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Entering in the BGC-Argo era: improvements of the Mediterranean Sea biogeochemical operational system

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Abstract: Biogeochemical Argo floats (BGC-Argo) provide an unprecedented availability of high-resolution biogeochemical and optical vertical profiles at near real time. The integration of biogeochemical and optical observations with marine ecosystem models allows to improve the model capability to describe marine ecosystem dynamics at different spatial and temporal scales, also resulting in an increase of the model skill.

Recent advancements and future upgrades of the Copernicus Marine Service (CMS) Mediterranean Sea biogeochemical modelling system include the use of BGC-Argo data for validation and assimilation of both biogeochemical and optical components.

The focus of this work is to present the upgrade of the BGC-Argo data stream quality check for the CMS Mediterranean Sea biogeochemical modelling system workflow and to discuss a novel skill assessment framework oriented to evaluate key biogeochemical processes and ecosystem dynamics (e.g. deep chlorophyll maximum depth, nitracline depth, minimum oxygen depth) and optical characteristics (bbp700 converted data) that benefit from the particularly rich and high quality level of the BGC-Argo network in this semi-enclosed sea.

1. INTRODUCTION

Monitoring the ocean biogeochemistry and the marine ecosystems, providing reliable present-state evaluations, short-term forecasts and long-term scenarios is an impelling challenge in a changing ocean. Ocean modeling and operational ocean forecasting systems have been widely recognized as important assets to increase our understanding of ecosystem processes and monitor the state of the ocean provided that the uncertainty level of model results are assessed by a proper validation framework and communicated. The BGC-Argo network, which has rapidly grown in recent years (Johnson and Claustre, 2016) contributed to solve the paucity of biogeochemical data in the global ocean, and allows to investigate the ocean interior status of biogeochemical variables and to assess several key physical processes impacting biogeochemistry. Thus, BGC-Argo can be effectively used in operational modeling frameworks and validation (Le Traon et al., 2017). The Mediterranean Sea has one of the first BGC-Argo networks with a sufficient density of floats to operationally implement BGC data assimilation systems (Cossarini et al., 2019). Furthermore, several studies based on BGC-Argo data enlightened vertical structures and dynamics of the biogeochemistry of this semi enclosed sea (Lavigne et al., 2015; D'Ortenzio et al., 2020). The present work aims to present some recent advancements of the introduction of the BGC-Argo high quality level dataset into the Mediterranean Sea biogeochemical modelling system embedded in the European Copernicus Marine Service (CMS) by devising an innovative validation scheme for evaluating biogeochemical processes along the water column. These developments benefit from the achievements carried out in the frame of two CMS Service Evolution projects (MASSIMILI and BIOPTIMOD), following the CMS continuous improvement philosophy.

2. DATA AND METHODS

The biogeochemical analysis and forecasts for the Mediterranean Sea at 1/24° of horizontal resolution (ca. 4 km) are produced for the CMS programme by means of the MedBFM model system (see Salon et al., 2019, for details and references), which includes the transport model OGSTM coupled with the biogeochemical flux model BFM and the variational data assimilation module 3DVAR-BIO (see details in Teruzzi et al., 2018, and Cossarini et al., 2019). Operating within the biogeochemical CMS Mediterranean Sea Monitoring and Forecasting Centre (Med-MFC BIO), MedBFM is off-line coupled with the NEMO-OceanVar model and produces seven days of analysis every week and ten days of forecast daily for a total of 14 biogeochemical variables (Feudale et al., 2021).

2.1 *Real Time and Delayed Mode of BGC-Argo float data:*

BGC-Argo has two data streams: “real-time” (“RT”) and “delayed-mode” (“DM”). The “RT” stream has a latency requirement of 24 hours between profile termination and data availability, and is expected to be free of gross outliers with an automated quality control and data checks. “DM” data, typically expected within 6-12 months (Bittig et al., 2019), include more sophisticated data adjustment and quality control procedures, involving sometime manual inspection, and provide the best quality data. During “DM” assessment (done usually after 5-10 cycles), any derived data adjustments (gain, drift, offset) can be fed back into the incoming “RT” stream, producing Real-Time Adjusted data (“A”).

While the use of “DM” data sounds safe, handling near real time (NRT) data for assimilation and validation in operational biogeochemical systems requires dedicated checks and procedures to ensure that only good data are integrated in model simulations. Considering the Med-MFC BIO operational system, the preliminary check on availability of “A” mode is combined with further check and corrections to deal with anomalous data and the presence of drift in time of sensor measurements. So far, chlorophyll (Chl) is the BGC-Argo float variable with the best “RT” Quality Control (Bittig et al., 2019): its adjusted mode already includes the quenching correction, recalibration at depth and a tuning correction of the manufacturer calibration fluorometer. Even if BGC-Argo oxygen (OXY) reports the largest improvement with currently 80% of all profiles adjusted and a large part of them passed in DM during 2020, the NRT use of oxygen data is still problematic. Our NRT oxygen quality check is done comparing the oxygen surface value with oxygen at saturation (Garcia and Gordon, 1992), and a threshold of 10 mmol/m^3 is used to discharge profiles. At NRT, the internal quality check of NO_3 includes: the discharge of “RT” mode and the correction of “A” mode nitrate based on availability of good quality oxygen data. Indeed, if good quality (“DM” or “A”) oxygen data are available, the nitrate correction is performed with the CANYON-B neural network results (Bittig et al., 2018), calculating the offset at 900m depth and applying a linear shift by this offset to the surface. In the case of no good quality oxygen data available, the offset at 600-1000m is computed from the Word Ocean Atlas 2018. Then, surface values are forced being at least 0.05 mmol/m^3. Optical data from Bbp700 sensor onboard the BGC-Argo are computed following the relationship of Bellacicco et al. (2019) to retrieve carbon biomass of phytoplankton (PhyC), and the 500-600m average off-set is removed from the profiles. For all variables, a further internal check is performed considering a threshold between model and observation misfit which is intended to spot observations that, even if good, cannot be handled by the model.

3. RESULTS

3.1 Process oriented metrics based on biogeochemical and optical BGC-Argo measurements.

A key element to establish a necessary confidence in the recent Med-MFC system improvements (Clementi et al., 2021) was to develop a validation framework that can evaluate both the quality of the biogeochemical variables values and the consistency of physical and biogeochemical processes. Thus, novel skill metrics have been implemented to monitor the quality of the products and validate the consistency of the ecosystem products with the physical ones (Salon et al., 2019), also considering the seasonality of ecosystem processes and highlighting the model capability to reproduce key elements of the vertical dynamics.

Model-float direct comparison is useful for verifying the model capability to predict the spatial-temporal distribution of oceanographic properties, critical for forecasting. For each BGC-Argo float, the vertical profiles of Chl, NO3, OXY and PhyC are matched-up with the model output at the same position and date, producing time series of paired profiles. Hovmoeller plots of model-float profiles highlight the time evolution of vertical biogeochemical processes involved in the euphotic layer and just underneath (e.g. see the top panels of Fig. 1). This direct comparison is published weekly in the medeaf.inogs.it website for the analysis of the previous week. From the match-up, a series of statistical metrics can be derived to evaluate state variables and emerging biogeochemical properties (i.e., deep chlorophyll maximum, nitracline, oxygen maximum), spotting ecosystem dynamics and physical-biogeochemical coupling processes. Regarding Chl, two seasonal metrics identifies the most important vertical modes of phytoplankton dynamics (Lavigne et al., 2015): (1) BIAS and root mean square of the difference (RMSD) between model and float of the deep chlorophyll maximum (DCM) depth and of its corresponding Chl value, and (2) BIAS and RMSD of the winter bloom layer (WBL) depth (details of DCM and WBL are in Salon et al., 2019).

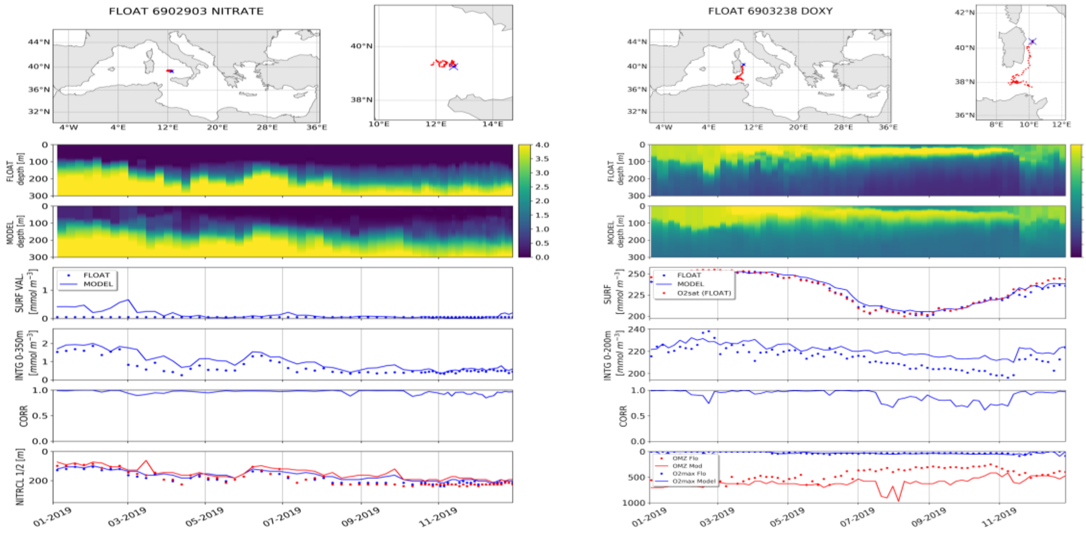

Fig. 1. Examples of Hovmoller diagrams of NO_3 (left) and OXY (right) of BGC-Argo floats (2nd panel) and model outputs (3rd panels) matched-up with float position (top) for year 2019. Left: time series of NO_3 indicators based on model and BGC-Argo floats comparison (4th-7th panel): NO_3 concentration at surface (SURF), 0-350m vertically averaged concentration (INTG), correlation between profiles (CORR), depth of the nitracline (NITRACL1/2). Right: Time series of OXY indicators based on model and BGC-Argo floats comparison (4th-7th panel): OXY concentration at surface (SURF) and OXY saturation from float (O2sat), 0-200m vertically averaged concentration (INTG), correlation between profiles (CORR), depth of the OMZ and of OXY maximum. Trajectories of the BGC-Argo floats are reported in the upper panels (red dots), with deployment position (blue cross).

	Chl			**PhyC**	**NO_3**		**OXY**	
	RMSD 0-200m mean [mg/m^3]	**RMSD DCM depth [m]**	**RMSD WBL depth [m]**	**RMSD 0-200m mean [mgC/m^3]**	**RMSD 0-200m mean [mmol/m^3]**	**RMSD NITRCL1 depth [m]**	**RMSD 0-200m mean [mmol/m^3]**	**RMSD max O2 depth [m]**
SWM	0.04	9	42	1.70	-	-	8.48	10
NWM	0.04	10	30	1.07	0.46	9	7.27	9
ION	0.03	27	18	0.52	0.26	11	3.18	25
LEV	0.02	17	17	0.43	0.32	36	7.93	5

Tab. I. Selection of multivariate skill metrics comparing model outputs and BGC-Argo floats data in the period January-December 2019 for south-western Mediterranean (SWM), north-western Mediterranean (NWM), Ionian Sea (ION) and Levantine basin (LEV).

Considering the photic layer, the BIAS and RMSD of the 0-200m vertical average (INTG) of Chl, NO_3, OXY and PhyC provide the assessment of model consistency to simulate the ecosystem productivity, biomass accumulation and oxygen balance. The productivity of the system is also assessed by the BIAS and RMSD of the depth of the oxygen maximum which spots the super-saturation condition occurring in the layer of maximum photosynthesis production.

The vertical transport of nutrients into the photic layer is highlighted by BIAS and RMSD of the depth of the nitracline, defined as the depth (1) where the nitrate concentration is 2 mmol/m^3 (NITRCL1) and (2) corresponding to the maximum nitrate vertical gradient (NITRCL2).

Furthermore, for OXY we identify: (1) BIAS and RMSD between model and float of the OXY maximum depth identified in the layer 0-200m, and (2) BIAS and RMSD between model and float of the oxygen minimum zone (OMZ) depth identified in the layer 200-600m.

Correlation (CORR) between each couple of Chl, NO_3, OXY vertical profiles from model and float provide an estimation of the consistency of vertical transport and biogeochemical processes simulated by the model. Results of the novel validation framework are reported as pseudo-lagrangian metrics following the BGC-Argo trajectories (Fig. 1) and then summarized in sub-basin statistics (Tab. I) in the specific product documentation available in CMS catalogue (Feudale et al., 2021).

3.2 Process-oriented metrics linking the impact of transport on biogeochemical vertical structure

Among BGC-Argo sensors, nitrate remains more limited due to high cost of sensors and technology limitations. However, inorganic nitrate is one of the important macronutrients for oceanic phytoplankton dynamics: it varies over timescales ranging from weekly to interannual and due to both physical and biological processes, and its vertical distribution and dynamics is paramount for understanding the new component of primary production and the ocean biological pump. Particular interest falls on possible relationships with physical processes from which might be possible to “extrapolate” its distribution (“process-oriented metric”). In particular, previous studies have revealed a relationship between density and nitrate distribution in the vertical (Johnson et al., 2010; Omand and Mahadevan, 2013; Ascani et al., 2013).

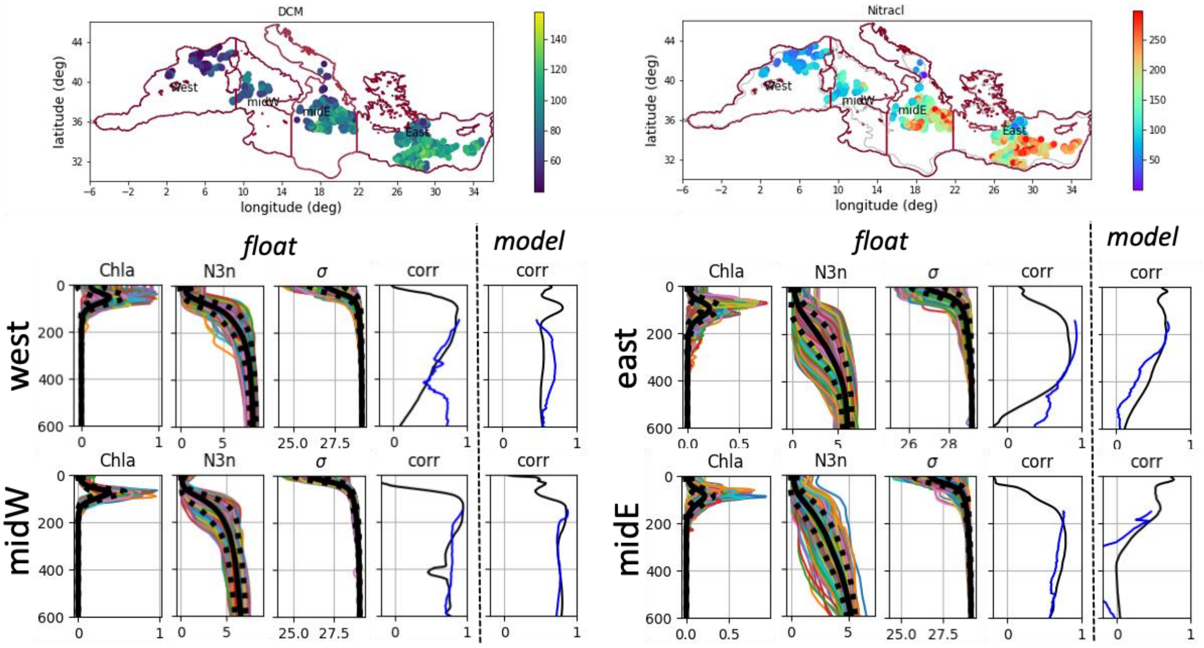

Fig. 2. Scatter plots of DCM [m] on the upper left and Nitracline [m] on the upper right based on BGC-Argo data of the 2013-2021 period. Multipanels below show from left to right, the vertical profiles of Chlorophyll, Nitrate, Potential Density (solid black thicker lines are the mean, dotted black lines are the standard deviation) and the correlation between nitrate with density (black) and isopycnals (blue) computed BGC-Argo float data. Last plot on the right of each panel shows the correlation between modelled nitrate and density. Analysis is repeated for the four sub-regions.

Taking advantage of 2013-2021 BGC-Argo floats equipped with nitrate and CTD sensors (Argo, 2020), profile correlation indexes are computed to characterize the density-nitrate relationship in four selected Mediterranean sub-regions, covering the zonal nitrate gradient and reproducing the deepening of the nutricline (Fig. 2, upper panels). The analysis focuses on the summer season (here defined as from April to September), when stratification and dynamics of the nutricline drives the DCM .

Results of the analysis show the presence of different physical-biogeochemical regimes in the different regions. Indeed, nitrate profile shapes are different in the four areas, from the shallower nutricline depth in the West and steeper slope (thinner nutricline thickness), and a nitrate pool at depth higher in the West, related to the well known oligotrophic West-East gradient.

Based on float data, nitrate correlation with potential density (computed following Ascani et al., 2013) is weak at surface where biogeochemical processes and near-surface variability might dominate, but increases with depth reaching values of 0.9 around 200m depth. The shape of correlation profile differs in the four regions: it is constant and high till 500m in the eastern sub-region, while it linearly decreases in the western area. In the two mid-west and mid-east sub-regions the correlation remains higher till 600m showing a consistent physical-biogeochemical dynamics far below the nutricline depth. Same calculations made with model output matching float trajectories are reported in the fifth plot referring to each sub-region. Results show that the model is consistently reproducing the physical biogeochemical coupled dynamics in all sub-regions but mid-East. In the mid-East region, the discrepancy between profile correlation of model and float might highlight possible model failure in reproducing the mixing and vertical position of different water masses in this complex area, where modified Atlantic water, Levantine intermediate water and outflow dense Adriatic water interact and are characterized by a different nutrient content.

4. CONCLUSIONS

The present work aims to highlight the benefits of the introduction of the high quality level dataset of the BGC-Argo network into the Copernicus Mediterranean Sea biogeochemical modelling system.

Beside the improvements in the data assimilation component (Cossarini et al., 2019), a novel metrics framework based on singular status parameters is defined evaluating emerging properties. Additionally, correlation metrics between nitrate and density at particular depths can be a promising validation technique in order to capture the nature of the physical processes which may influence the evolution of biogeochemical processes as well. Further, these relations, by spotting the dynamical coupling between transport and biogeochemical vertical profiles, could be adopted as a possible strategy in generating "synthetic" nitrate profiles where only physical variables are known, overtaking the problem of nitrate data paucity.

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