CMEMS Service Evolution 21-SE-CALL1

Development of a biogeochemical multi-data assimilation scheme to integrate Bio-Argo data with ocean colour data into CMEMS-MFCs (MASSIMILI)

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FINAL REPORT

FOREWORD

This document is the mid-term report for projects selected through the Service Evolution 21-SE-CALL1. As stated in the specifications of the call for tenders 21-SE-CALL1 “Mid-term and final reports shall provide a comprehensive description of the study results and a detailed analysis of the potential impact of these results on the CMEMS operational service.”
A single report is asked per project, even though the project could be carried out by a consortium. It should be sent by email to angelique.melet@mercator-ocean.fr (cc pierre-yves.letraon@mercator-ocean.fr).

Table of contents

1 Executive summary

The aim of the MASSIMILI project is the development of a multi-data assimilation framework for multi-variate biogeochemical parameters to be integrated into the CMEMS MED-MFC-Biogeochemistry model system.
The assimilation scheme adopted is a variational method (3DVarBio), which is the current assimilation scheme in use in the CMEMS MED-MFC-Biogeochemistry component.
The main achievements can be summarized in terms of the specific objectives and the corresponding expected results listed in the proposal, with the references to the specific sections of the report describing the results obtained so far:

Specific objectives	Achieved expected results	Sections in the report describing it
To develop and improve procedures of pre-processing of BGC-Argo for assimilation	Report describing BGC-Argo data and quality (D1.1) Draft of a manuscript describes the error quantification of BGC-Argo data. A proper operational procedure is implemented by the Med-MFC for downloading, quality checking and using the BGC-Argo floats data made available from LOV archiving facility.	3.1
To develop a biogeochemical multi-data assimilation scheme which combines ocean colour satellite data and BGC-Argo data	Code of the new 3DVarBio (D2.2) available through GITHUB Report and draft of a manuscript describing the implementation of a proper setup and evaluation of the feasibility of the assimilation of the BGC-Argo floats data.	3.2.1, 3.2.2, 3.2.3
To assess the potential impacts of the new multi-data assimilative scheme on the quality and accuracy of the biogeochemical CMEMS-MED-MFC products	New metrics operationally implemented at the Med-MFC; Final Report describing the impacts of the multi-data assimilation	3.3.1, 3.3.2, 3.3.3, 3.3.4, 4

The research and development activities carried out within MASSIMILI have been also presented in three manuscripts that are going to be submitted:

1) Teruzzi, A., Di Cerbo, P., Cossarini, G., Pascolo, E., Salon, S.: "Parallel implementation of a data assimilation scheme for operational oceanography: the case of the OGSTM-BFM model system", submitted to Computers & Geosciences;
2) Cossarini, G., D'Ortenzio, F., Feudale, L., Mariotti, L., Mignot, A., Salon, S., Taillander, V., Teruzzi, A.: "Toward an operational assimilation of BGC-Argo floats data into a biogeochemical model of the Mediterranean Sea: testing sensitivity of the 3DVARBIO variational scheme", to be submitted to Ocean Modelling;

3) Mignot, A., D'Ortenzio, F., Taillander, V., Cossarini G., Salon S.: "Error characterization in biogeochemical-Argo oxygen, nitrate and chlorophyll a concentrations", to be submitted to Limnology and Oceanography Methods.

Key messages:

1) BGC-Argo floats dataset - The continuous upgrade of the quality check protocols of the biogeochemical variables, provided by the BGC-Argo data management team (ADMT), is timely integrated in the project activities. Further, new possible protocols are going to be implemented and tested for the specificity of the BGC-Argo data of the Mediterranean Sea. A key element of the project is the estimate of the observation error covariance, which requires a deep knowledge of the functioning of the BGC-Argo sensors and of their data variability. The observation error accounts for the measurement errors and representation errors. The representation (or representativeness) errors, which account for unresolved scales or misspecification of the observation operator, have been estimated by two methods: the Triple Collocation method and the a-posterior error estimation method.
An operational data downstream from the BGC-Argo repository of LOV-UPMC to the Med-MFC-Biogeochemistry Production Unit (managed by OGS) has been implemented and is now routinely working, together with the integration of the BGC-Argo quality check procedures and observation error calculations.

2) Upgrade of the data assimilation scheme - The project has taken advance of the already existing 3DVarBio data assimilation scheme developed for the assimilation of surface chlorophyll data from satellite measurements within the CMEMS MED-MFC Biogeochemistry system. The code has been upgraded to include vertical profile observations in the assimilation scheme. Several operators of the 3DVarBio code (i.e. the observation operator, H, the vertical, horizontal and biogeochemical components of the background error covariance, Vv, Vh and Vb respectively, and the observation error covariance, R) have been re-designed and implemented for the assimilation of the BGC-Argo data vertical profiles. The 3DVarBio has been optimized using high performance computing protocols and libraries allowing the new code to be efficiently used in the contest of an operational system.

3) BGC-Argo data assimilation set-up - Several sensitivity tests on different key components of the 3DVarBio scheme (i.e. the operators of the background covariance and observation error covariance) showed that the most appropriate set up is the following:

- Use of a vertical covariance operator with 25 EOFs.
- Non-uniform correlation radius scale length (Lr).
- Observation error calibrated and time dependent.
- Frequency of assimilation shorter than 1 week and possibly daily.

4) Impact of the assimilation of BGC-Argo chlorophyll data - The impact of the new BGC-Argo data assimilation scheme was evaluated by quantifying the improvements in the output fields of the upgraded scheme through a series of indexes designed to spot intensity, shape and extent of the changes caused by the assimilation. Our results show that BGC-Argo data assimilation improves the description of the chlorophyll vertical structure, changing the concentration and shapes of profiles during the two most significant seasonal biogeochemical processes (winter surface bloom and summer deep chlorophyll maximum). Further, the observation error plays a major role in controlling the effectiveness of the assimilation. The estimated non-uniform correlation radius length scale, which is of the order of the mesoscale dynamics, together with the actual size of the BGC-Argo floats network allow to significantly constrain the phytoplankton dynamics up to 10% of the Mediterranean Sea area. We estimated that the frequency of the assimilation step can be optimized in order to enhance the persistence of the innovation and the consistency with the physical field. Our results also highlight the necessity of dedicated models and experimental integrations to optimize the future BGC-Argo floats deployments.

5) Multi-platform data assimilation - Results of the tests of the multi-platform assimilation show that BGC-Argo assimilation has local impacts, which are consistent along the water column, whereas satellite assimilation produces spatially homogeneous corrections. The most appropriate setup of the joint assimilation would be to assimilate separately satellite and float data (i.e. float assimilated daily and satellite assimilated weekly), and to assign a higher hierarchical rank to the float data over the satellite on a local basis by reducing the error of BGC-Argo float data. However, given the presence of model representative error (i.e., inconsistency of the model to properly reproduce the scales of observed processes) and of some inconsistency between satellite and BGC-Argo data, the multi-platform assimilation at different days produces a phytoplankton evolution characterized by a more jagged behaviour that might be not realistic.

6) Local versus large scale corrections - Results of the multi-data assimilation highlighted that BGC-Argo data assimilation has mainly a local impact compared with the basin wide impact of satellite data assimilation. This is due to the estimated correlation radius length scale (which is of same order of the mesoscale length scale) and the sparseness of the BGC-Argo floats network. However, a relevant part of the model error can be coherent at large scales (e.g. bias error of nutrient concentration at depth, or bias error of chlorophyll concentration in large scale surface blooms) and local observations, despite their sparseness, can help to correct it. As a possible solution, the 3DVarBio can be adapted by implementing a multiscale data assimilation: at the first step, large scale, coherent and smoothed correction would be triggered by a larger correlation radius length scale (e.g. values up to 100km or larger) and a larger observation error, and at the second step, the present configuration of the 3DVarBio would produce local scale corrections preserving the full impact of the vertical BGC-Argo data.
However, in order to avoid a too large isotropic correction, the anisotropy and non-stationarity of the correction can be accounted by including additional decorrelation terms in the horizontal covariance operator. Similarly to Nardelli (2002), the additional decorrelation terms of the $\mathbf{V_H}$ operator could be based on the surface chlorophyll or temperature fields (e.g. both observed by satellite or modelled), and would limit the correction in the direction perpendicular to fronts or other ocean horizontal structures which clearly separate different water masses.

7) Impacts of the multi-data assimilation of BGC-Argo floats to CMEMS – MASSIMILI project has evident impacts in different aspects of the CMEMS system:

- BGC-Argo protocols and data processing are continuously evolving at international level (note that, for example, name of the network changed from Bio-Argo to BGC-Argo during MASSIMILI lifetime). In particular, regional QC are not still implemented at global level. For this reason, for MASSIMILI, a parallel data flow was established, including all the state-of-the-art algorithms specifically dedicated to the Mediterranean area. This data set is completely free and available for the CMEMS community. Note, also, that in a relatively short time lap, all the algorithms used to process BGC-Argo for MASSIMILI (and then specific for the Mediterranean) will be implemented at global level (or replace with a more efficient data processing).

- The assimilation of BGC-Argo floats data improves the quality of the chlorophyll product (and, with some caution, of nitrate and phosphate). However the improvement appears currently limited to the areas covered by the BGC-Argo network. Further, the use of the BGC-Argo floats data as independent reference for the CMEMS biogeochemical products validation is beneficial for the assessment of their quality (new metrics have been also defined).
- Regarding the assessment of the effectiveness of the BGC-Argo network design in the Mediterranean Sea: we estimated that with a configuration of 15 BGC-Argo floats, the data assimilation may constrain up to 10% of the Mediterranean Sea surface; this network design is potentially strategic to monitor the biogeochemical processes in the areas of higher productivity (e.g. Gulf of Lyon Gyre, South Adriatic Gyre).
- The links with the biogeochemical data assimilation modelling community: the computational code including the new data assimilation scheme is publicly available, and we are open to support other modelling groups within CMEMS to upgrade their systems to assimilate the BGC-Argo floats data.
- The improvement of the representation of the mesoscale dynamics in the Mediterranean Sea biogeochemistry: our results show that the assimilation of the BGC-Argo floats data can potentially improve the description of the chlorophyll vertical structure related to the mesoscale dynamics, changing concentration and shapes of the vertical profiles during the typical seasonal processes (winter surface bloom, summer deep chlorophyll maximum autumn mixing).

MASSIMILI has not completely achieved all its objectives and there are still some open issues that has to be solved before the 3DVarBio can be implemented into the CMEMS operational system:

- Consistency between satellite and BGC-Argo float data is still an open issue. As a preliminary solution we proposed to assign a higher local rank to BGC-Argo in the hierarchy of the assimilated data. Further, it is worth to remind that the OGSTM-BFM model integration reacts as a filter by smoothly integrating the difference in the assimilated data.
- Multi-variate assimilation has to be finalized. The 3DAVAR-BIO code is ready and assimilation tests of nitrate have been performed. However, a proper setup of the multi-variate (chlorophyll and nitrate) assimilation simulation (i.e. hierarchy of the assimilated variables, observation error, depth and frequency of assimilated variables, multi-variate covariance Vb operator) has still to be tested and finalized. Assimilation of oxygen data has suffered from the lacking of a proper quality level of these observation, which has been reached only recently.
- The unavailability of enough independent insitu biogeochemical data remains an issue that prevents the proper evaluation of the improvement of CMEMS product at the mesoscale spatial scale due to the BGC-Argo assimilation.

2 Introduction

The main aim of MASSIMILI is the development of a multi-data assimilation framework for multi-variate biogeochemical parameters to be integrated into the CMEMS MED-MFC-Biogeochemistry model system. In particular, specific objectives of the project are:

- to develop and improve procedures of pre-processing of BGC-Argo data for assimilation;
- to develop a biogeochemical multi-data (i.e. multi-platform and multi-variate) assimilation scheme which combines ocean colour satellite data and BGC-Argo data;
- to assess the potential impacts of the new multi-data assimilative scheme on the quality and accuracy of the biogeochemical CMEMS-MED-MFC products.

3 Scientific results

The main scientific results achieved during the MASSIMILI project are presented following the project structure. MASSIMILI has 3 main tasks:

- Task 1 is dedicated to the implementation of novel protocols for using the BGC-Argo data;
- Task 2 is devoted to the development of the multi-data assimilation framework;
- Task 3 aims at assessing the impact of the new assimilation scheme.

3.1. Task 1: new protocols for the use and pre-processing of BGC-Argo data

This task was mainly devoted to the preparation and the use of the available BGC-Argo data in the Mediterranean area to test the assimilation scheme of the Task 2.
The activity principally focused on:

1. The continuous update of the QC methods for the Chlorophyll and Nitrate concentrations parameters, following the indication of the ADMT BGC-Argo working group. Methods to QC have continuously evolved during the last 5 years, and although they finally converged for the RT QC (Schmechtig et al., 2016), a constant re-processing of the Mediterranean data was performed for the MASSIMILI purposes. During the two years of MASSIMILI, then, a dedicated pre-processing data system was implemented at LOV. This data system diverged from the Coriolis system as data file included several additional fields, which were not still implemented at Coriolis. A complete description of the parameters and of the different QC methods of the two data systems is available as Google document[1]: a copy of the document is included in the Appendix A (MASSIMILI_appendixA_cook_book_BGC_Argo_File_V1.pdf).
   The LOV data system included several fields that are produced by using methods and algorithms not still validated at international level (i.e. at the ADMT), although already used in some publications specifically dedicated to the Mediterranean Sea (i.e. Pasqueron de Fommervault et al. 2015).
2. The elaboration and definition of methods to quantify the error on the BGC-Argo observations. The error on observations is a critical issue to perform realistic and

[1] https://docs.google.com/document/d/1_zoIujYyFG3GgYCsKIFGn7EyHd8HuA_gA5xNJahkNLM

efficient data assimilation and, in this sense, it was a main goal of MASSIMILI. Note, also, that the issue of the BGC-Argo observations error has been recently discussed at the international level in the last BGC-Argo Working Group of the ADMT. The same reasons that have selected the Mediterranean Sea as favourite assimilation test (i.e. high density of profiles, long deployments, systematic calibration procedures before, during and after the deployments) provided also an ideal test case to develop methods to determine (or at least evaluate) errors on BGC-Argo. This activity leads to the preparation of a publication (provided in Appendix B, Mignot et al.).

The main results, considerations and recommendations of the draft are summarized in the following.

BGC Argo observations suffer from systematic and random errors (or representativeness errors). Systematic errors are a type of error that deviates measurements from their true value by the same amount (hereinafter denoted *additive systematic bias or offset*) or the same fraction (hereinafter denoted *multiplicative systematic bias or gain*) all the time and in the same direction. Systematic errors are predictable and are introduced by imperfect initial calibration, decrease in the sensor stability or systematic changes in the environment during the measurement process. Random errors, on the other hand, are a type of error that shifts measurements from their true value in either direction by a random amount.

The systematic errors for BGC-Argo have been treated at the international level, and the developed algorithms (for the most based on existing peer review publication, level i.e. Johnson et al., 2017; Roesler et al., 2017; Xing et al., 2011) constitute the core of the RT QC procedures (Schmechtig et al. 2016).

On the contrary, representativeness or random errors, which account for the component of observation error due to unresolved scales, in float observations cannot be easily evaluated because of their randomness and unpredictability. Moreover, they cannot be characterized by the methods that are traditionally used to assess sensor accuracy. Sensor accuracy is usually assessed by dual comparison with discrete water samples collected with a rosette sampler from a ship during the deployment of the floats. In these comparisons, the ship samples are assumed to be perfectly calibrated and to represent the "truth" and all discrepancies between the floats and the ship data are attributed to the floats data. In reality, however, even though the ship measurements may be considered perfectly calibrated, they do include their own random errors. Consequently, the variability that can be observed between the ship and the float data does not necessarily result from the floats data alone. In this context, dual comparison with water samples collected from a ship is not adequate to quantify the random errors in BGC-Argo data sets and more elaborated tools are required.

In the framework of MASSIMILI, we tested the triple collocation (TC) analysis as a method for quantifying the random error standard deviation (hereinafter denoted root-mean-square error, RMSE) for O2, Chla and NO3 parameters. The TC method provides an estimation of the error of three data sets of the same geophysical variable (Stoffelen, 1998) by combining the covariances between the data sets. The TC analysis requires three spatially and temporally collocated data sets of the same target variable with uncorrelated random errors, but it does not require a high precision data set. If one data set is assumed to be perfectly calibrated, the TC analysis can also provide the optimal calibration coefficients (i.e., gains and offsets) of the

two other data sets (Stoffelen, 1998; Yilmaz and Crow, 2013). The formal definition of the TC method, as well as the literature associated, could be found in the paper Mignot et al. in the annex of this report.
The main limitation for the application of the TC analysis on measurements collected with the BGC-Argo floats is to find two more independent data sets collocated in space and in time with the float observation. To maximise the number of data for the TC analysis, we considered here all the BGC-Argo profiles of the Mediterranean Sea, which spawn from 2013 to 2017. We considered that the results should be further applied on the sub-sets of data used for the tests of assimilation.
The first independent data set used in MASSIMILI was the available ship measurements of O_2, NO_3^- and Chla performed at the time of the float deployments. We assumed that the ship data sets are perfectly calibrated, so that they can be used to determine the calibration coefficients of the floats data sets. In the considered period, 127 ship measurements of NO_3^-, 131 of O_2 and 131 of Chla were available.
For the second data set, we decided to use outputs of the MedBFM biogeochemical model system (i.e., CMEMS daily product MEDSEA_ANALYSIS_FORECAST_BIO_006_006), which provides, at high spatial and temporal resolution, vertical profiles of O_2, NO_3^- and Chla. The use of a model to estimate observations error is not anodyne and it could be considered inappropriate. However, TC methods have been efficiently used in the past with model data to estimate observations errors: for ocean wind speed and wave height (Caires, 2003; Janssen et al., 2007; Stoffelen, 1998), sea surface temperature (O'Carroll et al., 2008), soil moisture (Scipal et al., 2008), precipitation (Roebeling et al., 2012), sea surface salinity (Ratheesh et al., 2013) or sea-ice thickness (Scott et al., 2014).
The TC analysis requires a large number of samples to be able to provide a robust estimate of the covariance, which is not the case for our analysis. We followed then the approach of (Alemohammad et al., 2015), by performing a bootstrap analysis (Efron and Tibshirani, 1994) with 1000 replicates. For a given state variable, N bootstrap samples are obtained by randomly sampling with replacement from the N available samples. The TC analysis is then performed on this bootstrap sample, and the process is repeated 1000 times, producing 1000 RMSEs, gains and offsets. The mean and the standard deviation of the bootstrap estimates are then computed. If the sampling size is not too small, then the standard deviation will be much smaller than the mean. The standard deviations are also useful for comparing different estimators between data sets as it reflected their range of variability.
In the next, we present results only for the Chla parameter (see annexe for the NO3 and 02 results). Figure 3.1.1 shows the comparison between ship, float and model Chla. The calibration coefficients resulting from the application of the TC analysis are indicated as a regression lines. The mean and the standard deviation of the 1000 bootstrap estimates of the calibration coefficients and the RMSEs are indicated in Table 3.1.1.
The ship and float data sets are in favorable agreement with a gain of 1.1 and a negative offset of 0.06 mg m^{-3}. The model predictions, on the other hand, strongly underestimate the chlorophyll *a* concentrations when compared to the ship measurements. The model data set shows a gain of 0.42 and a negative offset of 0.03 mg m^{-3}.
The RMSEs in the ship, float and model data sets are 0.08, 0.03 and 0.08 mg m^{-3} respectively. Rescaling the float and model RMSEs (by applying the gain factor) reveals that Chl*a* concentrations are more precisely determined by fluorometers mounted on the floats than by ship-based measurements or predictions from the model.
The standard deviations of the bootstrap estimates are at least a factor of 3 smaller than the means, suggesting that the sampling size error is not important.

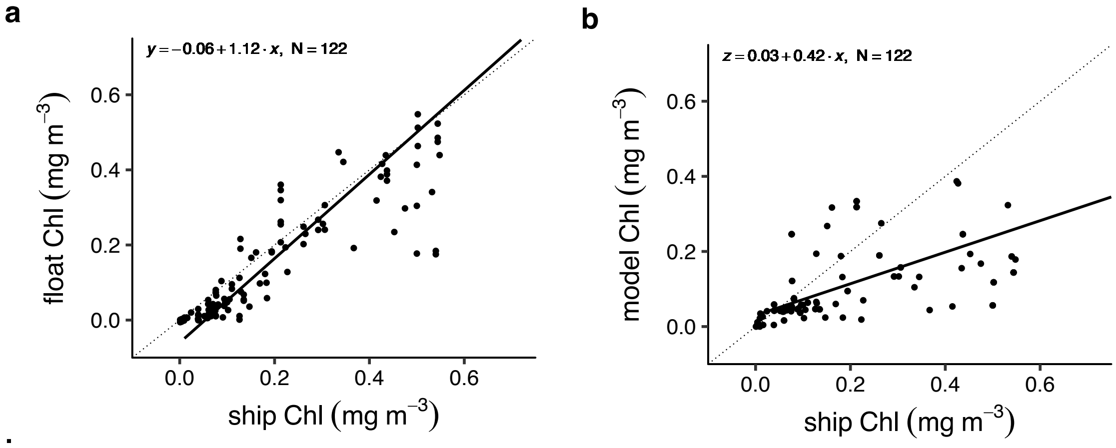


Figure 3.1.1. Scatter plots of float and model Chla as a function of ship data. a float (y) vs. ship (x) and b model (z) vs. ship (x). The dashed line represents the line 1:1. The plain lines are the linear regression lines between the two data sets considered in each panel.

data set	gain	offset (mg m^{-3})	RMSE (mg m^{-3})	rescaled RMSE (mg m^{-3})
ship	1	0	0.08 (0.01)	
float	1.12 (0.10)	-0.06 (0.02)	0.03 (0.01)	0.03 (0.01)
model	0.42 (0.06)	0.03 (0.01)	0.08 (0.01)	0.19 (0.03)

Table 3.1.1. TC estimates of the calibration coefficients (gain and offset), RMSE and rescaled RMSE for the ship, float, model Chla data sets. The mean and standard deviation (given in parentheses) of the 1000 bootstrap estimates are shown for each estimate, except for the calibration coefficients and rescaled RMSE for the ship Chla data set.

The TC analysis revealed that the accuracy of the quality-controlled profiles data sets is fairly good. The float O2, NO3$^-$ and Chl*a* data sets have a systematic additive bias of 1.8 μmol kg^{-1}, 0.35 μmol kg^{-1} and -0.06 mg m^{-3} respectively, and a systematic multiplicative bias close to 1.
The RMSE in the O2, NO3$^-$ and Chl*a* data sets were evaluated at 6.6 μmol kg^{-1}, 0.85 μmol kg^{-1} and 0.03 mg m^{-3}.
Normalized to the range of each data set (O2 : min =172.1 μmol kg^{-1} , max = 253.4 μmol kg^{-1}, range = 81.3 μmol kg^{-1}; NO3$^-$: min = -1.46 μmol kg^{-1} , max = 7.74 μmol kg^{-1}, range = 9.19 μmol kg^{-1}; Chl*a* : min =-0.01 mg m^{-3}, max = 0.55 mg m^{-3}, range = 0.55 mg m^{-3}), these estimates correspond to relative errors of 8.1 %, 9.2 % and 5.4 %.
Apart of the specific goals of MASSIMILI (i.e. estimation of the error on the Mediterranean BGC-Argo floats), the analysis presented in this section defines a theoretical framework to appreciate and evaluate the quality of the quality control procedures. Methods of QC are continuously evolving, by introducing corrections factors or improved data processing. The method presented here could be particularly efficient to highlight and quantify the amelioration introduced by a new QC protocol, by estimating the modification on the bias and of the RMSE.

A copy of the draft of the Mignot et al. manuscript is attached to the appendix B (MASSIMILI_ appendixB_error_definition_for_BGC_Argo_data.pdf).

3.2. Task 2: the development of the core of new 3DVarBio scheme

The 3DVarBio is a variational assimilation scheme (Teruzzi et al., 2014) derived from the original OceanVar code (Dobricic and Pinardi, 2008). The 3DVarBio is the actual assimilation scheme of the Med-MFC-biogeochemistry system for the assimilation satellite surface chlorophyll. The main achievement of the present task regards the upgrade of the 3DVarBio scheme to use BGC-Argo data. The results are presented into two submitted manuscripts briefly introduced in the next two sub-sections and attached to the final report, and in the sub-section 3.2.3 dedicated to the assimilation of nitrate BGC-Argo profiles.

3.2.1 Optimization of the 3DVarBio code

The new 3DVarBio code, a Fortran 90 code, has been optimized using modern HPC protocols and libraries in order to significantly reduce the execution time and enhance its modularity, allowing to integrate new different datasets.
The results of the upgrade of the code are presented in the manuscript "A parallel implementation of a Data Assimilation scheme for operational oceanography: the case of OGSTM-BFM model system" by A. Teruzzi, P. Di Cerbo, G. Cossarini, E. Pascolo, S. Salon, submitted to Computers & Geosciences as "Research Paper". A copy of the new code is now available at the gitlab repository git@gitlab.hpc.cineca.it:OGS/3DVar.git (branch WithVb: https://gitlab.hpc.cineca.it/OGS/3DVar/tree/WithVb) along with a test case and a manual.
The manuscript describes the parallelization and the optimization of the data assimilation scheme 3DVarBio implemented in the MedBFM model system embedded in the operational Med-MFC-Biogeochemistry component. The parallelization was performed using the domain decomposition with MPI, and adopting the PETSc/TAO library to perform the minimization of the cost function in parallel. The implementation of the sliced domain decomposition was carried out using the MPI_AlltoAll function. In single precision, a maximum scaling of 18.7 with 18 processes was obtained, whereas in double precision the best scaling was 8.8 with 18 processes.
To the best of our knowledge, this is the first efficient parallelization of a variational assimilation algorithm that includes a horizontal filtering scheme. This work may be significantly useful to reduce the time-to-solution of other operational models that adopt the same data assimilation approach, and therefore can be directly implemented within other CMEMS-MFCs.
As a result, one assimilation step at 1/24° horizontal resolution and 125 vertical levels grid (corresponding to the current Analysis and Forecast Med-biogeochemistry system, in a configuration of 20 cores) is executed between 5 and 10 minutes, which add to the 2 minutes for the activities of pre-processing (i.e. reading and checking data input) and post-processing (i.e. preparing the new initial conditions and setting for the OGSTM-BFM model). The use of 3DVarBio code for the multi-platform assimilation of satellite and BGC-Argo floats data rise the execution time (of 25% in summer and of almost 100% in winter) due to the increase of the number of iteration steps needed to reach convergence and compute the solution of the cost function. As a term of reference, a 1-week simulation of the OGSTM-BFM model at 1/24° has a computational cost between 1 h and 1 h 20 min.
A copy of the draft of the manuscript submitted is attached to the Appendix C (MASSIMILI_appendixC_parallel_implementation_of_3DVARBIO.pdf).

3.2.2 Upgrade of the 3DVarBio for chlorophyll BGC-Argo data assimilation

A manuscript entitled "Toward an operational assimilation of BGC-Argo floats data into a biogeochemical model of the Mediterranean Sea: testing sensitivity of the 3DVarBio variational scheme" describes the novel components of the assimilation scheme for the integration of the chlorophyll profiles from BGC-Argo floats.
In particular, results presented in the manuscript show that the assimilation of chlorophyll vertical profiles is feasible and effective in constraining a real ocean biogeochemical model simulation.
The paper introduces a series of indexes that are based on an objective and quantitative approach which aims at an operational use to assess the sensitivity and effectiveness of the assimilation of BGC-Argo floats data with respect to critical key factors of the assimilation (i.e. error of the observation, correlation radius length scale, frequency of the assimilation).
The results show that BGC-Argo floats data assimilation improves the description of the chlorophyll vertical structure, changing concentration and shapes of profiles during both winter surface bloom and summer deep chlorophyll maximum. The observation error plays a major role in controlling the effectiveness of the assimilation. The estimated non-uniform correlation radius length scale, which is of the order of the mesoscale dynamics, together with the actual size of the BGC-Argo floats network, allow to significantly constrain up to 10% of the Mediterranean Sea. The frequency of the assimilation step can be optimized in order to enhance the persistence of the innovation and the consistency with the physical field.
A copy of the draft of the manuscript is attached to the Appendix D (MASSIMILI_appendixD_Toward_an_operation_Assimilatin_of_BGC-Argo_floats.pdf).

3.2.3 Upgrade of the 3DVarBio for Nitrate BGC-Argo data assimilation

Typical nitrate vertical profiles in the Mediterranean Sea consist of low values at surface and constant and high values below a given depth. The zone of rapid nutrient change with depth is called nutricline (nitracline in case of nitrate) and represents a zone of potential source of a limiting nutrient and hence, a site of intense biological activity. Examples nitrate profiles are given Fig. 3.2.1. Thus, some specific upgrades of the 3DVarBio are necessary with respect to the version of chlorophyll in order to implement an effective assimilation of the BGC-Argo nitrate profiles. In particular, the upgrades of the 3DVarBio for the integration of nitrate BGC-Argo data consist of:

- H operator adapted for reading, preprocessing and interpolating of BGC-Argo nitrate into a common grid. Differently from the Chlorophyll assimilation, the nitrate assimilation has been set to integrate nitrate profiles down to 400m;
- Vv operator defined as a set of specifically computed EOFs using the same procedure defined in the manuscript presented in 3.2.2, see Appendix D
- Vh operator defined as maps of no-homogeneus correlation radius length scale computed from a reanalysis run carried out with MedBFM. As a result, the average at surface of the correlation radius length scale for nitrate is slightly bigger than that of chlorophyll, respectively: 15.5 and 15 km.
- Cost function of the 3DVarBio modified to compute the minimization in a multi-variate space.
- Observation error estimated for the new variable using the TC method (section 3.1).

As an example of the types of correction produced by the 3DVarBio, Figure 3.2.1 shows some cases of nitrate vertical profiles and their corrections produced for winter (left panel) and summer (right panel). In particular, the winter assimilation cases show correction of the concentrations at surface as well as at the deeper layers (a and b) while the summer assimilation cases reproduce a correction of the nitrate concentration in the deeper layers only (c) and a correction of the nitracline (d)

WINTER test cases	SUMMER test cases

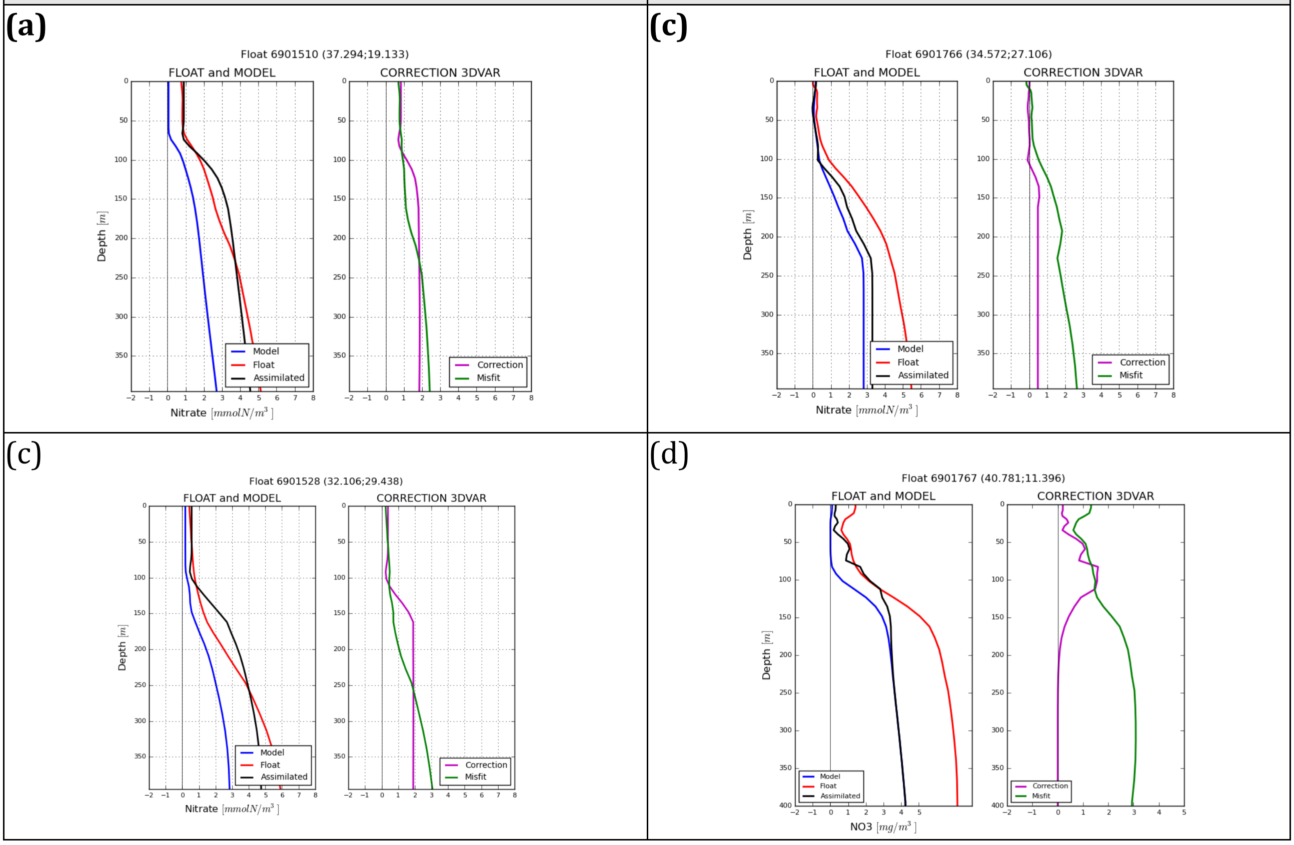


Figure 3.2.1. Summer nitrate assimilation test case for two different Bio-Argo floats. On the left plot of each panel: forecast (blue), observation (red) and new state or analysis state (black) profiles. On the right plot of each panel: misfit (green line) and innovation profiles (purple line).

3.3. Task 3: assessment of the multi-data assimilation framework

The Task 3 of MASSIMILI aims at evaluating the feasibility and the impact of the multi-data assimilation.

The CMEMS OC-TAC satellite chlorophyll Mediterranean product (CMEMS MED_CHL_L3_NRT_OBSERVATIONS_009-040) and the BGC-Argo float data are the datasets used either to be assimilated and for the validation of the multi-platform data assimilation simulations, according to different combination of the assimilated simulations. Further, a dataset of independent in-situ observations is used to evaluate the impact on CMEMS products.

3.3.1 Validation datasets and development of new metrics for the assessment of the multi-data assimilative runs

In situ data sets collected by ship in the Mediterranean Sea during the period interested by MASSIMILI have been gathered and provided to the MASSIMILI consortium (i.e. discrete measurements on the vertical of Chla, PO_4^{3-} and NO_3^-). In the following, we provide some details about the analytic methods used to estimate the concentrations on discrete samples collected on depth with Niskin bottles.
The HPLC method is used to estimate the Chla concentration: 2.27 L of the seawater samples were filtered onto glass fibre filters (GF/F Whatman 25 mm), and all filters were stored in liquid nitrogen then at -80°C to further analysis in laboratory. The chlorophyll-a and other accessory phytoplankton pigments were then extracted from the filters in 100% methanol, disrupted by sonification and clarified by filtration (GF/F Whatman 0.7µm) after 2 hours. Extracts were injected (within 24 hours after beginning of the extraction) on a reversed phase C8 column and 24 pigments were separated, identified and quantified according to the HPLC analytical protocol described by Ras et al. (2008). HPLC precision on Chla data is hard to quantify, as replicates are very infrequent. It is general assumed as error the detection limit of the Chla (i.e. 0.0001 mg/m3).
NO_3^- and PO_4^{3-} concentrations in seawater were estimated with the colorimetric method, on samples collected a few minutes after each cast directly at the tap of the Niskin bottles without tubing. Samples were poisoned with a HgCl2 solution and then stored in a refrigerator at 5°C and analysed on land by a standard automated colorimetric system.
The data available are reported in the following table:

Dataset	Period	Location	Chlorophyll	Phosphate	Nitrate
MOOSE-GE	10-27 July 2015	North West Med	451 samples 81 profiles	979 samples 81 profiles	709 samples 81 profiles
Dyfamed	Jan-Dec 2015	North West Med	0	105 samples 9 profiles	105 samples 9 profiles
Boussole	Jan-Dec 2015	North West Med	330 samples 33 profiles	0	0
BioArgoMed	12-31 May 2015	Med	60 samples 8 profiles	148 samples 14 profiles	123 samples 14 profiles

Table 3.3.1: in situ data availability for the validation task.

All the data were reprocessed with the correspondent geolocalisation (i.e. latitude and latitude), and completed with time information (i.e. date and hour of the cast) to obtain a homogenous data set, organized by cast as function of depth. This allows to apply the match up with the model output and to perform the skill assessment analysis of the assimilation simulation.
Although relatively small, the validation data set cover most of the Mediterranean Sea, and in particular, regions considered critical for the Mediterranean ecosystem functioning (i.e. NW area).

In the framework of MASSIMILI, we analyzed in details the question concerning the validation metrics, which could be pertinent in a data/model comparison. The discussion is not new (see for example the JMS special number completely dedicated to this question, Lynch et al., 2009),

although the recent availability of BGC-Argo profiles opens new perspectives and challenges for this topic.
Existing metrics are strongly biased by the availability of observation data. Most of the biogeochemical data/model comparisons are based on the surface Chla, as observed by ocean color remote sensing, which, despite of some intrinsic limitations (i.e. observations only during daytime, at cloud free conditions and limited to surface layer), represents the only data sets having the spatial and temporal resolutions close to the outputs of a biogeochemical model (at least at surface). Most of the data/model metrics have been then developed for the surface Chla (following GODAE classes approach in the framework of CMEMS).
The existing exceptions to the ocean color based metrics have been generally developed by comparing model and data at the location of the long term in situ stations (e.g. GODAE Class 2): OWP, PAPA, BATS, DYFAMED/BOUSSOLE. These programs, completely dedicated to ocean observations, have generated long term data sets (i.e. > 10 years) of vertical profiles of biogeochemically pertinent variables. Completely based on ship sampling, these data sets have generally monthly resolution and, consequently, they have been often compared to model outputs at climatological level (i.e. averaging over years or months).
Finally, comparisons have been developed using climatologies of in situ biogeochemical variables (i.e. WOA). However, spatial and temporal resolutions of in situ climatologies are often low or very low when compared to those of the existing models and, again, data/model comparisons have been generally carried out at climatological level (e.g. GODAE Class 1).
The availability of high frequency vertical profiles of biogeochemical variables collected with BGC-Argo floats could then solve most of the limitations of the existing data/model activity, under condition that existing metrics are adapted to the new data and that new approach, more specific to the floats observations, are developed (e.g. GODAE Class 4).
In the framework of MASSIMILI, then, we propose new methods and metrics, that we consider more efficient of the existing approaches to evaluate model outputs. The MASSIMILI metrics are roughly divided in two main categories, for the most based on the new information that could be provided by the BGC-Argo. In the next, we only provide a general overview of the new approaches, which are completely described (with examples) in the deliverable 3.1 of MASSIMILI.
Note that the new metrics have been developed in the specific case of the Mediterranean Sea and they have been tuned (in particular for the threshold values) on the Mediterranean physical and biogeochemical characteristics. Their application to other regions should require a verification and, eventually, a modification of the parameters that are used to compute the metrics (i.e. thresholds values). However, the philosophy and the rationale behind each metrics are, in our opinion, applicable to other regions.

Vertical Metrics
BGC-Argo data at high resolution on the vertical (i.e. from surface to 1000m) constitute certainly the most important information that could be used to enhance the data/model comparison exercise. In general, the "standard" profile comparison (or matchup) is carried out by comparing profiles of in situ data with model outputs at the same geographical location and at the same time period of the in situ stations (as defined by GODAE Class 4). These comparisons are generally carried out on the measured parameters (i.e. Chla and NO3 concentrations) at fixed depths.
Collected at high resolution on the vertical, BGC-Argo floats data have enough observations to allow the computation of the depth of specific layers, which could strongly inform on the skill of the model, as well as, of its capability to realistically simulate physical-biogeochemical

interactions. Comparing the depths could provide an efficient method to minimize any bias introduced by incorrect model parametrizations or erroneous calibration of BGC-Argo sensors. In MASSIMILI, we proposed following novel metrics:

- H_{DCM} (Depth of deep chlorophyll maximum),
- H_{MLB} (Depth of the layer involved in the winter mixed bloom),
- H_{Nit} (Depth of the nitracline).

Once depths of specific layers are computed, the integrated contents of biogeochemical variables over these layers could be evaluated for both the model and the data and then compared.

Temporal metrics

The elevated availability of in situ data provided by BGC-Argo floats allows to generate long time series of pertinent biogeochemical parameters that could be used to evaluate model skills. The Hovmoller diagram of BGC-Argo float and model output at the float position (similar to GODAE Class 2) can be generated to assess the model skill in reproducing time evolution of variables and specific events (dilution due to mixing, blooms, onset of DCM). In this graphical representation, specific events, which are considered critical for the physical-biogeochemical dynamics of the oceans, can be identified and compared between model and data. Moreover, these time series can be generated for a specific parameter (i.e. Chl), for its associated depths and for the related integrated contents, and classical skill metrics (bias, root mean square difference - RMSD) can be computed.

3.3.2 Assessment of the impact on the quality of CMEMS product

A one year (2015) simulation (DACHL2_2015) has been used to assess the impact of the BGC-Argo floats data assimilation on the quality of the CMEMS product.

According to the results of the Task 2 (section 3.2) the setup of the assimilation run consists of the following elements:

- Chlorophyll observation error is set constant in time and equal to 0.01 mg/m3. In this case a conservative approach is used (i.e., low observation error for all the year period) in order to ensure a high impact of the assimilation.
- Frequency of the assimilation step is set to 3 days. This represents a compromise considering the computational cost of the run and the opportunity of keeping the representative error in time as lower as possible.
- The Vv operator considers the set of 25 EOFs and the Vh considers the non-uniform correlation radius length scale (best choice of the setup as described in section 3.2).

The number of available BGC-Argo floats is 25, located mainly in the western Mediterranean Sea, north Ionian, and central and north Levantine sub-basin (Fig. 3.3.1). A total of 2150 chlorophyll profiles are assimilated with a mean of 15-17 profiles for each assimilation step.

A control run without any assimilation is used as the reference run (hereafter referred to as REF_2015). The MedBFM model system (that couples the OGSTM transport model and the BFM biogeochemical model) and its set-up for both the assimilation and reference run is that one currently operating in the CMEMS Med-MFC Analysis and Forecast configuration.

The results of the CMEMS Med-MFC analysis and forecast simulation (at 1/16 resolution, product CMEMS-MED-BIO-006-006) for the year 2015 are then used as term of comparison.

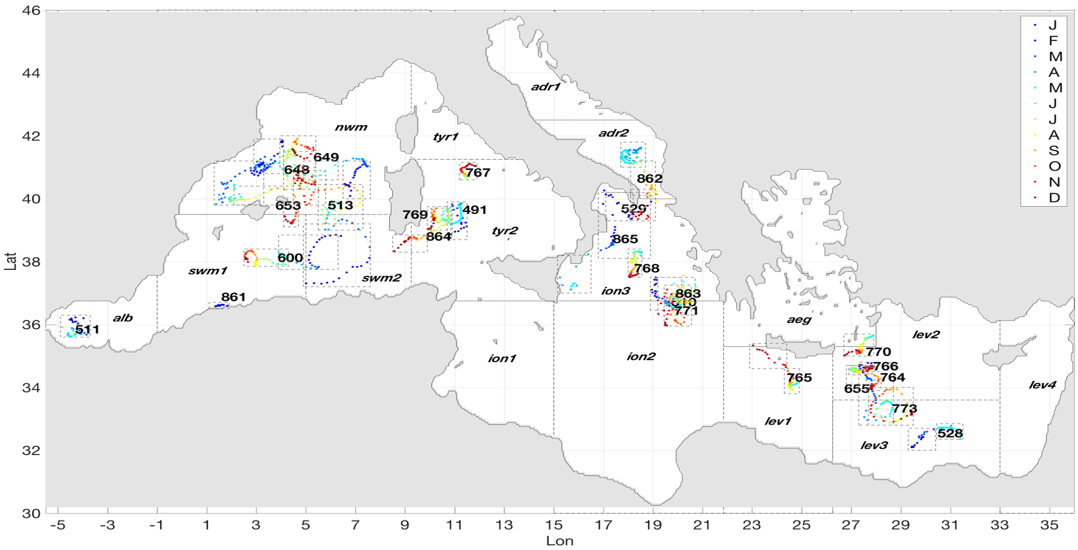
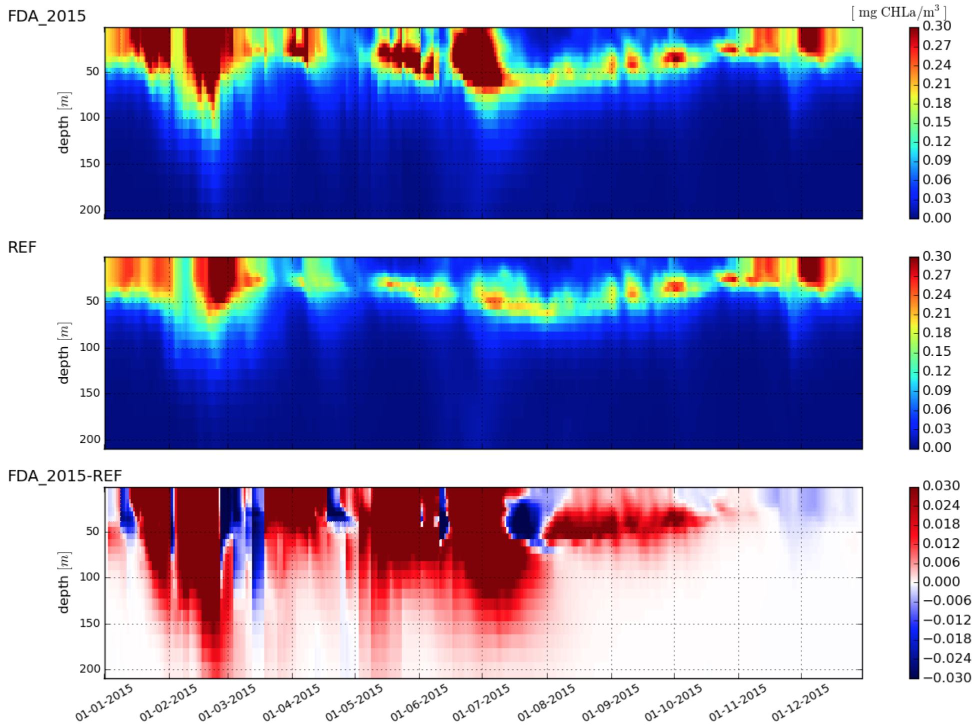


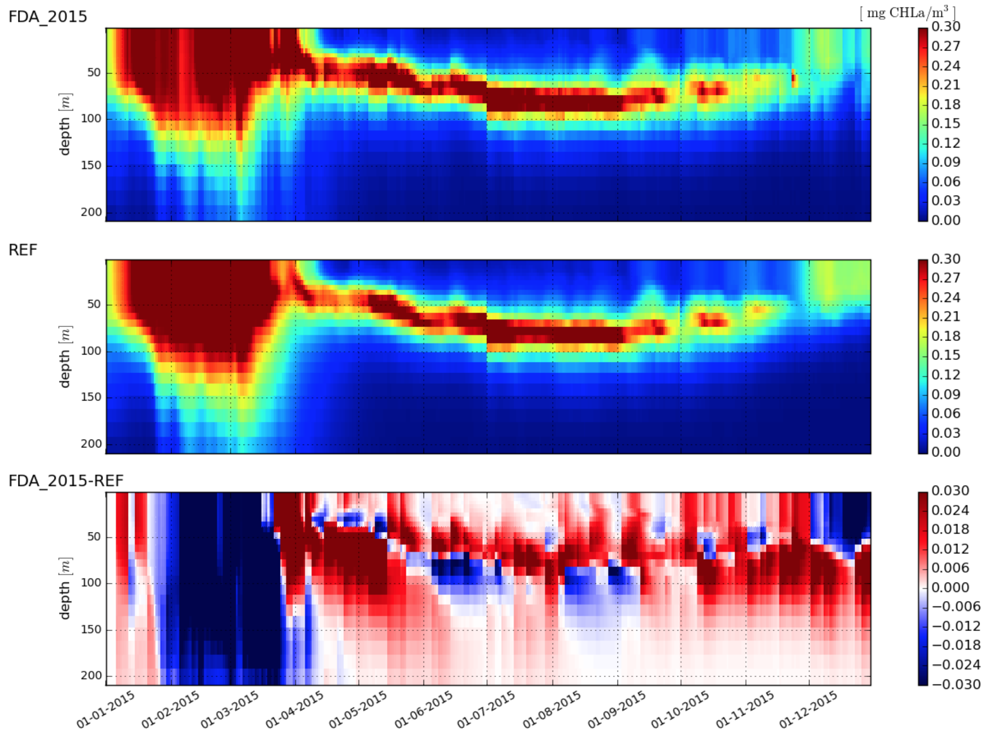
Figure 3.3.1: BGC-Argo float profiles available for the run DACHL2_2015. Float trajectories are reported in different colors highlighting the months of the sampling (see legend in the right side). Light grey dashed boxes indicate the areas used for computing the Hovmoller diagrams. Sub-basin names are reported in bold italic.

The Hovmoller diagrams of Fig 3.3.2 show, for four selected BGC-Argo floats, the daily evolution of the chlorophyll profiles of the reference simulation (REF_2015) and float assimilation simulation (DACHL2_2015 run, label FDA_2015 in Fig. 3.3.2). In general, the REF simulation has a very good qualitative performance in reproducing the known evolution of winter surface bloom, the onset of the deep chlorophyll maximum and the autumn mixing with vertically homogeneous chlorophyll blooms. The western to eastern gradient of the depth of the DCM (60-80 m in the western sub-basins and 100-120 in the eastern sub-basins) is another typical feature of the Mediterranean Sea biogeochemistry very well simulated by the REF simulation.
The assimilation of the BGC-Argo profiles produces correction of intensity and timing of bloom events, shape of the DCM and other small features, but the general picture of the chlorophyll dynamics is preserved.
The correction provided by the DACHL2_2015 run concerns on the improvement of the timing of local and short-lasting blooms during winter (e.g. Float 6901764 in Fig. 3.3.2d), the correction of the concentration of chlorophyll and the shape of chlorophyll profiles at DCM (alternation of positive and negative part of the vertical profiles of float 6901653, 6901768 and 6901764 in the FDA_2015 – REF_2015 difference plots of Fig. 3.3.2) and the adjustment of the timing of the autumn blooms (float 6901768 in Fig. 3.3.2c)
A specific evolution is simulated in the area of the Alboran subbasin delimited by the 6901551 box in Fig. 3.3.1, where impulsive signal of blooms are well simulated by the REF_2015 simulation. The assimilation of the BGC-Argo float 6901511 produces a correction of the intensity of the chlorophyll concentration and depth of the layer involved but small changes in the timing and duration of the blooms.

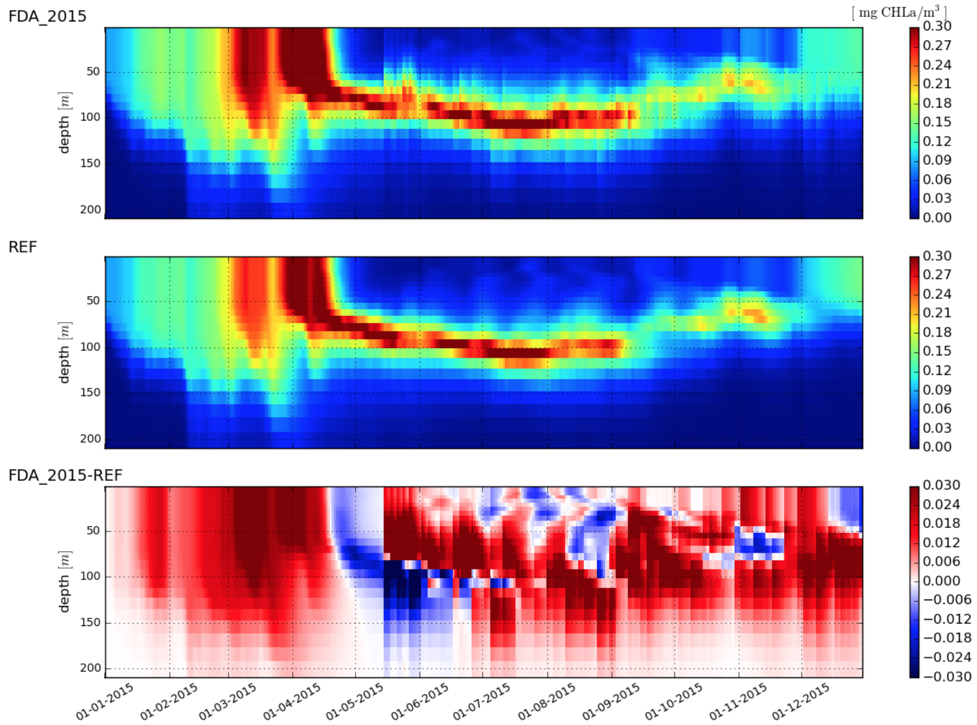
(a) FLOAT 6901511 - Alboran Sea



(b) FLOAT 6901653 - Northern western Mediterranean



(c) FLOAT 6901768 - Northern Ionian Sea



(d) FLOAT 6901764 - Northern Levantine basin

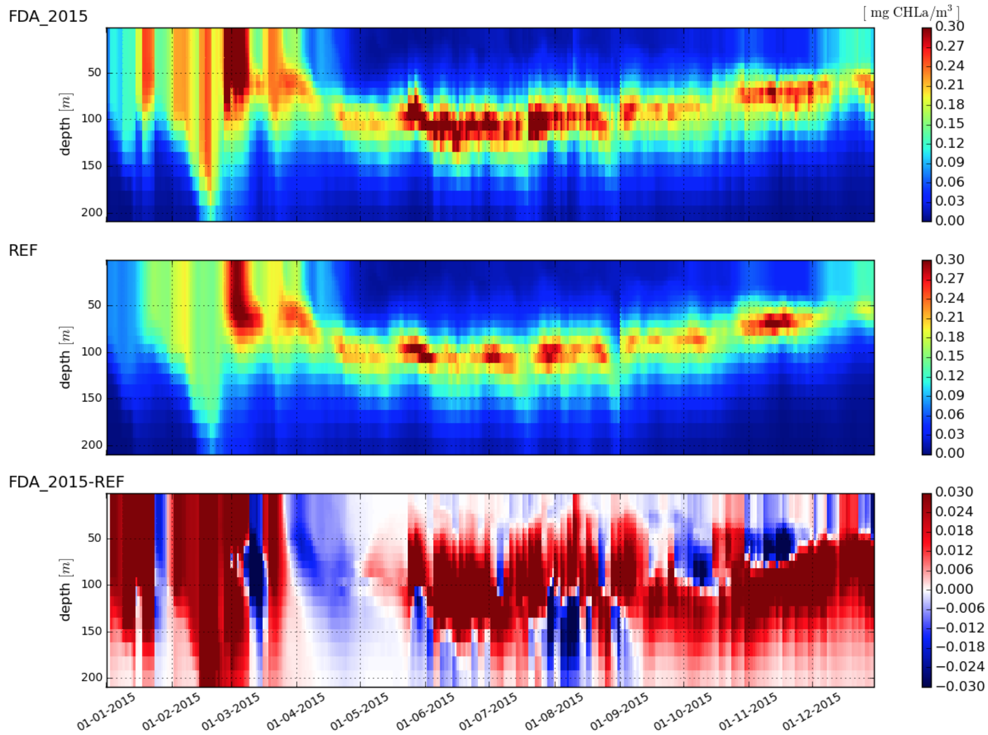


Fig. 3.3.2. Hovmoller diagram of the daily evolution of chlorophyll profiles in the areas surrounding the trajectories for some selected BGC-Argo floats.

In order to assess the potential impact of the BGC-Argo chlorophyll data assimilation on the CMEMS products two analyses are presented:

1) validation of chlorophyll, nitrate and phosphate against independent in situ data described in Section 3.3.1;
2) validation of chlorophyll against surface chlorophyll from satellite (dataset CMEMS OCTAC 008-040).

The chlorophyll validation of the reference (REF_2015) and the two assimilation simulations (DACHL2_2015 and CMEMS-MED-BIO-006-006) against in-situ observations (Tab. 3.3.2) shows that both the assimilation simulations performed slightly better than the reference simulation without assimilation. Further, the overall skill improvement of the DACHL2_2015 simulation is higher than that of CMEMS-006-006 product both in term of bias and RMSD.
Regarding the not-assimilated variables (i.e. nitrate and phosphate) the DACHL2_2015 simulation slightly improves the bias and RMSD of nitrate and the bias of phosphate, and increases of 3% the RMSD of phosphate. On the other hand, the statistics of nitrate and phosphate of CMEMS-006-006 are all slightly worse than that of REF_2015 simulation. In terms of sub-basin performance, the highest skill is mainly observed in lev or in ion (particularly for chlorophyll) for the DACHL2_2015 run, the worst in nwm for the CMEMS-006-006.

		Skill metrics against insitu data						**% variation with respect to REF**					
		CHL		**NITR**		**PHOS**		**CHL**		**NITR**		**PHOS**	
		RMSD	**bias**	**RMSD**	**bias**	**RMSD**	**bias**	**RMSD**	**bias**	**RMSD**	**bias**	**RMSD**	**bias**
CMEMS 006-006	**nwm**	0.332	-0.181	2.703	-2.072	0.098	-0.052	2	6	6	20	2	13
	tyr	0.144	-0.066	1.678	-1.237	0.057	-0.025	-2	10	4	18	-2	32
	lev	0.116	-0.065	1.621	-1.159	0.066	-0.036	2	-10	0	7	0	9
	ion	0.112	-0.065	1.138	-0.756	0.043	-0.012	-19	-36	1	6	2	33
	tot	**0.176**	**-0.094**	**1.785**	**-1.306**	**0.066**	**-0.031**	**-3**	**-7**	**3**	**14**	**1**	**17**
DACHL2_2015	**nwm**	0.323	-0.167	2.558	-1.654	0.097	-0.044	-1	-2	0	-5	1	-4
	tyr	0.135	-0.061	1.54	-0.969	0.063	-0.007	-8	2	-5	-8	9	-63
	lev	0.099	-0.058	1.617	-1.088	0.066	-0.033	-13	-19	0	0	0	0
	ion	0.098	-0.051	1.142	-0.712	0.044	-0.009	-29	-50	1	0	5	0
	tot	**0.163**	**-0.084**	**1.714**	**-1.10**	**0.067**	**-0.023**	**-10**	**-17**	**-1**	**-3**	**3**	**-13**
REF_2015	**nwm**	0.325	-0.17	2.56	-1.733	0.096	-0.046						
	tyr	0.147	-0.06	1.615	-1.052	0.058	-0.019						
	lev	0.114	-0.072	1.616	-1.084	0.066	-0.033						
	ion	0.139	-0.102	1.131	-0.71	0.042	-0.009						
	tot	**0.181**	**-0.101**	**1.7305**	**-1.145**	**0.066**	**-0.027**						

Tab. 3.3.2: overall statistics of the comparison between model output (REF_2015, DACHL2 and CMEMS 006-006 runs) and insitu observations. Percentage relative difference between the statistics of the two run is also reported.

The skill statistics (RMSD only) are computed for different layers (Table 3.3.3) in order to assess whether the float assimilation can improve the description of the vertical

characteristics of the chlorophyll and biogeochemical profiles. As reported in Table 3.3.3, the DACHL2_2015 simulation improves the chlorophyll performance from 1% to 38% depending on the sub-basin and the layer. Only in the case of tyr at surface the assimilation of BGC-Argo produces a slight worsening of the chlorophyll concentration.
Regarding the not assimilated variables (nitrate and phosphate), Table 3.3.3 shows that the assimilation of chlorophyll provides an improvement of phosphate at upper layer and of nitrate in the sub-surface layers. However, phosphate concentrations of the intermediate layer and of nitrate concentrations at the surface of the DACHL2_2015 simulation exhibit a slight worsening (positive numbers in Table 3.3.3).
It is worth to remind that despite this analysis provides a satisfactory picture, the number of observations, which might appear high at least for the nwm sub-basin, is indeed very low and the scarcity and sparseness of the observations along the one year simulation and the whole Mediterranean Sea might strongly limit the significance of this kind of assessment.

RMSD		Chlorophyll mg/m3				Phosphate mg/m3				Nitrate mg/m3			
		nwm	**tyr**	**lev**	**ion**	**nwm**	**tyr**	**lev**	**ion**	**nwm**	**tyr**	**lev**	**ion**
DACHL2	**0-30m**	0.185	0.059	0.041	0.045	0.016	0.009	0.017	0.006	0.93	0.615	0.197	0.086
	30-60m	0.471	0.178			0.033	0.007			1.177	0.131		
	0-100m	0.324	0.209	0.18	0.149	0.068	0.047	0.027	0.01	2	1.509	0.3	0.345
	100-150m	0.258	0.119	0.115		0.092	0.076	0.023		2.526	1.208	0.404	
	150-300m	0.057	0.022			0.112	0.087	0.044	0.04	3.169	1.277	1.265	1.074
REF	**0-30m**	0.185	0.058	0.042	0.073	0.016	0.01	0.018	0.007	0.719	0.518	0.19	0.089
	30-60m	0.476	0.188			0.032	0.008			1.157	0.097		
	60-100m	0.326	0.223	0.189	0.213	0.067	0.051	0.026	0.009	2.06	1.556	0.318	0.357
	100-150m	0.26	0.152	0.146		0.09	0.077	0.022		2.597	1.423	0.408	
	150-300m	0.057	0.025			0.113	0.058	0.044	0.038	3.173	1.669	1.268	1.076
PERCENTAGE RELATIVE DIFFERENCE	**0-30m**	**0**	**2**	**-2**	**-38**	**0**	**-10**	**-6**	**-14**	**29**	**19**	**4**	**-3**
	30-60m	**-1**	**-5**			**3**	**-13**			**2**	**35**		
	60-100m	**-1**	**-6**	**-5**	**-30**	**1**	**-8**	**4**	**11**	**-3**	**-3**	**-6**	**-3**
	100-150m	**-1**	**-22**	**-21**		**2**	**-1**	**5**		**-3**	**-15**	**-1**	
	150-300m	**0**	**-12**			**-1**	**50**	**0**	**5**	**0**	**-23**	**0**	**0**

Tab. 3.3.3: statistics of the comparison between model output (REF_2015 and DACHL2_2015 runs) and insitu observations. Percentage relative difference between the statistics of the two runs and number of observations. Sub-basins are defined as nwm, tyr (tyr1+tyr2), lev (lev1+lev2+lev3+lev4) and ion (ion1+ion2+ion3).

The validation against the satellite data is shown in Figure 3.3.3, which reports the time series of satellite observations (SAT), DACHL2_2015 and REF_2015 simulations for three selected Mediterranean sub-basins (SWM2, LEV2, and ION3), and in Table 3.3.4, which reports the statistics for all sub-basins. The three selected sub-basins are those with the largest difference between the two simulations since the density of BGC-Argo float profiles is the highest (see Fig. 3.3.1). Considering the three sub-basins shown in Fig. 3.3.3, the assimilation of BGC-Argo floats data increases the surface chlorophyll concentration (in several cases oppositely to satellite observations) in the first months (from January to March). During the summer months (May to September) the differences between the two runs are negligible, while during the autumn months DACHL2_2015 has many more points closer to the satellite observations than REF_2015.

Statistics of RMSD and bias between model chlorophyll and satellite observations for all sub-basins (Tab. 3.3.4) confirms the results of Fig. 3.3.3. In the reference simulation the winter bias is positive in all the sub-basins (excluding ALB and AEG), while the summer bias is negative everywhere. In summer, the values of bias of DACHL2_2015 are unchanged in 11 sub-basins and decrease of around 3% (except ALB, with -38%) in the other sub-basins with respect to the reference simulation. On the other hand, the winter bias of DACHL2_2015 is higher than that of REF_2015 in 7 sub-basins, while decrease only in 3 sub-basins (ALB, ION1 and AEG) and remains unchanged in the others (variation lower than 2%).

The RMSD of the DACHL2_2015 simulation is slightly higher than that of REF_2015 for the Mediterranean Sea both in winter and summer. However, at the sub-basin scale, the RMSD of DACHL2_2015 decreases in 5 sub-basins, increase in ALB (+7%) and remains unchanged in the other sub-basins. In winter, the percentage differences of RMSD are mainly positive (9 sub-basins) or null (3 sub-basins). Slight decreases of winter RMSD are present for only 4 sub-basins (SWM1, NWM, TYR2 and ION1). Overall, the skill analysis with satellite data returns a contrasting picture: the assimilation of floats data has not or negligible impact in many sub-basins, and the impact in the other sub-basins is mainly negative with a slight worsening of the skill metrics.

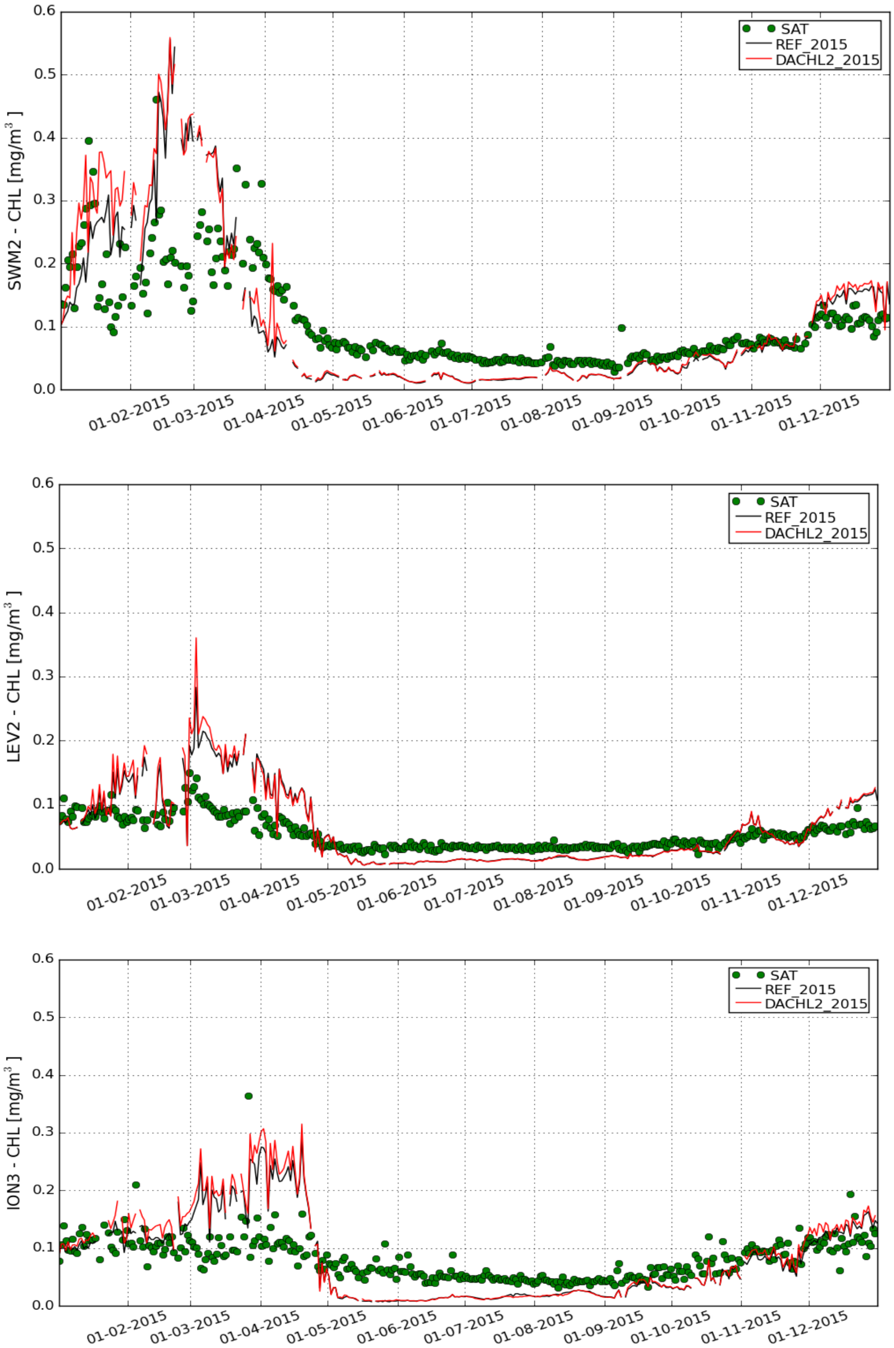


Fig. 3.3.3. Time series for three Mediterranean sub-basins of satellite observations (green points), and averaged chlorophyll over 0-10m of model output at the satellite location (i.e. cloud cover points are excluded) for the DACHL2_2015 (red line) and REF_2015 (black line) runs.

	REF_2015				DACHL2_2015				%DIFF			
	Winter		summer		winter		summer		winter		summer	
	RMSD	BIAS	RMSD	BIAS	RMSD	BIAS	RMSD	BIAS	RMSD	BIAS	RMSD	BIAS
ALB	0.178	-0.038	0.132	-0.076	0.217	0.003	0.141	-0.047	**21.9**	**-107.9**	**6.8**	**-38.2**
SWM1	0.129	0.013	0.035	-0.032	0.128	0.016	0.034	-0.031	**-0.8**	**23.1**	**-2.9**	**-3.1**
SWM2	0.153	0.028	0.03	-0.028	0.161	0.053	0.029	-0.027	**5.2**	**89.3**	**-3.3**	**-3.6**
NWM	0.221	0.099	0.043	-0.038	0.219	0.098	0.042	-0.038	**-0.9**	**-1.0**	**-2.3**	**0.0**
TYR1	0.145	0.045	0.033	-0.031	0.145	0.045	0.033	-0.03	**0.0**	**0.0**	**0.0**	**-3.2**
TYR2	0.142	0.059	0.031	-0.028	0.14	0.061	0.031	-0.028	**-1.4**	**3.4**	**0.0**	**0.0**
ADR1	0.059	0.021	0.054	-0.053	0.06	0.021	0.054	-0.053	**1.7**	**0.0**	**0.0**	**0.0**
ADR2	0.079	0.038	0.049	-0.047	0.081	0.039	0.048	-0.046	**2.5**	**2.6**	**-2.0**	**-2.1**
AEG	0.132	-0.004	0.059	-0.047	0.133	-0.002	0.059	-0.047	**0.8**	**-50.0**	**0.0**	**0.0**
ION1	0.081	0.042	0.023	-0.021	0.08	0.041	0.023	-0.021	**-1.2**	**-2.4**	**0.0**	**0.0**
ION2	0.066	0.042	0.018	-0.016	0.069	0.044	0.018	-0.016	**4.5**	**4.8**	**0.0**	**0.0**
ION3	0.088	0.047	0.035	-0.03	0.1	0.063	0.035	-0.03	**13.6**	**34.0**	**0.0**	**0.0**
LEV1	0.087	0.071	0.017	-0.015	0.09	0.074	0.016	-0.015	**3.4**	**4.2**	**-5.9**	**0.0**
LEV2	0.079	0.043	0.021	-0.019	0.088	0.05	0.021	-0.019	**11.4**	**16.3**	**0.0**	**0.0**
LEV3	0.07	0.057	0.011	-0.009	0.07	0.056	0.011	-0.009	**0.0**	**-1.8**	**0.0**	**0.0**
LEV4	0.056	0.02	0.02	-0.016	0.056	0.02	0.02	-0.016	**0.0**	**0.0**	**0.0**	**0.0**
MED	0.137	0.042	0.04	-0.028	0.142	0.047	0.041	-0.027	**3.6**	**11.9**	**2.5**	**-3.6**

Tab. 3.3.4. Mean RMSD and BIAS between REF_2015 and DACHL2_2015 runs and satellite observations for Mediterranean sub-basins for winter (January - April) and summer (July - September) periods. The last four columns report the percentage difference of DACHL2_2015 with respect to REF_2015.

3.3.3 Multi-platform assimilation

The present section reports the results of the multi-platform data assimilation experiments planned in the Sub-Task 3.2. The object is to assess the feasibility and the impact on the biogeochemical status of the lone and joint assimilation of chlorophyll observations from BGC-Argo floats and from satellite.

The code of the multi-platform data assimilation differs from the one presented in the section 3.2 since the **H** operator is now modified to read and integrate multiple upstream data sources (i.e. satellite data and BGC-Argo floats data). In particular, the **H** operator consists of

the match of the surface model grid point for satellite observation and of the match and interpolation of model vertical grid levels to the BGC-Argo float profile vertical resolution. As a result, the vector misfit ($\mathbf{y}$-$\mathbf{H}(\mathbf{x})$) consists of almost 50000 and 1500 values for satellite and BGC-Argo, respectively.
The setup of the 3DVarBio and OGSTM-BFM is those described in section 3.2 and the assimilation elements here tested are the selection of the assimilated datasets, the observation errors and the frequency of the assimilation (Table 3.3.5).
The simulations DACHL1 and DACHL2 assimilate satellite and BGC-Argo floats separately every 7 days according to the standard setup of the CMEMS Med-MFC-Biogeochemistry Analysis and Forecast system. Simulation DACHL3 is aimed to the joint or multi-platform data assimilation, while DACHL3_1D differs from the previous run since the assimilation of BGC-Argo is daily while that of satellite every 7 days. The observation error relative to BGC-Argo floats used in DACHL2 and DACHL3 is equal to the value computed in section 3.1, but it has been rescaled to the background error defined by the EOF in order to get an observation error that is lower than that of satellite. As it will be shown later, this means that the hierarchy of the assimilation gives a higher rank to the BGC-Argo floats data. A higher observation error of BGC-Argo (as defined in Section 3.2) is set for simulation DACHL2_err and DACHL3_err in order to verify the impact of a different hierarchy in the assimilation scheme.
Two 40-day test cases (i.e., January: 1/1/2015- 9/2/2015, and August: 1/8/2015- 5/9/2015) are produced for each simulation. As reported in section 3.2, the two test cases differ for the physical and biogeochemical conditions: vertically mixed profile and surface chlorophyll bloom for January, and vertically stratified profiles with the presence of a Deep Chlorophyll Maximum (DCM) for August.

RUN name	Observations assimilated	Assimilation frequency	Observation error
REF	-	-	-
DACHL1	Satellite chlorophyll	weekly	Sat: monthly map of st.dev
DACHL2	Float profiles (chl)	weekly	Float: 0.01 mg/m3
DAHCL3	Float profiles (chl) and satellite chlorophyll	weekly	Float: 0.01 mg/m3 Sat: monthly map of st.dev
DACHL3_1D	Float profiles (chl) and satellite chlorophyll	sat weekly float when available at daily basis	Float: 0.01 mg/m3 Sat: variance
DACHL2_err	Float profiles (chl)	weekly	Float: st.dev of float
DACHL3_err	Float profiles (chl) and satellite chlorophyll	weekly	Float: st.dev of float Sat: monthly map of st.dev

Table 3.3.5: List and setup of the multi-platform assimilative runs.

3.3.3.1 Cross-validation of the multi-platform assimilation

The assimilation performance of the different runs is first assessed using the same datasets that are assimilated. Thus when one dataset is not assimilated it represents an independent validation, whereas when the dataset is used for assimilation it represents a semi-independent validation. In particular, the RMSD reported in Tables 3.3.6 and 3.3.7 for January and August, respectively, is computed matching the daily model output with the datasets at the observation location: only at surface for the satellite, and along the profile at the float position for the floats.

The results show that when a dataset is assimilated the model performance computed on the same dataset improves of the order of 50-70%, which is, of course, an expected result.

On the other hand, assimilating only one type of data does not necessary improves the model performance with respect to the other dataset. Indeed, the RMSD of DACHL1 increase in the 0-150 m layer using the floats data validation, and the RMSD of DACHL2 remains unchanged in surface using the satellite validation.

Fig. 3.3.4 shows two examples of chlorophyll concentrations of float, satellite and model before and after the assimilation of DACHL2 at the location of the BGC-Argo float profile. The after assimilation profiles (black line) are, as expected, close to the float profile, however at surface the distance of the model from the satellite observation increases in both cases. For the 20th of January (right panel) the float measurement at surface and the satellite observation are respectively higher and lower than the model before the assimilation.

The results of the multi-platform assimilation (DACHL3) show that the validation assessment of winter test case mostly maintains the performance of the semi-independent validation calculations with possible slight decrease of the performance due to the negative impact of the multi-platform data assimilation. (e.g. RMSD of daily surface chlorophyll between MODEL and SATELLITE of DACHL3 is slightly lower than DACHL1, and the RMSDs of validation using float data of DACHL3 are slightly lower than DACHL1, Table 3.3.6). This is because satellite chlorophyll values and chlorophyll float values at surface, as described below, are slightly inconsistent (Fig. 3.3.5). On the other hand, during the August test case, three statistics of the joint assimilation simulation improve with respect the single assimilation simulations while the DCM statistics of DACHL3 worse with respect to that of DACHL2. It is worth to note that the absolute value of RMSD statistics are pretty low (Table 3.3.7) as well as the satellite-float inconsistency and the percentage differences among the simulations.

Considering the statistics of the novel metrics (i.e. depth of the layer influenced by the winter bloom -MLB- and depth of the deep chlorophyll maximum –DCM-, see section 3.3.1), only when the BGC-Argo data are assimilated (DACHL2, DACHL3 and DACHL3_1D) an improvement is achieved whereas the satellite assimilation (DACHL1) has a negative (January) and null (August) impact.

JANUARY	REF	DACHL1	DACHL2	DACHL3	DACHL3_1D	DACHL2_err	DACHL3_err
RMSD of the daily surface chlorophyll between MODEL and SATELLITE [mg/m³]	0.109	-45%	0%	-44%	-34%	0%	-45%
RMSD of the averaged 0-150 mchlorophyll between MODEL and FLOAT [mg/m³]	0.081	+5%	-76%	-62%	-82%	-58%	-33%
RMSD of the chlorophyll surface value between MODEL and FLOAT [mg/m³]	0.172	+19%	-48%	-42%	-48%	-31%	-15%
RMSD of the MLB computed between MODEL and FLOAT [m]	22.4	+58%	-2%	-14%	-14%	n.a.	n.a.

Tab. 3.3.6: Model performance for January test case, expressed as percentage difference of each simulation with respect to REF: RMSD of surface chlorophyll using satellite dataset, RMSD of the chlorophyll profile integral using BGC-Argo float data, RMSD of the surface chlorophyll using BGC-Argo float data, RMSD of Mixed Layer Bloom (MLB).

AUGUST	REF	DACHL1	DACHL2	DACHL3	DACHL3_1D	DACHL2_err	DACHL3_err
RMSD of the daily surface chlorophyll between MODEL and SATELLITE [mg/m³]	0.068	-47%	-1%	-50%	-50%	-4%	-50%
RMSD of the averaged 0-150 mchlorophyll between MODEL and FLOAT [mg/m³]	0.034	+4%	-42%	-49%	-59%	-15%	-13%
RMSD of the chlorophyll surface value between MODEL and FLOAT [mg/m³]	0.087	-71%	-22%	-68%	-59%	-1%	-71%
RMSD of the DCM computed between MODEL and FLOAT [m]	13	0%	-17%	-11%	-58%	n.a.	n.a.

Tab. 3.3.7: Model performance for August test case, expressed as percentage difference of each simulation with respect to REF: RMSD of surface chlorophyll using satellite dataset, RMSD of the chlorophyll profile integral using BGC-Argo float data, RMSD of the surface chlorophyll using BGC-Argo float data, RMSD for Deep Chlorophyll Maximum (DCM).

As exemplified in Figs. 3.3.4 and 3.3.5, the consistency of the two datasets assimilated might be a not trivial issue. The methods to estimate chlorophyll are different in the two data sources: optical fluorescence for BGC-Argo floats and optical algorithms based on remote sensed reflectance for satellite. Thus, precision and errors of the two datasets can be substantially different. The averaged difference between the two datasets, evaluated by comparing surface floats data and satellite data at the location of the floats in the two periods considered in the simulations (Fig. 3.3.5), is -0.04 and 0.01 mg/m3 in January and August, respectively. This result indicates that the differences between the two datasets, which are of the same order of the observations errors, are time dependent and the error distributions appear neither normal nor log-normal at the monthly scale. The lack of consistency between the datasets is an open issue and has not a straightforward solution, that would require a method for modifying a float profile using a single surface value (satellite data) or for modifying a map (or a portion of a map) of satellite values using a single point (float data at surface).
Regarding the observation error, it is worth to note that accurate estimates of the observation error for satellite data are not given, and the tuning method proposed by Teruzzi et al. (2014)

can be applied only for the case of the satellite assimilation alone. On the other hand, the observation error for BGC-Argo float has been estimated either by the TC method (section 3.1) or by a tuning procedure (section 3.2). However, an integrated estimate of the observation error of both datasets is still missing. Another point to consider is that the number of observations (which is much higher for the satellite if compared with floats data) impacts the computational burden of the cost function of the 3DVarBio, which will produce a convergence toward the minimization of the misfit of satellite observation. Thus, an appropriate recalibration of the observation errors (i.e. imposing a much lower observation error of the BGC-Argo floats) is necessary to objectively shift the hierarchy of the assimilation scheme toward the BGC-Argo floats data, at least locally, overcoming the need to resolve the issue of the consistency of the two datasets.

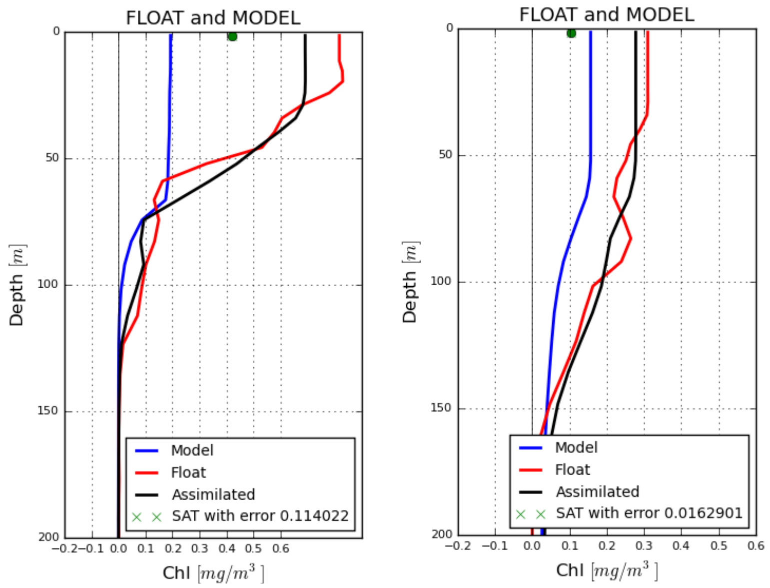


Fig. 3.3.4. Chlorophyll concentration over depth at the location of the assimilated float profile (left panel for float 6901513 and assimilation date 13 January, right panel for float 6901655 and assimilation date 20 January): model before the assimilation (BLUE line), float observations (RED line), model after the assimilation (BLACK line), and satellite observation at surface (GREEN)

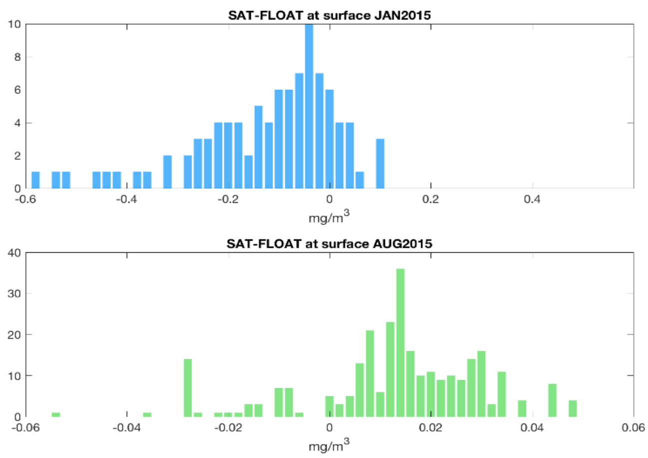


Fig. 3.3.5. Histogram of the differences of Satellite and BGC-Argo chlorophyll values at the surface of the float position for the two test cases: January (upper panel), August (lower panel).

Given the previous considerations, the DACHL3 simulation uses the datasets unchanged (i.e. without any inter-calibration of the data) and an observation error of BGC-Argo data much lower than that of satellite. As a result, the DACHL3 is characterized by corrections that are close to those of DACHL1 but with local effects in the neighborhood of the float positions (Figs. 3.3.6 and 3.3.7). This appears very evident in the anomaly map computed over a specific week (right column in Fig. 3.3.6 and 3.3.7), which has also a specific interest for operational purposes. When floats are assimilated at the daily frequency (DACHL3_1D) the local differences between the anomalies are more evident highlighting that the impact of the assimilation at the correct days is higher with respect to the impact of the weekly joint satellite-float assimilation. This can be seen also in Tables 3.3.6 and 3.3.7 where the statistics of DACHL3_1D show the highest improvement in the comparison indexes that use the float data. In fact, DACHL3_1D shows identical performance with respect to DACHL1 when satellite data is used (Tables 3.3.6 and 3.3.7) but an increase of the performance for the float-based skill assessment (see also Fig. 3.3.8). This is due to the fact that floats data assimilation occurs at different times of the assimilation of satellite (thus uncoupling the two assimilation streams) but at the same time of Argo physical variables (e.g. T and S), thus increasing the consistency with physical fields and possibly the persistence of the new biogeochemical status.

Two additional simulations, DACHL2_err and DACHL3_err (results not shown), that use a higher observation error of BGC-Argo (according to the estimates in section 3.1 and 3.2) produce results very similar to DACHL1 when the comparison is made with satellite data and a lower improvement with respect to DACHL2 when the comparison is made with the BGC-Argo data (Table 3.3.6 and 3.3.7). The use of the calibrated observation error for the BGC-Argo data (DACHL3_err e DACHL2_err) reduces the spatial impact of the assimilation of the chlorophyll profiles, highlighting the lower effectiveness of the BGC-Argo data when their hierarchy rank is decreased.

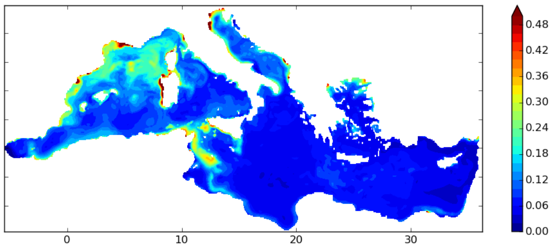
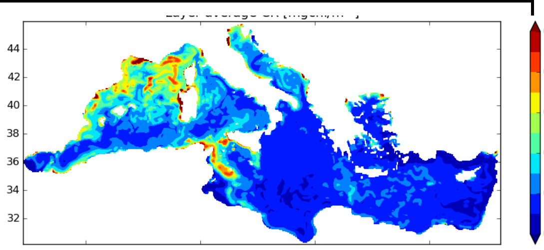
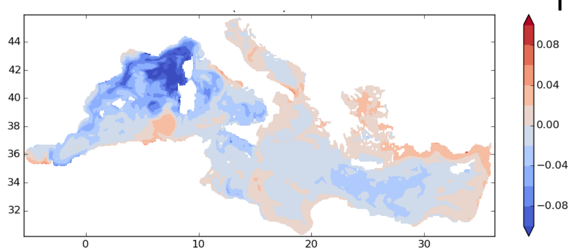
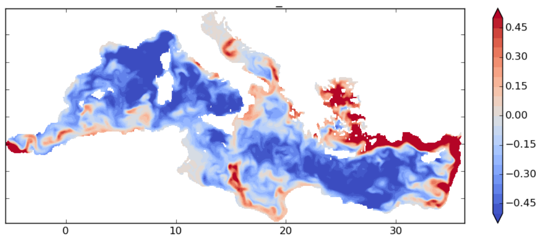
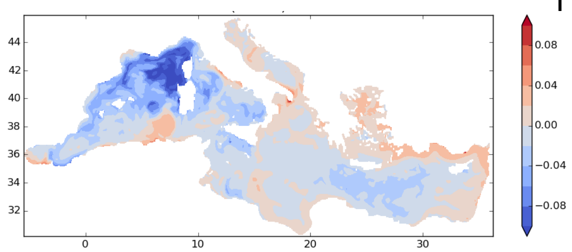
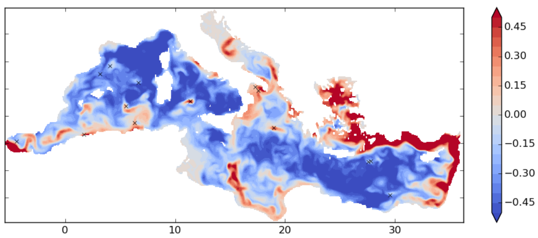
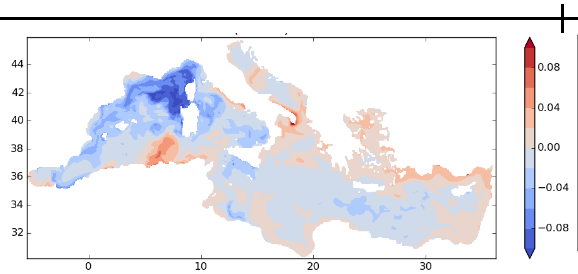
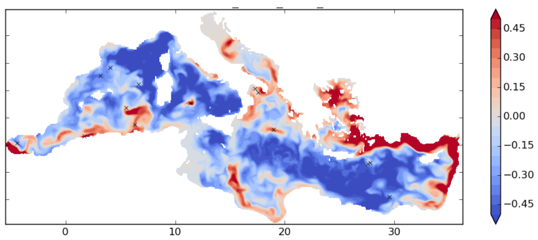
	monthly mean for January	weekly mean 20-27 Jan 2015
REF		
DACHL 1		
DACHL 3		
DACHL 3_1D		

Fig. 3.3.6. Maps of integrated chlorophyll concentration (mg/m3) in January for the REF run (first lines), and maps of the anomaly between REF and DACHL1 (second) and DACHL3 runs (third) and DACHL3_1D (fourth). Maps refer to the monthly mean (left column) and a specific weekly mean (right column). Float positions (x).

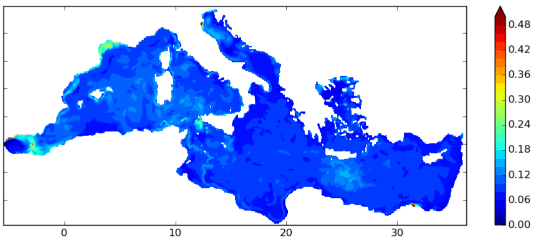
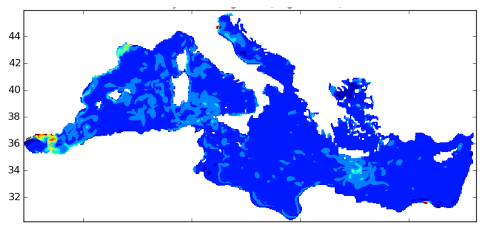
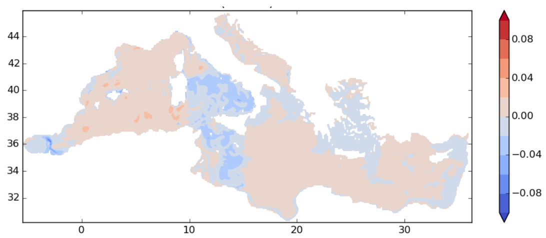
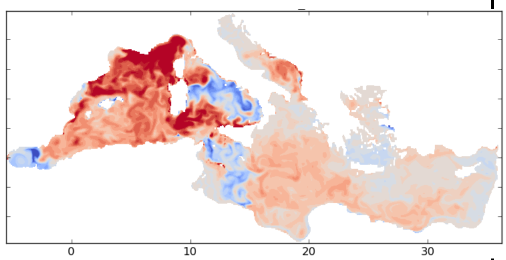
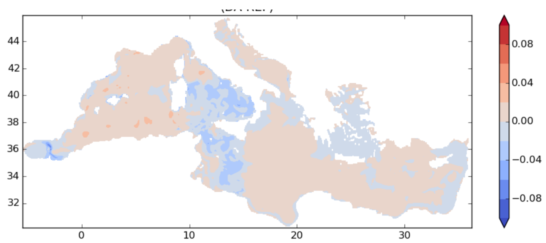
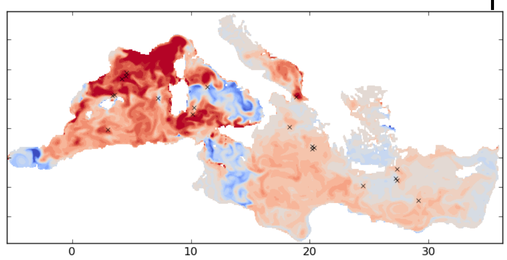
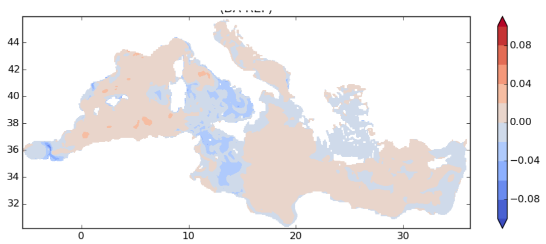
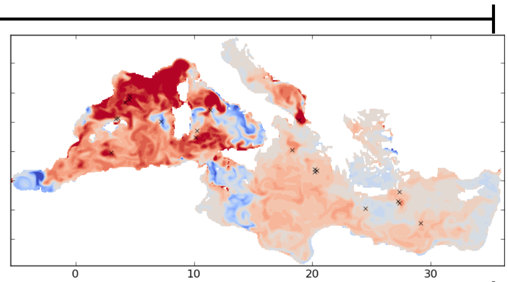
	monthly mean for August Chlorophyll (mg/m3) and absolute difference	weekly mean 24-39 Aug 2015 chlorophyll (mg/m3) and relative difference
REF		
DACHL 1		
DACHL 3		
DACHL 3_1D		

Fig. 3.3.7. Maps of integrated chlorophyll concentration (mg/m3) in August for the REF run (first lines), and maps of the anomaly between REF and DACHL1 (second) and DACHL3 (third) and DACHL3_1D (fourth). Maps refer to the monthly mean (left column) and a specific weekly mean (right column). Float positions (x).

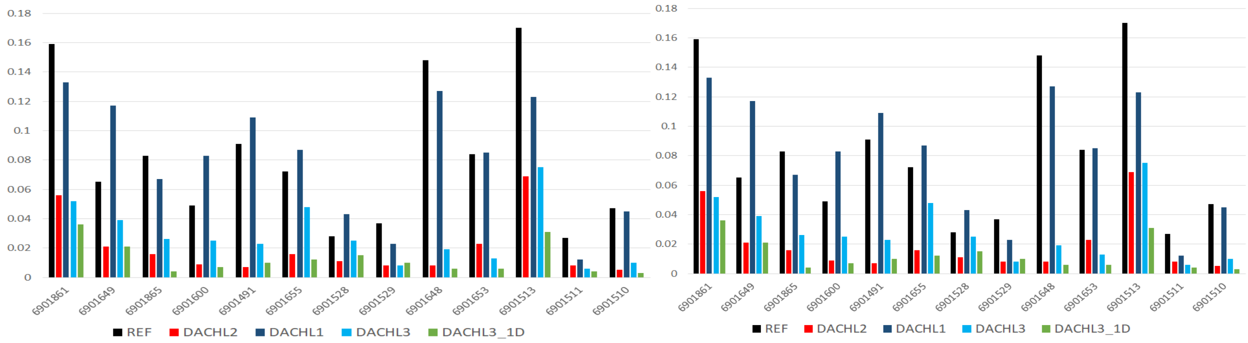


Fig. 3.3.8. RMSD [mgchl/m3] of integrated 0-150m chlorophyll between simulation and float data for each float and for the two test cases: January (left panel) and August (right panel).

3.3.3.2 Local effect of BGC-Argo float assimilation

The BGC-Argo floats data assimilation has a significant impact on the vertical structure of chlorophyll (and other phytoplankton variables) at local scale (i.e. in a neighborhood of the float positions). On the contrary, when surface satellite chlorophyll values are assimilated, the propagation of the correction along the vertical relays on a statistical a priori knowledge, through the Vv operator of the 3DVarBio. On the other hand, as shown in the section 3.2, the BGC-Argo floats have a very high density of observations along the water column that allows to efficiently constrain the modeled chlorophyll vertical profiles.

Considering the areas surrounding the float trajectories during the 1-month simulation (see section 3.2 for explanation on the definition of the dimension of the areas), the Hovmoller diagrams of Figures 3.3.9 and 3.3.10 show the evolution of chlorophyll profiles simulated by the reference and assimilation runs for two couples of floats. It can be noted that the assimilation of BGC-Argo profiles (DACHL2, DACHL3 and DACHL3_1D) provides higher temporal variability of the chlorophyll profile evolution with respect to the assimilation of satellite only (DACHL1). In some cases, when the area over which the model outputs are averaged is large enough (e.g. Float 6901767 in Fig. 3.3.10) DACHL3 has some more similarity with DACHL1 highlighting that the vertical propagation of correction due to surface satellite assimilation and the horizontal propagation of vertical correction due to float assimilation might combine together even at small scales.

The DACHL3_1D has the highest temporal variability showing often a high frequent fragmentation (e.g. evident during the summer DCM of float 6901767) of the temporal chlorophyll evolution, which is due to the occurrence of the alternation of satellite assimilation steps (every 7 days) and BGC-Argo float assimilation steps (usually every 5 days due to floats data availability).

In order to evaluate the importance of the assimilation at the local scale, the persistence index (ITP, see section 3.2) is computed for the areas surrounding the float trajectories for the different assimilation simulation. Results of the analysis, reported in Table 3.3.8, show that the joint assimilation (DACHL3) provides the highest values of ITP, in terms of number of events with divergent evolution and days of persistence. It is worth to note that the satellite assimilation has a higher impact than the float assimilation alone because of a positive neighboring effect. Indeed, the satellite correction is consistently extended to larger areas and the lateral transport (the major driver to decrease the persistence) has a minor impact.

Persistence of DACH3_1D is always higher than the frequency of the assimilation steps that, in the surrounding area of a float position, occur usually every 3 to 5 days.

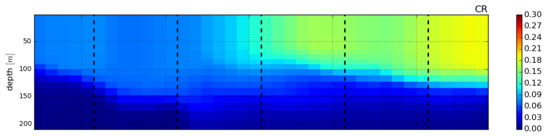
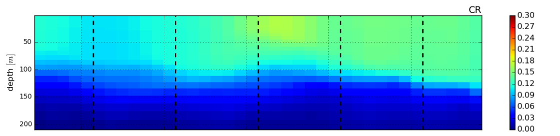
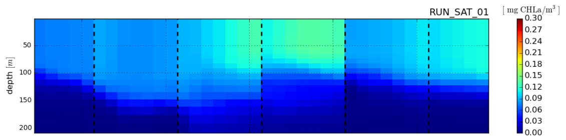
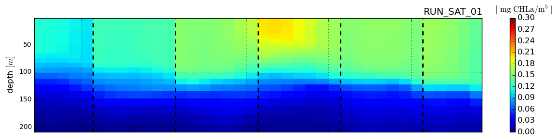
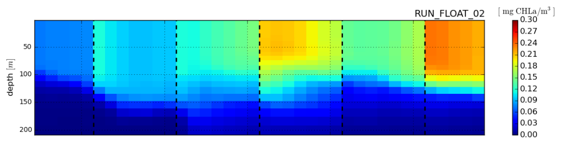
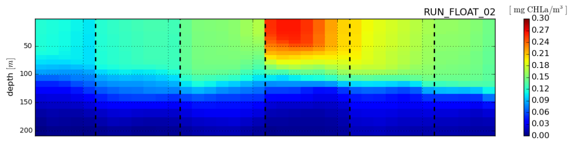
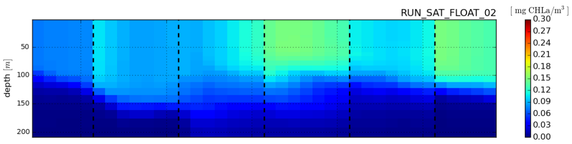
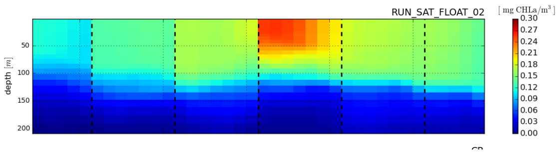
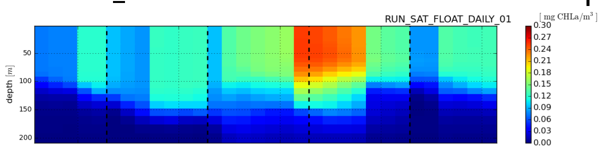
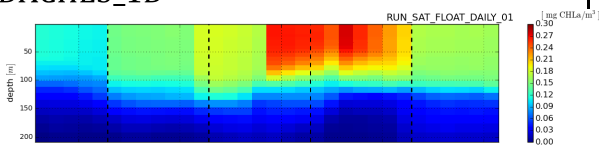
Float 6901655	Float 6901529
REF 	REF 
DACHL1 	DACHL1 
DACHL2 	DACHL2 
DACHL3 	DACHL3 
DACHL3_1D 	DACHL3_1D 

Fig. 3.3.9. Hovmoller diagram of chlorophyll concentrations (mg.m-3) for two selected floats for the reference and assimilation simulations of the January test case.

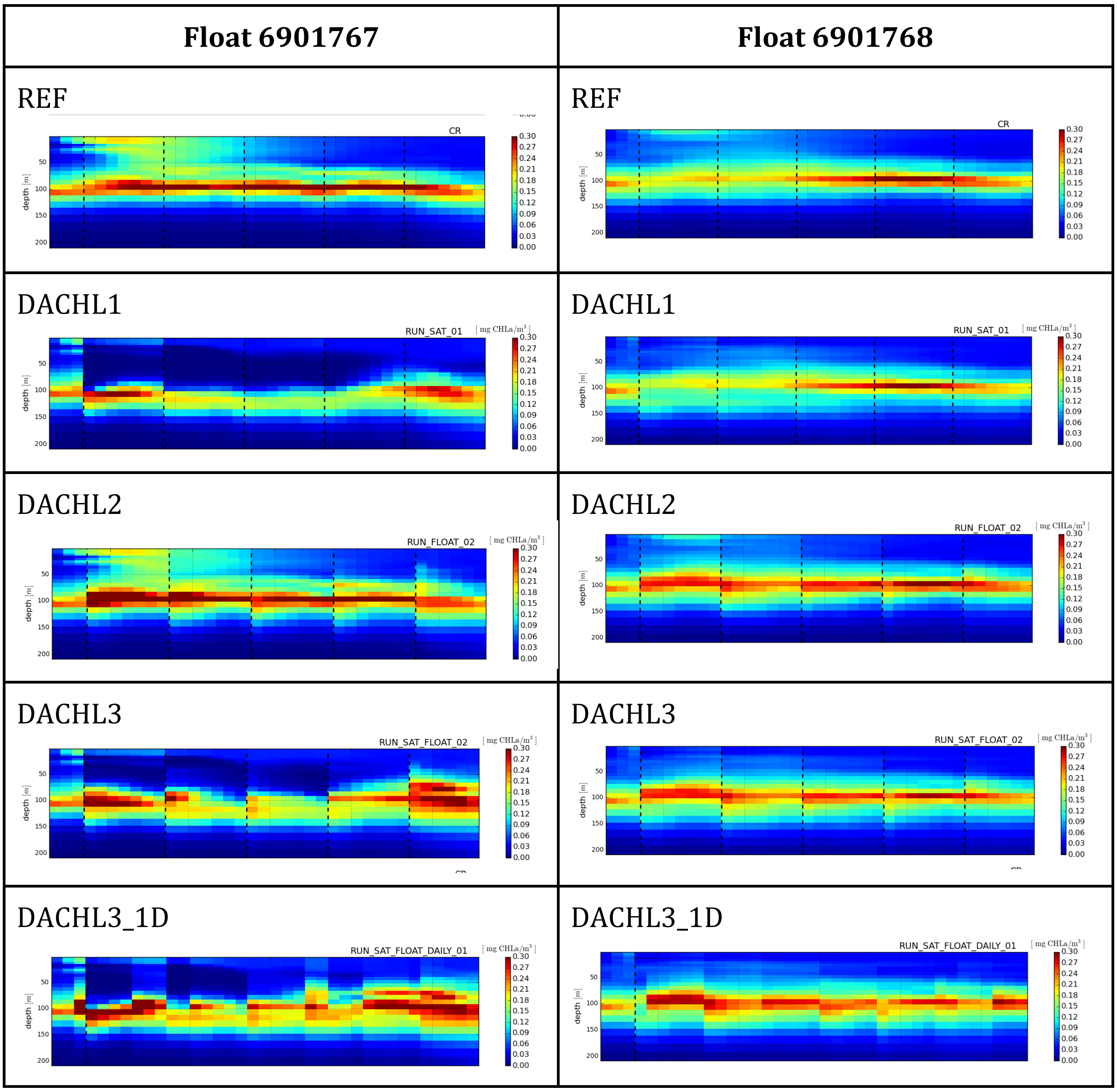


Fig. 3.3.10. Hovmoller diagram of chlorophyll concentrations (mg.m-3) for two selected floats for the reference and assimilation simulations of the August test case.

	assimilated observation and frequency of assimilation step	% of events with a divergent evolution (i.e. ITP>1)		Persistence index ITP<0.5 [days]	
		JAN	AUG	JAN	AUG
DACHL1	Sat: weekly	32%	39%	5.2	5.9
DACHL2	Float: weekly	18%	9%	4.3	3.7
DACHL3	Sat: weekly Float: weekly	38%	44%	5.4	5.8

Table 3.3.8. Persistence index (defined in Section 3.2) computed for the different simulations and the 2 test cases.

The analysis of the shape of the innovation profile (ISP index, details in section 3.2) shows that the impact of the BGC-Argo floats data assimilation (DACHL2) is local and spatially heterogeneous (maps of Fig. 3.3.11), due to the more accurate description of the vertical structure of the chlorophyll profiles. Satellite assimilation (DACHL1 in Fig. 3.3.11) produces maps with more homogeneous patterns, due to the fact that the propagation along the vertical direction of the surface innovation occurs through predefined statistical covariance (i.e. set of EOFs defined for each sub-basin, Teruzzi et al., 2014). The joint assimilation (DACHL3) produces maps of innovation profile pretty similar to that ones of DACHL1 but with the impact of the BCG-Argo floats prevailing at the local scale. Indeed, this increases the heterogeneity of the maps because often the BGC-Argo corrections and adjacent satellite corrections are different.
The histograms of ISP frequency (lower panel of Fig. 3.3.11) show that, despite the different spatial impact of BGC-Argo and satellite, DACHL2 and DACHL3 have a larger number of possible ISP values. In fact, the number of possible ISP of DACHL1 is 10 and 19 in January and August test cases, respectively, whereas the BGC-Argo float assimilation produces a much higher number of possible shapes: 22 in January and 23 in August test cases.

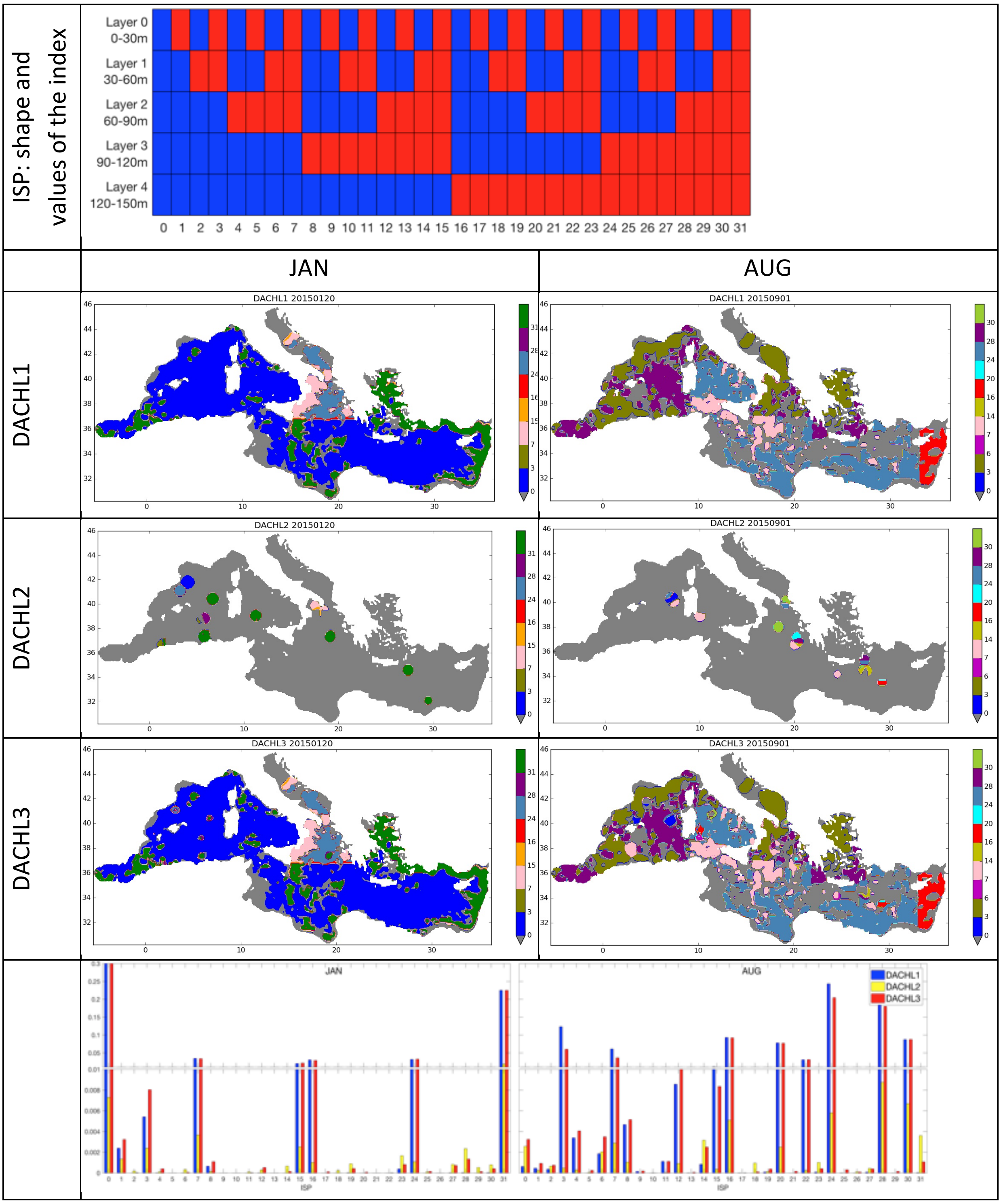


Fig. 3.3.11. Shape of innovation profiles (blue-red profiles) and value of ISP (from 0 to 31, upper panel), maps of ISP index for one assimilation step of the JAN (left column) and AUG (right column) test cases and for the three assimilation simulations (central rows: grey areas correspond to other than the most important ISP values and areas with innovation integral below a given threshold, 0.001 mg/m3). Histogram of the frequency of the ISP index for the two test cases (lower panel). Values of innovations higher than the threshold are used.

The 3DVarBio variational assimilation scheme acts as a filter, producing instantaneous changes of the updated variables (chlorophyll and phytoplankton variables) at the assimilation steps. This is visible in all assimilation simulations at the assimilation step (i.e. vertical dashed lines and sharp changes in the daily DACHL3_1D assimilation in Fig. 3.3.12). This phenomenon, which occurs also for the assimilation of physical variables of NEMO through the OceanVar scheme, is clearly visible in the Hovmoller diagrams of the T and S. In fact, it is possible to recognize several sharp temporal discontinuities in the evolution of the temperature and salinity due to the daily assimilation of the Argo floats (Fig. 3.3.12).
Since the physical assimilation produces changes in the evolution of temperature and density of the water column along with the transport proprieties (velocities and vertical diffusivities), we tested whether the biogeochemical assimilation produces changes that are consistent with the evolution of physical variables.
As an example, the Hovmoller float diagram in January (left column in Fig. 3.3.12) shows that temperature and salinity have a couple of harsh changes in the last two weeks that produce an enhancement of the vertical mixing (i.e. increase of phosphate in the upper layers of the water column in the bottom left panel of Fig. 3.3.12). Among the assimilation simulations, the DACHL1 and DACHL3 produce updates of chlorophyll that appear not fully consistent with the increase of phytoplankton that it would be expected, since the increase of the nutrient availability. On the other hand, the evolution of the shape and depth of the summer DCM in the plot of float 6901766 (right panels in Fig 3.3.12) shows a periodic oscillation due to the mesoscale summer dynamics around the Ierapetra gyre (location of the box encompassing the float 6901766 in Fig. 3.3.1). Oscillations appear also in the T and S evolution that are triggered, beside other factors, also by the assimilation of the Argo physical variables. The oscillation of the depth of the nutricline (i.e. depth at which phosphate concentration change abruptly, bottom right panel in Fig. 3.3.12) is the direct consequence of the physical forcing. Thus, among the biogeochemical assimilation simulations, DACHL2 seems to have a better consistency with the evolution of the physical variables. In order to verify whether the assimilation can provide a higher physical-biogeochemical consistency with respect to the ocean dynamics, the temporal correlation of the vertical integrated 0-80m (other depths are tested as well but with less clear results) is computed for all the floats and their average is reported in Table 3.3.9 for the different assimilation simulations.
Even if the variability of the correlation values among the simulations are pretty low, the assimilation of BGC-Argo float alone (DACHL2) is the one that provides the highest correlation, highlighting how the assimilation of satellite data might produce some inconsistency in the temporal evolution of the chlorophyll with respect to the physical fields.
The lowest values are computed for DACHL3_1D because in this case the frequent and alternated assimilation of satellite (every 7 days) and floats (every 5 days) produces the most disjointed evolution of chlorophyll, which might lose some consistency with the physical fields.

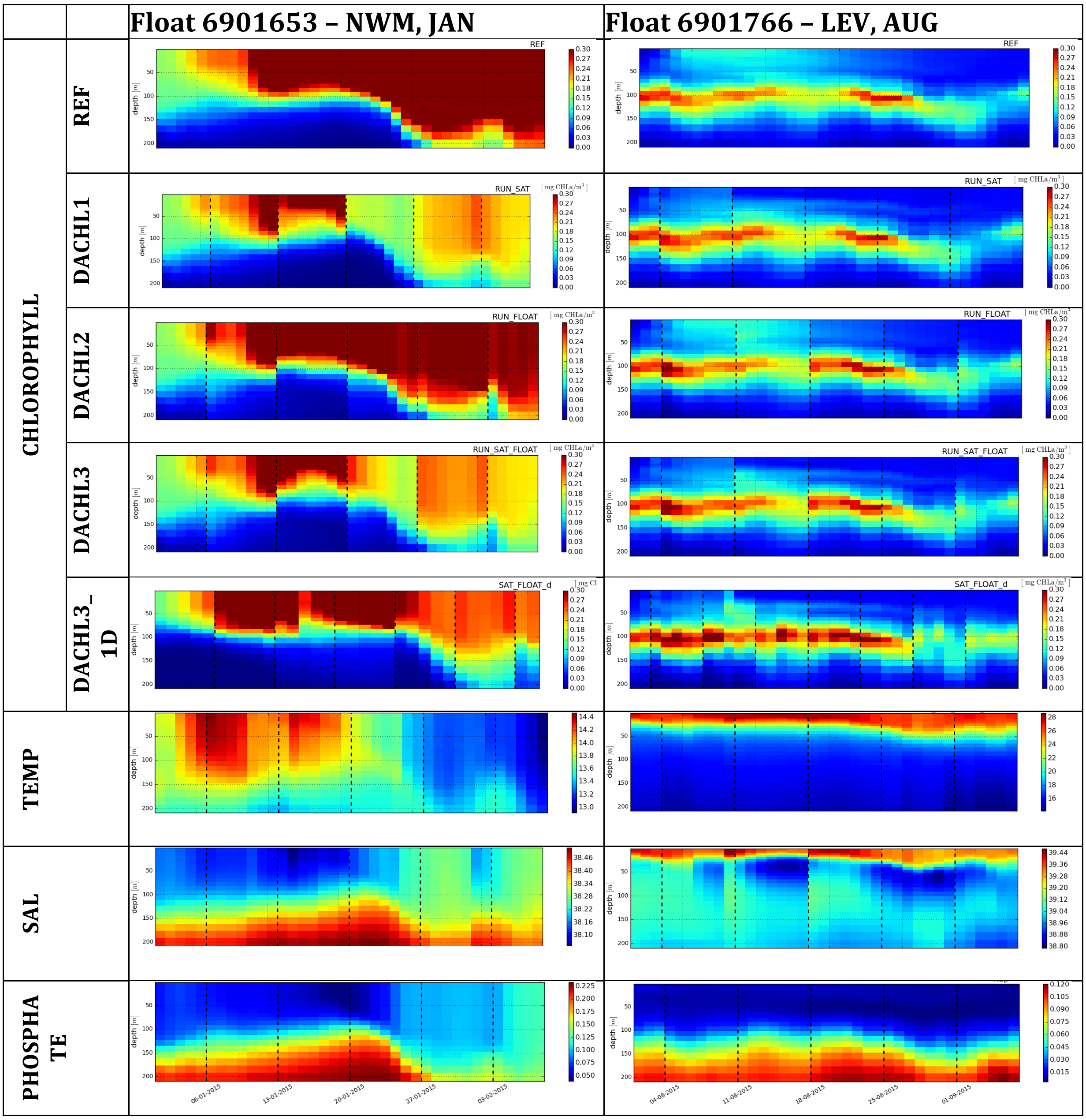


Fig. 3.3.12. Hovmoller diagrams of the evolution of chlorophyll for different assimilation simulations and of the evolution of Temperature, Salinity and Phosphate. Hovmoller plots are generated using the model outputs in the surrounding area of the BGC-Argo trajectory. The weekly and daily assimilation steps are designed by the vertical dashed lines.

Correlation with CHL		DACHL1	DACHL2	DACHL3	DACHL3_1D
PHOSPHATE	JAN	0.4266	0.4423	0.4329	0.3543
	AUG	0.4739	0.5335	0.5013	0.4408
TEMPERATURE	JAN	0.5185	0.5302	0.5137	0.4534
	AUG	0.3207	0.3263	0.3187	0.2954
SALINITY	JAN	0.5436	0.5240	0.5306	0.3984
	AUG	0.3628	0.5319	0.3729	0.3424

Table 3.3.9. Correlation between the temporal evolutions of the vertical integrated 0-80m chlorophyll concentration and the vertical integrated 0-80m concentration of phosphate, temperature and salinity.

3.3.4 Impact of the multi-platform assimilation on biogeochemical processes

The assimilation of chlorophyll directly updates 17 model state variables (i.e. the contents of the four phytoplankton groups of C, N, P, Chl and the Diatoms group in Si) and indirectly the dynamics of the biogeochemical processes. In order, to assess the impact of the multi-platform assimilation, the vertical integrated primary production is shown for one given week for the two test cases as an example (Fig. 3.3.13) and averaged over the 1-month runs (Table 3.3.10) in the different assimilation simulations.
At the basin scale, the satellite assimilation has clearly the largest impact, however given the high spatial heterogeneity of the primary production, due to the mesoscale and patched biological dynamics, the assimilation of chlorophyll profiles produces local changes that then propagate along the trophic chain. The differences in the simulations including the floats data assimilation are more evident in August, possibly due to the higher values of primary production and higher spatial variability due to mesoscale dynamics.

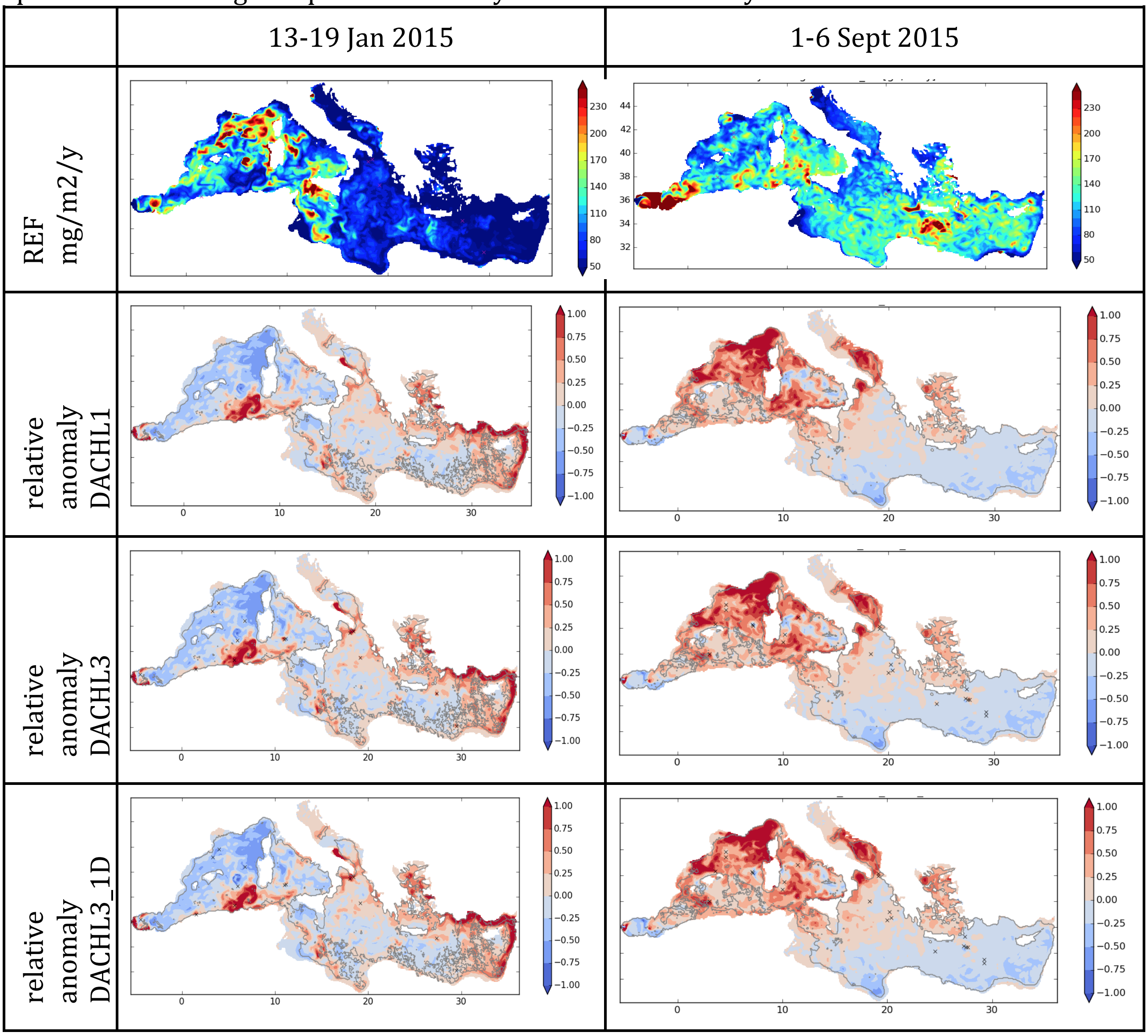


Fig. 3.3.13. Mean weekly maps of 0-200m vertically integrated primary production for the reference run (REF, first row) and maps of relative anomalies for the DACHL1 (second row), DACHL3 (third row) and DACHL3_1D (fourth row). Position of floats (x).

	REF NPP [mg/m²/y]	DACHL2	DACHL1	DACHL3	DACHL3_1D
Jan	83.1	-1.1%	-7%	-6.7%	-3.1%
Aug	277.2	-0.1%	-32%	-32.1%	-34.2%

Tab. 3.3.10. Vertically integrated (0-200 m) primary production of REF simulation (average over the Mediterranean Sea) and relative differences between the assimilation runs and the reference.

3.3.5 Impact of the multi-variate assimilation on biogeochemical processes

The assimilation of nitrate has been included in 3DVarBio with some changes with respect to what implemented for the assimilation of chlorophyll: the vertical operator V_V is specified on EOFs defined down to 450 m (rather than 200 m), the horizontal correlation radius of V_H is slightly larger than that used for chlorophyll assimilation, and the biological multi-variate covariance operator V_B is defined as monthly covariance matrix among nutrients. Further, the nitrate assimilation impacts on 3 state variables (nitrate, phosphate and silicate) rather than 17.
To assess the impact of the multi-variate assimilation, we started by running numerical tests with assimilation of the nitrate measurements only (note that only a part of the BGC-Argo floats provides NO3 data, see Tab. 3.3.11).
Figure 3.3.14 shows an example of the results obtained during the January test case: as plotted in the top 3 panels, the nitrate assimilation has an impact at the 3rd and 5th assimilation steps, with an increase in the nutrient pool below 100 m with respect to the REF simulation without assimilation. Such increment has a consequence on other non-assimilated variables: phosphate (which is updated through the updated operator V_B and also increases below 100 m) and the free variable chlorophyll (which is not updated by operator V_B but whose vertical profiles are significantly impacted in the following days after the assimilation due to the increase of the available nutrients).
To quantify the impact of the nitrate assimilation in terms of the spatial innovation (index of spatial innovation, ISI, measured as the area where the absolute difference of the innovation is larger than a selected threshold, defined around 1% of the average value, e.g. 0.001 mg/m^3 for chlorophyll and 0.01 mmol/m^3 for nitrate) and of the temporal persistence (ITP, section 3.3.3.2) we compared the runs with only chlorophyll assimilation and with only nitrate assimilation (Tab. 3.3.11), considering for both a weekly assimilation frequency. We computed ISI and ITP on different layers: 0-150 m for chlorophyll, and 0-200 m / 200-400 m for nitrate and phosphate. We can observe that the impact of the nitrate assimilation is potentially larger, with an area innovated that is twice that one for the only chlorophyll DA, and a persistence more than 10% longer in terms of days. This is related to the vertical structure of the nitrate, which contains most of the information below the nutricline, with larger covariance, wider horizontal scales, and longer time scales.
Therefore, from these preliminary tests we can conclude that the impact of the assimilation of nitrate data provided by the BGC-Argo floats has a potential impact which is higher than that estimated by the assimilation of chlorophyll data.

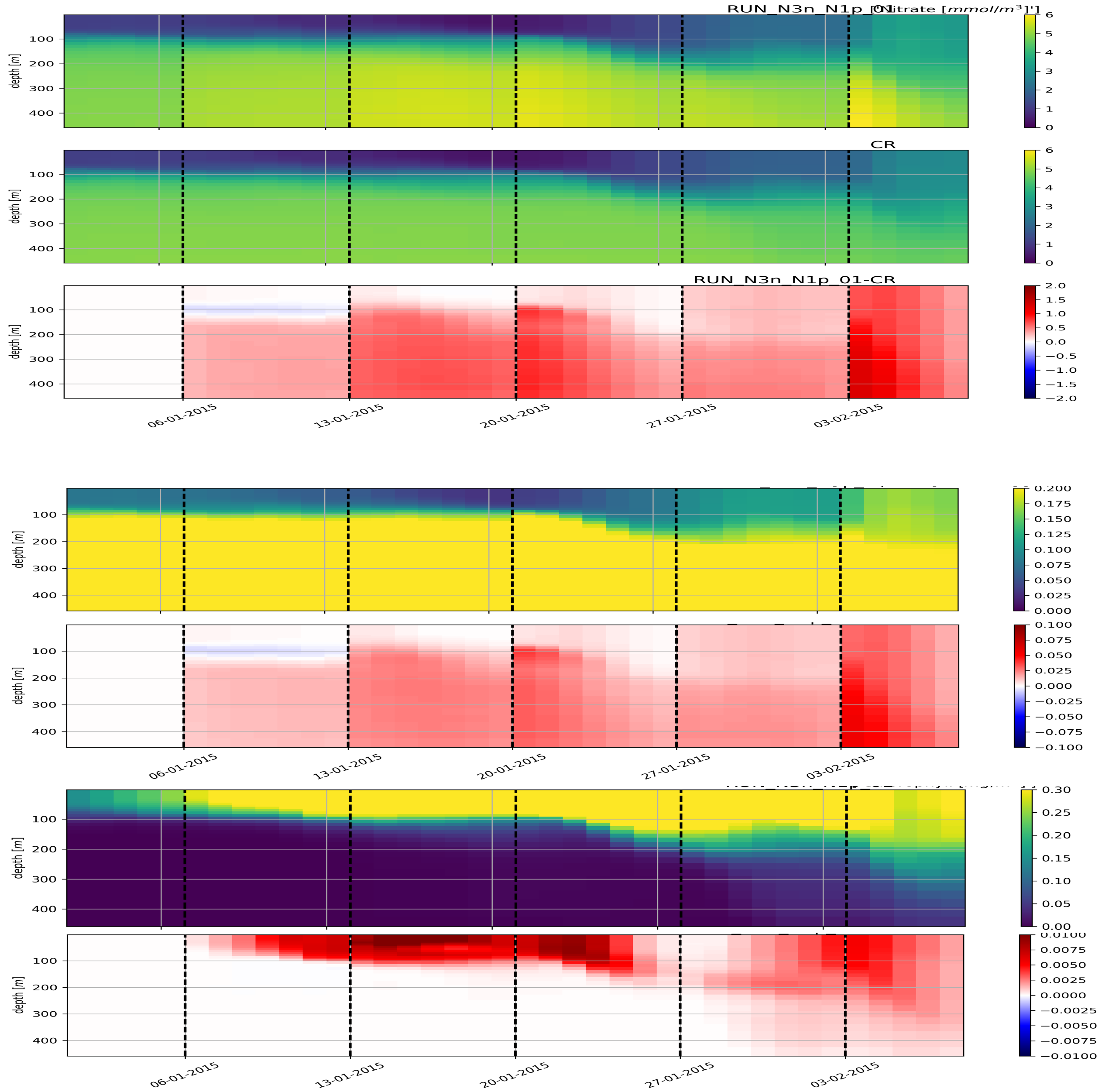


Fig. 3.3.14. Hovmoller diagrams of the evolution of nitrate (3 top panels: DA run, REF run, difference), phosphate (2 middle panels: DA run and difference with REF) and chlorophyll (2 bottom panels: DA run and difference with REF) for the nitrate assimilation simulation. Hovmoller plots are generated using the model outputs in the surrounding area of the BGC-Argo trajectory. The weekly assimilation steps are designed by the vertical dashed lines.

Assimilation of:	**n. of floats**	**Correlation radius [km]**	**Assim. frequency**	**Updated variable**	**Layers [m]**	**ISI [km2] per float**	**ITP [days]**
Chlorophyll	13-15	15.2	7 days	Chlorophyll	0-150	10050 (0.4)	4.1±2.0
Nitrate	3-5	15.5	7 days	Nitrate	0-200	19500 (0.8)	4.6±1.2
				Nitrate	200-400	23900 (1.0)	4.8±1.2
				Phosphate	0-200	19500 (0.8)	4.7±1.3
				Phosphate	200-400	23900 (1.0)	4.7±1.4

Tab. 3.3.11. Quantification of the impacts for nitrate only DA vs chlorophyll only DA. Number in parentheses of the ISI column refer to the % of the whole Mediterranean Sea area.

4 Potential impacts for CMEMS and transfer towards CMEMS

The main impact of MASSIMILI regards the **improvement of the quality of the next generation CMEMS biogeochemical products and services**.

This has been presented and discussed in Section 3.3.1 for chlorophyll assimilation. As a first key message, it must be noted that the assimilation of chlorophyll floats data has an impact at local scales and in small areas due to the low number of BGC-Argo floats.

Moreover, it has been shown that, given the possible inconsistency between chlorophyll float and satellite datasets, the positive impact of floats data assimilation cannot be fully evaluated by using satellite dataset only. Further, the very scarce in-situ and independent data make the evaluation of the positive impact of the floats data assimilation a not trivial task.

Another important impact on the CMEMS products quality is that BGC-Argo floats data, made available within MASSIMILI consortium through the strict collaboration between OGS and LOV teams, are now operationally used for the validation activities of the Med-MFC-Biogeochemistry component.

In particular, the operational validation activities now include the use of BGC-Argo floats for weekly quality assessment of CMEMS-MED-BIO products (chlorophyll, nitrate, oxygen). Results are weekly updated on the regional validation website medeaf.inogs.it (tab “Bio-Argo float” of the page http://medeaf.inogs.it/nrt-validation). All available data of the BGC-Argo floats are compared with the vertical profile corresponding to the closest model grid point, together also with vertical profiles of temperature and salinity.

As an example, Fig. 4.1 shows one of the plots that may be found on the medeaf.inogs.it website, with the comparison of vertical profiles of model results and BGC-Argo float data.

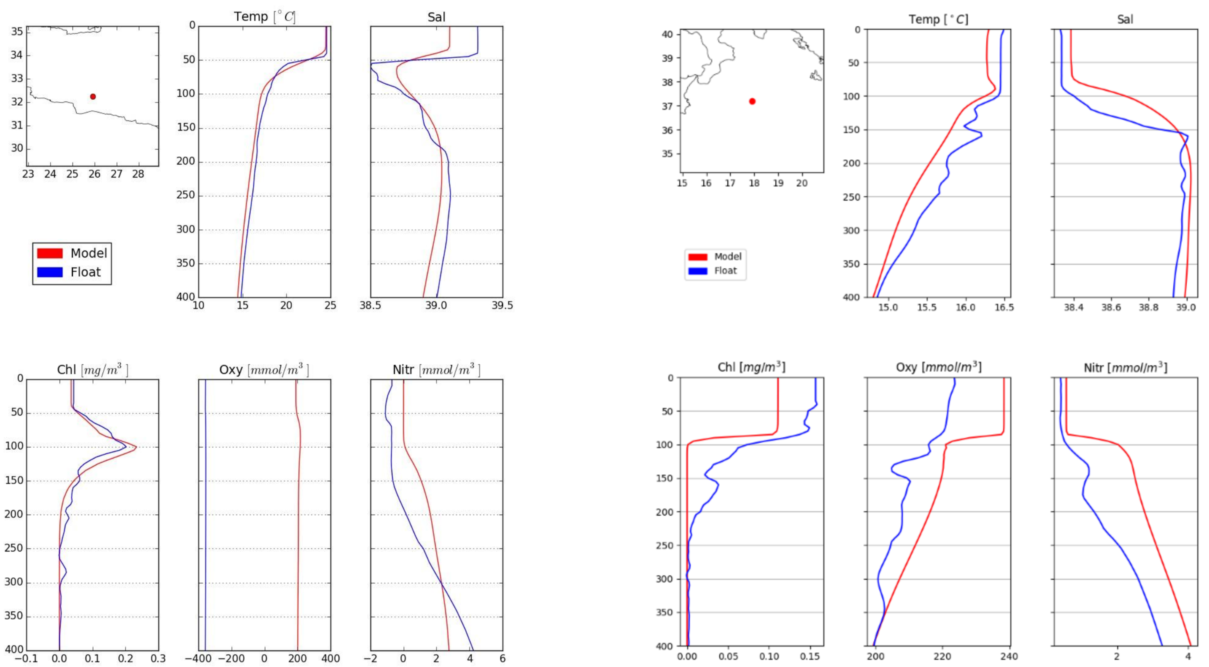


Fig. 4.1 – Examples of plots shown on the “NRT-validation” section of the medeaf.inogs.it website. BGC-Argo data (blue lines) and model output (red lines) for data extracted from the WMO 6901766 on 15 October 2017 (left panel) and the WMO 6901769 on 6 January 2018 (right panel). The position of the float is shown in the box at the top left position.

Further, MASSIMILI project allowed to develop and implement novel metrics to evaluate the performance of the MedBFM model system. Bias, root mean squared difference (RMSD), correlation and *ad hoc* new metrics between BGC-Argo profiles and the matching model output profiles (i.e. the model output at the time and location of the float profile, GODAE class 4 metric) were used to evaluate the model performance in reproducing the temporal evolution of the vertical dynamics of chlorophyll and nitrate in the Mediterranean Sea. The new metrics were estimated both for each specific float trajectory and as average statistics computed from all the matching pairs of model and observation profiles for selected layers and sub-basins. In particular, we defined the depth of the deep chlorophyll maximum (DCM), the 0-200 m vertical averaged chlorophyll values, the depth of the mixed winter bloom (MLB) defined as the depth at which chlorophyll concentration is 10% of surface concentration during winter period. Similar metrics were also defined for the nitrate.

A second major potential impact regards the **assessment of the effectiveness of the Bio-Argo network design in the Mediterranean Sea**.

MASSIMILI project was strategic to quantify which is the portion of the Mediterranean Sea area that can be affected by an operational assimilation of BGC-Argo floats data with the present BGC-Argo network: with a coverage of 15 BGC-Argo floats we can constrain maximum 10% of the total Mediterranean Sea extension for the chlorophyll field. Therefore, we can estimate how the number of platforms should increase to constrain a wider area. As a consequence, our results show that we may choose two solutions to enhance the impact of the data assimilation of BGC-Argo floats: increase the number of platforms or deploy the floats in the key points.

As potential impact, considering the difficulties to increase the number of active BGC-Argo platforms (related to multiple aspects such as funding, management and operations costs), we can highlight the key areas where we can envisage a significant impact of the assimilation of the BGC-Argo keeping their network configuration as in the current conditions: Balearic Front, Gulf of Lion Gyre, South Adriatic Gyre, Northern Tyrrhenian Gyre, Sicily Strait, Northern Ionian Cyclonic Gyre, Rhodes Gyre (names from Pinardi et al. 2015, Prog. Ocean 132). This strategy, besides constraining the operational data assimilation of the BGC-Argo floats, will potentially affect the monitoring of the biogeochemical processes in such areas. In this perspective, BGC-Argo floats should be deployed in those areas characterized by higher productivity, which have also an economical importance (related to Blue Growth strategy and fishery industry): operational biogeochemical models can thus support the BGC-Argo deployment strategy through the analysis of the product maps of primary productivity.

A third area of potential impact regards the **biogeochemical data assimilation modelling community**.

The MASSIMILI team is open to share the experience gathered during the development of the new data assimilation with other modelling teams within CMEMS. The evaluation of our results and of the technical problems encountered indicates that is necessary a period of about one year to finalize the operational implementation of the new assimilation scheme and to include it in the CMEMS-MED-BIO workflow. In any case, the impact is clear, since the development of the integration of the BGC-Argo floats data within an operational CMEMS-MFC has been successfully concluded, and the code of the new data assimilation scheme is publicly available. Moreover, the 3DVarBio code has been officially released. As potential impact, under the coordinated action of Mercator Ocean, we are ready to support other modelling groups within CMEMS to upgrade their data assimilation systems in order to integrate the BGC-Argo floats information.

A last area of potential impact regards the **improvement of the representation of the mesoscale dynamics in biogeochemical fields of the Mediterranan Sea**.

Our results proved that the observation error plays a major role in controlling the effectiveness of the assimilation, and that the estimated non-uniform correlation radius length scale, which is of the order of the mesoscale dynamics, together with the actual size of the BGC-Argo floats network allow to significantly constrain up to 10% of the Mediterranean Sea. The frequency of the assimilation step can be optimized in order to enhance the persistence of the innovation and the consistency with the physical field.

As potential impact, we conclude that improvements of the above described issues might be achieved by redesigning the biogeochemical state variable error covariance operator (Vb) in terms of multi-variate covariance or of physical-biogeochemical inverse model. Our results show that the assimilation of the BGC-Argo floats data can potentially improve the description of the chlorophyll vertical structure related to the mesoscale dynamics, changing concentration and shapes of the vertical profiles during the two most significant seasonal processes (winter surface bloom and summer deep chlorophyll maximum).

5 Communications

List of presentations reporting MASSIMILI project and its results:

NAOS meeting (Villefranche, 21-22 September 2016). Participants: F. D'Ortenzio and V. Taillandier. Dissemination of the MASSIMILI activities within the Bio-Argo community.

MONGOOS workshop: "Advances in Oceanographic Modelling in the Mediterranean Sea ", SPLIT (Croatia), 15 November 2016.
Cossarini G., Salon S., D'Ortenzio F., Mariotti L. Development of a multi-data assimilation scheme to integrate Bio-Argo floats data with Ocean Colour satellite data into the CMEMS MFC-Biogeochemistry.

1st CMEMS Service Evolution Coordination Meeting, Bergen, Norway, 1-2 December 2016, presentation of MASSIMILI project.

Mid Term Meeting at Mercator Ocean in Toulouse (27th January 2017), participation of OGS and LOV teams.

7th China-Italy Collaboration Workshop (Rome 11-13 April), presentation of the MASSIMILI project.

EGU, Wien, 24-28 April 2017
G. Cossarini, Salon S., D'Ortenzio F., Mariotti. Development of a multi-data assimilation scheme to integrate Bio-Argo floats data into the CMEMS MED MFC-Biogeochemistry.

EuroArgo user meeting, Paris, France, on 4-5 July 2017.
Mariotti L., Cossarini G., Salon S., D.Ortenzio F., Mignot A. A multi-data assimilation scheme of Biogeochemical-Argo data for the CMEMS Mediterranean Biogeochemical model.

EuroArgo user meeting, Paris, France, on 4-5 July 2017.
Mignot A., D'Ortenzio F., Taillandier V., Cossarini G. , Salon S., Mariotti L.
Estimation of BGC-Argo chlorophyll fluorescence and nitrate observational errors using the triple collocation method

Copernicus Marine Week (Bruxelles, 25-29 September 2017), Service Evolution section.
Cossarini G., D'Ortenzio F., Salon S., Taillandier V., Mariotti L., Mignot A., Teruzzi A., Feudale L. MASSIMILI: Development of a multi-data assimilation scheme to integrate Bio-Argo floats data with Ocean Colour satellite data into the CMEMS MFC-Biogeochemistry.

GODAE Joint DA-TT/OSEval-TT Meeting, La Spezia, October 2017
A.Teruzzi, L.Mariotti, L.Feudale, and G.Cossarini. A multi-data variational assimilation of BGC-Argo and satellite data into the CMEMS Mediterranean biogeochemical model

AGU, Portland, 11-15 February, 2018
Teruzzi A., Mariotti L., Cossarini G., Salon S., Crise, A., Solidoro, C. Use of Variational Assimilation of Multi-platform Observations for an Optimal Description of the Vertical Phytoplankton Dynamics in the Mediterranean Sea.

6 Miscellaneous

People involved and hired in the project.

A student (Pierluigi Di Cerbo) from the master course of HPC (high performing computing) of SISSA (Scuola Internazionale Superiore di Studi Avanzati) worked on the optimization and parallelization of the 3DVarBio code.

Two postdocs, Laura Feudale (March-June 2016, then maternity leave) and Laura Mariotti (September 2016 - October 2017, then maternity leave), and a researcher Anna Teruzzi (October 2017 – January 2018) from OGS along with Cossarini Gianpiero and Stefano Salon have been involved in the project for the development of the new multi-data and multi-variate assimilation scheme (Task 2) and the implementation of the assimilation simulations and the evaluation of the impact of BGC-Argo assimilation on the biogeochemical model of the Mediterranean Sea (Task 3).

One postdoc, Alexandre Mignot (Jan-Dec 2017) has been directly involved at LOV in the MASSIMILI project in particular on task 3.1 and 3.3. Fabrizio D'Ortenzio, Vincent Taillandier, Louis Prieur and Catherine Schmechtig have been also strongly involved in the project. Discussions with A. Mangin (ACRI) and C. Pinazo (MIO, FR) have been also extremely proficient.

Finally, the MASSIMILI consortium proficiently interacted with the operational team of MERCATOR Ocean devoted to biogeochemical simulations.

7 To be included in the website

MASSIMILI project aims at developing a multi-data assimilation framework for BGC-Argo float and Satellite observations to be integrated into the CMEMS MED-MFC-Biogeochemistry model system. The assimilation scheme adopted is a variational method (3DVarBio), which is the current assimilation scheme in use in the CMEMS MED-MFC-Biogeochemistry component.
Key operators of the 3DVarBio code (i.e. the observation operator, H, the vertical, horizontal and biogeochemical components of the background error covariance, Vv, Vh and Vb respectively, and the observation error covariance, R) have been re-designed and optimized for the assimilation of the BGC-Argo data vertical profiles. BGC-Argo data assimilation has a relevant impact on biogeochemistry by improving the description of the vertical structure. Regarding chlorophyll (Figure I), the novel DA changes the concentration and shapes of profiles during the two most significant seasonal biogeochemical processes (winter surface bloom and summer deep chlorophyll maximum). Further, the observation error (estimated by Triple Collocation method and *a-posterior* error estimate) plays a major role in controlling the effectiveness of the assimilation. The estimated non-uniform correlation radius length scale, which is of the order of the mesoscale dynamics, together with the actual size of the BGC-Argo floats network, allow to significantly constrain the phytoplankton dynamics up to 10% of the Mediterranean Sea area (Figure I, upper box). We estimated that the frequency of the assimilation step can be optimized in order to enhance the persistence of the innovation and the consistency with the physical field.
Regarding nitrate, the impact of the BGC-Argo data assimilation is much larger (in term of spatial scales) given the fact that the corrections change the profiles down to 500 m depth.

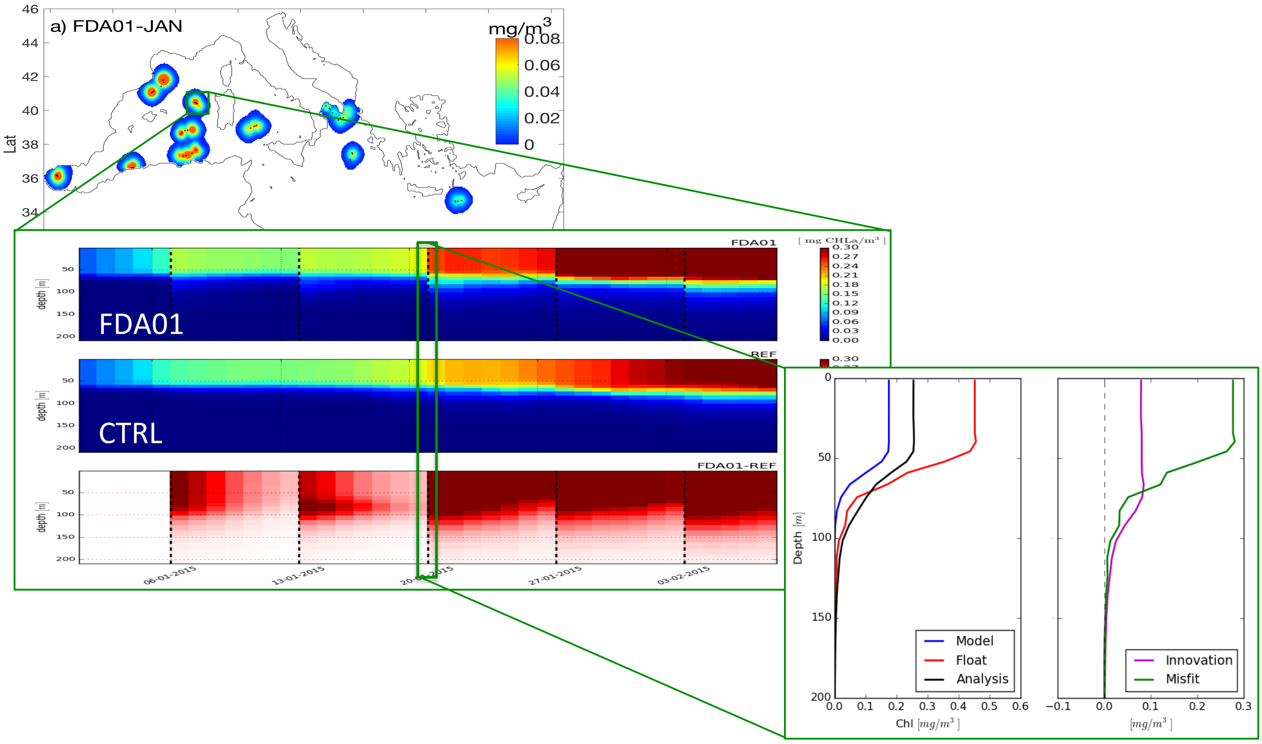
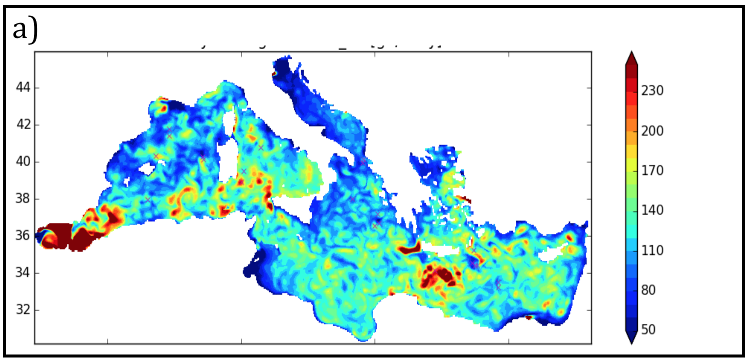


Figure I. Maps of the vertical integrated innovation of chlorophyll (upper box) and Hovmoeller diagrams of chlorophyll concentration (middle green box) of the assimilation run (upper), the reference run (middle) and their differences (lower) and the timing of the assimilation steps (dashed black vertical lines) are shown. The vertical chlorophyll profiles of the model forecasts (blue), float observations (red), analysis (black), misfits (green) and innovation (purple) for the assimilation step on the 20th of January are also shown in the lower green box.

The multi-platform assimilation (joint assimilation of BGC-Argo float and Satellite chlrophyll) shows that BGC-Argo assimilation has local impacts, which are consistent along the water column, whereas satellite assimilation produces spatially homogeneous corrections (example of the impact of assimilation on Primary Production in Figure II). The most appropriate setup of the joint assimilation would be to assimilate separately satellite and float data (i.e. float assimilated daily and satellite assimilated weekly), and to assign a higher hierarchical rank to the float data over the satellite on a local basis by reducing the error of BGC-Argo float data.



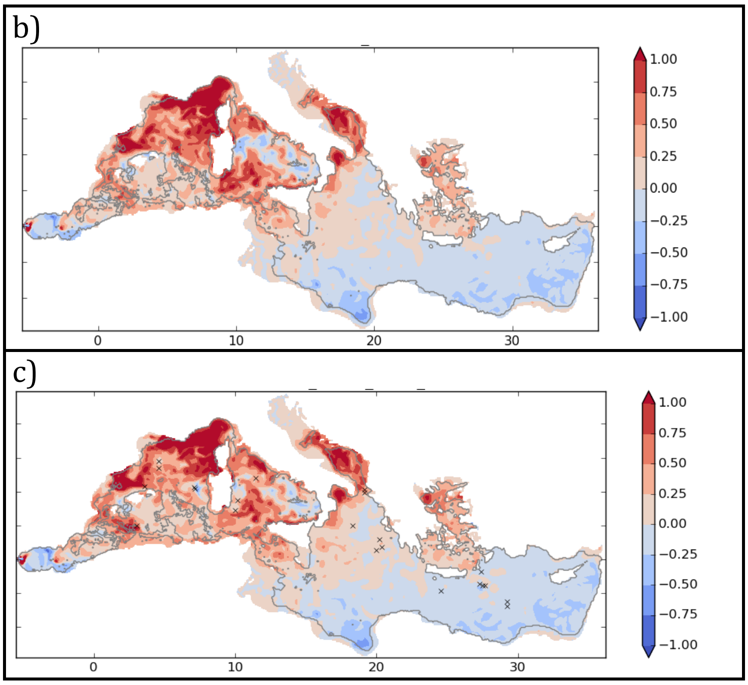


Figure II. Primary production (mgC/m2/y) averaged over 1 week of hindcast simulation (24-31 August 2015, upper panel), and relative anomaly of the analysis run with assimilation of satellite only (middle panel) and with joint assimilation of BGC-Argo and satellite data (lower panel).

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