front, and regions with strong horizontal strain.

Frontogenesis is commonly studied in terms of frontal tendency function $F$ (Hoskins and Bretherton, 1972; Capet et al., 2008c),

$$F = \frac{D|\nabla_h \rho|^2}{Dt} = Q \cdot \nabla_h \rho, \quad (2.2)$$

where $\rho$ is density, $Q$ is the Q-vector defined in equation (2.3) and $\nabla_h = \partial/\partial x \hat{i} + \partial/\partial y \hat{j}$. A positive sign of $F$ represents an increase in time of the magnitude of the density gradient indicating frontogenesis, while a negative sign indicates frontolysis.

The Q-vector (Hoskins, 1982),

$$Q = (Q_1, Q_2) = \left( -\frac{\partial u}{\partial x} \cdot \nabla_h \rho, -\frac{\partial u}{\partial y} \cdot \nabla_h \rho \right), \quad (2.3)$$

computed with the full horizontal velocities (geostrophic and ageostrophic), affects the evolution of the thermal wind components disrupting the thermal wind balance. The thermal wind balance is then compensated by a secondary ageostrophic circulation across the front. The resulting cross front circulation is described by the $\Omega$-equation which expresses the spatial distribution of the vertical quasi-
geostrophic velocity, $\omega$, as a function of the horizontal divergence of $Q$ (Hoskins et al., 1978; Giordani and Planton, 2000; Giordani and Caniaux, 2001),

$$N^2 \nabla^2 h \omega + f_0^2 \frac{\partial^2 \omega}{\partial z^2} = -2 \frac{g}{\rho_0} \nabla_h \cdot Q,$$

where $N^2$ is the Brunt-Väisälä frequency, $N^2 = b_z$ (subscript represents the partial derivative with respect to $z$), with $b$ the buoyancy $b = -g \rho / \rho_0$ and $\rho_0$ the reference density computed as the average density in the mixed layer of region A.

Examples of vertical recirculations indicative of frontogenetic activity during winter in subregion $S$ are shown in terms of $\omega$ for HR (Fig. 2.5a). Alternate bands of vertical velocity are evident along the fronts, spatially correlated to regions with large values of $F$ (not shown). Notice that $\omega$ is computed inverting the $\Omega$-equation, and therefore strictly speaking represents only the QG component of the frontal vertical velocity (Mahadevan and Tandon, 2006). Typical values of $\omega$, though, have magnitude on the order of 15 meters per day that accounts for most of the vertical velocity computed by HYCOM as divergence of the horizontal velocity field. These values compare well with observations ($10 \text{ m day}^{-1}$ Flament et al. (1985), $40 \text{ m day}^{-1}$ Dewey et al. (1991), $15 \text{ m day}^{-1}$ Pollard and Regier (1992)).
Figure 2.5: Vertical velocity $\omega$ [m s$^{-1}$] computed for HR (a) during winter at 60 m depth and (b) during summer at 5 m depth and (c) for LR during winter at 60 m depth. Depths are chosen in order to represent the mixed layer.

During summer, the frontal vertical recirculations appear significantly weaker, as shown by the snapshot in Fig. 2.5b. Values of $\omega$ are almost one order of magnitude smaller across the fronts with respect to the winter season, and the patterns do not show the typical bands of alternated positive and negative values at the flanks of the density fronts.

The $\omega$ vertical velocity has also been computed for the LR simulation in winter (Fig. 2.5c). Fronts appear significantly weaker in intensity (about 30% less) and
they occur mainly at the mesoscale, confirming that the structures in Fig. 2.5a emerge at increased resolution and they are linked to submesoscale.

The frontal vertical velocity can be quantified computing the average value of $|\omega|$ over region A, and can be regarded as a proxy for frontal intensity. The time series of the average $|\omega|$ at 5 m is shown in Fig. 2.6, indicating a clear seasonal cycle with maximum values during winter (around February) and minimum values in summer (around August).

![Figure 2.6](image.png)

**Figure 2.6**: Time series of the module of vertical velocity $|\omega|$ [m s$^{-1}$] computed as average values over region A at 4 m depth for the HR simulation.
2.2.2 Mixed Layer Instabilities

Once fronts intensify, instabilities of various types can occur (Haine and Marshall, 1998). Here we consider the general class of baroclinic mixed layer instabilities (MLI, Boccaletti et al. (2007); Stone (1966, 1970)), and we propose to diagnose them through their net effect, i.e. the conversion rate of APE to eddy kinetic energy EKE (Boccaletti et al., 2007; Fox-Kemper et al., 2008; Capet et al., 2008c).

The conversion of APE in EKE is common to all baroclinic instabilities, therefore, to ensure that only the submesoscale fraction is considered, quantities are filtered as described in Section 2.1.1. The release of APE can be quantified in terms of eddy vertical buoyancy flux $w' b'$ (where primes denote the SM residual) which is expected to show positive and negative values at the flanks of the front as the secondary ageostrophic circulation drives the density anomalies.

Computing $w' b'$ for subregion S (Fig. 2.7) shows that indeed positive and negative values are present at the two sides of the front. Overall larger values are found in the winter season (Fig. 2.7a) compared to summer (Fig. 2.7b) as expected due to the stronger vertical velocities found during winter that drive large buoyancy fluxes. For LR (Fig. 2.7c), values are comparable in magnitude to HR but only few relatively large features remain after filtering.
Figure 2.7: $w' b'$ [$m^2 s^{-3}$] for (a) winter at 60 m, (b) summer season at 5 m in HR and (c) for winter LR at 60 m.

In Fig. 2.8, a typical winter profile of $w' b'$ averaged over region A is shown. Average flux is always positive, with zero value at the surface (consistently with the boundary condition $w = 0$) and small values below 300 m, as expected given that the MLIs activity is confined in the mixed layer. A clear maximum can be seen at approximately 80 m, indicating the presence of a buoyancy flux vertical divergence, with negative vertical flux gradients contributing to a positive buoyancy tendency in the upper 80 m, and positive gradients below. The tendency
towards a lighter upper mixed layer and heavier lower mixed layer contributes to a net restratification effect. The pattern is consistent with results from idealized MLI numerical models (Boccaletti et al., 2007; Fox-Kemper and Ferrari, 2008) as well as with realistic models in the California Current and Argentinean shelf (Capet et al., 2008a), and it indicates that also in the GS region, heavily influenced by strong mesoscale and rings, the mixed layer dynamics is largely controlled by MLIs.

![Figure 2.8](image)

**Figure 2.8:** Vertical dependence of $w'b'$ ($[m^2 s^{-3}]$, equation (2.5)) averaged over region A for HR during winter season. The dots represent the mixed layer depth (and corresponding value of PK) for HR ($\sim 171$ m, red dot) and LR ($\sim 226$ m, blue dot).

In order to quantify the net release of APE we integrate over the mixed layer depth (MLD) the average of $w'b'$ over region A, obtaining the rate of conversion of APE in EKE, PK (Boccaletti et al., 2007; Fox-Kemper et al., 2008; Capet et al., 2008c),
\[ PK = \frac{1}{\text{MLD}} \int_{0}^{-\text{MLD}} \langle w'b' \rangle_{xy} dz. \]  

(2.5)

where the angle brackets \( \langle \cdot \rangle_{xy} \) represent the averaging over region A. MLD is computed by HYCOM as the depth at which the density difference with respect to the surface is equivalent to a 0.3°C temperature change (leaving salinity constant).

The value of PK corresponding to the snapshots in Fig. 2.7 in winter and summer for the HR simulation are \( 2.86 \cdot 10^{-8} \ [m^2 s^{-3}] \) and \( 1.25 \cdot 10^{-9} \ [m^2 s^{-3}] \) respectively, showing that values are overall larger during winter than during summer. Also values are typically larger on average in the HR simulation as features developing in LR are suppressed by the filtering. In Fig. 2.9 the complete time series of \( \langle w'b' \rangle_{xy} \) is computed, showing a clear seasonal cycle in phase with the seasonality of the vertical velocity \( \omega \). Sensitivity of the time series to different filtering length scales was tested using values of \( \lambda = 40 \ km \) and \( \lambda = 130 \ km \). Results show a seasonal cycle with values of the same order of magnitude of the current filter at 70 \( km \) but with smaller or larger values of PK for smaller and larger values of \( \lambda \). The time series for LR shows that a seasonal cycle in PK exists despite the filtering, meaning that a scale separation is not fully captured by the filtering or not present.
Figure 2.9: Time series of the conversion rate of available potential energy into eddy kinetic energy, PK \([m^2 s^{-3}]\), as computed in equation (2.5). PK is integrated over region A at 5\(m\) depth for HR (solid line) and LR (dashed line).

2.3 Diagnosing the characteristics of submesoscale features

Here we quantitatively describe the characteristics of the flow in the mixed layer with specific interest in the occurrence of submesoscale features which we expect to be particularly prominent in winter when the mechanisms of frontogenesis and MLI are more active. SM features are expected to be characterized by scales of the order of the mixed layer Rossby radius of deformation, with significant deviation
from geostrophy and high relative vorticity and Rossby number (Thomas et al., 2008). Various diagnostics are presented here to quantify the seasonality of SM.

### 2.3.1 Horizontal Length Scale

A way to quantify the scale of the features developing in the flow field is by computing spectra of kinetic energy. From these it is then possible to quantify the seasonality of the energy associated to the SM regime integrating, for each day, the kinetic energy spectrum over the SM wave numbers,

\[
KE_s(t) = \int_{R_{SM}^{-1}}^{2\Delta x^{-1}} KE(k,t)dk,
\]

where \( KE_s(t) \) is the portion of the total kinetic energy associated to the sub-mesoscale regime, i.e., the fraction of \( KE_s \) integrated over wave numbers from \( R_{SM}^{-1} \), where \( R_{SM} \) is the length scale of the submesoscale dynamics, to \( 2\Delta x^{-1} \), where \( \Delta x \) is the grid size. \( R_{SM} \) is a function of the Rossby deformation radius for the mixed layer, \( Rd_{ML} \) (Özgökmen et al., 2011),

\[
Rd_{ML} = \sqrt{MLD g \Delta \rho / \rho_0},
\]

where \( \rho_0 \) is the vertical average density across the mixed layer, \( \Delta \rho \) is the density jump across the mixed layer. In the following we considered a value of \( R_{SM} = 5Rd_{ML} \) as it has been suggested by Eldevik (2002).
Equation (2.6) has been estimated for both resolutions (Fig. 2.10), showing a clear seasonal cycle with larger values of KE associated to SM features in HR, as expected from the fact that the HR simulation resolves more small scale features and thus covers a broader range of wave numbers than LR.

![Figure 2.10](image)

**Figure 2.10:** Kinetic energy (KE, \([m^2 s^{-2}]\)) integrated over the submesoscale wave numbers computed from equations (2.6), for both HR (black line) and LR (blue line).

### 2.3.2 Deviation from gradient wind balance

A measure of how SM features are effectively unbalanced comes from the quantification of the deviation from gradient wind balance (McWilliams, 1985; Capet
where $\zeta$ is the vertical component of the relative vorticity and velocities are only horizontal ($\mathbf{u} = (u, v)$). The term $\mu = f\zeta_{\text{RMS}} + \rho^{-1}(\nabla^2_h p)_{\text{RMS}}$, where RMS indicates root mean square values, is added to the denominator to avoid situations dominated by Coriolis force from being identified as unbalanced. $\epsilon(x, t)$ can vary between 0, for completely balanced flows, and 1, for completely unbalanced dynamics. Snapshots of this diagnostic in the mixed layer for winter and summer in HR are shown for a subregion of region A in Fig. 2.11, indicating that deviations occur in both seasons but with different characteristics. In winter, the deviations are mostly in filaments and fronts, suggesting the presence of SM, while in summer they occur only in few regions near the large mesoscale structures.

2.3.3 Relative vorticity and Rossby number

SM features are expected to be significantly ageostrophic and characterized by high relative vorticity. A quantitative view of the seasonal and resolution dependent distribution of relative vorticity normalized by planetary vorticity, i.e. the Rossby number $Ro = |\zeta/f|$, can be observed in Fig. 2.12. In Fig. 2.12a $Ro$ is spatially averaged over region A and computed as a function of depth for
Figure 2.11: Unbalanced regions computed in region S for (a) winter at 60 m depth and (b) summer season at 5 m depth.
each resolution and season. Ro shows a clear intensification in the mixed layer, especially evident during winter in HR. This is consistent with a signature of the intensification of submesoscale features. The seasonal variations of Ro are also evident in Fig. 2.12b where the frequency of instances of Ro > 0.5 over region A has been computed throughout the year for the 5 m and 500 m depth at both resolutions. Fig. 2.12a and Fig. 2.12b show that most of the ageostrophic values of ζ occur in the mixed layer, mostly in HR, with maximum during the winter season.

More details on the distribution of ζ, including its sign, are shown by the PDFs of ζ/f₀ (Fig. 2.13). The difference between LR and HR, which is expected to be due to the emergence of submesoscale, is evident especially in the mixed layer and is characterized by enhanced deviation from a Gaussian distribution and development of strong tails especially in the positive side. The positive asymmetry is consistent with flows generating in presence of frontogenesis and MLI where large negative relative vorticity is dissipated in symmetric and centrifugal instabilities (Hoskins, 1982; Hoskins et al., 1978; Rudnick, 2001; Thomas and Lee, 2005; Klein et al., 2008).
Figure 2.12: (a) Vertical dependence of the Rossby number averaged over region A for summer (dashed lines), winter (solid lines), HR (black lines) and LR (blue lines). The red dots on the curves represent the mixed layer depth. (b) Seasonal trend of the frequency of instances of $Ro > 0.5$ over region A for both resolutions at $5\, m$ and $500\, m$ depth.
Figure 2.13: PDF of relative vorticity for winter season, HR (left panel) and LR (right panel), normalized over $f_0$. The solid lines are for PDFs at 10 m depth and the dashed line for PDFs computed at 500 m depth. The red lines represent the pdf of the normal distribution computed with the same standard deviation as the 10 m depth PDF and with zero mean.

2.3.4 Okubo Weiss parameter

We conclude the flow diagnostics computing the Okubo-Weiss parameter ($OW$). $OW$ is a metric used to identify elliptic (vorticity dominated) and hyperbolic (strain dominated) regions, that has been often applied to 2D or quasi-geostrophic quasi non divergent flows (Weiss, 1991; Okubo, 1970). For the general case of a non-null horizontal divergence field (Petersen et al., 2006; Zavalasanson and Sheinbaum, 2008) $OW$ can be written as,

$$OW = S^2 - \zeta^2 = \delta^2 + 4 \left( \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right) = \delta^2 - 4 Det(\nabla_h u). \tag{2.9}$$
where \( \mathbf{u} = (u, v) \), \( S^2 = S_1^2 + S_2^2 = (\partial u/\partial x - \partial v/\partial y)^2 + (\partial v/\partial x + \partial u/\partial y)^2 \), \( \zeta^2 = (\partial v/\partial x - \partial u/\partial y)^2 \) is the square of the relative vorticity, \( \delta = \nabla_h \cdot \mathbf{u} = \partial u/\partial x + \partial v/\partial y \) is the horizontal flow divergence and \( \text{Det}(\nabla_h \mathbf{u}) \) is the determinant of the velocity tensor gradient \( \nabla_h \mathbf{u} \). Notice that \( S^2 \) exactly corresponds to the determinant of the horizontal strain rate for divergence free fields, while in divergent flows, \( S^2 \) also includes a divergence component (Provenzale, 1999).

Fig. 2.14 shows two typical snapshots of \( OW \) computed in winter and summer in the mixed layer for HR and LR. The \( S^2 \) term appears dominant in winter HR (positive \( OW \)), therefore indicating a direct connection with the submesoscale field. As discussed above, \( S^2 \) is a signature not only of strain but also of divergence, that appears to be strongly increased in winter likely because of frontogenesis and MLI.

Seasonality of \( OW \) is quantitatively shown by the time series in Fig. 2.15, obtained computing \( OW, S^2, \zeta^2, \delta^2 \) integrating over region A at 5 m depth. Differently from what is expected for a divergent free closed flow (Petersen et al., 2006), \( OW \) appears to be significantly different from zero especially for HR during winter, showing mostly positive values.

In order to better understand the behavior of the integrated \( OW \), consider the following form of equation (2.9) in terms of the gradient (Zavalasanson and
Figure 2.14: Okubo-Weiss parameter ($OW$) normalized by $f_0^2$ computed at the surface (5 m) for winter (left column), summer (right column), HR (top row) and LR (bottom row).

Sheinbaum, 2008),

$$OW = \delta^2 - 2\nabla_h \cdot (u \delta) + 2\nabla_h(u \cdot \nabla_h u).$$  (2.10)

When equation (2.10) is integrated over a domain, the last two terms on the right hand side can be rewritten as closed path integrals which depend on the boundary conditions,

$$\int_A OW \, dA = \int_A \delta^2 \, d\mathbf{A} - 2 \oint \mathbf{u} \delta d\mathbf{r} + 2 \oint \mathbf{u} \cdot \nabla_h \mathbf{u} \, d\mathbf{r}.$$  (2.11)
Equation (2.11) implies that $OW$ is zero when the flow is non divergent and computed in a closed domain with no-slip boundary conditions. In our case, both components of the r.h.s. are expected to be different from zero, therefore contributing to a net value of $OW$. The $\delta^2$ component (shown in Fig. 2.15 in blue), is indeed of the same order as the total $OW$ (shown in red), suggesting that it is a predominant factor. The difference between $OW$ and $\delta^2$ is likely to be due to the boundary condition effects.

Ultimately the time series of $OW$ and its components shows that, while LR is essentially 2D and geostrophic, HR experiences a seasonal transition from a quasi 2D divergence free regime during the summer to a more three-dimensional regime during the winter season which is another indication of deviation from geostrophic balance. This transition is on top of an increased hyperbolicity of the flow field during the winter season as many filaments and fronts develop in the proximity of large and mesoscale features.
Figure 2.15: Temporal evolution of the components of the Okubo-Weiss parameter ($[s^{-2}]$, from equation (2.9)) integrated over region A at 5 m depth for (a) HR and (b) LR: $\text{OW}$ (Okubo-Weiss parameter, red line), $S^2$ (strain rate, black line), $\zeta^2$ (relative vorticity squared, gray line) and $\delta^2$ (divergence squared, blue line).
2.4 Role of stratification and mixed layer depth on submesoscale seasonality

In the previous sections, we have shown that submesoscale features are mostly present during winter and in the mixed layer. Here we investigate the main environmental parameters controlling the observed seasonality.

We build on the results of a number of previous works, mostly based on idealized numerical experiments, that investigated the relationship between the development of MLI and consequent occurrence of SM features in relation to ambient parameters (Boccaletti et al., 2007; Klein et al., 2008; Lapeyre et al., 2006; Thomas et al., 2008; Molemaker et al., 2010; Lévy et al., 2001; Özgökmen et al., 2011; Fox-Kemper et al., 2008; Fox-Kemper and Ferrari, 2008; Capet et al., 2008a; Badin et al., 2011). In particular, we focus on the works by Boccaletti et al. (2007); Fox-Kemper et al. (2008); Fox-Kemper and Ferrari (2008) who investigated the dependence of MLI from the parameters of several ideal flows, including a channel with mesoscale eddies and an isolated mixed layer front, varying in particular the main stratification and lateral density gradients.

MLIs are expected to be relevant in terms of transfer of buoyancy fluxes. The buoyancy equation for the total (meso and submesoscale) buoyancy can be written
as,

$$\frac{\partial}{\partial t}(\vec{b} + b') + \nabla \cdot [(\vec{u} + u') \cdot (\vec{b} + b')] = -\mathcal{F},$$

(2.12)

where \( \vec{u} \) is the three dimensional velocity, primes indicate the SM component and \( \mathcal{F} \) indicates the solar and diffusive fluxes. As reviewed in Section 3.2, the SM integrated vertical buoyancy flux term, \( w'b' \), is expected to be significant in presence of mixed layer fronts when MLIs develop, and is related to a transfer between APE stored in the fronts and EKE, leading to slumping of the fronts and re-stratification of the mixed layer. Fox-Kemper et al. (2008) proposed a simple parameterization for this term written as an overturning streamfunction with a given scaling and vertical structure. The scaling for the total APE conversion can be written as (Capet et al., 2008a),

$$PK = \langle w'b' \rangle_{xyz} \propto f^{-1} \langle |\nabla \vec{b}| \rangle_{xyz}^2 \langle MLD \rangle_{xy}^2,$$

(2.13)

where \( \langle \cdot \rangle_{xy} \) indicates horizontal averaging over region A, and \( \langle \cdot \rangle_{xyz} \) volume averaging over region A and over MLD. Equation (2.13) is valid under the assumption that the flow field is dominated by advection, as is the case of SM regime, and that horizontal velocities scale according to the thermal wind relationship. The complete parameterization by Fox-Kemper et al. (2008) has been tested using idealized model results (Fox-Kemper and Ferrari, 2008), while the validity of the
integrated scaling in equation (2.13) has been tested by Capet et al. (2008a) using a realistic model of the Argentinian shelf.

Conceptually, equation (2.13) assumes that there are two main parameters influencing MLIs and their effects: the presence of horizontal density gradients, i.e. fronts, in the mixed layer, and the depth of the mixed layer, MLD. Shallow mixed layer and strong surface stratification inhibit the formation of vertical recirculations along the flanks of fronts, while in presence of deep mixed layer and low surface stratification the cells are enhanced and a great reservoir of APE is available for MLIs giving rise to significant SM features.

In the following, we aim at quantitatively testing the integrated scaling (2.13). The GS region is expected to be different from the idealized settings analyzed before, and also from the coastal or upwelling dominated areas considered by Capet et al. (2008a,d), in so far it is influenced by very strong mesoscale nonlinearity and strain. In the next subsection we provide an analysis of the stratification and MLD seasonality in our GS model.

**2.4.1 Seasonality of surface stratification and MLD**

The seasonal variation of the upper ocean stratification is first qualitatively shown in terms of snapshots of vertical sections of potential density and monthly mean profiles (Fig. 2.16). During the winter season a weakly stratified and deep mixed
layer is established. This allows meso and large scale features to outcrop at the surface and generate deep fronts in the mixed layer. During the summer season on the other hand a strongly stratified and warm mixed layer is established which counteracts the outcropping of features from below the mixed layer. Strong density gradients are generated during spring at the base of the mixed layer when the relatively warm mixed layer interacts with cold mesoscale features generating in the thermocline. During the summer season (August) density gradients are high only at the very base of the mixed layer and the stratification becomes strong enough to inhibit mesoscale features from reaching the surface.

Seasonality of surface stratification is reflected on the MLD. Fig. 2.16 shows vertical density profiles and MLD averaged over one month period, confirming the presence of a deep mixed layer during the winter season and a shallow mixed layer during the summer season.
Figure 2.16: Density ($\sigma_2$) sections showing the vertical stratification for the winter (left panels) and summer (right panels) season in the HR simulation. In the top panels daily snapshots are shown, while averages for the same sections over one month are shown in the lower panels (dashed lines are the mean values plus or minus the standard deviation). Mixed layer depth is represented by a white line in the top panels and black line in the lower panels.
The seasonal cycle of MLD is shown in Fig. 2.17a for both HR and LR, indicating that the mixed layer depth reaches approximately 200 $m$ during winter, while it quickly becomes shallow in the spring, starting in April reaching a minimum of less than 10 $m$ by June. The difference in HR and LR MLD values reaches a maximum of the order of 50 $m$ during the winter season, with the LR MLD being deeper than the HR.

Since the only difference between the two simulations is resolution, with consequent occurrence of SM features in HR, this is a clear indication that indeed SM restratification tends to compact the isopycnals leading to a significant change in the winter MLD. We notice that such an effect is not observed in the simulations of Capet et al. (2008b) in the California Current, where the HR mixed layer does not become shallower, even though MLI flux divergence is clearly present. Capet et al. (2008b) argue that this is due to the fact that the increasing vertical flux is counterbalanced by an increase in vertical mixing, that tends to destratify the flow. They also suggest that this effect might be overestimated in their simulations because of their constant forcing. In our simulations, wind synoptic scales, seasonal flux variations and high variability in mesoscale fronts are likely to sustain MLIs effects over boundary layer turbulence. In particular wind has been shown to be able to intensify surface density fronts and to affect the magnitude
of the across front ageostrophic circulation (Thomas and Lee, 2005; Capet et al., 2008c; Cardona and Bracco, 2012). Nevertheless we did not observe the same strong correlation between the magnitude of \( \omega \) and down-front winds observed for example in the California Current by Capet et al. (2008c). This difference might be due to the presence of a strong mesoscale field in the GS region which ultimately controls the orientation and intensity of ML fronts.

The MLD seasonality is clearly linked to the atmospheric forcings. Both HR and LR simulations are forced with a realistic perpetual year forcing and seasonality can be quantified in terms of mean surface fluxes of heat \( (f_T [W/m^2]) \) and salinity \( (f_S [10^{-3} kg m^{-2} s^{-1}]) \) and a mechanical forcing represented by wind speed \( (u^* [m s^{-1}]) \).

In order to quantify the degree of the correlation between MLD and the atmospheric forcings, we computed the cross-correlation (defined as a sliding cross product by the \( \ast \)) between the time series of each forcing and mixed layer depth,

\[
\rho [t] = (f_{T,S}, u^* \ast MLD)[t] \equiv \sum_{m=0}^{365} f_{T,S}, u^*[m] \ MLD[m + t], \tag{2.14}
\]

Results are shown in Fig. 2.17b, where the cross correlation \( \rho [t] \) is computed for \( f_T \) (dashed line), \( f_S \) (dashed-dotted line) and \( u^* \) (dotted line). The red solid line represents the autocorrelation curve computed as the cross-correlation of MLD
with respect to itself and represents the ideal cross-correlation. Cross-correlation is computed based on the last 365 days of MLD and forcings.

![Figure 2.17](image-url)

**Figure 2.17:** (a) Temporal variability of the mixed layer depth [m] averaged over region A (black line, HR and blue line LR). (b) The correlation in time between surface forcings ($f_T$ dashed line, $f_S$ dashed-dotted line and $u^*$ dotted line) and mixed layer depth is shown for the last 365 days of the simulation. Red line in (b) represents the mixed layer autocorrelation function. The gray line in (a) represents the begin of the portion of the time series that has been used to compute $r[t]$.

The time series for MLD shows a good correlation (with maximum correlation of $r \sim 0.8$) with both buoyancy fluxes (dashed and dashed-dotted lines), while it is slightly lower for the wind (maximum correlation of $r \sim 0.6$). Time series of surface fluxes and mixed layer depth are shifted in time due to the fact that the maximum flux corresponds to the maximum time derivative of the ocean response. As a result, the maximum of mixed layer depth occurs $\sim 60$ days after the minimum of $f_T$ and the maximum of $f_S$. The time lag is nearly zero in the
case of the mechanical forcing \( (u^*) \). In summary the seasonality of MLD is forced by the fluxes of buoyancy and wind speed.

Figure 2.18: Time series of the terms in equation (2.13) for HR. \( \langle w'b \rangle_{xyz} \) in red, \( \langle |\nabla b| \rangle_{xyz}^2 \cdot \langle \text{MLD} \rangle_{xy}^2 \) in blue, \( \langle |\nabla b| \rangle_{xyz} \) in solid gray and \( \langle \text{MLD} \rangle_{xy} \) in dashed gray. All curves are normalized over the maximum value of each time series.

2.4.2 Dependence of MLIs on MLD

Here we quantitatively test whether the scaling in equation (2.13) is valid for our realistic GS simulation similarly to what has been done by Capet et al. (2008a) for the Argentinian shelf simulation. The various terms in equation (2.13) have been computed for the HR simulation and the corresponding time series are shown in Fig. 2.18. Sensitivity tests have been done for different values of the sine filter
wave length showing some sensitivity to the values of $\lambda$. In particular choosing a value of $\lambda = 40 \, km$ gives values of $w'b'$ too small during the spring and fall seasons.

The overall agreement between the two sides of equation (2.13) (blue and red lines) is satisfactory, indicating that the scaling holds, similarly to what found by Capet et al. (2008a). It is interesting to notice though that the horizontal gradient term $\langle |\nabla \bar{b}| \rangle_{xyz}$ shows a significantly different behavior with respect to MLD. While MLD is maximum in winter and very shallow from May to September, the horizontal gradient term has a less well defined and more complex structure. A minimum can be seen around August and September, when stratification is the strongest and effectively isolates the mixed layer from the internal mesoscale structure, but during spring and autumn there are clear peaks. The term has a very high variability over monthly scales, likely due to oscillations of the large scale Gulf Stream fronts and formation and advection of mesoscale eddies and rings. We can compute the autocorrelation of the timeseries in Figure 2.18 to quantify the degree of agreement between the terms (Figure 2.19) and we confirm that correlation between $\langle w'b' \rangle_{xyz}$ and $\langle |\nabla \bar{b}| \rangle_{xyz}$ is in fact smaller than with $\langle MLD \rangle_{xyz}^2$. 
Figure 2.19: Autocorrelation between the timeseries of $\langle w'b' \rangle_{xyz}$ and $\langle \text{MLD} \rangle_{xy}^2$ solid line, $\langle w'b' \rangle_{xyz}$ and $\langle |\nabla \bar{b}| \rangle_{xyz}$ dashed line and $\langle w'b' \rangle_{xyz}$ and $\langle |\nabla \bar{b}| \rangle_{xyz}^2 \cdot \langle \text{MLD} \rangle_{xy}^2$ dotted line.

From the physical point of view, the results indicate that the limiting and controlling factor in SM formation in the GS region is indirectly MLD. Horizontal gradients and surface fronts are present in this area almost during the whole year, but the stratification inhibits the formation of deep recirculating cells and significant MLIs. This is different from what found by Capet et al. (2008a) in the Argentinian shelf where lateral gradients have a maximum approximately in phase with MLD, and they are both related to atmospheric forcing. Here atmospheric forcings are still the main controlling factor, but only through the control of MLD. Horizontal gradients are provided by the vigorous mesoscale field that is present
during the whole annual cycle, except for a brief period at the end of summer when stratification shuts them down in the mixed layer.

2.5 Concluding remarks

Results from a realistic high resolution (HR) simulation of the region of the Gulf Stream recirculation are presented, with the goal of investigating submesoscale (SM) processes in the mixed layer and their seasonality. Results show that during the winter season, deep vertical recirculations are observed to develop associated to fronts outcropping from mesoscale eddies and rings into the mixed layer. Mixed layer instabilities (MLIs) are generated at these fronts, leading to the formation of a vigorous submesoscale field. During summer, on the other hand, the occurrence of vertical recirculations and MLIs appear damped, and the SM field is much weaker.

The characteristics of the mixed layer flow and the occurrence of SM features have been quantitatively characterized in statistical terms. SM features, with scales of the order of the mixed layer Rossby radius, appear characterized during winter by a clear deviation from geostrophy, high Rossby number, with prevalently positive vorticity, and significant divergence.

Results of the HR simulations are compared to results from the LR simulation where submesoscale features are not resolved. In the LR results, seasonality of
the mixed layer flow is much reduced and the field is dominated by mesoscale
during the whole year, with relatively small deviations from geostrophy and a
quasi 2D behavior.

We then investigate what are the main environmental parameters that control
the observed SM seasonality, building on previous results from idealized numer-
ical studies and realistic simulation (Özgökmen et al., 2011; Badin et al., 2011;
Boccaletti et al., 2007; Capet et al., 2008c,b,d,a; Fox-Kemper and Ferrari, 2008;
Fox-Kemper et al., 2008; Molemaker et al., 2010).

The flow field is filtered to separate meso and larger scales from SM. Isolating
the SM anomalies allows to apply the scaling of the total SM vertical buoyancy
flux in the mixed layer, PK, proposed by Fox-Kemper et al. (2008). PK quantifies
the APE release associated to MLIs and can be considered as a measure of the
presence of SM features in the field. The scaling by Fox-Kemper et al. (2008)
and Capet et al. (2008a) links PK with the presence of mesoscale surface lateral
gradients in the mixed layer, indicative of surface fronts, and with the magnitude
of mixed layer depth MLD. Direct testing with our results shows that the scaling
is appropriate, following the same seasonal variations as the observed PK. The
governing factor appears to be MLD, while horizontal gradients appear present
during the whole year because of the presence of mesoscale eddies and rings. This
result is different from what obtained by Capet et al. (2008a) in the Argentinian Shelf, where the seasonality of both horizontal gradients and MLD contributes to the scaling, and both are induced by atmospheric forcing. In our case, atmospheric fluxes and wind forcing are still the cause of SM occurrence, but mostly through their action on MLD. While surface fronts are always available, the deep MLD during winter provides a much greater reservoir of APE, that allows MLIs to develop a vigorous SM field.

The importance of MLIs on the large scales is suggested by the comparison between the mixed layer in HR and LR. The mixed layer in HR is shallower than in LR of approximately 50 m, i.e. of a significant $\sim 25\%$, suggesting that the restratification induced by SM is the cause of mixed layer shoaling.

We notice that this finding is different from what shown in Capet et al. (2008d,b,c) in the California upwelling simulations, where MLD did not change significantly between HR and LR simulations. As suggested by Capet et al. (2008b), this is likely due to their numerical setting characterized by constant forcing, that allows destratifying effects by vertical mixing to counteract the stratifying effects of MLIs. In our simulations, instead, atmospheric variability and mesoscale induced frontal variability appear to maintain MLI activity and their stratifying effects.
Appendix

2.5.1 Surface fluxes parametrization

Thermal energy flux into the ocean ($f_T [W/m^2]$) is computed by HYCOM from the balance between incident radiation and emitted ocean radiation ($\mathcal{R}$), the latent heat transfer ($\mathcal{H}$) and the sensible heat transfer due to evaporation ($\epsilon$),

$$ f_T = \mathcal{R} - \epsilon - \mathcal{H}. \tag{2.15} $$

$\mathcal{R} ([W/m^2])$, the net solar radiation (as well as its short and long wave components), is positive into the ocean and is provided as forcing. The surface radiation budget also includes a black body radiation correction flux, proportional to the difference between the surface temperature and the air temperature of the data used for the forcing (ERA40).

Latent heat transfer due to evaporation, $\epsilon$, is computed from

$$ \epsilon = L_E \rho_a u^* C_L (T_s - T_w), \tag{2.16} $$

where in equation (2.16), $L_E$ is the latent heat of evaporation coefficient ($2.47 \cdot 10^6 [j/kg]$), $\rho_a$ is the air density computed from air temperature, $u^*$ is the 10 m wind speed, $C_L$ is the latent heat flux coefficient computed from a polynomial expression, function of stability and temperature difference between atmosphere and
ocean (Kara et al., 2000; Fairall et al., 2003), and \( T_s \) and \( T_w \) are respectively the saturation mixing ratio (from a polynomial expression, function of surface temperature) and water vapor mixing ratio which is provided as part of the (ERA40) forcing.

The last term in the expression of \( f_T \) is the sensible heat transfer, \( \mathcal{H} \), obtained from

\[
\mathcal{H} = C_{P_{air}} \rho_a C_S u^* (T_{sur} - T_{atm}),
\]

where \( C_{P_{air}} \) is the specific heat of the air at constant pressure \([j\ kg^{-1}\ deg^{-1}]\), \( C_S \) is the sensible heat flux coefficient computed by Kara et al. (2000) as 0.9554 \( \cdot C_L \), \( T_{sur} \) is the model sea surface temperature and \( T_{atm} \) is the air temperature.

The salinity flux into the ocean, \( f_S \) \(([10^{-3}kgm^{-2}s^{-1}])\), is quantified in the model as

\[
f_S = (E - P) \cdot (S \cdot 10^3),
\]

where \( E \) the is evaporation rate

\[
E = \epsilon \cdot 10^{-3}/L_E,
\]
$P$ is precipitation (given as a forcing) and $S$ is the salinity at the surface. In addition, a relaxation of sea surface salinity to climatology is included.

In Fig. 2.20a the seasonal variability of $f_T$ averaged over region A is shown. Values are negative during the winter season and positive during the summer representing a heat flux from the ocean to atmosphere during the winter and a net heat gain of the ocean during the summer. Analogously, in Fig. 2.20b, the spatially averaged values of $f_S$ in time are shown with maxima and minima shifted of approximately half period with respect to $f_T$. Average values of $f_S$ are always positive in region A, being evaporation larger than precipitation; $f_S$ contributes to the mixed layer being saltier during winter and fresher during summer.

![Graphs showing seasonal variability of heat, salinity, and wind speed](image)

**Figure 2.20:** (a) Temporal variability of the bulk fluxes of (a) heat [$W m^{-2}$], (b) salinity [$10^{-3} \text{kg m}^{-2} \text{s}^{-1}$] and (c) wind speed [$m s^{-1}$] averaged over region A. The gray line represents the first point of the time series considered.

During the winter season, negative values of $f_T$ act to increase density reducing the ocean temperature, while positive values of $f_S$ contribute to increase salinity...
and thus density. During the summer season on the other side, $f_S$ is nearly zero due to weak evaporation, and density is driven only by $f_T$ which is positive into the ocean. Buoyancy fluxes ultimately affect MLD by stratifying the upper ocean during summer and destratifying the mixed layer in winter.

Wind speed ($u^*$) enters in the equations as a factor in the formulation of sensible heat and evaporation. The wind speed seasonal cycle (Fig. 2.20c) shows a maximum in winter and a cycle similar to $f_S$. Wind speed enters in the formulation of both $f_s$ and $f_T$ favoring the latent heat transfer due to evaporation (2.16) and thus producing a loss of heat (2.15) and a gain of salinity (2.19) at the surface.
Chapter 3

Material Transport in Ocean Eddies

SM features have been described as important factors affecting primary production in the oceans. The vertical velocity associated to SM fronts and eddies could in fact be responsible to significant vertical transport from below the photic zone, in the water column, where nutrients are abundant and primary production is inhibited by the lack of light, to the upper ocean where nutrients become available to phytoplankton.

The vertical transport of nutrients has been suggested to take place in ocean eddies, where the vertical structure of the eddy could represent a pathway for vertical fluxes of nutrients. The details and the mechanism of such transport are yet not fully understood and the subject of this chapter. In particular we focus on two processes: SM pumping and Eddy-Ekman pumping. These are the
two main processes isolated by Siegel et al. (2011) which would affect vertical transport in stable and steady eddy. On top of these, vertical velocities and mixing in ocean eddies has been shown to be generated by the breaking of near-inertial waves (Jaimes and Shay, 2010; Jaimes et al., 2011; Cardona and Bracco, 2012). We investigate these processes via an idealized numerical simulation of an anticyclonic eddy.

Ultimately, the objectives of this study can be summarized as follows.

1. to quantify the relative importance of SM pumping and Eddy-Ekman pumping;

2. to assess the role of near-inertial waves on vertical transport;

3. to investigate the anatomy of the vertical transport in ocean eddies.

In the present work we study the vertical transport of ocean eddies via a high resolution non-hydrostatic numerical simulation of an anticyclonic eddy. In order to quantify Lagrangian transport we release synthetic particles at the eddy core. We run a set of experiments based on an anticyclonic eddy isolated from a HYCOM simulation of the GS during the summer season (Mensa et al., 2013) which, due to the shallow mixed layer, does not present submesoscale activity. The state without submesoscale is used a reference against which to study dif-
ferent processes. From this original eddy we extract a density profile which we use to initialize and axisymmetric eddy in MITgcm. This simulation is compared against the same initial conditions with wind forcing and against a winter configuration with deep mixed layer, with and without wind forcing. The winter simulation is produced from the summer case but has a thick mixed layer. Details on the initialization are provided in the next section. The goal is to produce four simulations which cover the cases of SM induced transport, Eddy-Ekman induced transport and the combinations of the two.

The present work is divided as follows. In the first part we describe the model configuration. Next we present results from an Eulerian prospective. We describe the evolution in time of the eddy, its vertical structure, vertical velocities and internal waves field. We conclude the results with the core of the work where we focus on the Lagrangian vertical transport of the four experiments. Final remarks and conclusions follow in the last section.

3.1 Methods

In order to fully and accurately resolve the vertical velocity field inside a warm core eddy we use the non-hydrostatic model MITgcm. The model is configured to run in cylindrical domain of 200 km side and 900 m depth. Model resolution
is of 1.25 km in the horizontal and from 2 to 50 m in the vertical. Details on the model equations and configuration follows in this section.

3.1.1 Model equations

MITgcm solves the incompressible Buossinesq equations,

\[
\frac{D\mathbf{u}_h}{Dt} + f_0 \hat{k} \times \mathbf{u}_h + \frac{1}{\rho_0} \nabla_h p' = A_h \nabla^2 \mathbf{u}_h + \mathbf{F}_r, \tag{3.1a}
\]

\[
\frac{\partial w}{\partial t} + \frac{g \rho'}{\rho_0} + \frac{1}{\rho_0} \frac{\partial p'}{\partial z} = A_v \frac{\partial^2 w}{\partial z^2}, \tag{3.1b}
\]

\[
\frac{\partial w}{\partial z} + \nabla_h \cdot \mathbf{u}_h = 0, \tag{3.1c}
\]

\[
\frac{DS}{Dt} = A_{vs} \frac{\partial^2 T}{\partial z^2}, \tag{3.1d}
\]

\[
\frac{DT}{Dt} = A_{vt} \frac{\partial^2 S}{\partial z^2} + \mathbf{F}_\theta. \tag{3.1e}
\]

where \( D/Dt = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \) is the total derivative operator, \( \mathbf{u}_h = (u, v) \), \( f \) is the Coriolis parameter, \( p' \) is the dynamic pressure, \( g \) being the gravitational acceleration, \( \rho_0 \) reference density and \( \mathbf{F}_r \) the wind forcing term later defined. The simulations are performed on a f-plane with \( f_0 = 10^{-4} \text{s}^{-1} \) in order to avoid the eddy from propagating westward. This approximation is justified by the work from Dewar et al. (1999) who did not find significant difference in stability of warm core eddies evolving in a beta-plane. In the vertical dimension, the model
is run in non-hydrostatic mode. In the tracer equation, $T$ is temperature and $F_\theta$ is buoyancy forcing defined in the next section.

Horizontal diffusivity in $T$ and $S$ is implicit while horizontal viscous term is harmonic and uses a Leith eddy viscosity coefficient (Leith, 1996, 1968),

$$A_h = \left( \frac{L}{\pi} \right)^3 |\nabla \bar{\zeta}| \tag{3.2}$$

where $L$ is the length scale of the grid and $\bar{\zeta}$ is the vertical component of the relative vorticity of the resolved velocities. This allows to parameterize the unresolved enstrophy dissipation at the small scales.

In the vertical, eddy viscosity ($A_v$) and diffusivities ($A_{v_S}, A_{v_T}$) are set by KPP. Tracers advection scheme is a 3rd order direct space time with flux limiter.

The perturbation density $\rho'$ in $\rho = \rho_0 + \rho'$ is expressed through a linear equation of state that depends on temperature and salinity

$$\rho = \rho_0 [1 - \alpha \, T + \beta \, S], \tag{3.3}$$

where the reference density is $\rho_0 = 999 \, Kg \, m^{-3}$, thermal expansion coefficient $\alpha = 2.0 \times 10^{-4} \, ^\circ C^{-1}$ and haline contraction coefficient $\beta = 7.4 \times 10^{-4} \, psu^{-1}$. 
The model is configured to run four experiments (Table 3.1): two with deep mixed layer (WW and W), simulating a winter condition, and two with a shallow mixed layer simulating a summer condition (SW, S). All simulations are forced by a buoyancy flux at the surface with daily cycle while SW and WW are also forced by a wind stress.

<table>
<thead>
<tr>
<th>Wind/No Wind</th>
<th>Summer</th>
<th>Winter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wind</td>
<td>SW</td>
<td>WW</td>
</tr>
<tr>
<td>No Wind</td>
<td>S</td>
<td>W</td>
</tr>
</tbody>
</table>

Table 3.1: Characteristics of the four experiments conducted. Two experiments are wind forced (SW,WW) and two experiments have a deep winter mixed layer (W, WW).

3.1.1.1 Forcing and Boundary Conditions

All simulations are forced with a heat flux $F_\theta$ at the surface with daily cycle,

$$F_\theta = -\frac{Q_0}{C_p \rho_0 \delta z}$$  \hspace{1cm} (3.4)

where $C_p = 4000 \text{ J Kg}^{-1} \text{ K}^{-1}$ is the specific heat capacity, $\delta z$ is the top layer thickness (2 m) and $\rho_0$ the reference density. The daily cycle of $Q_0$ is idealized and inspired by observations from Price et al. (1986) and Brainerd and Gregg (1995).
\[ Q_0 = \begin{cases} 
-250 & \text{if } \text{time} < 2 \\
Q_{\text{Max}} \times (\text{time} - 2) - 250 & \text{if } \text{time} < 3 \\
Q_{\text{Max}} - Q_{\text{Max}} \times (\text{time} - 3) - 250 & \text{if } \text{time} < 4 
\end{cases} \]  
(3.5)

with \( Q_{\text{Max}} = 1000 \text{Wm}^{-2} \) and \( \text{time} = t/3600.0 \mod(24/6) \), where \( \mod() \) is the modulo operator. The resulting profile of \( Q_0(t) \) is shown in Figure 3.1. The heat flux constructed in this way is null over the 24 hours period.

**Figure 3.1:** Daily cycle of the neat surface heat flux \( Q_0 \).

Mechanical forcing is applied to the top surface of the wind forced simulations \( SW \) and \( WW \),

\[ F_h = \frac{\tau_{x,y}}{\rho_0 \delta z} \]  
(3.6)

where wind stress \( \tau_{x,y} \) is computed from,

\[ \tau = \rho_a C_D |u_{10}| u_{10}, \]  
(3.7)
where $\rho_a = 1.3 \, \text{Kg m}^{-3}$ is the air density, $C_D = 1.5 \times 10^{-3}$ is the drag coefficient, for the assumed neutral meteorological boundary layer and $u_{10}$ is the wind velocity vector. Wind velocity magnitude is constant $7 \, m \, s^{-1}$. Wind forcing is uniform in space but direction changes in time and rotates CCW with a period of 3 days. This is to avoid the wind pushing the eddy in one preferential direction. Wind rotation is in the opposite direction of the eddy rotation which results in an increased surface stress. Wind forcing corresponds to a state with relatively calm winds, typically generating a surface oceanic current on the order of $0.1 \, m \, s^{-1}$ (Hunkins, 1966; Price et al., 1987).

Boundary conditions are free-slip at the sides and at the bottom and free surface at the top.

3.1.2 Initial conditions and spin-up

In order to reproduce a semi-realistic configuration the model is initialized from a temperature and salinity profile extracted from a HYCOM simulation (Mensa et al., 2013). The original eddy detached from a meander of the Gulf Stream during the summer season. The eddy was confined between the Gulf Stream jet and the continental slope. Because of the position, the eddy developed in relatively shallow waters ($\sim 900 \, m$). The original eddy presented a complicated flow field (Figure 3.2) and in order to simplify the problem we select a section
of the eddy and project it in an axisymmetric configuration. Temperature and Salinity are taken directly from the HYCOM model while velocities are computed in thermal wind balance from the initial density profile. This configuration was not perfectly stable so we allowed the simulation to adjust for one week without forcing and we re-initialize the model with the fields averaged over the initial spin-up. A temperature section of the summer eddy after spin-up is plotted in Figure 3.3a.

In order to simulate a similar eddy in winter conditions we prescribe a uniform mixed layer extruding temperature and salinity from the 100 m depth. This allows to have a winter eddy with identical configuration than the summer simulation below the 100 m mark but with a deep mixed layer. The winter simulation is also averaged after a week of spin-up in order to produce a more stable initial condition. A temperature section of the winter configuration is shown in Figure 3.3b.
Figure 3.2: Potential density section of the warm core eddy extracted from HYCOM. The black lines represent the slice used to initialize the model in the Summer configuration.

3.2 Results

The goal is to study the characteristics of vertical transport in the presence of sub-mesoscale features, Ekman pumping and internal waves. The different processes are reproduced in separate model configurations in order to study the individual effects. Ultimately vertical transport is assessed with Lagrangian techniques.

In the following we describe the Eulerian characteristics of the four simulations while in the last part we focus on material transport.
Figure 3.3: Temperature section [°C] for the (a) summer and (b) winter configurations after spin-up.

3.2.1 Eulerian Dynamics

Summer eddies (S and SW) present a very stable density profile and retain their structure even after several months of integration. Figure 3.4 shows a temperature section at 50 m depth after 30 days of integration with no visible sign of baroclinic instabilities developed.

The wind forced eddy shows a similar surface temperature structure than S but SW shows a warmer core than S due to the formation of a thin mixed layer in SW which mixes the warmer waters above the shown depth (Figure 3.4b).
Winter simulations (W and WW) are characterized by a much more complex surface signature. At the beginning of the simulation features develop around the eddy core in form of filaments. These are presumably submesoscale features as they develop in the mixed layer with small scales. After few weeks these structures become part of larger scale features (Figure 3.4c). These structures develop from the steep density profile of the mixed layer which produces filaments detaching from the boundaries of the eddy. Filaments are roughly organized in two cyclonic eddies developing at the boundary of the main anticyclone in a tripole configuration. Tripoles have been documented in the ocean (Pingree and Le Cann, 1992), numerical experiments (Carton and Legras, 1994; Carnevale and Kloosterziel, 1994; Killworth et al., 1997; Chavanis and Sommeria, 1998; Dewar et al., 1999; Carton et al., 1989) and laboratory experiments (Kloosterziel and van Heijst, 1991). In particular their formation is associated to instabilities of the eddy profile. These features originate in the mixed layer and with small scales but their signature can be observed also at larger depths.

The wind forced winter simulation (Figure 3.4d) presents very similar temperature signature than W although we expect submesoscale features to interact with the wind and to generate stronger submesoscale features (Thomas and Lee, 2005).
Both wind forced simulations shows the effect of the wind forcing at the boundaries of the domain, where water is forced away from the boundary pulling colder waters from below the surface. This is an artifact of the simulation but boundaries are kept far from the eddy core.

\begin{figure}[h]
\centering
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure3a.png}
\caption{(a)}
\end{subfigure}\hfill
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure3b.png}
\caption{(b)}
\end{subfigure}
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure3c.png}
\caption{(c)}
\end{subfigure}\hfill
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure3d.png}
\caption{(d)}
\end{subfigure}
\caption{Temperature sections $^\circ$C at 50m depth for all four experiments at 30 days into the simulation.}
\end{figure}
Structures in the winter simulations develop in the mixed layer and are mostly confined in the upper ocean and around the eddy but a signature of their structure can be found up to 500 m depth. In Figure 3.5 we compute temperature anomalies respect the summer simulation $S$ for day 30 of $SW$, $W$ and $WW$. Wind forced summer simulation $SW$ has a similar temperature structure than $W$ (Figure 3.5b) while both winter simulations show significant density anomalies at the 500 m mark (Figure 3.5c and 3.5d). Baroclinic instabilities develop from the steep isopycnals of the winter mixed layer but in proximity of the eddy core can penetrate at depths far deeper than the prescribed mixed layer. As it will be shown later, this can affect the whole structure of the eddy.
Figure 3.5: Difference between temperature [°C] at 500 m depth for all four experiments at 30 days into the simulation.

The horizontal velocity structure is shown computing horizontal speed $|\mathbf{u}|_{θ,t} = \sqrt{u^2 + v^2}$ averaged in the azimuthal direction and over a period of 24 hours (Figure 3.6). Values of $|\mathbf{u}|_{θ,t}$ are computed 30 days after spin-up and are shown as anomalies respect to the unforced summer simulation $S$. In all simulations, averaged horizontal speed shows an intensification in the upper ocean near the
eddy core where the horizontal density gradient is steeper driving a stronger thermal wind. In the summer simulations $S$ and $SW$, the maximum speed is observed at about 100 m depth. In the wind forced summer simulation $SW$, the velocity maximum is slightly weaker at the eddy core and stronger at the eddy boundary due to the formation of a shallow mixed layer which shifts the outcropping isopycnals towards the boundary of the eddy.

In the winter simulations, velocities are similar in magnitude to the summer simulations but positive and negative anomalies are observed near the surface and at the flanks of the eddy. Surface anomalies are expected due to the presence of mixed layer structures near the surface. Features are roughly organized in two cyclonic structures at the boundaries of the eddy (Figure 3.4). The result is a positive velocity anomaly at the eddy boundaries and a negative anomaly closer to the core where the cyclonic pole and the anticyclonic core collide. Velocity anomalies propagate to up to 500 m depth consistent with the deep temperature anomalies observed in Figure 3.5.
Figure 3.6: Vertical sections of averaged horizontal velocity magnitude and anomalies respect to $S \overline{|u|^{\theta,t}} [m/s]$. (a) Exp. S (b) Exp. SW-S, (c) Exp. W-S and (d) Exp. WW-S after 30 days after spin-up. Contours represent the isothermal surfaces.
Figure 3.7: Vertical sections of the averaged vertical velocity magnitude $|w| [m s^{-1}]$ for (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW after 30 days after spin-up. Contours represent the isothermal surfaces.
In Figure 3.7 we compute sections of the azimuthally and time averaged vertical velocity magnitude $|w^{\theta,t}|$.

The summer unforced simulation $S$ shows very weak vertical velocity throughout the water column. The eddy is near geostrophic balance and vertical velocities are very weak. Introducing wind in $SW$ enhances vertical velocities at the eddy core. Internal waves and Ekman pumping are expected to develop in proximity of the eddy core because of the wind forcing. Ekman pumping and near inertial waves can develop near the surface due to the effective wind stress generating from the interaction of the wind with the eddy surface current.

In both winter simulations, we observe large velocities near the surface in the proximity of the mixed layer fronts. These velocities are associated to the secondary ageostrophic circulation of the surface density fronts which in a regime of weak stratification produces strong ageostrophic velocities (Hoskins, 1982; Capet et al., 2008b; Mensa et al., 2013). Stronger velocities are observed also at depth. Density anomalies generating in the mixed layer, and found at depths close to 500 m, can affect the vertical ageostrophic circulation of the interior and explain the larger velocities of the interior.
In $WW$ vertical velocities show also the signature of the internal waves and
Ekman pumping near the eddy core similarly to $SW$. More on the dynamics of
the different processes will be discussed in the next section.

Figure 3.8: Sections of instantaneous vertical velocity $[ms^{-1}]$ at 50 $m$ depth for
(a) Exp. $S$, (b) Exp. $SW$, (c) Exp. $W$ and (d) Exp. $WW$ 30 days after spin-up.
The dot represents the probe location used to compute frequency spectra.
Figure 3.9: Sections of instantaneous vertical velocity $[ms^{-1}]$ at 500 m depth for (a) Exp. $S$, (b) Exp. $SW$, (c) Exp. $W$ and (d) Exp. $WW$ 30 days after spin-up. The dot represents the probe location used to compute frequency spectra.
Instantaneous vertical velocities are shown over a section at 50 m depth (Figure 3.8) confirming the very weak vertical velocities in the summer simulation $S$ and the presence of strong vertical velocities at the eddy core in the wind forced summer simulation $SW$. Again, at the eddy core, especially near the surface, we expect to see the superposition of the Eddy-Ekman pumping and the signal of internal waves. In the next section we will address the nature of the internal wave field studying time series of vertical velocities recorded at probes located around the eddy (blue dots in Figure 3.8 and Figure 3.9).

The winter simulations $W$ and $WW$ are characterized by bands of positive and negative vertical velocities typical of submesoscale filaments. These are the signature of a secondary ageostrophic circulation developing around the eddy in the mixed layer. The wind forced winter simulation $WW$ presents a similar structure than $W$ with slightly larger vertical velocity across the fronts. This is expected given, that, as described by Thomas and Lee (2005), down front wind can enhance the secondary ageostrophic circulation in density fronts by moving dense water over the less dense side of the front. The eddy interior is surrounded by the strong vertical velocities of the filaments developing at the eddy boundaries and it is not clear whether vertical velocities due to Eddy-Ekman pumping or internal waves are present at the eddy core.
At 500 \( m \) depth (Figure 3.9) vertical velocities in \( S \) are as expected very small while \( SW \) presents again larger vertical velocity near the eddy core presumably due to a combination of Eddy-Ekman pumping and/or internal waves. In \( W \) vertical velocities are larger at the eddy core as observed in Figure 3.7c. This again is associated to the deep penetration of features developing from the instability of the mixed layer. With wind, consistently with Figure 3.7d, vertical velocities are similar to \( W \) in magnitude but present some noise typical of internal waves. In the next sections we will discuss the processes responsible of these vertical velocities focusing in particular of the secondary ageostrophic circulation driving vertical velocities in density fronts, Eddy-Ekman pumping and internal waves generated by the action of wind on the ocean surface.

### 3.2.1.1 \( \Omega \)-equation

Especially in the winter simulations (\( W \) and \( WW \)) we observe strong vertical velocities associated to density fronts whether these are in the mixed layer or at depth. Across front velocities are described by the \( \Omega \)-equation where vertical velocities are a function of the divergence of the Q-vector (Hoskins et al., 1978; Giordani and Planton, 2000; Giordani and Caniaux, 2001),

\[
N^2 \nabla_h^2 \omega + \frac{f^2}{\rho_0} \frac{\partial^2 \omega}{\partial z^2} = -2 \frac{g}{\rho_0} \nabla_h \cdot Q, \quad (3.8)
\]
where $N^2$ is the Brunt-Väisälä frequency, $N^2 = b_z$ with $b$ the buoyancy $b = -g\rho/\rho_0$ and the subscript represents the partial derivative with respect to depth. $Q$ is defined as (Hoskins, 1982),

$$Q = (Q_1, Q_2) = \left( -\frac{\partial u}{\partial x} \cdot \nabla_h \rho, -\frac{\partial u}{\partial y} \cdot \nabla_h \rho \right).$$

Vertical velocities $\omega$ are then solutions of the elliptic equation (3.8) where larger values of $\nabla_h \cdot Q$ propagate correspond in first approximation to large vertical velocities.

Computing $\nabla_h \cdot Q$ for $S$ and $W$ (Figure 3.10) shows that large values are observed in the mixed layer of the winter simulation. These result is consistent with the idea that the mixed layer is characterized by submesoscale features with large vertical ageostrophic velocities.

Large values of $\nabla_h \cdot Q$ are also observed at depth explaining the large vertical velocities observed in the horizontal and vertical sections in Figure 3.9 and Figure 3.7. We conclude that features developing in the winter mixed layer, reach significant depth, as shown in Figure 3.5, forcing vertical velocities via divergence of the Q-vector.
Figure 3.10: Q-vector divergence \(g \rho_0^{-1} \nabla_h \cdot Q\) [m\(^{-1}\)s\(^{-3}\)] for the (a) summer and (b) winter configurations after 30 days.

At the eddy core values of \(\nabla_h \cdot Q\) are small suggesting that other mechanisms have to be in place in order to produce the observed vertical velocities.

### 3.2.1.2 Ekman-Eddy pumping

In order to assess the contribution to the total vertical velocity of the Eddy-Ekman pumping, we can compute the magnitude of the wind induced vertical velocity from,

\[
w_e = \frac{1}{\rho f_0} \left( \frac{\partial \tau_y}{\partial x} - \frac{\partial \tau_x}{\partial y} \right),
\]

(3.10)

where wind stress \(\tau = (\tau_x, \tau_y)\) is the product of the interaction between wind forcing and eddy velocity and can be parameterized as,

\[
\tau = \frac{\rho_a K_a}{(1 + \epsilon)^2} |u_a - u_0|(u_a - u_0),
\]

(3.11)
where $\rho_a = 1.3 \, kg \, m^{-3}$ is the air density, $K_a$ is the drag coefficient of the air over the ocean and $u_a = (7 \, m \, s^{-2}, 0)$ and $u_0$ are the wind and ocean current velocity which change in time.

$\epsilon^2$ is the ration $\rho_a/\rho_0$ such that in our simulation $\epsilon \sim 0.036$. $K_a$, the drag coefficient can be approximated by (Smith, 1980)

$$K_a = (0.61 + 0.063|u_a|) \times 10^{-3}.$$  \hspace{1cm} (3.12)

In our case, with a wind forcing with uniform magnitude of $7 \, m \, s^{-1}$, $K_a = 1.051 \times 10^{-3}$.

The computed wind stress is a measure of the effective stress on the ocean surface meaning the product of the constant wind stress applied as forcing and the ocean currents.

Computing the average $w_e$ over a 6 days period (two wind revolutions around the eddy) for the wind forced simulations (Figure 3.11), $SW$ and $WW$, shows vertical velocities about one order of magnitude weaker than the total vertical velocity computed in Figure 3.8 and Figure 3.7.

Nevertheless the Eddy-Ekman pumping could potentially provide for a constant up-welling in contrast to the up-welling associated to the vertical velocities
across the density fronts which oscillate in time. The role of Ekman-Eddy inter-
action on vertical transport will be addressed in the last section.

**Figure 3.11:** Wind induced time average vertical velocity $w_e \ [ms^{-1}]$ at the surface for (a) Exp. SW and (b) Exp. WW after 30 days of spin-up.

### 3.2.1.3 Near-Inertial Waves

In the upper ocean velocities typically show energetic oscillations with frequencies near the inertial period. In the mixed layer these oscillations are often associated to fluctuations in the wind stress forcing (Ferris, 1968; Weller, 1982; D’Asaro, 1985b). Numerous observations and experiments have then suggested that the oscillations generating in the mixed layer can propagate downward exciting near inertial oscillations in the water column Pollard and Millard (1970); Leaman and Sanford (1975); D’Asaro (1985a).

The internal wave field is studied here recording vertical velocity at given locations around the eddy and for each model layer (black dots in Figure 3.8)
and Figure 3.9). Velocities are recorded at three locations around the eddy: one close to the eddy core \((p_0, [210 \text{ km}, 200 \text{ km}])\), one at the eddy boundary \((p_1, [240 \text{ km}, 200 \text{ km}])\) and one outside the eddy \((p_2, [322.5 \text{ km}, 200 \text{ km}])\). Time series of the vertical velocities at the probe locations are shown in the Hovmöller diagrams in Figure 3.12.

Near inertial oscillations develop with a period near the inertial period \((IP)\) which for the present simulations is \(IP = \frac{2\pi}{f_0} \approx 17.5 \text{ hrs}\).

Hovmöller diagram for the summer simulation \(S\) shows the presence of alternated bands of positive and negative vertical velocity with a period near the inertial period and no vertical variability. All simulations present this background oscillation which is an inertial oscillation residual of the eddy adjustment to the geostrophic state.

Wind \((SW)\) introduces a strong signal at the eddy core \((p_0)\) in the first few hundred meters as it was observed in Figure 3.7. This signal shows an upward phase propagation and a downward energy propagation originating from near the surface. This signal has a period of \(\sim 3 \text{ IP}\) similar to the atmospheric forcing rotation around the eddy and we associate it to the Ekman pumping. Oscillations develop at the base of a shallow mixed layer and extend through the whole water column remaining confined in the first \(\sim 500 \text{ m}\) of the eddy.
Figure 3.12: Hovmöller diagram of vertical velocity $w$ $[\text{ms}^{-1}]$ for the probes $p_0$, $p_1$ and $p_2$ for all simulations. Time is in inertial periods $IP \simeq 17.5\text{hrs}$. All diagrams are computed starting 30 days after spin-up.
In the winter simulation \( W \) the Hovmöller diagram is dominated by an oscillation with period of \( \sim 6 \) IP \((p_0 \text{ and } p_1)\). This is associated to the secondary ageostrophic circulation at the eddy boundaries observed in Figure 3.9. The wind forced winter simulation \( WW \) shows a similar oscillation plus an oscillation in \( p_0 \) which resembles the one with period \( \sim 3 \) IP observed in \( SW \) in the upper part of the eddy.

In Figure 3.13 we compute frequency power spectra of vertical velocity \( w \) at 160 \( m \) and 500 \( m \) depth. Spectra show a variety of signals at different depths and probe locations but they all share a a continuum of frequencies in the internal waves band with larger amplitudes close to the inertial frequencies.

The vertical velocity frequency power spectrum for \( S \) (first row in Figure 3.13) show a peak in the inertial frequency with larger amplitudes for the probe at 500 \( m \) depth consistently with the inertial oscillation observed in Figure 3.12. For the probes near the eddy center \((p_0 \text{ and } p_1)\), the frequency spectrum shows a slower oscillation \((2/pi/7 \times 10^{-6} \text{ s}^{-1} = 10 \text{ days})\) associated to the revolution of the eddy itself. This peak disappears outside the eddy in \( p_2 \).
Figure 3.13: Vertical velocity power spectra for all experiments and all probes. The vertical lines represent the inertial period (dashed line), the forcing period of 3 days (solid thin line) and two harmonics (solid thin lines).
In \( SW \) (second row in Figure 3.13) on top a similar internal wave spectrum observed in \( S \) there is the clear sign of Ekman pumping in the 160 \( m \) spectrum. This signal disappear at 500 \( m \) for reasons not completely clear yet. The oscillation has a dominant harmonic with frequency of \( f_\tau = 3 \text{ days}^{-1} \) (thin line in Figure 3.13) but also two more harmonics are visible \( (2f_\tau \text{ and } 3f_\tau) \). The presence of this signals is related to the nature of the wind eddy interaction. In Figure 3.14 we compute the time series of wind-current stress \( \tau \) as expressed in equation 3.11 for the different probes. This shows a complex timeseries with harmonics coinciding with the peaks in Figure 3.13.

In the winter simulation \( W \) sub-inertial frequencies present a similar profile then the summer simulations but the spectrum of the sub-inertial frequencies is more energetic suggesting that faster evolving energetic features with strong vertical velocities dominate the power spectrum. In particular, at the eddy boundary \( (p_1) \) the spectrum presents almost a continuum of time scales with the largest amplitudes observed at the time scale of the eddy revolution. Outside the eddy \( (p_2) \), vertical velocity amplitudes for periods larger than the inertial period are similar to the summer simulation \( S \) with the exception of few peaks at lower frequencies presumably associated to inertial gravity waves radiated by the eddy.
In the winter wind forced simulation $WW$, a combination of the sub-inertial signals in $W$ and the signals associated to the Ekman pumping in $SW$ is observed although the contribution of the wind-eddy induced vertical velocity is smaller compared to the signal of sub-inertial processes. Here the influence of wind is less striking than in the summer simulation.

The role of the different processes on vertical transport of nutrients will be investigated in the next section.

![Figure 3.14: Time series of the net surface stress magnitude $|\tau|$ for $SW$ at different probe locations.](image)

**3.2.2 Material Transport**

Vertical velocities show larger values in the wind forced simulations both in the mixed layer and at depth. The wind forced simulations show strong vertical ve-
locities near the eddy core while winter simulations show larger vertical velocities at the eddy boundaries near the surface and at depth. Nevertheless, this does not say much about the transport associated to the different processes.

In order to examine how vertical velocities contribute to material transport, we release artificial particles in all simulations. Particles are released 30 days after spin-up and advected offline using a fourth-order Runge-Kutta scheme with a 1 hour timestep. The total integration time is 90 days. Trajectories are computed for particles advected in 3D and spaced every 10 m meters in the vertical and 10 km in the horizontal for a total of \( \sim 150000 \) particles.

Figure 3.15 shows the final vertical location density of particles released at different depths \((0 \text{ m}, 50 \text{ m}, 150 \text{ m}, 250 \text{ m}, 500 \text{ m}, 800 \text{ m})\). Particles tend to move along isopycnals which results in the slantwise displacements observed at depth. For the summer simulation \( S \), most of the displacement is at depth and there is no neat displacement near the surface where velocities are almost zero.

In the summer wind forced simulation \( SW \) (Figure 3.15b) similar displacements are observed at depth but the mixed layer shows larger displacements at the eddy core. In particular, close to the surface the wind forced simulation \( SW \) shows the result of Eddy-Ekman pumping with particles displaced near the surface at the eddy core. Eddy-Ekman pumping seems to be confined in the upper
part of the eddy. The vertical oscillations observed at the probe \( p_0 \) and associated to the Ekman-pumping at the base of the mixed layer in Figure 3.12 do not seem to contribute to vertical transport below the 50 m.

Winter simulations \( W \) and \( WW \) show a similar vertical displacement at depth than the summer simulations but much larger vertical displacements in the mixed layer. Vertical transport associated to submesoscale features is as expected located at the boundaries of the eddy (Siegel et al., 2011) and shows much larger values than the displacement due to the Eddy-Ekman pumping observed in \( SW \). Results confirm the observations by Martin and Richards (2001). Similarly to \( SW \) in \( WW \) there is sign of Eddy-Ekman pumping at the eddy core.
To further study the pathways of the vertical transport we compute final displacement of the particles in the horizontal at 50 m depth (Figure 3.16). Again, the summer simulations do not show significant vertical transport with displace-
ments almost one order of magnitude smaller than the corresponding winter simulations. Nevertheless, \( SW \) shows the clear signature of upwelling at the eddy core with a band of downwelling particles all around the eddy.

A similar annular structure, but with much larger displacements is observed in the winter simulations. Vertical transport here is primarily due to mixed layer fronts which are in fact characterized by upwelling and downwelling velocities which would explain the observed structure. Also, at the core of the wind forced winter simulation \( WW \) we observe a similar upwelling region with displacements similar to the summer counterpart although these displacements are much smaller than those due to submesoscale features.

Vertical displacements at 500 \( m \) depth are the largest (Figure 3.17) with particles that in three months cover displacements larger than what observed in the mixed layer. There is not much difference between summer and winter simulations despite the observed larger vertical velocity in the winter simulations (Figure 3.9). The observed cross front velocities are linear oscillations which do not contribute to material transport and the observed particle displacement is likely due to the net deformation of the eddy in time.
Figure 3.16: Final vertical displacement respect to 50 m release depth after 30 days and advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. Positive values mean upward displacement.
Figure 3.17: Final vertical displacement respect to 50 m release depth after 30 days and advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. Positive values mean upward displacement.
3.2.2.1 Vertical net and total transport

The question of whether the observed vertical transport can provide a mechanism for the transport of nutrients in and out the euphotic zone is addressed here.

We identify two processes important for biological activity: (i) the advection of nutrients from below to inside the euphotic zone and (ii) the replenishment of nutrients from the water column. In the first case, we focus on the processes that within the mixed layer, can transport nutrients in and out the euphotic zone while the second process is responsible for the replenishment of fresh nutrients from below the mixed layer. The latter process requires that the euphotic zone is not isolated from the water column.

In general the euphotic zone has a depth ranging between 10 m-100 m. In our winter simulations this means that the euphotic zone is contained in the mixed layer which poses the question of whether the mixed layer is a dynamically isolated domain or not.

We investigate both processes computing the total and the net particle flux across depths. We define the two quantities as, $|P|$ and $\overline{P}$ respectively. Where $P$ is the number of particles crossing upward minus those crossing downward, $|P|$ is the number of particles crossing in either direction and the over bar represents the horizontal averaging of $|P|$ and $P$ at a certain depth $z$. For $|\overline{P}| = 0$ there is
then no net-exchange at the interface and $|\mathbf{P}|^z \neq 0$ means that there is exchange but does not say in which direction.

Total particle flux across depths $|\mathbf{P}|^z$ in the mixed layer for all simulations is shown in Figure 3.18. This is an azimuthal mean of vertical displacements for particles released at a given point in the radial direction and depth. Results show that for the summer simulation $S$ total flux is small as there is no mechanism able to effectively transport nutrients across the euphotic zone. For the wind forced summer simulation $SW$ on the other side some vertical transport at the eddy core is observed which is linked to the Eddy-Ekman pumping.

In the winter simulations, total particle flux $|\mathbf{P}|^z$ is large in the mixed layer and in particular at the eddy boundaries. Noticeably, we can identify two major transport pathways around the eddy in proximity of the eddy boundary at the main density front. This suggests that the mixed layer is not isolated from the water column. More on this will be investigated later in terms of net particle flux $\mathbf{P}^z$. The winter forced simulation, similarly to $W$ shows large vertical displacements with larger values at the top and base of the mixed layer. This is the result of the Eddy-Ekman interaction and the wind intensification of submesoscale filaments.
Figure 3.18: Total particle flux $|\mathbf{P}|^2$ for each release depth for particles advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW.

While the summer simulations show very little vertical transport the winter simulations show relatively large vertical displacements. The question then is
whether the vertical velocities are confined to the mixed layer or if nutrients can be advected from the water column to the upper ocean. We address this question computing the azimuthally averaged net particle flux across depths $\bar{P}^z$. In particular, $\bar{P}^z$ has units of a vertical displacement and we can define the quantity,

$$w_L = \frac{\bar{P}^z}{T}$$  \hspace{1cm} (3.13)

where $w_L$ is an integrated transport vertical velocity which represents the average velocity at which particles travel the displacements $\bar{P}^z$ in the integration time $T$. If we then assume that the eddy is axisymmetric, we can study the flow on the radial-depth plane $(r, z)$ and compute the second component of the velocity field $u_L$ from continuity,

$$\frac{\partial w_L}{\partial z} + \frac{\partial u_L}{\partial r} = 0,$$  \hspace{1cm} (3.14)

where $u_L(z)$ is the azimuthal averaged radial transport velocity. We can then plot the velocity field $u_L, w_L$ (Figure 3.19). Results show that for the summer season a weak vertical circulation is present at the base of the mixed layer but does not approach the interior of the mixed layer. In the summer forced simulation, some vertical transport is observed at the eddy surface but also no vertical transport is observed at the base of the mixed layer which implies that if Eddy-Ekman pumping can facilitate vertical transport of nutrients within the mixed layer, it
does not provide for a replenishment mechanism from the water column. In the winter simulations of the other side, a vertical circulation is observed at the base of the mixed layer which extends in the mixed layer itself. This is a crucial difference respect to the summer simulation as the mixed layer in this case is not isolated from the water column but exchanges particles with it. Similarly, but with stronger velocities, we observe vertical transport across the mixed layer in the winter forced simulation.
Figure 3.19: Net particle transport trajectories computed from equation 3.13 and 3.14 for each release depth for particles advected for 50 days in (a) Exp. S, (b) Exp. SW, (c) Exp. W and (d) Exp. WW. Colors stand for temperature.
3.3 Concluding remarks

In the present work we investigated vertical transport in an anticyclonic eddy focusing in particular on the role of Eddy-Ekman pumping and SM pumping. The study was carried on with a set of non-hydrostatic numerical simulations in order to isolate the individual role of each process.

Results showed that SM features develop in the two winter simulation and that strong near-inertial wave signal develops in the two wind forced simulations. The presence of a deep mixed layer has implications on the whole circulation of the eddy enhancing vertical velocities at depth. Wind forced transport on the other side is localized mostly in the upper part of the eddy and presents very weak velocities.

In order to study Lagrangian transport, 3D particles have been released in the four simulations. Trajectories show the presence of pathways in the winter eddy reaching and crossing the mixed layer base. This result suggest that mixed layer dynamics is not isolated from the water column and that SM features can effectively drive vertical transport in the eddy. On the other side, wind induced Eddy-Ekman pumping is too weak to provide significant vertical transport.
To conclude, findings support the idea that ocean eddies can effectively provide nutrients to the euphotic zone and that SM pumping is a leading factor in this process.
Chapter 4

Material Transport in the Mixed Layer

In this Chapter we investigate the properties of the flows developing at scales below the SM. These are characterized by a further weakening of the geostrophic constrains and by flows which are almost fully isotropic. Features developing at these scales are still largely understudied due to the breaking of the hydrostatic approximation which requires the use of complex and computationally expensive numerical models. Observations of processes at these scales are also challenging as satellites do not resolve the scales of motion and direct observations suffer the fast evolution and transient nature of these processes.

Of all the scales developing below the SM, here we present results from a study of the scales just shorter than the SM. This implies that at these scales rotation and stratification are still important. These are scales characterized by
a relatively high aspect ratio which cannot be considered fully isotropic but that nevertheless present many of the characteristics of the fully 3D dynamics.

Other studies that investigated these scales have mostly focused on extreme cases such as the insurgence of Langmuir turbulence in relatively strong wind conditions. Here the focus is on the conditions typical of the weakly forced upper ocean.

The objectives of this study are to address the following questions:

a) Which types of features characterize flows driven by moderate wind speeds of $5\, ms^{-1}$ and regular buoyancy forcing in the ocean mixed layer?

b) What are the regimes in relative dispersion and scale-dependent relative diffusivity attained by these flows? How do these results compare to canonical scaling laws, e.g. those by Richardson (1926); Okubo (1970).

c) When these flows are sampled by more traditional and readily available near-surface 2D drifters, as opposed to fully Lagrangian 3D floats, what types of differences can be noted in relative dispersion and scale-dependent diffusivity?

The Chapter is structured as it follows. In section 2, the numerical model and experiments are described. The goal is to explore two regimes: a case of pure
convection and both buoyancy and wind-forced case. Results are divided into two segments. In section 3, general dynamics are described, while in section 4, we focus on material transport, including comparison to scaling laws and previous findings. The main advances in our understanding are summarized in section 5.

4.1 Methods

Modeling and observation of the fluid flow at scales smaller than the submesoscale is challenging. Most of the numerical models developed by the oceanographic community solve the hydrostatic primitive equations while this regime requires non-hydrostatic models. Non-hydrostatic solvers are computationally expensive (Scotti and Mitran, 2008), stimulating development of hybrid hydrostatic/non-hydrostatic methods (Botelho et al., 2009). From the point of view of the observations, only few instruments exist that can sample the mixed layer in 3D, such as the Lagrangian floats developed by D’Asaro and Farmer (1996); D’Asaro et al. (2011).

In order to study the problem of material transport in the upper ocean, active mixed layer flows are generated under the forcing of buoyancy fluxes and wind stress. These flows are likely to contain high vertical velocities. Therefore, a non-hydrostatic solver is needed. We use the finite element Boussinesq equation solver Fluidity-ICOM (Imperial College Ocean Model, Piggott et al. (2008)).
4.1.1 Numerical model and configuration

Fluidity-ICOM is configured to integrate the following equations:

\[
\begin{align*}
\frac{D\mathbf{u}}{Dt} + 2\Omega \times \mathbf{u} &= -\frac{1}{\rho_0} \nabla p' + \rho' \mathbf{g} + \nabla \cdot \mathbf{\nu} \nabla \mathbf{u} & \quad (4.1a) \\
\nabla \cdot \mathbf{u} &= 0, & \quad (4.1b) \\
\frac{DT}{Dt} &= \nabla \cdot (\mathbf{k} \nabla T) + \frac{F_T}{\rho_0 C_p}, & \quad (4.1c) \\
\frac{DC}{Dt} &= \nabla \cdot (\mathbf{k} \nabla C), & \quad (4.1d)
\end{align*}
\]

where \( D/Dt = \partial / \partial t + \mathbf{u} \cdot \nabla \) is the total derivative operator, \( \mathbf{u} = (u,v,w) \), \( \Omega \) is the planetary angular velocity vector, \( p' \) is the dynamic pressure, \( \mathbf{g} = (0,0,-g) \) with \( g \) being the gravitational acceleration, \( T \) is temperature, \( C \) is a passive scalar field, \( \mathbf{\nu} = (\nu_h, \nu_h, \nu_z) \) with \( \nu_h = 5 \times 10^{-2} \text{m}^2\text{s}^{-1}, \nu_z = 5 \times 10^{-4} \text{m}^2\text{s}^{-1} \) and \( \mathbf{k} = (k_h, k_h, k_z) \) with \( k_h = 5 \times 10^{-2} \text{m}^2\text{s}^{-1}, k_z = 5 \times 10^{-5} \text{m}^2\text{s}^{-1} \) are respectively the kinematic viscosity and thermal diffusivity vectors. \( F_T \) is the surface heat flux forcing, and \( C_p = 4000 \text{J K}^{-1} \text{g}^{-1} \) is the heat capacity. The perturbation density \( \rho' \) in \( \rho = \rho_0 + \rho' \) is expressed through a linear equation of state that depends only on temperature: \( \rho = \rho_0 [1 - \alpha (T - T_0)] \), where the reference density is \( \rho_0 = 1027 \text{Kg m}^{-3} \), thermal expansion coefficient is \( \alpha = 1.5 \times 10^{-4} \circ \text{C}^{-1} \), and reference temperature is \( T_0 = 10 \circ \text{C} \).
Table 4.1: Domain and mesh sizes in the numerical experiments. $L_x$, $L_y$, and $H$ are the horizontal and vertical domain sizes, $\Delta x$ and $\Delta z$ are the horizontal and vertical mesh sizes.

Discretization in Fluidity-ICOM is based on first-order discontinuous Galerkin approximation for tracers and momentum, and second-order continuous Galerkin for pressure (Cotter et al., 2009). The model is capable of adaptive (moving) meshes, but here the mesh is fixed; unstructured in the horizontal and structured in the vertical, in that elements are vertically aligned. Meshing on the horizontal plane is done with Gmsh (Geuzaine and Remacle, 2009) while the extrusion in the vertical is performed inside Fluidity-ICOM.

Domain size is 8 km by 8 km for both simulations with 50 m depth. In the horizontal, the element size is 25 m while the vertical layers are evenly spaced every 1 m in the upper 20 m and every 2 m near the bottom.

The computations are conducted on 512 cores on an IBM cluster at the University of Miami. Both attain a simulated vs wall clock time ratio of about two, for the resolutions and computing resources used. In both simulations, boundary conditions for the velocity are doubly-periodic in the horizontal and no-slip at the bottom. The top boundary has a free-surface condition described in Kramer.
et al. (2010) and a mechanical stress in the experiment forced by wind. A Neumann boundary condition for temperature is applied to the top boundary as part of the buoyancy forcing and at the bottom boundary is insulated. The simulations are initialized from rest with an idealized temperature profile that presents weak stratification in the first 45 m and a stronger stratification near the bottom (Figure 4.1a).

4.1.2 Forcing

All simulations are forced by a surface heat flux with a diurnal cycle. Heat flux is decomposed into a short wave and a long wave radiation which contribute to the heat budget equation as described by Kraus and Turner (1967)

$$F_T = -\frac{\partial wT}{\partial z} + \frac{\partial Q_s}{\partial z},$$

(4.2)

where $Q_s(z, t)$ is the short wave radiation intake. The first term on the right hand side of equation (4.2) represents the surface fluxes of infrared radiation, sensible heat and evaporation enforced in the model as a Neumann boundary condition defined following Large and Yeager (2004)

$$wT = \frac{Q_L}{\rho_0 C_p}.$$  

(4.3)
where $Q_L$ is the outgoing long wave radiation which is assumed negative (surface cooling) and constant in time since its variations are normally over a time scale of several days (Price et al., 1986) (Figure 4.1c).

The second term on the right hand side of equation (4.2) depends on depth and represents the heating due to the short wave radiation, which changes throughout the day. The depth of penetration of the short wave radiation depends on the properties of the mixed layer and is parameterized as described by Paulson and Simpson (1977)

$$Q_s(t, z) = Q_0(t) \left( R e^{z/\beta_1} + (1 - R) e^{z/\beta_2} \right), \quad (4.4)$$

where for negative values of $z$, $Q_0(t)$ is the magnitude of the short wave surface radiation at the surface (Figure 4.1c) and $R$ is the short wave absorption coefficient.
Figure 4.1: (a) The initial condition for temperature (blue) and the corresponding Brunt-Väisälä frequency $N$ (red). (b) Daily cycle of penetrating short wave radiation $Q_s$. Cooling at the surface is constant in time and balances the short wave radiation. (c) Daily cycle of short wave radiation at the surface $Q_0$ (solid) and long wave radiation $Q_L$ (dashed).

The parameters $\beta_1$, $\beta_2$ and $R$ depend on the turbidity of the mixed layer. The mixed layer is assumed to contain Type 1B water according to the classification
by Jerlov (1968). This corresponds to a relatively clear mixed layer with values of $R = 0.67$, $\beta_1 = 1.0$ and $\beta_2 = 17$. The daily cycle of $Q_0(t)$ is taken from Price et al. (1986); Brainerd and Gregg (1995)

$$Q_0 = \begin{cases} 
Q_0 & \text{if } time < 2 \\
Q_{Max} \times (time - 2) & \text{if } time < 3 \\
Q_{Max} - Q_{Max} \times (time - 3) & \text{if } time < 4 
\end{cases} \quad (4.5)$$

with $Q_{Max} = 1000 \text{Wm}^{-2}$ and $time = t/3600.0 \mod(24/6)$, where mod() is the modulo operator. The resulting profile of $Q_s(t, z)$ is plotted in Figure 4.1b.

The integrated heat budget (right hand side of equation 4.2) is set equal to zero over a 24 hours period in order to arrive at the value of the surface cooling flux $Q_L$ compensating the incoming short wave radiation $Q_s$. The resulting surface heat flux, assuming no flux at the bottom boundary, is equal to $Q_L = -245.64 \text{Wm}^{-2}$, which is within the observed range in the ocean (Gregg, 1989).

In Exp. BW, wind forcing is applied to the top boundary in form of a stress vector $\mathbf{\tau} = (\tau_x, \tau_y)$ computed from

$$\mathbf{\tau} = \rho_a C_D |\mathbf{u}_{10}| \mathbf{u}_{10}, \quad (4.6)$$

where $\rho_a = 1.3 \text{Kgm}^{-3}$ is the air density, $C_D = 1.5 \times 10^{-3}$ is the drag coefficient and $\mathbf{u}_{10}$ is the wind velocity vector. Wind is zonal with magnitude of $5 \text{ms}^{-1}$ and constant in time. This corresponds to a state with relatively calm winds,
typically generating a surface oceanic current on the order of 0.1 $ms^{-1}$ (Hunkins, 1966; Price et al., 1987).

Compared to more complete parameterization of the surface fluxes (Gill, 1982), in the present work, the turbulent fluxes do not take into account the wind and SST dependence of the latent and sensible heat fluxes. This simplification is made in order to have identical buoyancy forcing in both Exps. $B$ and $BW$, and to isolate the role of wind forcing in the dynamics.

## 4.2 Dynamics

### 4.2.1 Buoyancy-driven mixing

Pure convection (e.g., Rayleigh-Bénard instability) is a well-studied process in laboratory experiments (Rossby, 1969; Jones and Marshall, 1993; Bodenschatz et al., 2000; Grooms et al., 2010). Even though the absence of any wind forcing is rare in the oceans, convection is the norm and the current simulation can be used to study material transport in the limiting case of vanishing vertical shear (Shay and Gregg, 1986).

The daily heat flux generates alternating phases of convection and restratification in Exp $B$ (Figure 4.2). Starting from a state of weak stratification, plumes develop due to surface cooling and grow linearly in a classic Rayleigh-Bénard instability (Bodenschatz et al., 2000). After 12 hours, plumes are already well
developed (Figure 4.2a) while the short wave radiation starts heating the water column inducing partial restratification. At 24 hours, surface heating is absent and the cycle starts again (Figure 4.2b). During the second and successive cycles, the mixed layer is not quiescent anymore, thus plumes do not develop uniformly but preferentially where the stratification is weaker (Figure 4.2c, 4.2d). In the vertical, plumes develop with a classic mushroom shape, while in the horizontal the surface plumes are organized in polygons, similar to those observed in laboratory experiments (Veronis, 1959; Grooms et al., 2010). The cellular surface structure similar to that reproduced in Figure 4.2 was revealed using airborne remote sensing by Marmorino et al. (2009).

4.2.2 Buoyancy and wind driven mixing

Similarly to the purely convective case Exp. B, the wind-forced mixed layer Exp. BW undergoes phases of strong convection and restratification (Figure 4.3). The surface signature of the convective plumes is organized by wind in that they are elongated to the right of the direction of the wind.
Figure 4.2: Temperature field for the simulation Exp. B during the first two convective cycles: at the beginning of the surface heating ((a) at 12 hours and (c) at 36 hours) and at the end of the cycle ((b) at 24 hours and (d) at 48 hours). The animation is available from: http://youtu.be/QtOrKF2z2gw.
Figure 4.3: Temperature field in Exp. BW (a) after 12 hours, during the first cooling event, (b) after 24 hours, at the end the first day, (c) at 36 hours during the second cooling event and (d) at 48 hours at the end of the second day. The animation is available from: http://youtu.be/TYYI6VvB34Y.

Speed (Figure 4.4a) and vertical velocity (Figure 4.4b) during convection reveal surface intensified jets. The flow field is organized into elongated structures
separating regions of stronger horizontal and vertical velocities. These jets are associated with convergence zones developing on top of convective plumes. Similar structures have been generated by Moeng and Sullivan (1994) in a model of the atmospheric boundary layer and by Heitmann and Backhaus (2005) in a model of the oceanic mixed layer, namely on both boundary layers across the air-sea interface. Airborne remote sensing images by Marmorino et al. (2009) and in-situ observations by Soloviev (1990) also detected similar features at the ocean’s surface.

In that sense, there seems to be some support that modeled flows under moderate atmospheric have relevance to the oceanic mixed layer. Next we proceed to focus on material transport in these flow fields using passive tracer, 2D passive particles and 3D fully neutrally-buoyant particles. This is the main original aspect of the study, to the authors’ knowledge.
Figure 4.4: (a) Speed \([m \, s^{-1}]\) and (b) vertical velocity \([m \, s^{-1}]\) at the end of the second convective event (at 36 hours) in Exp. \(BW\).

Time evolutions of mean horizontal and vertical speeds allows us to make a decision about how long the spin-up of the flow field lasts; it seems reasonable to assume a spin-up of 72 hours (Figure 4.5). It is also noted that the horizontals speed is an order of magnitude is larger in Exp. \(BW\) while vertical speeds are comparable between Exps. \(B\) and \(BW\). Thus, vertical flows are driven by convection in both, while the surface field is driven by the wind in Exp. \(BW\).
Figure 4.5: Time evolutions of domain averaged (a) horizontal speed \([m \ s^{-1}]\) and (b) vertical speed \([m \ s^{-1}]\) for the entire integration time for both Exps. \(B\) (red) and \(BW\) (blue). The dashed lines mark the spin-up period.

4.3 Material Transport

Our simulations appear to contain many of the characteristics that can be found in the oceanic mixed layer, namely intense vertical shear, near-surface horizontal divergence and strong vertical velocities. In this section, these flows are characterized in terms of Lagrangian dispersion and scale-dependent diffusivity using 2D and 3D particles, as well as passive tracer releases.

4.3.1 Passive scalar transport

4.3.1.1 Evolution of scalar gradients

Consider the concentration (density) of a conservative tracer, \(C_{\rho}(x, t)\), (initially uniformly distributed) transported by a two-dimensional surface velocity field \(\mathbf{u}(x, t)\). Neglecting diffusive effects for simplicity, the evolution is described by
the advection equation,

\[
\frac{\partial C_\rho}{\partial t} + \nabla \cdot (uC) = 0, \quad (4.7)
\]

Since the velocity field is not necessarily solenoidal, this becomes:

\[
\frac{\partial C_\rho}{\partial t} + u \cdot \nabla C_\rho = - (\nabla \cdot u) C_\rho, \quad (4.8)
\]

The divergence of the vector field acts as a multiplicative forcing on the concentration field and the linear PDE is simply:

\[
\frac{\partial C_\rho}{\partial t} + u \cdot \nabla C_\rho = - (\nabla \cdot u) C_\rho = f(x, t) C_\rho \quad (4.9)
\]

For uniform initial conditions and \( f(x, t) = 0 \), Eq. (4.9) has the unique solution of \( C_\rho(x, t) = C_0 \), and therefore, the initially uniform field remains so. In fact, the only means of creating scalar gradients from an initially uniform scalar field is via the velocity divergence. This can be confirmed by using an initially uniform distribution for the scalar density. For area preserving flows, (horizontal divergence \( \nabla \cdot u = 0 \)), initially uniform scalar density fields remain uniform. However, if there are spatial gradients of scalar density, then these gradients may be amplified by solenoidal velocity fields, namely by typical Lagrangian chaos. Taking the gradient of Eq. (4.9) yields:

\[
\frac{\partial \nabla C_\rho}{\partial t} + (u \cdot \nabla) \nabla C_\rho = - \left( [\nabla u]^T + (\nabla \cdot u) \right) \nabla C_\rho - C_\rho \nabla (\nabla \cdot u) \quad (4.10)
\]
Eq. (4.10) shows that scalar gradients (indicative of clustering of surface material) can only be directly produced from initially uniform scalar fields by the velocity divergence. In fact, the production of scalar gradients requires that the gradient of the velocity divergence be non-zero. Spatially uniform divergence simply changes the density field in a spatially uniform manner.

Consider a uniform scalar field - Eq. (4.9) shows that $C_\rho(x,t)$ will grow (decay) exponentially in regions of convergence (divergence). Thus, very rapidly, the initially uniform $C_\rho$ field will develop spatial gradients. Eq. (4.10) shows that these gradients will be advected by the velocity field and amplified by three distinct mechanisms: (1) production by stretching (2) production by divergence (3) production by gradient of the divergence.

4.3.1.2 Numerical results

It is of great interest to explore how the strain induced by the movement of coherent structures and horizontal divergence interact in near-surface flows, as modeled here. Some of these concepts have been demonstrated using passive particles by Schumacher and Eckhardt (2002), but we specifically explore these in the context of oceanic mixed layer dynamics. We also use a passive tracer release since, as demonstrated in section 4.1.1, the temporal evolution of a concentration field from a uniform release is perfectly suitable to explore the issue.
In Exp. B, plumes are well organized at the surface and show regular structures of few hundred meters width. These structures are separated by convergence zones of cold temperature fronts at the boundaries of convective plumes. These structures remain relatively coherent throughout the simulated period. A passive tracer is released after 48 hours over the first 3 m near the surface with a uniform concentration of \( C = 1 \) in order to explore whether the divergence field has any impact on the subsequent distribution of the tracer. It is found that the tracer rapidly evolves along the converge zones in both Exps. B (Figures 4.6a, 4.6b) and BW (Figures 4.7a, 4.7b).

In order to quantify this visual similarity, the time evolution of the correlation between the tracer concentration and horizontal divergence fields is computed from

\[
\text{corr}(C, \nabla \cdot u) = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \frac{(C_{ij} - \langle C \rangle) \cdot (\nabla \cdot u_{ij} - \langle \nabla \cdot u \rangle)}{\text{std}(C) \text{std}(\nabla \cdot u)},
\]

(4.11)
Figure 4.6: (a) Divergence \([s^{-1}]\) of the horizontal velocity field at 1 m depth and (b) passive tracer concentration 3.1 hours after the release in Exp. \(B\).

Figure 4.7: (a) Divergence \([s^{-1}]\) of the horizontal velocity field at 1 m depth and (b) passive scalar concentration 1.5 hours after the release in Exp. \(BW\).
where $\langle C \rangle$ is the spatially-averaged tracer concentration averaged over the release depths from 1 to 3 m, $\nabla \cdot u$ is the horizontal velocity divergence at 2 m depth and $std(C)$ and $std(\nabla \cdot u)$ are the corresponding standard deviations.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure4.8.png}
\caption{Time dependence of the spatial correlation between the horizontal velocity divergence and tracer concentration for Exp. $B$ (solid) and Exp. $BW$ (dashed).}
\end{figure}
Figure 4.9: Time dependence of tracer concentration normalized variance for Exp. $B$ (solid) and Exp. $BW$ (dashed).

The time series show that the highest amplitude correlation is attained just after 1 to 3 hours after the release for both cases (Figure 4.8). Exp. $BW$ shows considerable weaker correlation than Exp. $B$. Tracer variance $\langle (C - \langle C \rangle)^2 \rangle$ is also plotted (Figure 4.9). Larger variance for $B$ supports the view that surface tracer concentration is driven mainly by horizontal divergence while in Exp. $BW$ horizontal advection is important and responsible for the weaker correlation with $\nabla \cdot u$.

From the passive tracer release with initially uniform concentration, we arrive at the clear result that horizontal divergence by convection has a major influence on the distribution of surface material in mixed layer flows. This is a fundamentally different transport mechanism than stretching induced by wind or existing
background coherent structures. Both stretching and horizontal divergence result in filamentation, or generation of scalar gradients. Our results suggest that filamentation can be generated with a matter of a few hours in the oceanic mixed layers. These features are of great interest in practical applications such as oil spills, because this inhomogeneity can influence response efforts and effectiveness of the resources deployed.

4.3.2 Lagrangian transport

In order to study horizontal dispersion in our simulations, particles were released after 72 hours of spin-up and advected offline using a fourth-order Runge-Kutta scheme in 2D (constant z-level) as well as in 3D. The justification for this approach is that while near-surface drifters were commonly employed in the ocean (Davis, 1983), these were not fully Lagrangian in that they do not follow the 3D velocity field. The differences between 2D and 3D measurements could be particularly significant in a forced oceanic mixed layer and carry importance in applied problems motivating this investigation. In advecting particles, velocities were updated every 1440s. 1440 s. Particles are seeded in box of 5 km by 5 km in the middle of the domain every 10 m in both horizontal directions. 2D releases were conducted at three selected depths of 5 m, 10 m, 15 m, which were in the general
range typical depths used in oceanic drogued drifters (Lumpkin and Pazos, 2007). A total of 750,000 particles were advected in each flow field.

Plumes were generated due to surface cooling at the top of the mixed layer, resulting in complex three-dimensional structures that determine vertical transport and mixing. This regime poses challenges for oceanic Lagrangian observations due to the presence of strong vertical velocities and horizontal divergence (D’Asaro et al., 2002, 2011). Because of the prominence of 3D motion, it is important to investigate whether there is a difference between 2D and 3D sampling, and where exactly these fields were sampled at depth. Since surface waves were not included in our computations, the dynamics of the surface sublayer potentially influenced by the wave motion is necessarily excluded from consideration.

In Exp. B, 2D particles (Figure 4.10a) behave in a manner consistent with tracer releases and cluster together in the form of filaments and small eddies, under the influence of convergence regions. No significant difference is visible between 5 m and 15 m releases, indicating that the effect of the convergence regions in aggregating fixed-depth particles prevails at depth. Such filaments and streaks were of great interest for the behavior of 2D drifters in the field, as well as trapping of buoyant pollutants that remain close to the ocean’s surface, such as oil. In comparison, 3D particles show a far more homogeneous distribution in the depth
average sense (Figure 4.10b), again lacking a significant visual difference between releases conducted from different depths. 3D particles were free to move vertically and were advected inside convective plumes, where they travel to different depths spreading in a more homogeneous fashion. Perhaps most interestingly, there is a striking similarity between the overall extent of particle dispersion from 2D and 3D releases; in other words, the outer bounds of dispersion seems similar, while the interior patterns were significantly different, with 2D releases being characterized by patterns of clustering leading to substantial deviations from the mean pattern.

In Exp. $BW$, the addition of wind introduces significant depth dependence. For 2D releases, the near-surface pattern still shows clustering consistent with tracer results (Figure 4.10c, while for particles at the edge of the wind-influenced layer ($15\, m$), the clustering effect is largely diminished, or evolving far more slowly. There is also significant vertical shear, on top of the cross-wind Ekman transport, propelling surface particles in the along-wind direction and implying that coherent structures would be rapidly tilted and decorrelated in the vertical. This indicates the importance of vertical shear dispersion. Qualitatively similar patterns were visible from 3D particles releases (Figure 4.10d).
Figure 4.10: Horizontal location of a subset of particles released in a $1 \text{ km} \times 1 \text{ km}$ box in the center of the domain in Exp. $B$ (a) using 2D advection, and (b) using 3D advection of particles released at 5 m (blue) and 15 m (red) depth after 144 hours of integration. Same for Exp. $BW$ in the case of (c) for 2D and (d) 3D particles after 14 hours of advection.
4.3.2.1 Vertical dissipation, dispersion and diffusivity

The daily cycle of the convective mixed layer has been extensively studied in both lakes, oceans and numerical models (Imberger, 1985; Brainerd and Gregg, 1993a,b; D’Asaro et al., 2002; Nagai et al., 2005; Yeates et al., 2013). A quantity of interest is the kinetic energy dissipation rate $\epsilon$ [W Kg$^{-1}$].

Figure 4.11: Temporal and vertical variability of the horizontally-averaged kinetic energy dissipation rate $\log(\epsilon)$ [W Kg$^{-1}$] for (a) Exp. $B$ and (b) Exp. $BW$ over three days after the spin-up.
Considering the full expression for $\epsilon$ (Hinze, 1959),

$$\epsilon = \nu \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \frac{\partial u'_i}{\partial x_j},$$

(4.12)

and given that $\nu$ is a diagonal tensor $\nu = (\nu_h, \nu_h, \nu_z)$ we obtain an expression for $\epsilon$,

$$\epsilon = 2 \nu_h \left( \frac{\partial u'}{\partial x} \right)^2 + 2 \nu_h \left( \frac{\partial v'}{\partial y} \right)^2 + 2 \nu_z \left( \frac{\partial w'}{\partial z} \right)^2,$$

(4.13)

where $u'$, $v'$ and $w'$ are turbulent fluctuations. Anomalies are calculated respect to the mean computed in space over $x,y$ and in time over the three days period so that the resulting mean is a function of depth only.

Brainerd and Gregg (1993a) make the distinction between a mixed layer, generated on a seasonal scale and mostly quiescent, and a mixing layer where active convection is forced by daily buoyancy fluxes. While the mixed layer extends throughout the first 45 m of the domain, depth of the mixing layer depends of the penetration of convective plumes. Surface cooling forces convection in the mixed layer at night, while during the day the penetrating short wave radiation forces restratification inhibiting convection and reducing turbulent dissipation.

Overall the daily cycle of the dissipation rate is similar to what observed in the real ocean under similar conditions (Brainerd and Gregg, 1993a) and presents a relatively stable cycle in time (Figure 4.11). Kinetic energy dissipation rate
for $BW$ and $B$ show qualitatively the same time dependency with deepening of
the mixing layer at night and restratification during the day. The values were
more than one order of magnitude larger for $BW$ in the upper 10 m, where the
vertical shear is stronger. In Figure 4.12 we compute the horizontally averaged
vertical shear $\langle \log (du/dz + dv/dz)^2 \rangle$. Values are about two orders of magnitude
larger in $BW$ than $B$ accounting for the difference observed in the kinetic energy
dissipation rate.

![Figure 4.12: Horizontally averaged vertical shear after 72 hours for Exps. $B$ and $BW$.](image)
A second method to estimate vertical eddy diffusivity is directly from passive particle releases at different depths. Vertical diffusivity $K_z$ can be computed from (Babiano et al., 1990)

$$K_z = \frac{1}{2} \frac{d\sigma_{D_z}^2(t)}{dt}, \quad (4.14)$$

where $\sigma_{D_z}^2(t)$ is vertical relative dispersion

$$\sigma_{D_z}^2(t) = \langle (z_1(t) - z_2(t))^2 \rangle, \quad (4.15)$$

where $z$ is the particle depth, and subscripts refer to particle pairs. Relative dispersion allows to define different dynamical regimes in particular Figure 4.13 shows that $\sigma_{D_z}^2(t) \sim t^3$ consistently with Richardson scaling. This suggests that transport is dominated by features with scales comparable to the scale of the particle separation. The transition to Richardson regime is faster for particles released in $BW$ than $B$ due to the strong vertical shear and generation of smaller scale features by the anisotropy induced by wind, both of which enhance pairs separation statistics.
Figure 4.13: Relative vertical dispersion $\sigma_{D_z}^2(t)$ computed from 3D particle released at 5 m depth. The black line has slope $t^3$ characteristic of Richardson regime and the inset shows normalized dispersion.
Figure 4.14: Diffusivity versus length scale for particles released at $t = 72\,hr$ in both experiments. The canonical Richardson slope $\ell^{4/3}$ is shown for comparison. The symbol $X$ represents the value of eddy viscosity computed from inverse Ekman theory ($K_z \approx 6 \times 10^{-4}\,m^2s^{-1}$) against the mixed layer depth of $50\,m$. 
Figure 4.15: (Upper panel) Vertical diffusivity $K_z(t)$ in Exps. B (red line) and BW (blue line). The circles indicate the instances when particles were released in the flow field. (Lower panel) Time series of surface buoyancy forcing.
In order to define the scale dependence of eddy diffusivity, we compute $K_z$ against the length scale $\ell = 3\sigma_{D_z}$. The factor 3 comes from the fact, that assuming a Gaussian distribution, 3 standard deviations from the mean cover 99% of the particle’s patch.

Results are shown in Figure 4.14 for particles released at $t = 72 h$ at 5 m depth in both simulations. Eddy diffusivity plateaus at scales of about $\sim 50 m$ which corresponds to the full vertical extent of the domain.

Diffusivity shows Richardson scaling (Richardson (1926), $K_z \sim \ell^{4/3}$) right after the release which is consistent with the Richardson regime observed in Figure 4.13.

Overall, we find that vertical diffusivity changes by more than one order of magnitude from $\sim 2 \times 10^{-6} m^2 s^{-1}$ to $\sim 8 \times 10^{-4} m^2 s^{-1}$ where the maximum value, reached at the length scale of the mixed layer, is very close to the $K_z \approx 6 \times 10^{-4} m^2 s^{-1}$ obtained from inverse estimation using Ekman theory (black X in Figure 4.14) where the length scale of $K_z$ is taken equal to 50 m. This result suggests that eddy viscosity computed from Ekman theory is a measure of the diffusivity acting at the scale of whole mixed layer which is then the maximum vertical eddy viscosity that can be attained in the domain at a given time.
We estimate time-dependent variations of $K_z$ for both experiments computing $d\sigma_{D_z}^2(t)/dt$ with 3D particles released every two hours at 5 m depth (Figure 4.15).

$K_z$ here is computed averaging values of instantaneous eddy viscosity between 20 hour < $t$ < 22 hour after release which corresponds to the middle of the Richardson regime (Figure 4.13).

Both experiments show a clear daily cycle, indicating that vertical diffusivity is influenced by the surface buoyancy forcing. Highest $K_z$ is attained at the end of the nightly surface cooling, and the lowest $K_z$ coincides with the end of the daily heating cycle (i.e., cross over point to cooling).

Vertical diffusivity changes in the range of $5 \times 10^{-4} \text{m}^2\text{s}^{-1} \leq K_z \leq 9 \times 10^{-4} \text{m}^2\text{s}^{-1}$ for BW and $2 \times 10^{-4} \text{m}^2\text{s}^{-1} \leq K_z \leq 4 \times 10^{-4} \text{m}^2\text{s}^{-1}$ for B. The average values are $K_z \approx 5 \times 10^{-4} \text{m}^2\text{s}^{-1}$ for BW and $K_z \approx 2 \times 10^{-4} \text{m}^2\text{s}^{-1}$ for B.

4.3.2.2 Horizontal relative dispersion

Relative dispersion $\sigma_{D_H}^2(t)$, a metric for horizontal dispersion, is computed,

$$\sigma_{D_H}^2(t) = \langle (\mathbf{r}_1(t) - \mathbf{r}_2(t))^2 \rangle,$$

(4.16)

where $\mathbf{r}$ is the particle position vector, and subscripts refer to particle pairs. Spreading is denoted non-local when it is dominated by features at scales larger than particle pair separation scale (Bennett, 1984). In the non-local dispersion
regime, $\sigma_D^2 \sim exp(t)$. When particles are sufficiently separated, $\sigma_D^2$ transitions to a \textit{local} regime, where dispersion is driven by processes with the same scale as pair separation. This regime is characterized by the Richardson law, $\sigma_D^2 \sim t^3$. When the scale of separation is much larger than the scale of the eddies, the diffusive regime, $\sigma_D^2 \sim t$ can be attained. Sometimes, also a ballistic regime emerges, where particle dispersion is dominated by horizontal shear ($\sigma_D^2 \sim t^2$) (Iudicone et al., 2002).

Given that relative dispersion can show a super-diffusive character with such different growth rates, it has been a topic of investigation both in classical fluid mechanics and physical oceanography.

Of particular interest is the Richardson’s regime, which is observed in 2D turbulence (Babiano et al., 1990) as well as 3D turbulence (Boffetta and Sokolov, 2002) in classical fluid dynamics. Nevertheless, oceanic flows contain multi-scale flows driven by a large number of processes (as reviewed in Section 1), and it is a natural question to ask whether and over which scales Richardson’s law would remain valid. Richardson law has been observed for mesoscales using floats (deep measurements) by LaCasce and Bower (2000); Ollitrault et al. (2005) in the North Atlantic, using 15 to 30 m drogued drifters in the Gulf of Mexico LaCasce and
Ohlmann (2003), in the nordic seas by Koszalka et al. (2009) and in the Ligurian Sea by Schroeder et al. (2011).

There has been measurements indicating that the Richardson scaling extended into the submesoscale regime, most notably in studies by Lumpkin and Elipot (2010) in the North Atlantic and Schroeder et al. (2012) in the Ligurian Sea, but also different results were put forward (e.g., Berti et al. (2011) in the Brazil Current). Modeling studies (Poje et al., 2010; Özgökmen et al., 2012; Haza et al., 2014) have demonstrated that the primary challenge in pinning down the statistical regime has been that the number of drifters were either too low, or that the positioning accuracy needed for submesoscale dispersion is hard to attain in oceanic measurements. These obstacles have been overcome recently, and results consistent with the Richardson law were found in the northern Gulf of Mexico (Poje et al., 2014). The next frontier is to identify what types of scaling laws can be expected for mixed-layer flows modeled here, especially given the challenge that measurement of relative dispersion with adequate statistical accuracy is likely to be limited to the use of surface drifters, since the use of hundreds of Lagrangian floats (D’Asaro et al., 2002) is likely to be prohibitively expensive for the foreseeable future.
Figure 4.16: Relative dispersion $\sigma_D^2(t)$ for (a) 2D particles (released at $5 \text{m}$ solid, $10 \text{m}$ dashed, $15 \text{m}$ dashed-dotted) and (b) 3D particles in Exp. B. The slope $t^3$ shows the Richardson regime for reference. The insets show relative dispersion normalized by the Richardson regime.
Figure 4.17: Relative dispersion $\sigma_D^2(t)$ for (a) 2D particles (released at 5 m solid, 10 m dashed, 15 m dashed-dotted) and (b) 3D particles in Exp. BW. The slope $t^3$ shows the Richardson regime for reference. The insets show relative dispersion normalized by the Richardson regime.
In Exp. $B$ (Figure 4.16) particles were released after the spin-up period (72 hours) and initially show an exponential regime because particle pair separation distances ($10 \text{ m}$) were much smaller than the scale of the convection cells ($\mathcal{O}(100 \text{ m})$). Transition to a well-defined Richardson regime starts after 6 hours for 5 m releases and after 12 hours for 15 m releases. The Richardson scaling persists throughout the remainder of the analysis period, as also shown in the normalized ($\frac{\sigma_D^2}{t^3}$) plot in the inset of Figure 4.16a. Sampling using 3D particles, initialized at a depth of 5 m (Figure 4.16b) shows very similar results to the 2D sampling. Even though the distribution patterns of 2D and 3D particles were significantly different as discussed above, relative dispersion captures the amount of the overall spreading and other metrics were needed to identify the clustering behavior.

In comparison, Exp. $BW$ (Figure 4.17) shows the following differences. 2D particles near the surface make a faster transition to Richardson scaling, after 4 hours, for particle releases at 5 m depth, because of the wind creates anisotropic features with a smaller dynamical scale helping the transition to local dispersion. Thus, 2D sampling has a more pronounced depth dependence (with deeper releases showing a delayed transition to Richardson’s regime) in Exp. $BW$. In addition, the amplitude of relative dispersion is approximately an order of mag-
magnitude larger in Exp. BW than in Exp. B. Furthermore, the transition to Richardson scaling emerges after a full 24 hours of the release of 3D particles in Exp. BW.

**4.3.2.3 Scale-dependent horizontal diffusivities**

In his seminal work, Richardson (1926) pioneered the concept of scale-dependent diffusivity based on the notion turbulence consists of eddies of difference sizes and velocities at different scales, as a tracer patch encounters ever larger scales of motion while spreading. He proposed the so-called 4/3-law (thereafter, the Richardson law) on the basis of remarkably few observations. Okubo (1970) compiled results from a series of measurements in lakes and coastal oceans, and estimated the scale-dependent diffusivity $k_D$ from

$$k_D = \frac{\sigma_D^2}{4t}. \quad (4.17)$$

According to Richardson (1926), the slope of $k_D$ with respect to the length scale $\ell$, should follow $k_D \sim \ell^{4/3}$, which is fundamentally consistent with the 3D turbulence theory by Kolmogorov (1941). This is remarkable in that both formulations rely on the assumption of constant turbulent kinetic energy dissipation rate $\epsilon$ throughout the kinetic energy wavenumber spectrum, irregardless of the direction of the cascade. The diagrams compiled by Okubo (1970, 1971) did not match the
Richardson law. When the relationship between $k_D$ and $\ell = 3 \sigma_D$ is plotted from a number of experiments, Okubo found

$$k_D \approx 0.0103 \ell^{1.15},$$

(4.18)

where the exponent 1.15 is a little less steep than the Richardson’s regime. As discussed in Okubo (1970), Richardson regime is observed for individual experiments but not when the full collection of observations was considered.

The possible emergence of the Richardson law is the central focus from a large surface dispersion experiment conducted in the northern Gulf of Mexico recently. These results, discussed in Poje et al. (2014), covered larger separation scales than Okubos and is found perfectly consistent with the Richardson scaling.

The difference in the scale-dependence coefficient of 1.15 vs 1.33 is quite small, nevertheless, this issue can still benefit from further investigation, in particular about how it depends on 2D vs 3D sampling.

The scale-dependent diffusivity for Exp. $B$ (Figure 4.18a and 4.18b) shows overall smaller values (by up to an order of magnitude) for both 2D and 3D particles respect to Okubos results. Apparently, the horizontal dispersive effect of wind missing in Exp. $B$ is quite important to get results that were consistent with
previous oceanic estimates for scale-dependent diffusivity. 3D sampling shows a slope which is closer to the Richardson power law.

Figure 4.18: Scale-dependent relative diffusivity $k_D(\ell)$ for Exp. $B$ (upper panels (a), (b) 3D)) and Exp. $BW$ (lower panels, (c), (d) 3D) using 2D sampling (left panels) and 3D sampling (right panels). Diffusivity is computed from particles released at 5 m (red), 10 m (green) and 15 m (blue) depths. Okubo’s (1970) curve is plotted for reference in solid line. The dashed line marks Richardson’s scaling of $k_D \sim \ell^{4/3}$. 
When the wind is added (Figures 4.18c and 4.18d) a better agreement with Okubo (1970) is attained in terms of the amplitude of $k_D$. Vertical shear and overall larger horizontal velocities substantially contribute to diffusivity. 2D sampling exhibits some depth-dependence in that particles released near the surface show a better agreement to Richardson scaling, while particles released at 15 m depth have diffusion that is half of what is measured by Okubo (1970). Finally, with 3D sampling of the case with both buoyancy and wind forcing, the amplitude of $k_D(\ell)$ is close to Okubo’s measurements at all depths while the scaling is consistent with the Richardson power law.

### 4.4 Concluding remarks

In this chapter, motivated by the importance of transport processes in the upper ocean mixed layer, most notably those involving biogeochemical tracers, and buoyant pollutants such as oil, we investigate the properties of a forced mixed layer at scales below the SM. The study is carried out with a non-hydrostatic numerical model able to capture the 3D motion driven mostly by convection due to buoyancy fluxes. We focus on a regime that is not well investigated, namely on flows subject to low wind speeds of $5 \text{ms}^{-1}$, because it is a common state in the ocean. Thereby, the numerical model does not require the vortex force used
to parameterize the wind-wave effect, which is thought to generate Langmuir circulations at wind speeds above 10 m s$^{-1}$ (Craik and Leibovich, 1976).

Once a fairly realistic upper ocean flow field under moderate forcing conditions is generated, the primary objective of this study is to characterize transport and dispersion in these flows. These notions are most naturally explored, and most directly applicable to problems of interest outlined earlier, in the Lagrangian framework. Therefore, we mostly focus on the use of 2D and 3D passive Lagrangian particles, which readily provide quantitative information on metrics such as relative dispersion, vertical diffusivity and scale-dependent horizontal relative diffusivity, for which scaling laws based on theory and prior observations exist for comparison. Passive tracer releases are also used for visual guidance.

We find that the horizontal flow divergence that is generated by convective cells near the surface has a tremendous control on particle motion in that it leads to the accumulation of surface material along these convergence zones. This is counter to traditional LCS thinking that material transport is controlled by the temporal variability of 2D non-divergent coherent vortices and jets, leading to barriers to transport that are invisible in any snapshot of the velocity field. What is seen here in contrast is that the material lines are very much visible through the surface horizontal divergence field. A high correlation is established within hours after the
release of the surface tracer with the horizontal divergence field. This correlation lasts 12 hours, after which the tracer is fully homogenized through the mixed-layer circulation. It should be noted however, that the modeled flows do not contain the larger scale strain fields that can be exerted by submesoscale or mesoscale flows on the surface clustering by convergence zones. As such, the question of such a multiscale interaction is a ripe area for a future study. The factors determining the distribution of surface material in the ocean have important practical implications, bringing dynamical support to the adage “90% of the oil in 10% of the area” (Oil in the Sea: Inputs Fates and Effects, 2003).

We then proceeded to explore differences between 2D and 3D particle sampling of the mixed layer. 2D sampling is not only applicable to the motion of buoyant surface material, but it is also the only technique that is presently available through the use of massive drifter arrays (Poje et al., 2014). 3D sampling is possible using the innovative Lagrangian float (D’Asaro and Farmer, 1996) but not in large enough numbers needed to capture adequately the degrees of freedom in a turbulent flow field. We do not address the practical limitations facing a real sampling strategy, but focus on dispersion regimes given an adequately high number of sampling points. Poje et al. (2014) clearly demonstrated that advances in measurement techniques are possible by scaling the resources, if the statistical
requirements are estimated a-priori on the basis of metrics and flows patterns of interest. Such a statistical sensitivity study may be attempted at a future time.

In both modeled cases, we observe a clear emergence of a Richardson regime in relative dispersion. Sampling of the flow field by 2D and 3D particles did not result in a significant difference in Exp. $B$, but the depth dependence in dispersion is pronounced in Exp. $BW$, with surface releases transitioning to the Richardson’s regime faster, due to larger shears in the upper 20 m. In addition, relative dispersion in the wind-forced case is about an order of magnitude larger than in the buoyancy-forced case, implying the importance of wind forcing in these measurements. We have not observed emergence of a diffusive regime and it is not realistic to maintain steady winds longer, in face of seasonal variations that come in at longer time scales.

It is also of great interest to compare the scale-dependent diffusivity associated with various upper ocean processes because of the remarkable consistency of the transport theory by Richardson (1926) with turbulent energy cascade laws of Kolmogorov (1941), as well as the existence of a canonical tracer data set by Okubo (1971) and recent results from a large dispersion experiment (Poje et al., 2014). Values of scale-dependent diffusivity are similar to Okubo’s results when the simulation is forced by both wind and buoyancy forcing. In the case of Exp.
diffusivity is about one order of magnitude smaller than Okubo’s values. For 2D particles, good agreement in diffusivity is reached only for particles released close to the surface. This is consistent with the findings of Poje et al. (2014) from surface drifters at 1 m depth. When 3D sampling is used, the slope of the scale-dependent diffusivity steepens from Okubo’s \(k_D \sim \ell^{1.15}\) to Richardson’s \(k_D \sim \ell^{4/3}\) estimate, and all curves seem to collapse. This result implies a somewhat reduced diffusivity for surface-bound tracers, even though the differences are admittedly small.
Chapter 5
Conclusions

The goal of the present work is to investigate the properties of the flows developing at the scales of the SM and below. The ocean presents a variety of scales ranging from the scale of the large scale ocean circulation to the isotropic scales of 3D turbulence. Historically research focused on understanding the large scale processes but the development in observational techniques and computational power allowed to push the scientific focus towards much smaller scales. The push towards smaller scales is motivated by the understanding that there is a wide gap between the scales of the mesoscale and the scale of the processes experienced by human activities. The fine structure of the sea is something which has not yet been investigated despite being potentially very important from an anthropocentric prospective. In this context with this dissertation we want to contribute to
the description and understanding of SM processes and push the investigation towards scales below the SM.

5.1 Mechanisms and Implications of the SM Dynamics

In the second chapter we presented a picture of SM dynamics in the complex GS region, characterized by strong nonlinear mesoscale interactions. One of the main results is that frontogenesis and MLIs appear to be one of the main mechanisms leading to a vigorous winter SM field, mostly due to deepening of the mixed layer and increased available potential energy reservoir. The dependence of SM formation on the properties of the mixed layer explained the observed seasonality.

This work represented the first evidence of seasonality of SM features. Nowadays SM features are well studied and their existence is recognized but their role on the ocean dynamics is a question that remains mostly unanswered.

While theoretical considerations and numerical experiments suggest that SM might represent a turning point in the energy cascade there is, as of today, no definitive evidence of this. On the other side, Lagrangian observations have recently proven that SM can play an important role on material transport Poje et al. (2014). In particular a key role could be played on the vertical transport of
biogeochemical tracers where the large vertical velocities of the SM could explain
the observed large primary production of the oceans.

5.2 Role of SM on vertical transport of nutrients in mesoscale eddies

In the third chapter we investigate the role of SM features on the vertical trans-
port of an anticyclonic eddy. Ocean eddies are thought to behave like pathways
between the deep ocean and mixed layer driving nutrients from the water col-
umn to the euphotic zone. A clear picture of the involved mechanisms is still
missing and in particular it is not possible to explain the observed large primary
production in terms of mesoscale dynamics alone.

Klein and Lapeyre (2009) and Siegel et al. (2011) discussed the different pro-
cesses that could affect and enhance vertical transport in ocean eddies where SM
features could be one of the leading processes. In the present work we have con-
firmed this hypothesis showing that a thick mixed layer developing SM features,
can in fact drive the circulation of nutrients from the water column to the upper
ocean. Developing close to the surface and acting as active boundary conditions
in the eddy dynamics, SM and in general mixed layer processes, can contribute
to the dynamics of ocean eddies.
Lagrangian techniques have been proven very effective in studying SM processes as they sample scales ranging from the release scale to the scale of entire basins. Nevertheless most of the current techniques have been develop in order to study ∼2D flows and might not apply to the ∼3D mixed layer processes.

In the fourth Chapter of this work we investigated the Lagrangian properties of a convective mixed layer showing that in fact at these scales, 2D drifters suffer from strong convergence and vertical shear underestimating in some cases particle dispersion and diffusion. Pushing the investigation towards smaller scales such as the experiments described in Chapter 4, allowed to investigate processes which are almost fully 3D. These are the scales characterized by convection, vertical shear and inertial oscillations. At these scales the flow is far from 2D but not quite 3D yet which is yet another intermediate regime between the fully isotropic turbulence and the early loss of balance of the SM dynamics. Little is known about the material transport of these scales and the present work represent to our knowledge the first attempt in this direction.

Future research will necessarily go in the direction of bridging the gap between SM and isotropic scales. Some research has been done in this direction but probably the most important questions will remain unanswered for years. A complete understanding of the energy pathways in the oceans and the corresponding La-
grangian transport regimes requires resolving all the scales of the oceans at once. This will require new computational tools able to resolve the non-hydrostatic nature of the mixed layer but also to retain little diffusion in the ocean interior. In this direction some hope might come from the finite element modeling approach.

The quest towards the SM has been rewarded with a deeper understanding of the mixed layer dynamics and material transport. The hope is that approaching even smaller scales will get us closer to answer some of the biggest questions in oceanography.
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