Combining In Situ and Satellite Observations to Retrieve Salinity and Density at the Ocean Surface

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ABSTRACT

Monitoring sea surface density (SSD), sea surface salinity (SSS), and sea surface temperature (SST) allows for investigating important aspects of the earth system dynamics, with relevant implications on both local/regional short-scale processes and global climate. Different approaches combine in situ measurements and satellite data to provide gap-free SSS at regular spatial and temporal resolution, aiming to resolve ocean mesoscale. Depending on the application, however, knowing SSD would be more useful than SSS and/or SST alone. Indeed, even if density can be obtained by combining SSS and SST maps at the same nominal resolution, this procedure can lead to spurious features and larger errors when SSS and SST are obtained from different observations and interpolation techniques, especially at the mesoscale. A multidimensional covariance model is applied to interpolate either in situ salinity or in situ density measurements and to build dynamically coherent surface fields, using satellite SST differences as an additional parameter in the optimal estimate. SSS/SSD level 4 (L4) maps are reconstructed over the North Atlantic area, analyzing one month of data. The L4 data are validated using data from the first Salinity Processes in the Upper Ocean Regional Study (SPURS-1) field campaign. The root-mean-square error (RMSE) ranges between 0.03 and 0.13 for the SSS L4 data, and between 0.09 and 0.32 kg m$^{-3}$ for the SSD L4 data, with improvements of up to 20% with respect to standard products. A holdout validation provides similar values for the SSS RMSE (0.13 ± 0.07) and the SSD RMSE (0.13 ± 0.17 kg m$^{-3}$). The limitations and advantages of the two approaches are further discussed and analyzed by looking at spatial wavenumber spectra, showing that the multidimensional optimum interpolation (OI) method significantly increases the L4 effective resolution.

1. Introduction

Ocean salinity, temperature, and related density are fundamental physical variables to investigate global ocean dynamics. They are clearly related to the earth hydrological cycle and contribute to global ocean circulation, potentially affecting climate processes also (e.g., Baumgartner and Reichel 1975; Schmitt 2008; Yu 2011).

Sea surface salinity (SSS) is largely controlled at the global scale by the balance between evaporation and precipitation, but it is also significantly modified by ocean circulation and mixing. Moreover, freshwater from rivers and groundwater discharges, and freezing and melting in polar regions also change salt concentration in the upper layers. Similarly, sea surface temperature variations are mostly driven by latent and sensible heat fluxes and by radiative fluxes at the air–sea interface, but then are further modulated by ocean currents and mixing.

Salinity and temperature are the main variables driving seawater density changes, and sea surface density (SSD) changes can be transferred to the deep ocean by several
advection and diffusion mechanisms, acting on very different scales [from small-scale turbulence to (sub)mesoscale processes, etc.]. Variations in density modulate the ocean thermohaline circulation, which contributes to the redistribution of a huge amount of heat and regulates ocean–atmosphere coupling, with potential consequences on the climate change over the continents (e.g., IPCC 2007). As an example, El Niño–Southern Oscillation (ENSO), primarily affecting the SST in the central and eastern equatorial Pacific, is considered as one of the major sources of interannual climate variability and its improved prediction could have an enormous socioeconomic impact. Ballabrera-Poy et al. (2002) first showed that SSS estimates play a significant role in 6–12-month predictions of ENSO. Their analysis was further confirmed by Hackert et al. (2011), who applied a hybrid coupled model to forecast ENSO dynamics, showing the impact of SSS observations on the seasonal variability of tropical dynamics. More recently, Zhu et al. (2014) investigated the role of SSS in the medium- and low-frequency variability of Pacific climate through its effects on SSD, which is associated with horizontal pressure gradients and stratification. Similarly, a significant impact on North Atlantic Ocean salinity in driving the decadal variability of the North Atlantic meridional overturning circulation (MOC) has been observed (e.g., Frankignoul et al. 2009).

Besides, knowing the distribution of surface tracers would not only help monitor large-scale processes but also investigate ocean dynamics at smaller scales. For example, the availability of high-resolution SSD fields (and/or associated dynamically coherent SST and SSS) would improve the observation-based reconstruction of 3D dynamics at the mesoscale, presently carried out through a number of different techniques (e.g., Pascual and Gomis 2003; Isern-Fontanet et al. 2008; Buongiorno Nardelli et al. 2012; Mulet et al. 2012; Buongiorno Nardelli 2013; Pascual et al. 2015), as well as the tracking of water masses of different origins (e.g., Sabia et al. 2014).

However, the low number of observations available has significantly limited the study of SSS and SSD variability. In fact, in situ measurements are very sparse and only with the advent of autonomous profilers could they provide an almost global coverage. In practice, even combining all available in situ data, only the large-scale signals can be effectively resolved (e.g., Gaillard et al. 2009a,b). More recently, the availability of Soil Moisture Ocean Salinity (SMOS) and Aquarius/Satellite de Aplicaciones Científicas-D (SAC-D) remotely sensed observations allowed for significantly increasing the number of SSS measurements, even though their resolution, on the order of 100–200 km and 10–30 days, is still not sufficient to resolve the mesoscale (Font et al. 2013; Yin et al. 2012, 2013). As an example, Melnichenko et al. (2014) have used an optimal interpolation technique to map SSS from Aquarius level 2 along-track data, taking into account long-wavelength errors. Their analysis, covering the North Atlantic area, can only be considered as “eddy permitting,” mapping the SSS field at a spatial scale $O(150$ km) and time scale $O(1$ week).

Different approaches have thus been proposed to further increase the effective resolution of SSS level 3 (L3, merged) and level 4 (L4, interpolated) products, both merging in situ and satellite SSS data and/or combining one or both data with the information that can be extracted from other parameters that can be sampled at a higher resolution, more specifically, using satellite-derived SST data as a sort of “template.” In fact, many studies have shown that different ocean variables can be significantly correlated at relatively local scales, or even possess the same multifractal structure of singularity fronts (e.g., Umbert et al. 2014). Starting from similar considerations but adopting a different approach, Buongiorno Nardelli (2012) proposed a high-resolution optimal interpolation (OI) method combining the in situ SSS observations with the information extracted from satellite SST L4 data. This method takes into account the local correlation between SSS and SST through a multidimensional covariance function, and it has also been adapted to include SMOS data as input (Buongiorno Nardelli et al. 2016).

To get an estimate of SSD, one might thus apply the equation of state of seawater combining any of the available SSS and SST L4 data. SSD could then be used to describe and analyze specific aspects of the surface dynamics and/or to project surface information onto the vertical (e.g., Pascual and Gomis 2003; Buongiorno Nardelli et al. 2012; Mulet et al. 2012; Buongiorno Nardelli 2013; Pascual et al. 2015). However, depending on the in situ data sparseness and area considered, the combination of SSS and SST maps obtained from different input datasets (e.g., SSS obtained from in situ data and SST from satellite data) and/or the different interpolation algorithms can introduce spurious features and gradients into the resulting SSD field. Therefore, even when L4 data are retrieved exactly on the same spatial grid, the SSD field must be carefully reconstructed, especially in areas where strong gradients are present. Concerning the multidimensional OI technique proposed by Buongiorno Nardelli (2012), which takes advantage of the high-resolution satellite SST L4 retrievals to interpolate in situ SSS, problems are likely to appear if too few SSS input data are present along the strongest SST fronts, due to the intrinsic smoothing associated with the OI technique and error propagation issues. An example of how the combination of incoherent SSS and SST retrievals can lead to spurious SSD features is presented in Figs. 1–3. Figure 2, in particular, shows that when density is obtained...
FIG. 1. (left) SSS and (right) corresponding gradient intensity obtained from (top) first guess, interpolated through (middle top) method 1 and (middle bottom) method 2, and (bottom) from Mercator. This example refers to 15 Mar 2013. Gradient intensities at each pixel are estimated from neighbor pixels as the Euclidean norm through central differencing.
FIG. 2. (left) SSD and (right) corresponding gradient intensity obtained from (top) first guess, interpolated through (middle top) method 1 and (middle bottom) method 2, and (bottom) from Mercator. This example refers to 15 Mar 2013. Gradient intensities at each pixel are estimated from neighbor pixels as the Euclidean norm, through central differencing. A zoom over a portion of the Gulf Stream is displayed to show the spurious structures created by estimating the SSD with method 1.
by applying the equation of state to interpolated SSS and SST in the North Atlantic, the dense water found along the Gulf Stream is split in two well-separated veins, while it should appear as a unique water body. Hence, inconsistencies in the effective resolution and interpolation errors between SSS and SST easily reflect “dynamical” incoherencies when looking at the SSD.

In this paper, two complementary approaches to obtain SSD and SSS L4 images at high resolution (1/10°, daily) are investigated and compared. Both methods are based on a combination of in situ measurements and satellite SST estimates. The first one (method 1) is the technique proposed by Buongiorno Nardelli (2012) that generates SSS fields, and the corresponding SSD field is simply obtained by combining the interpolated SSS and SST fields using the standard equation of state for seawater density. Method 2 uses the same covariance model as method 1, but it directly interpolates in situ SSD measurements. In that case, a dynamically coherent SSS field (namely, an SSS field that provides correct density gradients once combined with the SST) can be obtained by inverting the equation of state to get salinity from density and temperature pairs. This is done by preliminary compiling a lookup table of salinity, temperature, and density values.

The fields obtained with the two methodologies are validated with independent data and analyzed in terms of spatial spectral content, discussing their potential contribution to the analysis of the large-scale circulation and mesoscale turbulence.

The paper is structured as follows: Section 2 provides an overview on in situ and satellite datasets considered and provides a general description of the multidimensional covariance algorithm used for the optimal interpolation. Section 3 presents the results, the validation methods, and an analysis of spatial wavenumber spectra. Section 4 provides the main conclusions and a brief discussion of possible further improvements of our analysis.

2. Data and methods

The datasets used as input to the high-resolution multivariate interpolation, for the successive validation and the interpolation method itself, are briefly described below. The domain selected for our tests is the North
Atlantic area (20°–45°N, 35°–80°W) and the analysis was carried out on one month of data (March 2013).

a. In situ observations

Different in situ measurements have been used as input to the OI and for validation.

1) The objectively analyzed SSS and SST data generated by the Coriolis In situ Analysis System (ISAS) in the framework of the MyOcean project (Gatti 2013) and presently distributed through the European Copernicus Marine Environment Monitoring Service (CMEMS, http://marine.copernicus.eu/) were used here. The ISAS SSS field was used as the background (first guess) for method 1. Method 2 requires an SSD background field, which was obtained by applying the United Nations Educational, Scientific and Cultural Organization (UNESCO) equation of state for seawater to ISAS SSS and SST fields. These data have an original resolution of 1/8° and have been increased to our final grid at 1/10° through a cubic-spline interpolation. The ISAS analysis uses 30 days of quality-controlled in situ observations (from Argo floats and CTD) centered on the interpolation date.

2) The surface values of the quality-controlled in situ data (from Argo floats and CTD) ingested by the ISAS objective analysis were used as input to our OI. The salinity and temperature profiles in this dataset are binned at standard depth levels and only the surface measures have thus been taken. The SSD input data, in the method 2 case, are computed by the UNESCO equation from ISAS salinity and temperature surface measures.

3) To validate the SSS/SSD L4 products, different datasets provided by the first Salinity Processes in the Upper Ocean Regional Study (SPURS-1) field campaign data (http://podaac.jpl.nasa.gov) from the NASA SPURS (http://spurs.jpl.nasa.gov/SPURS/) project were used. The campaign involved a series of five cruises during 2012–13 seeking to characterize salinity information in a region of the subtropical North Atlantic. Selected data sources are described below.

   (i) Data acquired by thermosalinographs (TSGs), automated measurement systems that are coupled to research vessel water intake and GPS system to provide continuous along-track surface temperature and salinity measurements. The TSG data are sampled every 5–10 s and subsampled to every minute. Measurements were calibrated using onboard salinometers during the cruises.

   (ii) Standard Surface Velocity Programme drifters equipped with salinity sensors (SVPS/S) deployed during the SPURS-1, measuring SSS and SST (at about 0.5-m depth) every 30 min (see also Hormann et al. 2015; Centurioni et al. 2015).

   (iii) Waveglider data provided by six wavegliders (ASL2, ASL3, ASL4, ASL22, ASL32, and ASL42) deployed in September 2012 and finally recovered in September 2013. Each waveglider has one CTD near the surface (~0.5 m) and a second one at 6-m depth.

The spatial coverage for each of these datasets in March 2013 is shown in Fig. 4.
b. Satellite SST

The satellite SST L4 dataset used is the ODYSSEA version 2 (V2) product developed by the Institut Français de Recherche pour l’Exploitation de la Mer (Piolé and Autret 2011). This dataset provides daily estimations of the high-resolution SST over a \( \frac{1}{10}^\circ \times \frac{1}{10}^\circ \) grid for the global ocean and is based on a global multisensor L3 product built from both infrared and microwave measurements and distributed through CMEMS (http://marine.copernicus.eu/). They represent the foundation measurements and distributed through CMEMS (http://marine.copernicus.eu/). They represent the foundation measurements and distributed through CMEMS (http://marine.copernicus.eu/). They represent the foundation measurements and distributed through CMEMS (http://marine.copernicus.eu/).

A comparison between ODYSSEA and other similar products has been carried out by Buongiorno Nardelli et al. (2012) by computing zonal wavenumber spectra. In their Fig. 8a, it is evident that ODYSSEA displays the highest variance up to scales between \( \frac{1}{16}^\circ \) and \( \frac{1}{8}^\circ \).

c. Mercator

The output of the Mercator Ocean Global Ocean numerical model \( \frac{1}{8}^\circ \) (distributed through CMEMS; see also Drillet et al. 2015) has been used as a reference to compare spatial wavenumber spectra of surface salinity, temperature, and density. The Mercator model uses the Nucleus for European Modelling of the Ocean, version 3.1 (NEMO 3.1), modeling system; it is forced every 3 h using atmospheric fields from ECMWF operational analyses and forecasts with empirical bulk formulas. It assimilates jointly satellite sea level anomaly [Jason-2, CryoSat-2, Satellite with Argos and Ka-Band Altimeter (Altika; SARAL)] and sea surface temperature (Reynolds \( \frac{1}{8}^\circ \) L4), and in situ profiles of temperature and salinity.

d. The multidimensional OI technique: Implementation

Optimal interpolation is a fairly straightforward but powerful data analysis method used to estimate geophysical variables from sparse observations. An optimal analysis \( \mathbf{x}_{\text{analysis}} \) is obtained as a weighted sum of the anomalies of the observations \( \mathbf{y}_{\text{obs}} \) with respect to a first-guess field \( \mathbf{x}_{\text{first guess}} \) [see section 2a(1)]. The weights provide the minimum expected estimate error (in a least squares sense) and the estimate is unbiased (i.e., it has the same mean as the true field):

\[
\mathbf{x}_{\text{analysis}} = \mathbf{x}_{\text{first guess}} + \mathbf{C}(\mathbf{R} + \mathbf{C})^{-1}(\mathbf{y}_{\text{obs}} - \mathbf{x}_{\text{first guess}}).
\]  

(1)

In (1) \( \mathbf{C} \) represents the first-guess error covariance, \( \mathbf{R} \) represents the observation error covariance (that is assumed diagonal, so that observation errors are uncorrelated and defined by constant values per each observation type/platform):

\[
\mathbf{C} = E\{e_{fg}e_{fg}^T\} = E\{(\mathbf{x}_{\text{first guess}} - \mathbf{x}_{\text{true}})(\mathbf{x}_{\text{first guess}} - \mathbf{x}_{\text{true}})^T\}
\]  

(2)

\[
\mathbf{R} = E\{e_{o}e_{o}^T\} = E\{(\mathbf{y}_{\text{obs}} - \mathbf{x}_{\text{true}})(\mathbf{y}_{\text{obs}} - \mathbf{x}_{\text{true}})^T\}.
\]  

(3)

In the implementation considered here, the observation error covariance is actually expressed as a noise-to-signal ratio (dividing it by signal variance). In the classic OI technique, the covariance function is generally estimated as a function of distance (thus defined in a bidimensional Euclidean space). However, depending on the input data available, covariance models are easily extended to multidimensional spaces (e.g., considering space–time variability) simply by introducing generalized distances in the covariance function. Here, the same multidimensional covariance model developed by Buongiorno Nardelli (2012) has been applied to interpolate either in situ SSS or in situ SSD measurements, that is, method 1 and method 2, respectively. This extended OI method can be considered as an approximation of a multivariate approach including both the SST and the SSS (or the SSD) in the state vector. The cross terms in the resulting covariance matrix are thus approximated by defining a covariance function that depends on both space–time distance and (high-pass filtered) thermal differences. In practice, this particular covariance model gives more weight to the observations found on the same (high-pass filtered) isothermal of the interpolation point with respect to the observations found at the same spatial and temporal separation but characterized by different SST values. As the SST L4 data contain information at the mesoscale, this algorithm is thus able to increase the effective resolution of the SSS/SSD L4 (see also section 2e). The covariance function used is a simple Gaussian function of the form

\[
\mathbf{C}(\Delta r, \Delta t, \Delta SST) = e^{-(\Delta r/L)^2}e^{-(\Delta t/\tau)^2}e^{-(\Delta SST/T)^2},
\]  

(4)

where \( \Delta r, \Delta t, \) and \( \Delta SST \) are the spatial, temporal, and thermal separations, respectively, while \( L, \tau, \) and \( T \) are the spatial, temporal, and thermal decorrelation terms, respectively.

Here, the values used for the decorrelation scales and the in situ noise-to-signal ratio are those defined in Buongiorno Nardelli (2012) and Buongiorno Nardelli (2013). The decorrelation scales are thus taken as \( L = 500 \text{ km}, \tau = 7 \text{ days}, T = 2.75 \text{ K}, \) and the in situ observations noise-to-signal ratio was fixed at 0.1. The analysis was run daily, using high-pass-filtered (<1000 km) SST L4 (see section 2b) data to compute the OI weights.
e. The multidimensional OI technique: Hypotheses and implications

The assumptions and the limits of applicability of the multidimensional covariance model described in section 2d are briefly recalled below. Optimal interpolation assumes that the covariance of the parameter to be interpolated is statistically stationary and known a priori. Moreover, standard models often make additional assumptions on covariance isotropy. However, classical space or space–time SSS/SSD true covariances are generally spatially anisotropic and nonstationary. In fact, SSS/SSD are sensibly modified across fronts and in mesoscale features, and the resulting covariance scales, in turn, change significantly between the cross-front and alongfront directions. These structures are also subject to intense temporal variability. On the other hand, SSS and SSD associated with a specific water mass are basically modified by isopycnal mixing, thus occurring at larger space/time decorrelation scales.

Part of this nonstationarity and anisotropy can be recovered by representing the covariance as a function of space, time, and (high-pass filtered) SST separation. In practice, this multidimensional covariance automatically adapts to the mesoscale field evolution/frontal displacements. In fact, assuming that different water masses are characterized by different SST/SSS (and SSD) values, this model implies that SSS/SSD variations at small scales are correlated to SST variations, filtering out the effects of large-scale freshwater/heat fluxes. This is a reasonable assumption in the open ocean, where surface exchanges mostly occur at the atmospheric scales. However, SST and SSS/SSD variations are not necessarily well correlated near the coast, where air–sea interactions and terrestrial freshwater fluxes can result in localized input.

In practice, it is assumed here that residual high-pass-filtered SSS/SSD variations are exclusively due to advection and mixing, but also that SST, SSS, and SSD mixing are driven by the same dynamics (which is a reasonable assumption in the upper layers, where mixing is mostly driven by turbulent fluxes).

The drawback of this covariance model is that if the water masses are characterized by the same temperature but have different salinities/densities, then the interpolation will reduce to a standard space–time algorithm (simply because no local SST anomalies are present).

3. Results

The validation and analysis of the SSD and SSS L4 data obtained with the two different configurations of the multidimensional OI (methods 1 and 2) were carried out following three different approaches. In the first one, independent measurements provided by the NASA SPURS project [see section 2a(3)] have been used to compute the statistics of the differences between L4 data and collocated in situ observations. In the second approach, a holdout validation technique has been applied to evaluate the accuracy of the SSD L4 fields. Finally, spatial wavenumber spectra have been estimated from the first guess, the interpolated fields, and the output of a numerical general circulation model (see section 2c).

a. SSS/SSD validation versus independent SPURS-I data

The two multidimensional OI techniques (methods 1 and 2) have been validated by comparing the accuracy of the interpolated SSS and SSD data with respect to the precision of the background SSS and SSD fields. To compute the two SSS/SSD fields and the corresponding gradient intensities, the three different types of independent observations provided by the NASA SPURS project [described in section 2a(3)] were used. The accuracy has been evaluated by computing the root-mean-square error (RMSE), the mean bias error (MBE), and the standard deviation error (STDE) between the independent observations and the collocated interpolated values. Collocation was defined as a ±12-h interval centered on the L4 nominal time (0000 UTC). A Monte Carlo approach (Efron and Tibshirani 1993) was applied to estimate confidence intervals (σ) for the RMSE, MBE, and STDE. The results obtained from each validation dataset are summarized in Tables 1–3, respectively. As expected, the errors with SSS retrieval with method 1 are always lower than those obtained with method 2 (and the opposite for SSD). In detail, the MBE values are generally quite low (<0.006 for the SSS with method 1 and <0.06 kg m⁻³ for the SSD with method 2), when considering drifter and waveglider validation data. Conversely, they display higher values than the first-guess MBE when considering TSG validation data and SSD retrievals. The RMSE obtained from the validation with TSG data are then approximately 0.1 for the SSS and 0.3 kg m⁻³ for the SSD (Table 1). These values are higher than those obtained from the waveglider data, which attain around 0.03 for the SSS and 0.09 kg m⁻³ for the SSD (Table 3). However, they always display lower values with respect to the first-guess RMSE. These results reflect the different representativeness and coverage of the validation datasets. More specifically, part of the differences can be explained by the fact that the nominal depth of the TSG measurements lies between 3 and 5 m, while the waveglider measurements are collected at 0.5-m depth—much closer to that of the Argo.
data used in input to the OI. On the other hand, the results obtained looking at the drifter data, collected at about 0.2-m depth, show a smaller RMSE than the TSG case for salinity but bigger for density (Table 2), and the differences are thus likely due to the different areas covered by the instruments.

Overall, the statistics computed starting from the different datasets (TSGs, drifters, wavegliders) thus present minor discrepancies, which are mostly explained by the different layers sampled by each instrument and to their different space–time coverage. However, all numbers give the same message: multidimensional OI directly applied to the target variable significantly improves RMSE with respect to the first guess (up to a 35% reduction when looking at drifter data). Conversely, deriving SSD from interpolated SSS and SST fields may significantly worsen the accuracy of the retrieval (and equivalently retrieving the SSS values from interpolated SST and SSD). The gradients estimated for both variables with any of the multidimensional configurations significantly improve with respect to the first guess.

b. SSS and SSD holdout validation

As independent in situ measurements display a quite uneven spatial (and temporal) distribution, a simple kind of cross-validation analysis, known as holdout validation, has been carried out. This method, also called “test sample estimation,” splits the dataset into two subsets mutually exclusively—an input set and a holdout or test set—each of which is used as a fully independent validation dataset.

| Table 1. Statistics obtained from TSG validation dataset (March 2013). |
|----------------|----------------|----------------|
| MBE SSS       | STDE SSS       | RMSE SSS       |
| OI (method 1) | 268 472        | 0.0028 ± 0.0004 | 0.0995 ± 0.0009 | 0.0995 ± 0.0009 |
| OI (method 2) | 268 472        | 0.0461 ± 0.0004 | 0.0971 ± 0.0008 | 0.1075 ± 0.0007 |
| First guess   | 0.0003 ± 0.0005 | 0.128 ± 0.002  | 0.128 ± 0.002  |
| OI (method 1) | 192 360        | 0.0780 ± 0.0007 | 0.117 ± 0.002  | 0.210 ± 0.001  |
| OI (method 2) | 192 360        | 0.1421 ± 0.0005 | 0.119 ± 0.002  | 0.185 ± 0.002  |
| First guess   | 0.00243 ± 0.0002 | 0.0494 ± 0.0001 | 0.00479 ± 0.00009 |
| OI (method 1) | 266 431        | 0.000216 ± 0.00002 | 0.0047 ± 0.0001 | 0.00521 ± 0.00009 |
| OI (method 2) | 266 431        | 0.00174 ± 0.00002 | 0.00446 ± 0.00009 | 0.00479 ± 0.00009 |
| First guess   | 0.00243 ± 0.0002 | 0.00494 ± 0.0001 | 0.00555 ± 0.0001 |
| OI (method 1) | 192 360        | 0.000304 ± 0.00002 | 0.0057 ± 0.0004 | 0.0064 ± 0.0003 |
| OI (method 2) | 192 360        | 0.00329 ± 0.00002 | 0.0057 ± 0.0004 | 0.0065 ± 0.0003 |
| First guess   | 0.000359 ± 0.00002 | 0.0057 ± 0.0003 | 0.0067 ± 0.0003 |

| Table 2. Statistics obtained from drifter validation dataset (March 2013). |
|----------------|----------------|----------------|
| MBE SSS       | STDE SSS       | RMSE SSS       |
| OI (method 1) | 27212          | 0.0063 ± 0.0008 | 0.0661 ± 0.0009 | 0.0664 ± 0.0009 |
| OI (method 2) | 27212          | 0.059 ± 0.001   | 0.0892 ± 0.0009 | 0.107 ± 0.001   |
| First guess   | 0.0093 ± 0.0008 | 0.0664 ± 0.0009 | 0.0670 ± 0.0009 |
| OI (method 1) | 27212          | 0.075 ± 0.004   | 0.310 ± 0.002   | 0.319 ± 0.003   |
| OI (method 2) | 27212          | 0.035 ± 0.004   | 0.011 ± 0.003   | 0.307 ± 0.002   |
| First guess   | 0.109 ± 0.004   | 0.296 ± 0.002   | 0.297 ± 0.002   |
| OI (method 1) | 7294           | 0.0022 ± 0.0001 | 0.0044 ± 0.0003 | 0.0049 ± 0.0003 |
| OI (method 2) | 7294           | 0.0016 ± 0.0001 | 0.0047 ± 0.0003 | 0.0049 ± 0.0003 |
| First guess   | 0.0023 ± 0.0001 | 0.0044 ± 0.0003 | 0.0050 ± 0.0003 |
| OI (method 1) | 22169          | 0.0047 ± 0.0001 | 0.0086 ± 0.0003 | 0.0098 ± 0.0003 |
| OI (method 2) | 22169          | 0.0049 ± 0.0001 | 0.0086 ± 0.0003 | 0.0099 ± 0.0003 |
| First guess   | 0.0052 ± 0.0001 | 0.0086 ± 0.0003 | 0.0100 ± 0.0003 |
Table 3. Statistics obtained from waveglider validation dataset (March 2013).

<table>
<thead>
<tr>
<th>SPURS-1 waveglider validation</th>
<th>MBE SSS</th>
<th>STDE SSS</th>
<th>RMSE SSS</th>
</tr>
</thead>
<tbody>
<tr>
<td>OI (method 1) matchcup = 1167</td>
<td>0.001 ± 0.002</td>
<td>0.029 ± 0.004</td>
<td>0.029 ± 0.004</td>
</tr>
<tr>
<td>OI (method 2) matchcup = 1167</td>
<td>−0.020 ± 0.002</td>
<td>0.032 ± 0.003</td>
<td>0.037 ± 0.003</td>
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<tr>
<td>First guess</td>
<td>0.008 ± 0.002</td>
<td>0.032 ± 0.005</td>
<td>0.033 ± 0.005</td>
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<tr>
<td>OI (method 1) matchcup = 1167</td>
<td>0.019 ± 0.005</td>
<td>0.09 ± 0.01</td>
<td>0.09 ± 0.01</td>
</tr>
<tr>
<td>OI (method 2) matchcup = 1167</td>
<td>0.004 ± 0.005</td>
<td>0.09 ± 0.01</td>
<td>0.09 ± 0.01</td>
</tr>
<tr>
<td>First guess</td>
<td>−0.051 ± 0.005</td>
<td>0.08 ± 0.01</td>
<td>0.098 ± 0.008</td>
</tr>
<tr>
<td>OI (method 1) matchcup = 698</td>
<td>0.0010 ± 0.0001</td>
<td>0.0013 ± 0.0002</td>
<td>0.0017 ± 0.0002</td>
</tr>
<tr>
<td>OI (method 2) matchcup = 698</td>
<td>0.0002 ± 0.0001</td>
<td>0.0017 ± 0.0002</td>
<td>0.0017 ± 0.0002</td>
</tr>
<tr>
<td>First guess</td>
<td>0.00115 ± 0.00009</td>
<td>0.0012 ± 0.0002</td>
<td>0.0017 ± 0.0002</td>
</tr>
<tr>
<td>OI (method 1) matchcup = 942</td>
<td>0.0037 ± 0.0005</td>
<td>0.008 ± 0.002</td>
<td>0.009 ± 0.002</td>
</tr>
<tr>
<td>OI (method 2) matchcup = 942</td>
<td>0.0041 ± 0.0005</td>
<td>0.008 ± 0.002</td>
<td>0.009 ± 0.002</td>
</tr>
<tr>
<td>First guess</td>
<td>0.0043 ± 0.0005</td>
<td>0.008 ± 0.002</td>
<td>0.009 ± 0.002</td>
</tr>
</tbody>
</table>

The holdout validation has been applied here on both SSS and SSD interpolated fields. For each interpolation day, the in situ observations relative to the same day have been taken out as the holdout dataset and all remaining observations were used as input. The interpolated fields have thus been computed using only the input dataset, and the accuracy has been assessed by evaluating the MBE, STDE, and RMSE of the differences between L4 data and the corresponding values in the holdout set (containing a total of 1707 elements).

The statistics associated with the holdout validation are reported in Table 4.

The results of this holdout validation partially agree with what was found with SPURS data: the SSD RMSE for the OI (method 2) is 0.13 kg m\(^{-3}\), improving with respect to 0.16 kg m\(^{-3}\) of the first guess, while the SSS RMSE for the OI (method 1) is 0.13, thus showing the same value found for the first guess. However, the holdout data were not used for the multidimensional OI, but they were included in the first-guess field derivation, so this validation is automatically penalizing the former with respect to the latter.

c. Spatial wavenumber spectra

The last analysis carried out was based on the estimation of the spatial power spectral densities. For simplicity, this has been done here concentrating only on a land-free portion of the domain and considering only a sample date. The analysis aimed to evaluate the effective resolution of the data and to compare the different products in terms of spatial spectral information, complementing the more qualitative comparisons between the spatial gradients presented above. Spatial wavenumber spectra were computed by taking latitudinal variations only and averaging the results obtained at each longitude to obtain a single spectrum. To reduce spectral leaking, a Blackman–Harris windowing function has been applied before computing the fast Fourier transform.

Analyzing spatial wavenumber spectra is not trivial for a number of different reasons. First of all, most of the theoretical analyses on ocean surface variability are focused on the analysis of the energy spectrum, which clearly differs from the variance spectrum that can be estimated from tracer fields (Vallis 2006). Then, even when looking at the energy spectrum, the direction of the energy cascade cannot be univocally determined just by looking at the spectral slope, but it would rather require the direct estimation of spectral fluxes as, for example, the same \(k^{-5/3}\) behavior is expected both in the inverse cascade of two-dimensional turbulence and in the direct cascade of three-dimensional turbulence. On the other hand, several investigations based on either (mostly satellite) observations and/or numerical
modeling, and further theoretical arguments related to the knowledge of the ocean stratification, identified a net inverse cascade (in the mesoscale range and larger), consistent with two-dimensional turbulence, and the presence of kinetic energy sources at scales close to the deformation radius, consistent with linear instability theory (e.g., Scott and Wang 2005; Klein et al. 2008). This picture is further complicated when considering the smoothing/filtering effect related to the processing and interpolation of satellite data or the impact of satellite data assimilation on model surface fields (see also Arbic et al. 2014). A very clear example of the reduction of the signal variance caused by SST interpolation (and subsequent slope steepening) can be seen in the comparison carried out by NASA between original 1-km-resolution SST data (measured with infrared sensors) and interpolated SST fields (see https://podaac.jpl.nasa.gov/Multi-scale_Ultra-high_Resolution_MUR-SST).

In our case, given the resolution of the output grid, the latitudinal range, and the processing applied, we expect to resolve only the scales larger than the internal deformation radius, not even approaching the submesoscale range, and can anticipate surface kinetic energy spectral slopes on the order of $k^{-5/3}$ or flatter [coherently with surface quasigeostrophic (QG) turbulence]. In the inertial range, a relationship between the kinetic energy spectral slope and the spectral variance of a conservative passive tracer can then be deduced (Vallis 2006; Callies and Ferrari 2013). If the kinetic energy spectral slope scales like $k^{-n}$, then for $n < 3$ the associated passive tracer variance spectrum is $\sim k^{-(n-5)/2}$; so that in surface QG turbulence, the inverse energy cascade results in a passive tracer variance slope of $k^{-5/3}$ or steeper.

The wavenumber spectra obtained from the numerical model (Fig. 5) are in fact compatible with the inverse cascade scenario, displaying a $k^{-5/3}$ slope in the low-frequency range ($<0.5$ deg$^{-1}$), gradually changing to approximately $k^{-2}$ around 0.8 deg$^{-1}$. At smaller scales, ($>2$ deg$^{-1}$), the slope gets steeper, possibly due to the smoothing associated with the data assimilation procedures adopted in the Mercator model. In the background fields, as expected, an abrupt variance drop is found already at low wavenumbers (larger scales, ~500 km; Figs. 5a,b). Conversely, a significant part of this variance is efficiently recovered through the multi-dimensional OI, leading to an effective resolution of about twice the grid resolution, namely, between $\frac{\lambda}{2}$ and $\frac{\lambda}{8}$. Then, the SSD spectrum obtained with method 2 displays a higher variance level at the small scales (spatial frequency > 1.5) with respect to the spectrum computed from method 1 (Fig. 5a). In fact, a $k^{-3}$ slope is found all along the spectral range up to approximately $\frac{\lambda}{2}$ wavelength, where noise finally flattens the spectrum.
considered (Fig. 5b). Unfortunately, it thus seems that the spectra alone cannot be used to discriminate which one of the configurations performs best. On the other hand, significant improvements in terms of retrieved spatial variance at the mesoscale are always obtained with respect to standard OI methodologies by using the multidimensional covariance model.

4. Discussion and conclusions

The combination of satellite and in situ data represents a powerful approach to extract as much information as possible from available observations and to describe better the environmental parameters characterizing the ocean surface with respect to monoparameter-/monosensor-based approaches. Synergistic approaches are especially needed if aiming to resolve the signals associated with ocean mesoscale.

In this work, a multivariate optimal interpolation technique has been used to combine the high-resolution space–time information provided by satellite SST measurements with in situ measurements of salinity and density, in order to get a more accurate description of both parameters at the sea surface (a nominal resolution of \(1/10^3\) daily). This OI method is based on a multidimensional covariance model originally proposed by Buongiorno Nardelli (2012) to interpolate in situ SSS, and it provides an effective increase of interpolated fields’ spatial resolution compared to classical univariate OI methods. While this technique has been already extended to ingest satellite salinity measurements from SMOS (Buongiorno Nardelli et al. 2016), here it has been extended to the direct interpolation of SSD measurements. The implications of combining SSS L4 and SST L4 or working directly with SSD L4 fields were further discussed depending on the target application (the differences between method 1 and method 2). Interpolated fields have been validated with NASA SPURS independent data and through a holdout cross-validation approach. They display increased accuracy with respect to corresponding first-guess fields in terms of both absolute values and the ability to describe spatial gradients. The analysis of the spatial wavenumber spectra finally demonstrated that the multidimensional approach is able to effectively increase the resolution of the L4 fields, reproducing the tracer spectral behaviors expected in well-known geostrophic turbulence models and reproduced by numerical ocean general circulation models up to about half-degree wavelengths.

The methods described in this paper will be used to derive a new reprocessed SSS/SSD L4 dataset with global coverage at weekly temporal resolution in the framework of the European Copernicus Marine Environment Monitoring Service.

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