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Executive summary

The accuracy of the Copernicus Marine Environment and Monitoring Service (CMEMS) ocean analysis and forecasts are highly dependent of the availability and quality of observations to be assimilated. In situ observations are complementary to satellite observations that are restricted to the ocean surface. Higher resolution forecast model and improved observation coverage are needed to better fit the users of the CMEMS global and regional ocean analysis and forecasts.

In this task, numerical data assimilation experiments with the regional $1/36^\circ$ resolution and global $1/12^\circ$ resolution systems will be conducted to assess and improve the impact of in situ physical observations assimilated in open ocean and coastal areas. Improved version of the forecasting physical ocean model and assimilation scheme are under development. The focus will be on assessing the benefit of Argo array extension to deep ocean and tropical mooring increased vertical resolution for the global ocean and high frequency in situ profiles such as delivered by gliders in coastal regions.

Biogeochemical in situ profile observations, mostly from Argo, will be used to optimize the parameters of the global CMEMS biogeochemical model.

1. Introduction

In this task, we assess the impact of in situ observation in improved/future Copernicus Marine Environment and Monitoring Service (CMEMS) ocean analysis and forecasting systems. We are considering in situ physical and BioGeoChemical (BGC) observations to be assimilated in a global system but also in a regional system since they are specific physical observation data sets that are important for regional ocean monitoring. The numerical experiments are running with improved versions of the CMEMS global and regional IBI (Iberian Biscay Irish) systems compared to the one running operationally today. Those versions should allow to better benefit from observation information.

2. Global physical observing system experiments

Enhancements of the in situ ocean observing network in terms of additional or improved instruments and/or sensors have been carried out in the Atlantic Ocean for several decades. This Task 4.1 will specifically focus on the assessment of the in situ observation impact, in order to better integrate and make the best use of in situ observations that will be available in real-time for the Copernicus systems. This exercise will also be of interest to improve the operational system at Mercator Ocean.

2.1. In situ observations

The main in situ components of the global ocean observing system are the global mooring array and the global Lagrangian floats, which are key elements for global ocean monitoring systems. Those observations must be first identified in the CMEMS through the so-called *In Situ* Thematic Assembly Center (TAC). This *in situ* TAC, Coriolis, collects and distributes observations mainly from EuroGOOS. Only observations that are transmitted in real time to the Coriolis data centre will be available for assimilation in real time analysis and forecasting systems. An initial work is needed in collaboration with *in situ* networks involved in WP3 to determine that the number of good-quality data is consistent with observations having been post-processed with the more advanced quality control. Then, based on the inputs from the *in situ* networks (discussions are ongoing to identify the new/improved observations) impact studies will be defined depending on the status of the platform deployments, their availability and the data quality.

2.2. Experimental system

Mercator-Ocean is operating the Copernicus global ocean monitoring and forecasting system in real-time, at $1/12^\circ$ horizontal resolution. This system produces an analysis each week and a series of 10-day forecasts, in which satellite (i.e., sea surface height and sea surface temperature) and *in situ* temperature and salinity observations are assimilated. The *in situ* observations used for the assimilation come from the Copernicus *In Situ* Thematic Assembly Center (Coriolis). However, the computation cost of global numerical experiments at such high spatial resolution is too high, and a numerical experimental system based on a similar system but at lower resolution (at $1/4^\circ$ horizontal resolution) is used to assess the impact of in situ observations. This experimental system with the same up-to-date assimilation and modelling techniques allows to perform cost-effective numerical experiments, with expected conclusions transferable to the operational system. Impact of physical observations will be assessed using physical metrics informing on the ability of in situ observations to reduce forecast error on ocean state variables (e.g., Temperature, Salinity) and derived quantity (e.g., Steric Height, Ocean heat content). Comparison of model forecasts with regards to observations will be conducted as well as estimation of the forecast error reduction due to the assimilation of each component of the in situ global ocean observing system. The relevance of in situ observations for short-term ocean analysis and prediction will be determined by comparing different simulations with regards to assimilated and non-assimilated observations. Note that independent observations are key for the model evaluation and analysis and forecast validation process (e.g., current velocity from mooring)

2.3. Observing System Experiments

An experimental procedure will be applied based on numerical experiments called “observing system experiments” (OSE), which consist in comparing ocean states obtained by different simulations with and without the assimilation of specific set of observations. Differences between

the different ocean estimates with and without assimilation of a given set of observation will inform on the change or influence of those data in constraining different EOVS and regions. Misfit to observations (one of the usual metrics informing on the difference between observation and model analysis) is a complementary diagnostic to inform if modifications improve or degrade the ocean estimate.

As previously mentioned, the main components of the in situ ocean observing system are:

1. The Argo network and its extension in depth. For several years, deployments of Argo floats sampling the upper and the deeper ocean (200 dbar and deep enhancement of floats to 4000dbar or 6000dbar) have been carried out in the Atlantic Ocean. After the identification of these physical observations in the data sets provided by the data center (TAC in situ), their role in reducing the forecast error model at depth will be assessed. Note that discussions with researchers from the Argo array are very important, because these new observations of the deep ocean require high precision measurements and accurate calibration techniques to provide high-qualified measurements available for operational systems.

2. In addition to the deep Argo floats, the vertical resolution of Thermo-Conductivity sensors in the mixed layer of tropical moorings (i.e., PIRATA in the Atlantic) has been increased for several years following international recommendations. Those moorings are located at 0°N-35°W, 0°N-23°W and 0°N-10°W. By looking at the observation misfits, the impact of the enhanced vertical resolution on reducing the model forecast error could be estimated in this region.

More concretely, the main plan is to perform four 1-yr experiments in order to test the contribution of the deep Argo and the mooring arrays. The period will be chosen depending on the availability of recent ocean observations.

Assimilated data	Satellites (SST, SLA)	In Situ without moorings & Deep Argo	Moorings	Deep Argo
OSE0	No	No	No	No
OSE1	Yes	Yes	No	No
OSE2	Yes	Yes	Yes	No
OSE3	Yes	Yes	Yes	Yes

Plan of global experiments to assess the contribution of mooring and deep Argo

2.4. Expected outcomes

These numerical experiments will help to:

(i) identify the contribution of global in situ observations in constraining the ocean circulation with the state-of-the-art monitoring system,

- (ii) adapt assimilation procedures to improve benefits of these new in situ data sets,
- (iii) provide elements of the relative role of the evolution of the components of the global ocean observing system in ocean monitoring systems.

3. CMEMS Biogeochemical model optimization using BGC-Argo float data

In this task, we aim to find an optimal set of parameters for the biogeochemical model PISCES, (the model used in CMEMS global BGC hindcast and forecasting systems) using an ensemble-based data assimilation technique together with BGC-Argo floats data.

First, a 1D configuration of NEMO-PISCES (hereinafter denoted PISCES 1D) was set up in the North Atlantic along the trajectory of a BGC-Argo float (Figure 1a). We have selected a float that sampled the North Atlantic in a region with weak water masse contrasts, so we can safely assume that the biogeochemical dynamics observed by the float are driven by 1D processes. Along the trajectory of this float, daily vertical profiles of temperature, salinity, vertical mixing coefficient (K_z), as well as the mixed layer depth (MLD) and atmospheric forcing from a $1/4^\circ$ coarsened version of CMEMS global ocean physic forecasting system were extracted. Then, an “offline” version of PISCES 1D were forced using these hydrographic and atmospheric fields.

PISCES 1D is a good approximation of the CMEMS global ocean BGC forecasting system (hereinafter denoted PISCES 3D). Figure 1b compares the seasonal time series of the mixed layer depth (MLD), the average mixed layer concentration of Chlorophyll-a (Chla), nitrate (NO_3) derived from the BGC-Argo floats observations (blue), from PISCES 3D (yellow) and from PISCES 1D (red). Moreover, the temporal dynamics of Chla and nitrate are reasonably well approximated by the two models with the timings of minima, maxima and the onset of the bloom being correctly represented. The winter-Chla -minimum and winter-nitrate-maxima are also properly estimated by the model. However, the summer- Chla -maximum is underestimated and the summer- NO_3 -minimum is overestimated. The main expectation of the parameter optimization experiment for this particular case is to improve the skill of the model in simulating the summer conditions.

An ensemble of 534 members (grey lines in Figure 1) was generated by perturbing 89 parameters of PISCES by -90%, -70%, -50%, +50%, +70%, +90%. The next scheduled work will be:

- 1) Find an optimal set of parameters using a particle filtering algorithm that optimizes PISCES-1D for this particular float.
- 2) Compare the optimized parameters with the existing literature to ensure that the results are realistic.

3) Repeat the parameter optimization experiment in diverse oceanic regions in order to derive a regional map of PISCES parameters.

4) Test whether this new set of parameters improves the skill of CMEMS global ocean BGC forecasting system in simulating BGC variables at the global scale. The CMEMS global ocean BGC system will be compared to satellite observations (such as ocean color), and in situ data not use in the optimization experiments.

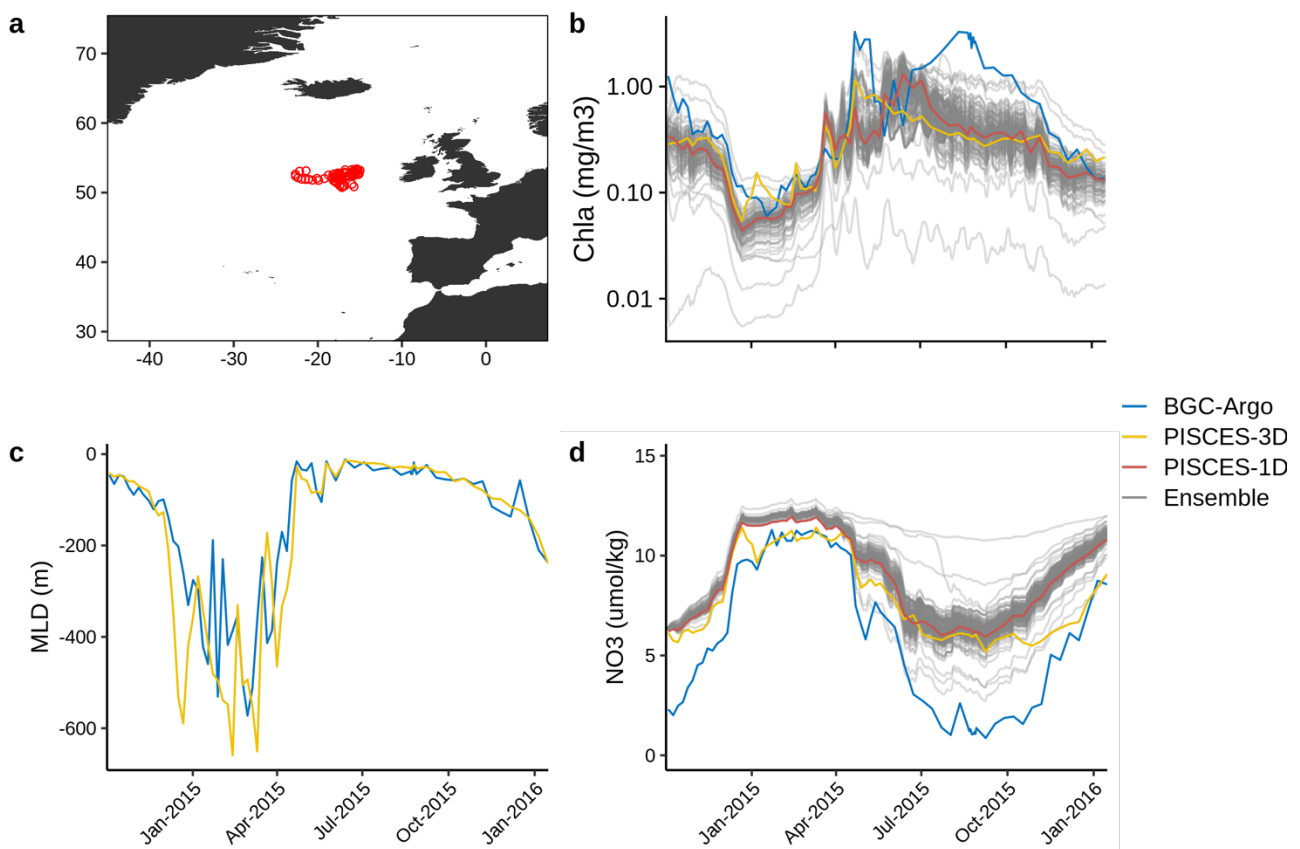


Figure 1. (a) Float trajectory of a BGC-Argo float located in the North Atlantic. Time series of (b), mixed layer depth, (c), Chla, (d), NO₃, derived from the BGC-Argo floats observations (blue) and from PISCES-3D (yellow), PISCES-1D (red) and the ensemble (grey).

4. Regional observing system experiments

The Observing System Experiments (OSE) for the global system are focusing on the impact of observing networks relevant to monitor the variability of the open ocean at global scale, here we focus on a regional CMEMS ocean monitoring and forecasting system to assess and improve the benefit of assimilating observations on the shelf. Compared to the open ocean, the variability on the shelf is at higher resolution and frequency and, in parallel, observing platforms are quite different, with different sampling strategy. Different processes are driving the coastal ocean variability, such as tide, compared to the open ocean. In this task, we are trying to better understand

and improve the assimilation of coastal observations in the regional Iberian Biscay Irish (IBI) system to increase their benefit in regional analysis.

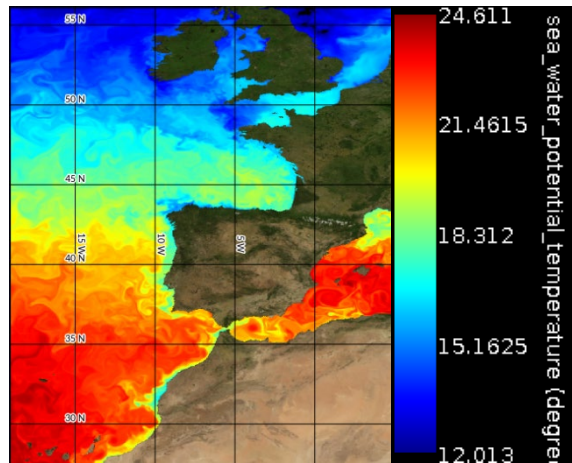


Figure 2. IBI domain, with a daily mean temperature field.

The operational IBI Ocean Analysis and Forecasting system (daily run by Nologin in coordination with Puertos del Estado and with the support, in terms of supercomputing resources, of CESGA) provides a 5-day hydrodynamic forecast including high frequency processes of paramount importance to characterize regional scale marine processes (i.e. tidal forcing, surges and high frequency atmospheric forcing, freshwater river discharge, wave current coupling in forecast, etc.). A weekly update of IBI downscaled analysis is also delivered as historic IBI best estimates. The system is based on a (eddy-resolving) NEMO model application run at $1/36^\circ$ horizontal resolution, with 50 vertical levels. The data assimilation system (Mercator Ocean assimilation system SAM2) allows constraining the model in a multivariate way toward satellite Sea Surface Temperature (SST), together with all available satellite Sea Level Anomalies (SLA), and in-situ observations profiles and times series of temperature and salinity.

In this task, we will take the future version of the IBI system to assess and improve the benefit of specific observing networks to reduce forecast error on the shelf. This future version will assimilate higher resolution along track altimetry observations (7 km) as well as higher resolution collocated SST product ($1/10^\circ$). Thanks to those increased resolution satellite observations, finer scales in the forecast should be better constrained. The assimilation of in situ observations will be revisited to “capture” more efficiently their information content, especially at higher frequency than today and ensure the coherency with satellite observations. Today, temperature and salinity observations from Argo, automated ship-based observations, drifters, gliders and moorings are assimilated in the system. However, they are strongly subsampled to avoid a too high number of observations. Only one profile per day and within 10 km are kept. This subsampling does not allow to follow the high

frequency variability. This subsampling strategy will be revisited, as well as the observation error specification in the assimilation scheme.

We plan to focus first on glider observation impact since they provide high (spatial) frequency temperature and salinity observations along vertical transects. They are the only platforms on the coastal zone that sample at high frequency the water column. Gliders are remotely driven in targeted area and can regularly sample some predefined section of interest. They are already extensively used along the US and Australian coast to monitor the coastal environment but also in the Western Mediterranean Sea. Observing System Experiments (OSE) consists of running two similar numerical assimilation experiments. In one of them the data set of interest is not assimilated. The difference between the two simulations is then representing the impact of the withheld data set.

We will run OSEs on the Atlantic coast of IBI where tidal dynamic is important to see the impact of glider data assimilation.

Since the IBI domain is covering also the western Mediterranean Sea, we are currently discussing within our work package (WP4) to run similar OSE experiments for Mediterranean gliders than the ones planned with Mediterranean forecasting system in the task 4.2. As the IBI and Mediterranean forecasting systems are based on very different assimilation schemes, it will allow to get more robust conclusion on their impact in different monitoring and forecasting systems. It is well known that observation impact is highly system dependant. Having their impact assessed in different systems will allow to identify similarities and differences.

We expect to get different impact of glider data assimilation in the Atlantic and in the Mediterranean Sea as the ocean circulation is dominated by different processes in those two areas.

All those OSEs, with different systems and in different regions will help to refine the sampling strategy of coastal zones.

The work plan is:

- 1) Document the glider data available in the CMEMS Coriolis database on the IBI domain (Figure 3). This was done in concertation with Coriolis team (WP3).
- 2) Revisit the observation error for their assimilation, with WP3, and the associated model representativity error which contains the error due to inability of the forecasting model to represent some physical processes that are observable by the data.
- 3) Run the assimilation experiments (OSEs)
- 4) Analysis of the OSEs to estimate how the additional observations are improving the analysis and forecasts.

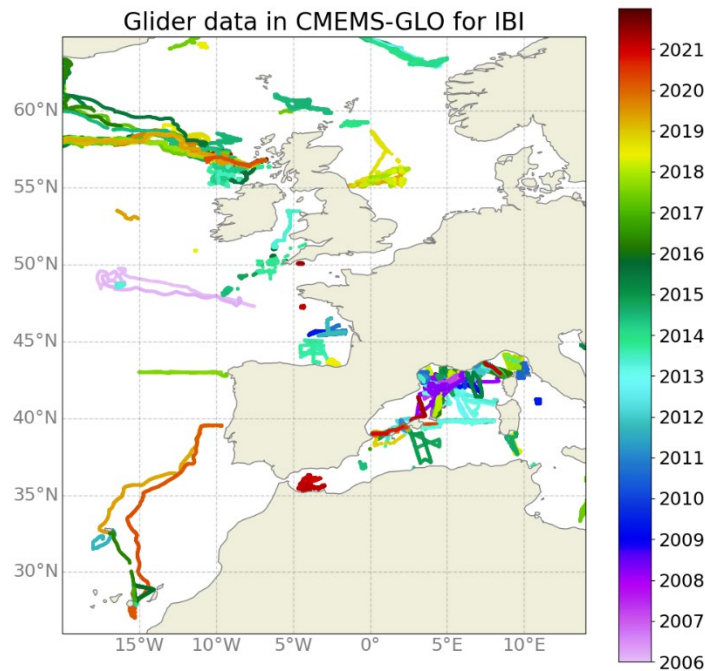


Figure 3. Positions of glider observations in the Real Time Coriolis database from 2006 to today. Colour is associated to the date of the observations.

The period for the OSEs will be chosen depending on the characteristics of glider observations (frequency sampling, maximum depth) within the IBI domain. The assimilation of gliders is an ongoing effort in different monitoring systems, discussions are ongoing to identify areas of collaboration (common period for OSE, definition of common impact diagnostics...).

Three different experiments are planned (Table 1). In one of them no data are assimilated (OSE0). That will give the model ability to represent the ocean dynamic when no data are constraining it. In the OSE1, satellite SST and SLA and in situ observations from the Coriolis database will be assimilated, except glider data. In OSE2, the drifter observations will also be assimilated. The comparison of the OSE1 and OSE2 will give the impact of the drifter data assimilation.

Table 1. Data assimilated in the different Observing System Experiments

Assimilated data in the different experiments	Satellite Sea Surface Temperature	Satellite Sea Level Anomaly	ARGO, drifters, XBT, CTD, moorings, automated ship-based observations	Gliders
OSE0	No	No	No	No
OSE1	Yes	Yes	Yes	No
OSE2	Yes	Yes	Yes	Yes

Additional short OSEs will be run to test different settings/parametrization in the assimilation system.

5. Conclusion

The numerical data assimilation experiments to be carried within this task are now well defined. Their goal is to assess the impact of improved in situ observation networks on global and regional ocean analysis and prediction delivered by CMEMS. The focus is on the impact of deep Argo floats and tropical mooring observations for the global ocean and gliders observations for the regional system.

The global and regional physical forecasting systems used for those experiments were improved to increase the benefit of assimilating in situ physical observations compared to the systems operated in real time today. The BioGeoChemical model will benefit from optimized parametrization thanks to Argo float observation comparisons.

The numerical experiments will be carried out in 2022 and their analysis will be presented in the deliverable "Assessment of impact of observations (D4.8)".