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Report on the prototype BGC models and their 1D simulations in CMEMS MFC sites

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1. Scope

The present deliverable presents results from *Task 2.1a, Task 2.1b, Task 2.1c* and results from *Task2.3a*. The overall objective of this deliverable, as well as of the above-mentioned Tasks, is to include all SEAMLESS biogeochemical models and their case site setups into the 1D prototype. It is worth to remind that this is a prerequisite for all the SEAMLESS activities based on the 1D prototype and allows to carry out data assimilation experiments consistently throughout the CMEMS systems.

2. Introduction

The SEAMLESS 1D prototype consists of the coupling between all CMEMS biogeochemical models (i.e., ERSEM, BFM, PISCES, ERGOM, ECOSMO) and the physical GOTM model through the FABM tool package (Bruggeman and Bolding, 2014; http://fabm.net). The GOTM physical component has been chosen here because of its widespread use, large number of mixing schemes and user friendliness. Thus, it provides a widely usable prototype system that can be representative for the different physical models used in CMEMS.

At the start of the project, the FABM framework included ERSEM, ECOSMO and ERGOM only (Table 2.1). Two subtasks of Task 2.1 were devoted to the porting, debugging and testing on 0D or 1D setups of the biogeochemical models PISCES (Task 2.1a) and BFM (Task 2.1b) into FABM:

- *Task 2.1a*: BB ported the PISCES model into FABM; then integrated and tested it within the prototype system and compared it with NEMO-PISCES
- *Task 2.1b*: OGS ported the BFM model into FABM with support by BB and implemented a setup for BFM in the prototype system.

An additional subtask of Task 2.1 was devoted to the preparation of a specific setup of GOTM-FABM with ERGOM in the prototype system for the Baltic Sea as a blueprint for the DA implementation (Task 2.1c, AWI)

Model	Coupling with FABM	SEAMLESS 1D setup
PISCES	This project (section 3.1)	BATS (section 4.2)
BFM	This project (section 3.2)	BOUSSOLE and BGC-Argo (sections 4.3 and 4.4)
ERGOM	Already in FABM	Arkona (section 4.1)
ERSEM	Already in FABM	L4 (section 4.5)
ECOSMO	Already in FABM	M (section 4.6)

Table 2.1. SEAMLESS biogeochemical models and stations for the reference simulations of the 1D prototype.

Additionally, the SEAMLESS 1D prototype includes specific setups for regional case sites which are used in the sensitivity and data assimilation experiments of WPs 3-6 of the project. The partners configured their own biogeochemical model systems at the different representative sites (Task 2.3). All the partners prepared a working setup of the prototype system for reference simulations at the fixed stations in the different CMEMS regional seas (Arkona Basin, BATS, BOUSSOLE Station, Stations M and L4; Table 2.1 and Figure 2.1) and for the pseudo-lagrangian data (BGC-Argo float, Figure 2.1).

All the implementations performed in this activity are developed in git-based versioning system platforms.

The main outcome of this Task is the preparation of a working GOTM-FABM version of the biogeochemical models used by each partner in the different sites and its qualitative validation with respect to the observed dynamics in the selected sites. The validation is based on visual comparison of model output with observed variables using Hovmoeller diagrams. It is worth to remind that, at this stage of the project, a working setup of the 1D prototype in a specific site should be considered as a model simulation that can reproduce consistently the mean values and seasonal cycle of the observed variables. The model consistency at the regional sites is a preliminary result of the project, while the assimilation of observations (WP4 and WP5) and the model calibration (WP 6) will have the objective to improve the model capability to reproduce quantitively values and dynamics of the *seven SEAMLESS target indicators* (e.g., primary production, POC) in the different sites.

The deliverable is subdivided in two parts:

- Section 3 presents the inclusion of new models into the FABM framework and the quality control of the porting with respect to the CMEMS version of the models;
- Section 4 presents, for each SEAMLESS model, the regional sites, the implementation of the 1D prototype system for the CMEMS regional sea sites and the qualitative validation.

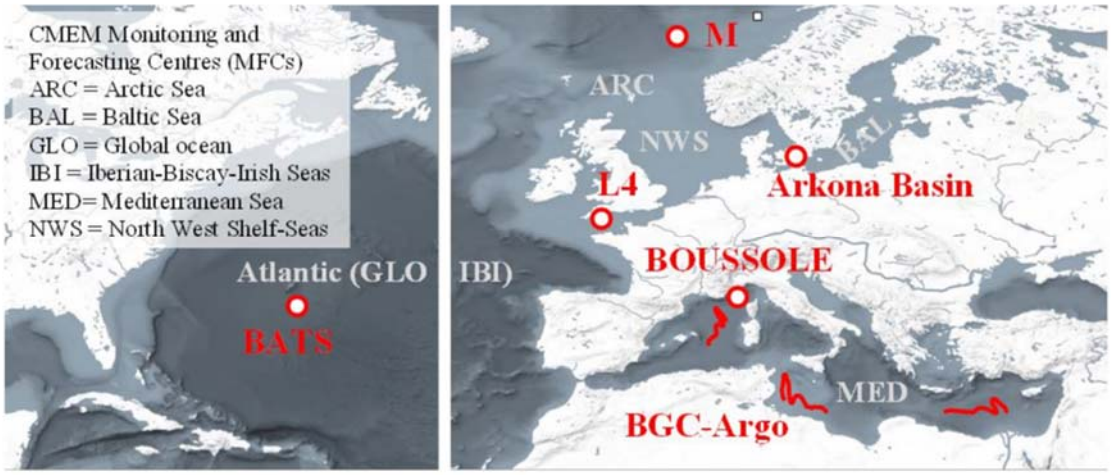

Figure 2.1 Sites (red circles) of the CMEMS Monitoring and Forecasting Centres (MFC) used for reference simulation of the 1D prototype. The red lines represent the trajectories of the biogeochemical-Argo floats (BGC-Argo) simulated with the pseudo-Lagrangian configurations of the prototype.

3. Porting new models into FABM

This section reports the inclusion of the two models PISCES and BFM into the FABM framework and the quality control done on the new codes to verify their consistency with the model versions used in the CMEMS Monitoring Forecast Centers.

3.1 Porting the PISCES model to FABM (Task 2.1a)

Author: Jorn Bruggeman (BB)

3.1.1 Background and model presentation

The FABM port of the PISCES biogeochemical model is based on the code that comes with the r4.0-HEAD.r13720 version of NEMO, which is the version currently used in the CMEMS GLO MFC. As part of this port, the PISCES code has been modularised further to support two specific use cases in the future:

1. a runtime-configurable (as opposed to hardcoded) number of phytoplankton types, zooplankton types, and particulate organic matter classes
2. exchange of process models for e.g., carbonate chemistry, optics, particulate organic matter, and the benthos with other FABM-based biogeochemical models such as ERSEM, BFM, and ECOSMO.

An overview of the modules of the default configuration, as well as the underlying code, is given in Fig. 3.1.1.

The FABM-PISCES code is available from a public GitHub repository:

https://github.com/BoldingBruggeman/fabm-pisces

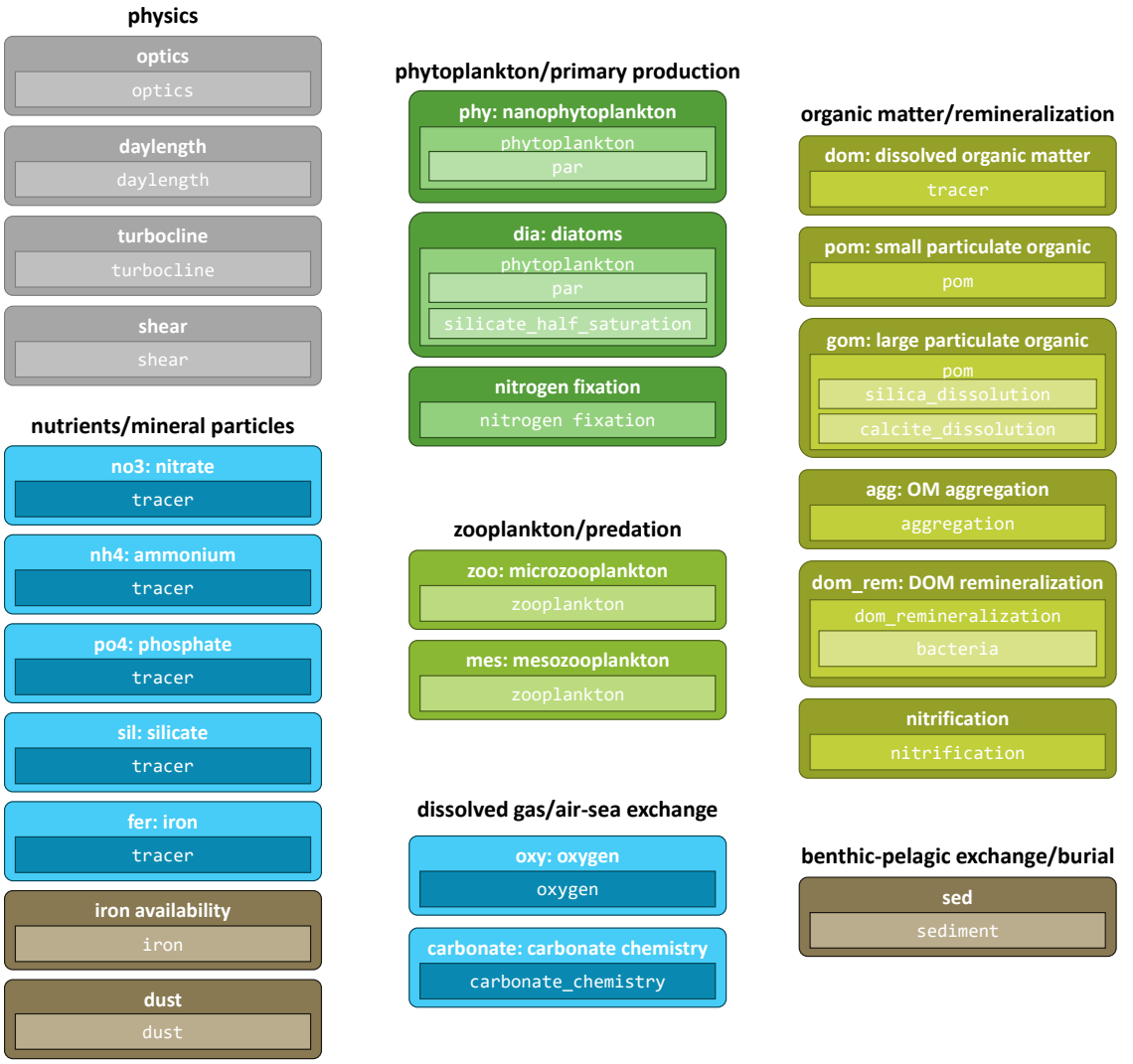

Figure 3.1.1. Overview of the default set of modules of the FABM port of the PISCES biogeochemical model. Rounded rectangles correspond to the modules defined at runtime by the user in the fabm.yaml configuration file. The contained rectangles indicate the underlying Fortran types that describe the relevant processes and behaviours; these map to source files in the src subdirectory in the repository. In some cases, such a type contains nested types, e.g., each phytoplankton module has a "par" submodule that computes the experienced photosynthetic active radiation, determined by irradiance as well as the absorption coefficients of that specific phytoplankton group. In several cases, a single Fortran type is used for multiple ecosystem components. For instance, nanophytoplankton and diatoms share the same "phytoplankton" type (though each is represented by a different instance of this type, with different parameters). Likewise, micro- and mesozooplankton share the same "zooplankton type", small and large particulate organic matter share a single "pom" type, and nutrients and dissolved organic matter are all represented by a generic "tracer" type.

3.1.2 Implementation of the porting

As part of the PISCES port, the original code was carefully studied, compared with the original publication (Aumont et al., 2015), and where necessary discussed with its seminal author, Olivier Aumont (olivier.aumont@ird.fr). This has produced an extensive list of differences between the NEMO-PISCES code and the original publication, and in a few cases led to corrections or bug fixes that

were not yet present in the r4.0-HEAD.r13720 version of NEMO-PISCES. Both are documented in the readme file within the FABM-PISCES repository. The fixes to the original code are the following:

- Nitrogen fixation has been corrected to conserve carbon by adding a loss term for dissolved inorganic carbon (issue confirmed by Olivier Aumont, 2021-09-07)
- The sign of the alkalinity contribution of calcite dissolution in zooplankton gut, associated with flux/filter feeding, has been changed (issue confirmed by Olivier Aumont, 2021-07-15)
- The time scaling of the pdust diagnostic has been corrected (issue confirmed by Olivier Aumont, 2021-09-09)

For naming of variables and coding style, we closely follow the original PISCES implementation, even where that means that the value of process parameters is hardcoded. This was done to maximize the similarity between new and old code, thereby aiding review of the code by PISCES' original contributors at a later stage.

Detailed instructions for compilation and use are given in the readme of the repository. In short, the FABM-PISCES codebase can be included in a standard FABM compilation by providing two arguments when calling cmake:

- `-DFABM_INSTITUTES="<LIST>"`, in which `<LIST>` is a semi-colon separated list of model categories to include. At minimum this list must include `pisces`.
- `-DFABM_PISCES_BASE=<PISCESDIR>`, in which `<PISCESDIR>` is the path to the PISCES source code (the root of the repository, containing among others CMakeLists.txt).

This basic procedure is the same for all hydrodynamic models from which FABM can be used, e.g., GOTM, NEMO, ROMS, HYCOM, FVCOM.

At runtime, FABM reads its configuration from a `fabm.yaml` configuration file. This file describes the set of biogeochemical/ecosystem modules that will be active during the simulation, along with their parameter values, default initial values, and the coupling/sharing of variables between modules. A `fabm.yaml` file describing the default PISCES configuration is included in the testcases directory of the repository. It is worth noting that most PISCES parameters have a recommended default value set in the code; only parameters with a value that differs from the default are currently included in the fabm.yaml example.

3.1.3 Quality control of the porting

FABM offers a mechanism to check conservation on a per-module basis. This mechanism is activated by adding `check_conservation: true` to the `fabm.yaml` configuration file. FABM will then sum up the rate of change in the total of every conserved quantity (carbon, nitrogen, phosphorus, silicon) per module (i.e., the rate of change associated only with the processes described by that module) and make these rates available as diagnostics that can be included in model output. This output can then be analysed to determine whether each module conserves mass; in this case, each saved diagnostic should be (numerically) indistinguishable from zero.

In this manner, it has been verified that all FABM-PISCES modules are fully mass conservative, except:

- The nitrogen fixation module is a non-conservative source of nitrogen in the pelagic, as it produces nitrogen (ammonium, DON, PON) from a source (dissolved dinitrogen gas) that is not tracked in the model.
- The nitrogen fixation module includes a non-conservative source of phosphorus in the pelagic. This process is stimulated by light and DOM and inhibited by phosphate; it was included to enable phytoplankton use of dissolved organic phosphorus in phosphate-poor regions, a phenomenon that a fixed-stoichiometry model such as PISCES cannot natively represent (Olivier Aumont pers. comm. 2021-09-03)
- The carbonate chemistry module is a non-conservative source/sink of carbon at the ocean surface, as dissolved carbon dioxide (part of the DIC pool) is exchanged with the untracked atmospheric pool of carbon dioxide.
- Denitrification in the sediment module is a non-conservative sink of nitrogen, as pelagic nitrate is used to fuel anaerobic remineralisation. In this process, nitrate is converted into nitrogen compounds (e.g., dinitrogen) that are not tracked by the model
- Burial in the sediment module is a non-conservative sink of carbon, nitrogen, phosphorus. This is controlled by an environment-dependent buried fraction (variable `zbureff`). In addition, part of the deposited particulate silicon is buried (a hardcoded 3%), as well as part of the deposited calcite (40%). The former constitutes a sink of silicon, the latter another sink of carbon.
- The sediment module makes no effort to conserve iron: deposited iron in POM is not tracked (i.e., it is lost); instead an unrelated iron source term representing release of sedimentary iron to the pelagic is introduced.

These processes are all non-conservative by design in the original PISCES implementation. Their behaviour is reproduced here in the FABM-PISCES port. The behaviour of the FABM-PSICES code in a more realistic setting is explored in section 2.3a.

3.2 Porting of the BFM model into FABM

Authors: Eva Álvarez, Anna Teruzzi, Paolo Lazzari, Gianpiero Cossarini (OGS); Jorn Bruggeman (BB)

3.2.1 Background and model presentation

The development of a prototype of the porting of BFM in FABM has been based on a modular approach. In particular, different subroutines and FABM models are related to the different plankton functional types (PFTs, e.g. phytoplankton, zooplankton) and chemical processes (e.g., light, denitrification) that are included in the ecosystem model. Since models are classified according to reference Institute in FABM, a new folder, named OGS, has been created to include the BFM code customized for FABM. The porting of BFM into FABM has been developed starting from the original style and structure of the official BFM code preserving also credits (original BFM code and manual can be retrieved from https://bfm-community.github.io/www.bfm-community.eu/). The version of BFM

included in FABM is the one described in (Cossarini et al., 2015; Lazzari et al., 2021, 2016, 2012). Name of the routines for plankton function types and ecosystem processes are those of BFM official release (Table 3.2.1).

3.2.2 Implementation of the porting

The work of coding with respect to BFM official version has been mainly related to the inherent structure required by FABM (e.g.; headers, initialize, do, do_surface structure of each model). In FABM each modular component is *per se* defined as a model. The models we introduced in the framework are rjv2Sk|wr/#rjv2ShdEdf/#rjv2Plfur]rr/#rjv2Phvr]rr/#rjv2ShdFkhp/#rjv2FddflwhGlvvroxwlrq/#rjv2ShdR{|jhq, rjv2ShdljlfFV\V/#rjv2djkwbvshfwudd#and also#the general routines#rjv2eipbshdljlfbedvh#and vkduhgII<3.## New headers for type extension based on type_ogs_bfm_pelagic_base have been defined in the new routing ogs/bfm_pelagic_base.

The relationships between the modular components (FABM models) are defined in the fabm.yaml file. Hence, a specific fabm.yaml file for BFM has been configured to run the model with 4 phytoplankton groups, 1 heterotrophic bacteria, 2 microzooplankton groups, and 2 mesozooplankton groups.

Table 3.2.1 New biogeochemical model units introduced in the OGS folder.

models	Module name	Type extension
Phyto.F90	eipbSk|wr	w|shbrjvbeipbsulpdu|bsurgxfhu
PelBac.F90	eipbShdEdf	w|shbrjvbeipbshdljlfbedfwhuld
MicroZoo.F90	eipbPlfur]rr	w|shbrjvbeipbplfur}rr
MesoZoo.F90	eipbPhvr}rr	w|shbrjvbeipbphvr}rr#
PelChem.F90	eipbShdFkhp#	w|shbrjvbeipbShdFkhp#
CalciteDissolution.F90	eipbFddflwhGlvvroxwlrq	w|shbrjvbeipbFddflwhGlvvroxwlrq
PelOxygen.F90	eipbShdR{|jhq	w|shbrjvbeipbShdR{|jhq#
PelagicCSYS.F90#	eipbShdljlfFV\V#	w|shbrjvbeipbShdljlfFV\V#

We specified for each model, Tab.3.2.1, the relevant entries of the type extension sections based on BFM variables, parameters and diagnostics:

- identification of state variables of other models required;
- environmental dependencies;
- identifiers of diagnostic variables;
- parameters (described in subroutine initialize, below).

In the module *initialize procedure* we included all the parameters using the same formalism of BFM (i.e., parameters have prefix "p_"). We set up the *register state* variables by adding the specific constituents for each model (e.g.: for phytoplankton carbon 'c', nitrogen 'n', phosphorus 'p', chlorophyll 'chl' and silicon 's'). Moreover, we included a diagnostic variable for each biogeochemical process to be able to check if the FABM-BFM prototype was consistent with respect to the official BFM version.

In the do procedure we replicated the structure of BFM (i.e., the original code opportunely adapted and comments are included) and we set a diagnostic for each process included.
Few changes with respect to the original BFM structure have been included:

1) a nutrient stress sinking process in phytoplankton was added to the Phyto model through two specific functions *get_sinking_rate* and *get_vertical_movement;*
2) the terms of alkalinity sink/source have been directly included in Phyto, PelChem, PelBac, MicroZoo and MesoZoo;

As a result of the activity, the developed new code of BFM has been released (available to SEAMLESS members upon request) at the following link of the git code versioning repository: git@github.com:inogs/bfmforfabm.git .

The FABM/BFM porting include two configurations: a simple mono spectral configuration (rjv2ljkw) and a multispectral configuration (rjv2ljkwbvshfwdq. The monospectral model includes only self-shading by chlorophyll. The multispectral model accounts for absorption, downward and upward scattering and it is based on the three-stream approach (Lazzari et al., 2021). In the initialization phase of the multispectral model rjv2ljkwbvshfwdq the bio-optical parameters of optically active constituents are loaded from specific ascii files and include sea water, phytoplankton, detritus and CDOM characteristics. These files must be provided in the *bcs* folder where model is executed. CDOM absorption can be read from file or alternatively computed online according to the exponential law of absorption dependence on wavelengths, this choice can be useful to evaluate the sensitivity of biogeochemical processes to the parameters used to describe optical properties of CDOM. The solver of the 3-stream optical model (function *solve_direct*) is linked in FABM as a library. The library is a development of the BIOPTIMOD project tool (https://www.mercator-ocean.fr/en/portfolio/bioptimod/).

3.2.3 Quality control of the porting

In order to test the accuracy of the BFM porting we used both the python coupling (https://github.com/fabm-model/fabm/wiki/python) and the 0D FORTRAN setup (fabm/src/drivers/0d/) and a 2-phase check was implemented. In the first phase we performed a test checking that all the diagnostics were identical up to machine precision between the two FABM configurations. In the second phase, we performed a check of the integration in time by setting up a 10 day simulation using the original BFM in a standalone model (https://bfm-community.github.io/www.bfm-community.eu/bfm-quick-guide/) and the BFM-FABM 0D configuration. The two configurations had the same initial conditions, the same constant environmental forcings (i.e., constant light, T, atmospheric CO2 and wind speed) and the time step of 864 s. Output were saved at each time step to avoid differences arising from interpolation in time. Results show an extremely satisfactorily agreement between the two configurations for all state variables, see examples shown in Fig.3.2.1. This indicates that the task has been successfully finalized and that the FABM/BFM is functionally equivalent to the original BFM (i.e., the version implemented in the CMEMS Med-MFC BGC system).

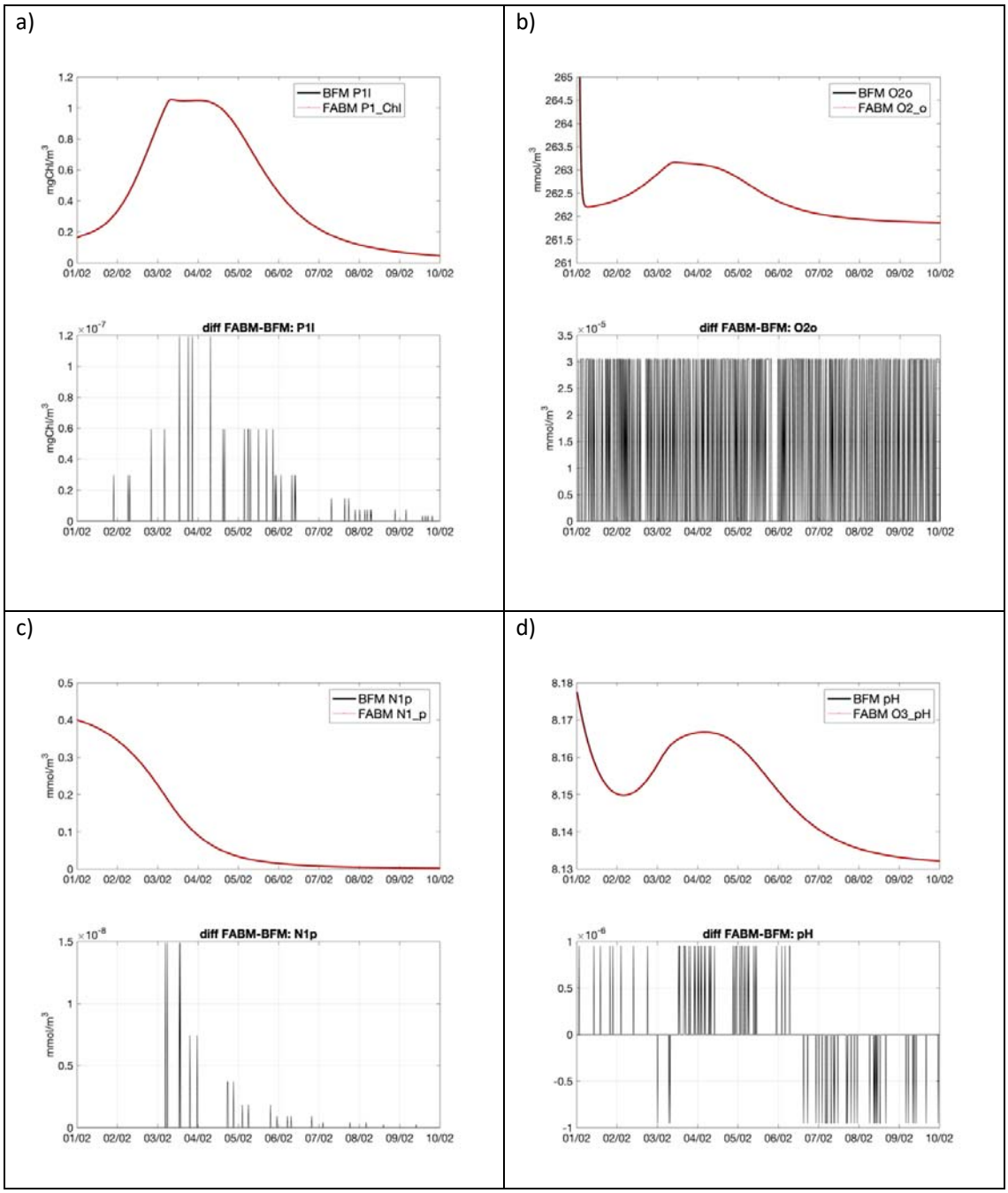

Figure 3.2.1 Results for the comparison between BFM official configuration and FABM coupled BFM. All state variables have been checked and here a subset is proposed, chlorophyll content in Diatoms a), Oxygen b), PO_4 c) and pH d). Each panel shows a 10 days timeseries of BFM standalone (black line) with super imposed FABM-BFM (red line). Each timeseries is shown along with the differences between the two simulations (diff FABM-BFM).

4. Implementation of the 1D prototype in the regional sea stations.

This section reports the implementation of the 1D prototype of the five SEAMLESS models (Table 2.1) in the CMEMS regional sea stations. For each SEAMLESS model, the subsections report: (i) a brief introduction of the specific site and of available observations and input data, (ii) the model implementation for the simulation at the specific site, and (iii) the visual comparison of model results with the available observations. The validation results aim to show that the SEAMLESS model setups implemented in the 1D prototypes qualitatively reproduces the physical and biogeochemical behaviours consistently with that expected at each site by providing mean values, vertical variability, and seasonal cycle consistent with observations of available variables. This represents a prerequisite for the use of the 1D prototype in the sensitivity studies planned in WP3 and assimilation experiments planned in WPs 4, 5 and 6.

4.1 GOTM-FABM-ERGOM at Arkona station

Authors: Farshid Daryabor and Lars Nerger (AWI)

This section reports the work performed in Task 2.1c (setup of GOTM-FABM with ERGOM in the prototype system for the Baltic Sea as a blueprint for the DA implementation) and Task 2.3a (first setup the prototype system for reference simulations at the Arkona station). The work of both tasks was strongly related and the purpose of Task 2.1c was mainly to make the early development of the setup explicit in the project flow. Task 2.3a was then aimed at the validation.

4.1.1 Site description and input data

The setup of GOTM-FABM with ERGOM in the prototype system has been configured for the location of the MARNET station 'Arkona Basin' of the German Marine Monitoring Network (See Fig. 4.1.1). The station is located in the Baltic Sea at Longitude 13.87^{o} E and Latitude of 54.88^{o} N in the Arkona Basin. The basin has a size of nearly 40 by 60 nautical miles and a maximum depth of 45 m. It is connected with the Kattegat through the Great Belt and the Belt Sea in the west and through the Oresund in the northwest. The connections are rather narrow and shallow with sill depths of only 18 m at the Darss Sill and 8 m at the Drogden Sill, respectively. At the station the depth is 46 m. While the water in the basin is brackish in the upper layers (around 8 to 9 psu), the salinity increases close to the bottom to around 14 psu. Occasionally, the region can be influenced by inflow events of water of higher salinity in the bottom layers from the North Sea.

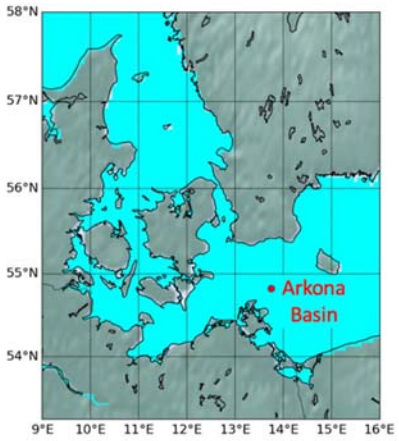

Figure 4.1.1: Location of Station Arkona Basin.

GOTM-FABM-ERGOM requires ocean variables (temperature and salinity), as well as meteorological variables, including hourly data on 2-meter elevation air temperature (°C), humidity (estimated from 2-meter dew-point temperature), 10-meter horizontal eastward and northward wind components (m/s), mean sea level pressure (Pa), and total cloud cover as a fraction (0–1), to estimate the temperature distribution in the water column, stratification, and mixing between the water layers. The diagnostic hydrographic and biogeochemical data for the model initialization are derived from the German Marine Monitoring Network (MARNET). Likewise, the input variables air temperature, humidity, 10-meter horizontal eastward and northward wind components, are derived from MARNET.

4.1.2 Model implementation

The model was implemented using the ERGOM model version MSI_ERGOM that was already available within GOTM-FABM (Lessin et al., 2014). The biogeochemical model (ERGOM) by (Neumann et al., 2002) consists of 10 state variables. The nutrient state variables are dissolved ammonium, nitrate, and phosphate. Primary production is provided by three functional phytoplankton groups: diatoms, flagellates, and cyanobacteria. A dynamically developing bulk zooplankton variable provides grazing pressure on phytoplankton. Dead particles are accumulated in a detritus state variable. The detritus is mineralized into dissolved ammonium and phosphate during the sedimentation process. A certain amount of the detritus reaches the bottom, where it is accumulated in the sedimentary detritus. Detritus in the sediment is either buried in the sediment, mineralized or resuspended into the water column, depending on the velocity of near-bottom currents. The development of oxygen in the model is coupled to the biogeochemical processes via stoichiometric ratios. Oxygen concentration controls processes as denitrification and nitrification.

The model was first run for a spin-up period of the two years 2010 to 2011. Subsequently the model is configured for a period of five years 2012 to 2016 with relaxation to climatology temperature and salinity observation. Figure 4.1.2 shows the development of the concentration of chlorophyll-a over the years 2012-2016. Visible is a short but strong bloom in mid-July of each year. The maximum concentration as well as the depth of the bloom varies in between the years following the

environmental conditions. Such short and strong bloom is also visible in satellite observations of total surface chlorophyll-a.

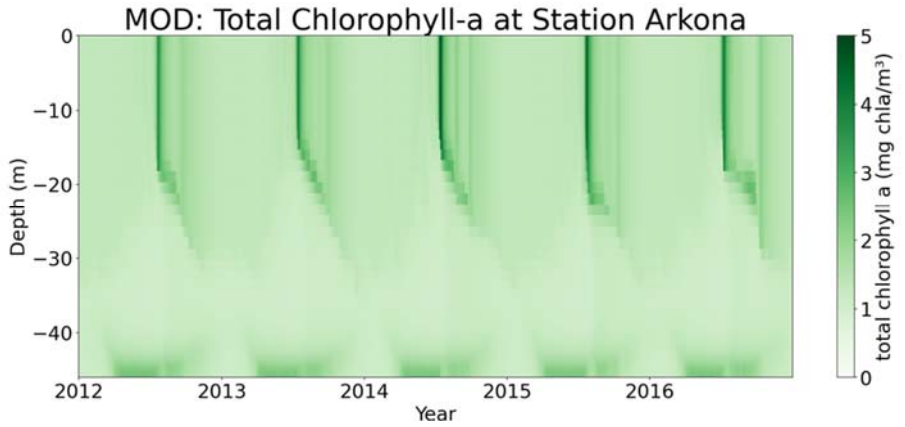

Figure 4.1.2: Total chlorophyll-a (mg chla/m3) at the station Arkona Basin for the years 2012 – 2016.

4.1.3 Model validation

For the validation of the model, MARNET station data is used. Here we focus on the single year 2015 and perform the validation qualitatively. Figure 4.1.3 shows Hovmoeller diagrams of temperature and salinity for this year. The left column shows observed values, while the right one shows the simulation. The simulated temperature and salinity are generally consistent with the observations. However, the observations are much smoother, which is caused by time-space interpolation of the data. Thus, in the modeled temperature the time development of the mixed layer is more clearly visible. The minimum and maximum temperatures occur at comparable time in the model and the observations. The higher temperature in summer reached further down in the model than in the observations, indicating a somewhat deeper mixed layer. The salinity is generally lower down to about 35m. It is particularly low during the summer due to the freshening by rain and river intakes. The bottom salinity is somewhat higher in the observations than the model.

Figure 4.1.4 shows the Oxygen at the station Arkona. For this variable only monthly observations are available. Further the observations only reach down to 25 m. Generally, the model and observations show similar concentrations and a similar seasonal cycle. However, in early spring (March/April) the surface concentration of Oxygen is higher in the observations. In August and September, the Oxygen concentrations are particularly low below 20m depth in the observations, while the model shows the smallest concentrations between the surface and 20m depth.

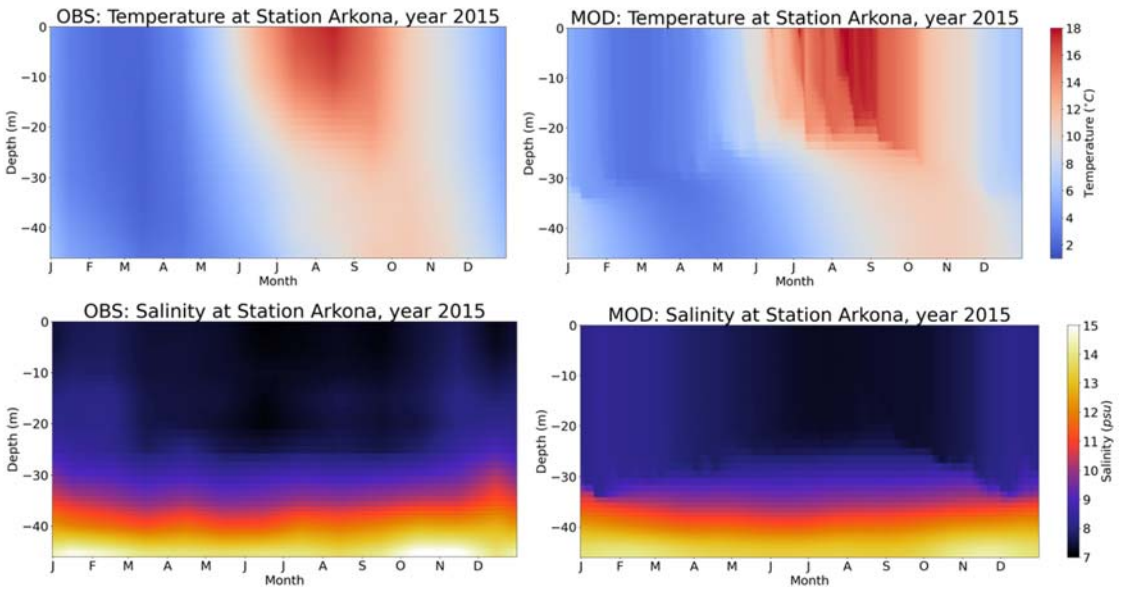

Figure 4.1.3: Temperature (top) and salinity (bottom) at the station Arkona Basin for the year 2015. The observations (interpolated station data) are shown on the left; the right shows the modeled field.

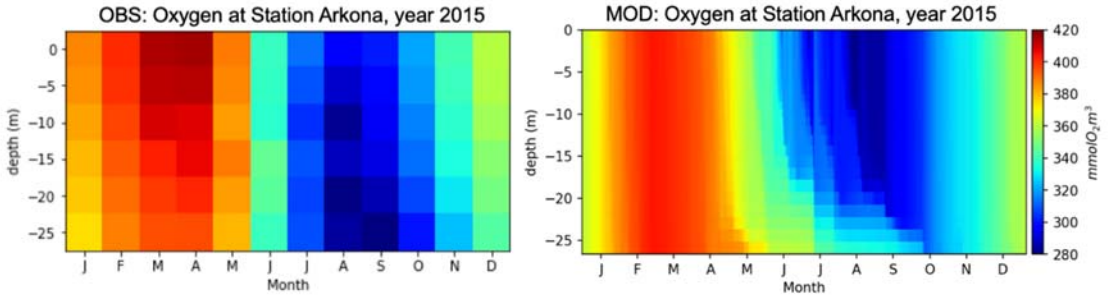

Figure 4.1.4: Oxygen for the year 2015. The left shows monthly observations, while the right shows the model result.

4.2 GOTM-FABM-PISCES prototype at BATS.

Authors: Arthur Capet and Pierre Brasseur (IGE)

This section reports the work done in task 2.3a (first setup the prototype system for reference simulations) for BATS station, located in the North Atlantic sector of the GLO MFC domain of CMEMS. This large domain covers a number of ecological provinces (Longhurst 2007) characterized by different environmental conditions. Ideally, the GOTM-FABM-PISCES should be tested in the different provinces, however the BATS site was selected in SEAMLESS because of the existence of long time

series collected at BATS, providing comprehensive datasets to assess the behaviour of biogeochemical and ecosystem models (e.g. Smith et al., 2021).

4.2.1 Site description and input data

The Bermuda Atlantic Time-series Study (BATS) (Steinberg et al., 2001) site is located in the Sargasso Sea (31◦40' N, 64◦10' W, Fig 4.2.1), within the North Atlantic subtropical gyre. The site is part of the US Joint Global Ocean Flux Study (JGOFS) program and benefits from data collection since 1988. It presents a typical oceanic oligotrophic biogeochemical regime. Winter mixing allows nutrients to be brought up into the mixed layer, producing a phytoplankton bloom between January and March. As thermal stratification intensifies over the summer months, this nutrient supply is cut off and a subsurface chlorophyll maximum is observed near a depth of 100 m (Steinberg et al., 2001). In contrast with other oligotrophic sites, stoichiometric ratios of carbon, nitrate, and phosphate are often non-Redfield and phosphate is considered as the dominant limiting nutrient.

Input data are used in the BATS setup for two purposes: (i) as 1D initial and surface forcing conditions for the GOTM-FABM-PISCES model, and (ii) to build a reference climatology for validation of the mean state and seasonal variability simulated by the model.

In-situ data were obtained from the ascii data file freely accessible at the BATS website. The datasets bats_bottle.txt and bats_pigments.txt were used to extract temperature, salinity, oxygen, nitrate, phosphate, silicate, dissolved inorganic carbon, alkalinity, particulate organic carbon, particulate organic nitrogen, particulate organic phosphorus, dissolved organic carbon, dissolved organic nitrogen, dissolved organic phosphorus, and chlorophyll. These data were monthly aggregated and discretized in layers to produce climatological initial conditions and to be used for comparison purposes. The methodology to create the climatology is freely accessible on github.

In addition to the physical and biogeochemical *in situ* data collected at BATS station, we also need surface atmospheric data, such as 10 m wind speed and photosynthetically active radiation (PAR) obtained from atmospheric reanalyses. Real-time forcing conditions were extracted from ECMWF ERA5 datasets for the simulation period (Hersbach et al., 2020). The complete framework can be obtained from the documented testcase.

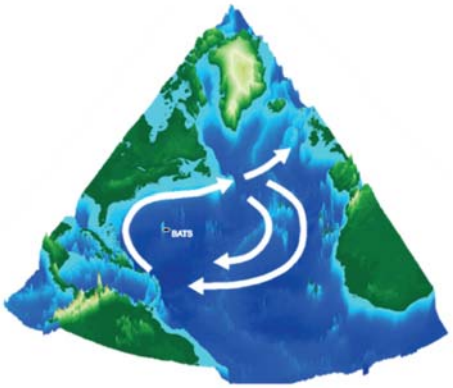

Fig. 4.2.1 BATS station location in the Sargasso Sea and Atlantic Ocean currents.

4.2.2 Model implementation

The GOTM-FABM-PISCES system has been implemented at BATS for reference simulations of the prototype system. We considered interannual simulations for the period [2014-2018]. The reference code is as described in section 3.1 here above.

The 1D vertical grid consists of 218 cells with heights varying from 0.12 m (surface and bottom) to 90 m (2500-3000 m). The vertical resolution is always better than 20m (resp. 10m) in the upper 300m (resp. 200m) to ensure sufficient resolution of the euphotic layer.

Oxygen, nitrate, phosphate, silicate, dissolved inorganic carbon, alkalinity, temperature and salinity were initialized for Jan 1st of 2014, using the January climatology. A factor of 10% was applied to initialize the detrital large and small organic carbon pools of the model from the observed particulate organic carbon (POC), assuming a 95-5% ratio between these size fractions. The 10% ratio is justified by the different nature of POC in the model and observation (e.g. living components and refractory material are not in the simulated POC pool) and was obtained empirically. In an attempt to minimize the impact of missing lateral influences, a small relaxation term (with a time scale of 1 year) has been set for salinity, temperature, and all biogeochemical variables initialized from climatology files (except detrital pools), based on the same climatological conditions

4.2.3 Model validation

This section presents the assessment, through visual comparison, of 5 years of simulations with respect to the repeated observed climatology for physics, nutrients, oxygen, dissolved inorganic carbon and chlorophyll. The physical environment (Fig. 4.2.2) appears as reasonably well constrained, although winter mixing seems to reach excessive depths, in particular for 2016 and 2017.

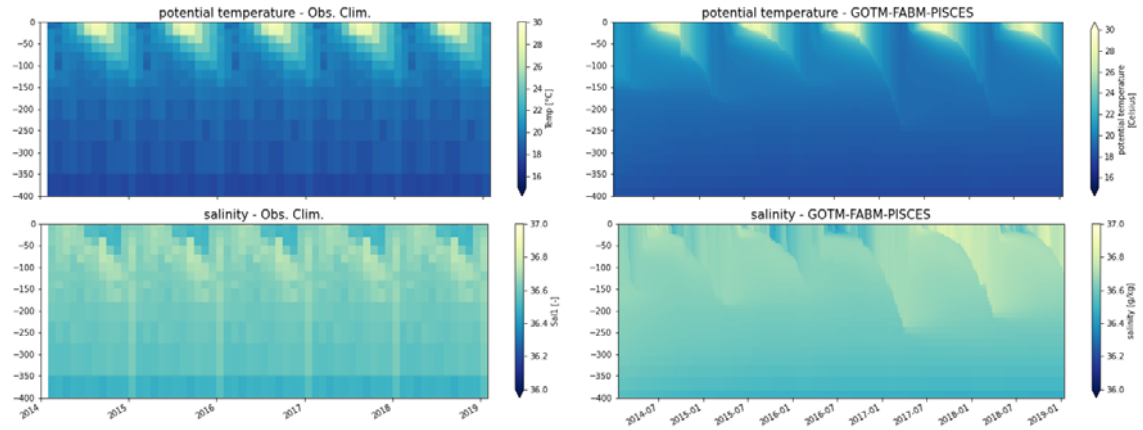

Fig. 4.2.2 (Left) repeated climatology and (right) model results for potential temperature and salinity.

The general range of nutrients availability in the surface layer (Fig. 4.2.3) is in agreement with observations, as far as can be said from the climatological compilation of observations. A slight overestimation of nitrate and phosphate concentration in the 150-300 m depth range is observed.

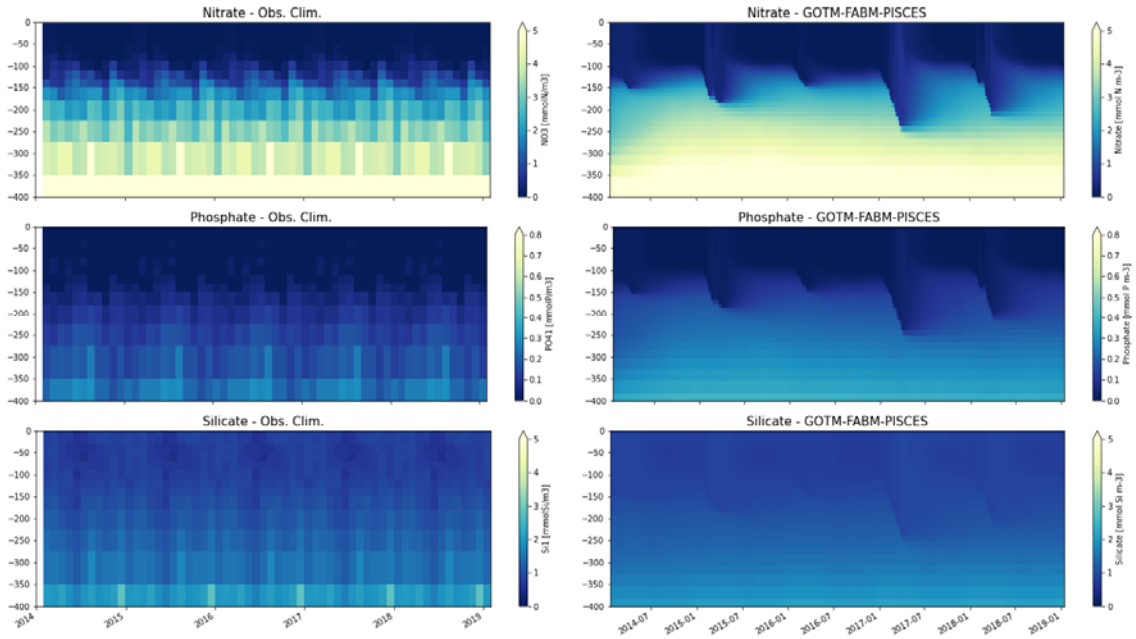

Fig. 4.2.3 (Left) repeated climatology and (right) model results for nitrate, phosphate and silicate.

As such, the system appears as well balanced, free of systematic drifts or significant recovery transition from the initial conditions. For instance, the oxygen minimum layer around 700-900m (Fig. 4.2.4), which is also a maximum layer for CO2, is stable and does not increase nor decrease in its vertical extent.

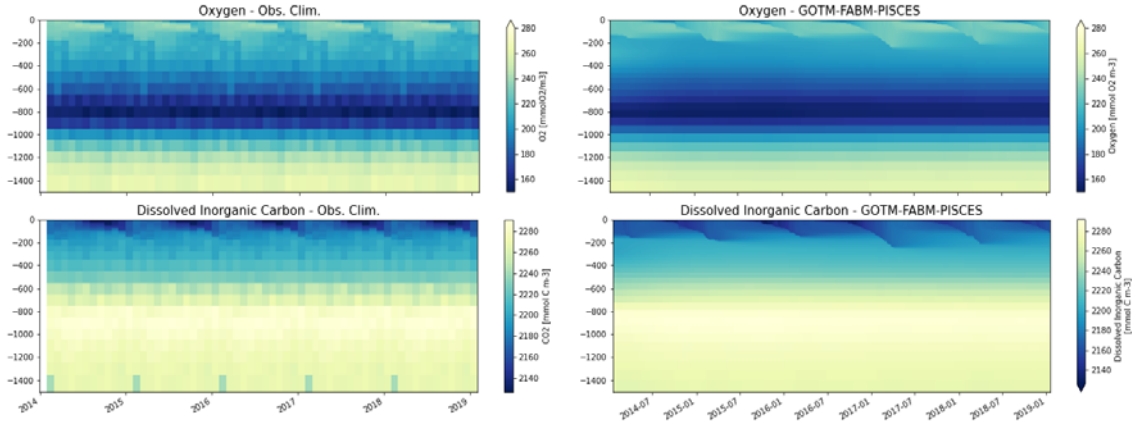

Fig. 4.2.4 (Left) repeated climatology and (right) model results for oxygen and dissolved inorganic carbon.

Finally, the DCM structure is well visible in the Chlorophyll seasonal pattern (Fig.3.5.5), at a depth slightly deeper (90-120 m) than observed (75-110 m). Noteworthy, the strong winter mixing of 2017 and 2018 induce high surface chlorophyll content during the summer period. In average, the simulated summer surface chlorophyll content appears higher than in the climatology.

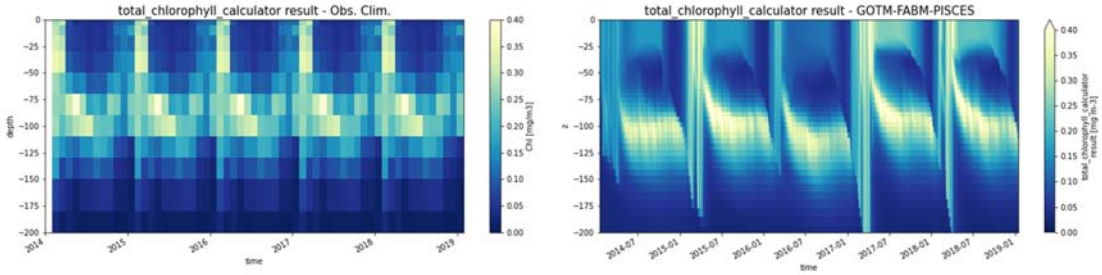

Fig. 4.2.5 (Left) repeated climatology and (right) model results for chlorophyll.

Additional diagnostics (not shown here) computed from the model outputs indicate that the simulated net primary production seems in agreement, but rather on the lower side, with former *in situ* estimates obtained in 2000 by the Bermuda Institute of Ocean Science.

In general, these results show that the BATS setup implemented in the prototype (i) qualitatively reproduces a behaviour consistent with that expected at BATS with notably an early bloom followed by a DCM, (ii) quantitatively provides a mean state and a seasonal cycle consistent with observations, (iii) does not produce significant drift over a 5-year simulation. We can therefore consider that it meets the criteria for conducting the sensitivity studies foreseen in WP3 task 3.2.

4.3 GOTM-FABM-BFM at BOUSSOLE and Lagrangian data (BGC-Argo float).

Authors: Eva Álvarez, Anna Teruzzi, Paolo Lazzari and Gianpiero Cossarini (OGS) and Jorn Bruggeman (BB)

The Mediterranean case study of the GOTM-FABM-BFM prototype consists of two sites: the BOUSSOLE buoy (described in this section 4.3) and the pseudo-lagrangian BGC-Argo float (section 4.4).

4.3.1 Site description and input data

The BOUSSOLE case study consists of the data collected in the offshore BOUSSOLE buoy (http://www.obs-vlfr.fr/Boussole/html/project/boussole.php) and in the DYFAMED station (http://sodyf.obs-vlfr.fr/). The BOUSSOLE buoy data are complemented by DYFAMED data due to the proximity of the two mooring. The area is located in the Ligurian sea, one of the sub-basins of the Western Mediterranean sea (Fig. 4.3.1a). The water depth is varying between 2350 and 2500 m in this area and the site has been selected in particular because currents are extremely low. This peculiarity is due to the position close to the center of the cyclonic circulation that characterizes the Ligurian sea. At the DYFAMED site monthly cruises collect data since 1991 that are made available to the entire scientific community (CTD casts, HPLC pigments, nutrients, oxygen, COD, short-time 14C incubation primary production). The BOUSSOLE site comprises a mooring, deployed at 7°54'E,43°22'N where the depth is 2440m, and collect optical data at high temporal resolution, and monthly cruises that collect biogeochemical variables. The DYFAMED buoy, located at 7.87°. 43.42°, consists of physical and biogeochemical variables of which we used NO_2, NO_3, PO_4 and SiO_4 for model validation.

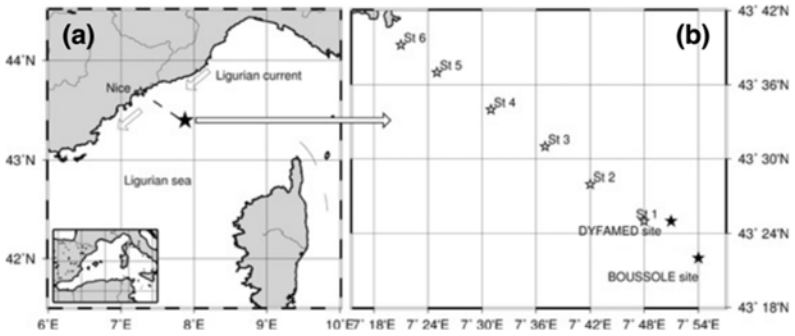

Figure 4.3.1 (a) the northwestern Mediterranean Sea, with indication (clack star) of the location of the work area. (b) Zoom from the genral map, showing the position of the BOUSSOLE and the DYFAMED sites.

4.3.2 Model implementation

The 1D GOTM-FABM-BFM with mono-spectral light configuration was run at the BOUSSOLE site location (43.37N, 7.90E, 2438m) using, as forcing, the iGOTM atmospheric forcings (Hersbach et al., 2020) and initialized with CMEMS Mediterranean reanalysis product (Cossarini G. et al., 2021; Escudier R. et al., 2021) at the same location and prescribing the nudging for temperature, salinity and nutrients. The timestep was 600s and the output was exported daily from 2000-01-01 to 2019-01-01.

Figure 4.3.2 shows a general overview of model behaviour in terms of daily available irradiance at ocean surface (Fig. 4.3.2a), stratification and mixing (Fig. 4.3.2b-c) and the formation of a deep chlorophyll maximum (DCM)(Fig. 4.3.2d) during the simulated period.

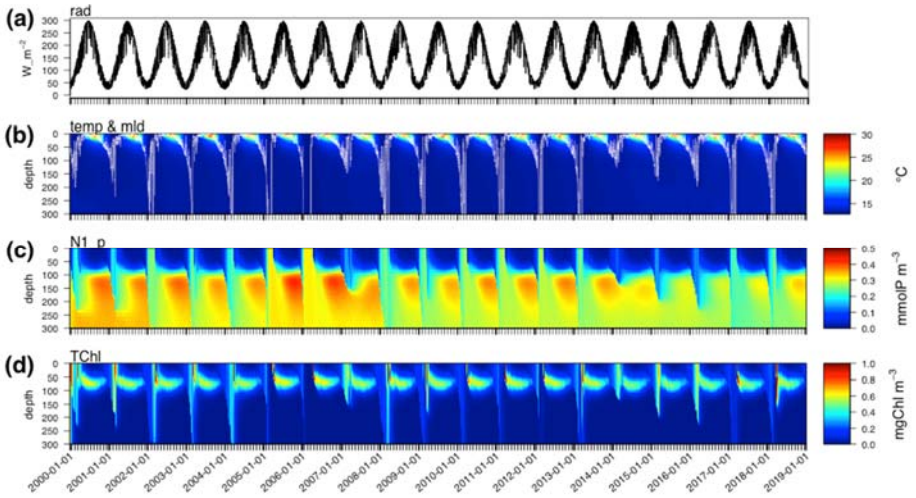

Figure 4.3.2 GOTM-FABM-BFM run at the BOUSSOLE location from 2000 to 2019: (a) Irradiance at ocean surface, and depth profiles of (b) temperature, (c) phosphate and (d) total chlorophyll.

4.3.2 Model validation

This section presents the assessment, through visual comparison, of one year of simulation with respect to the observed climatological values for physics, nutrients and chlorophyll for the layer 0-300m. The Fig. 4.3.3 shows distribution of temperature and main nutrients (nitrate, phosphate and silicate) as a climatological mean of observations taken at the Dyfamed site and simulated by GOTM-FABM-BFM for the year 2004. Climatologies are computed by averaging observation at 1 week basis and a common vertical discretization. Simulated values are consistent with the typical seasonal evolution and vertical gradients shown by the annual climatology of temperature and nutrients. A model underestimation can be observed for nitrate+nitrite and phosphate subsurface values, however depth of the nutricline (i.e., the sharp transition between the depleted surface layer and the high value subsurface layer) is reasonably well reproduced by the model.

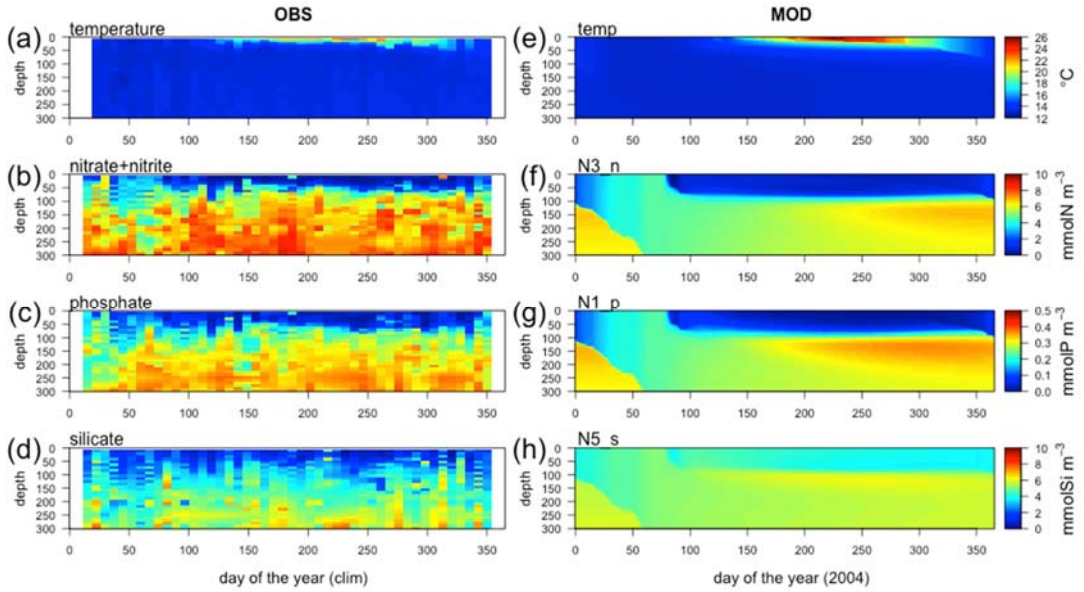

Figure 4.3.3 Hovmöller plots at Dyfamed site (OBS, left) and simulated by BFM (MOD, right) of (a, d) temperature, (b, e) nitrate, (c, f) phosphate and (d, h) silicate.

Figure 4.3.4 shows the distribution of total and size-fractionated chlorophyll as a climatological mean of observations taken at the BOUSSOLE site and simulated by GOTM-FABM-BFM. Consistent with the climatology, the main biogeochemical processes simulated by the GOTM-FABM-BFM model are the surface winter/early spring bloom, the spring formation of a deep chlorophyll maximum and its presence at a depth of 60-80m during the whole summer period.

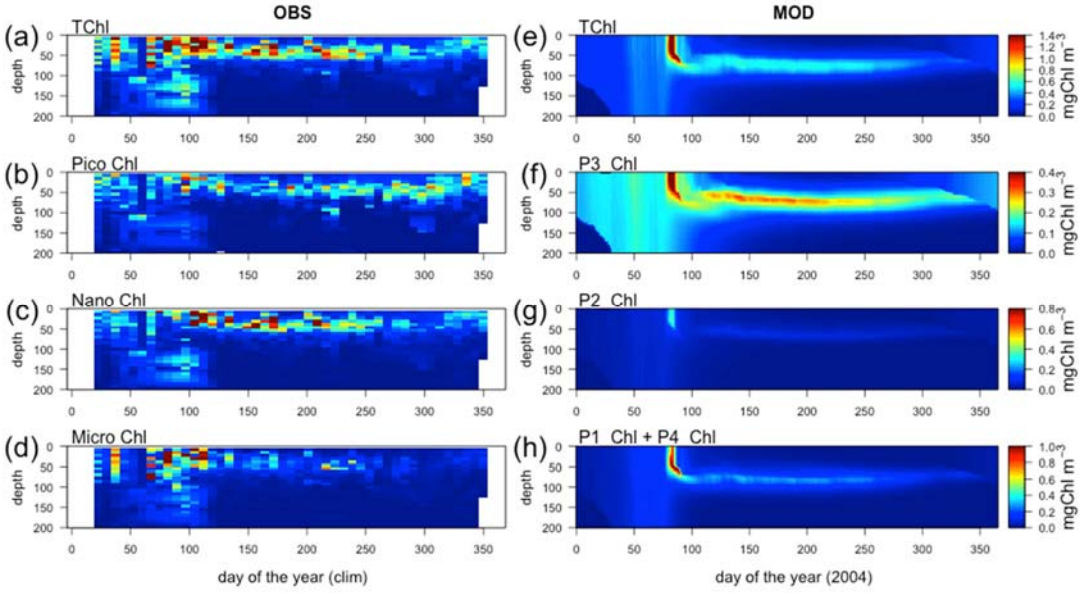

Figure 4.3.4 Hovmöller plots at BOUSSOLE site (OBS, left) and simulated by BFM (MOD, right) of (a, e) total chlorophyll, and chlorophyll of (b, f) pico- (c, g) nano- and (d, h) microphytoplankton.

4.4 GOTM-FABM-BFM at the East-Mediterranean pseudo-lagrangian BGC-Argo

Authors: Eva Álvarez, Anna Teruzzi, Paolo Lazzari and Gianpiero Cossarini (OGS)

4.4.1 Site description and input data

The second Mediterranean case study consists of the pseudo-Lagrangian simulations to reconstruct the biogeochemistry along BGC-Argo float trajectories. In this case, we used the capability of GOTM to be relaxed with respect to observed data, introducing a simplified data assimilation methodology. We upgraded the methodology which was based on BFM presented in previous studies, (Terzić et al., 2019), by using the capability of GOTM to resolve the mixing along the water column. In contrast to the simplified mixing model used in (Terzić et al., 2019), the GOTM-FABM-BFM simulation used the state-of-the-art mixing schemes of GOTM, the relaxation with measured temperature (converted to potential temperature) and the outputs from iGOTM for the atmospheric forcing using the average coordinates of the BGC Argo float trajectory.

We created a python tool to interface the data measurements from BGC-Argo float to GOTM model (https://github.com/plazzari/BGC_ARGO_GOTM_FABM) and we initialized the model using reanalysis output from MedMFC CMEMS service (Cossarini G. et al., 2021) for all the BFM biogeochemical variables (52) with the exclusion of CDOM, that is set to low values for these preliminary tests. The BFM implementation of the CMEMS reanalysis do not include, yet, CDOM and therefore the evolution of its components is not solved. The trajectory of the BGC-Argo considered is reported in Fig. 4.4.1.

Figure 4.4.1: Trajectory of the BGC-Argo float lovbio066d (WMO code 6901655) considered in the present simulation, Starting date is 2014-04-04, and the end date is 2015-05-20.

4.4.2 Model implementation

The GOTM-FABM-BFM implementation for BGC-Argo used the monochromatic light model accounting only for chlorophyll self-shading. High frequency relaxation (1 week) with respect to BGC-Argo temperature and salinity measurements is applied. This is consistent with the average profiling frequency of BGC-Argo floats. The number of vertical levels is 197 and the time step is 600s. Evolution of biogeochemical parameters, such as nutrients and chlorophyll, is without any relaxations. As shown in Fig. 4.4.2, the BGC-Argo float implementation allows to examine a biogeochemically different area with respect to BOUSSOLE, we selected the instrument with WMO code 6901655 (lovbio066d), deployed in the Levantine basin with average coordinates (34.12 ° E, 28.04 ° N) and a displacement standard deviation (±0.40 ° E, ±0.63 ° N) for the activity duration of the float. In particular, the simulation starts at August 2014 and stops at the end of May 2015. The implemented simulation

includes one winter vertical mixing period (Fig. 4.2.2b-c), which supplies nutrients to the surface layer (Fig. 4.2.2e and f). Additionally, the simulated chlorophyl (Fig. 4.2.2d) show the winter/spring surface bloom and the presence of a deep chlorophyll maximum structure during the summer periods.

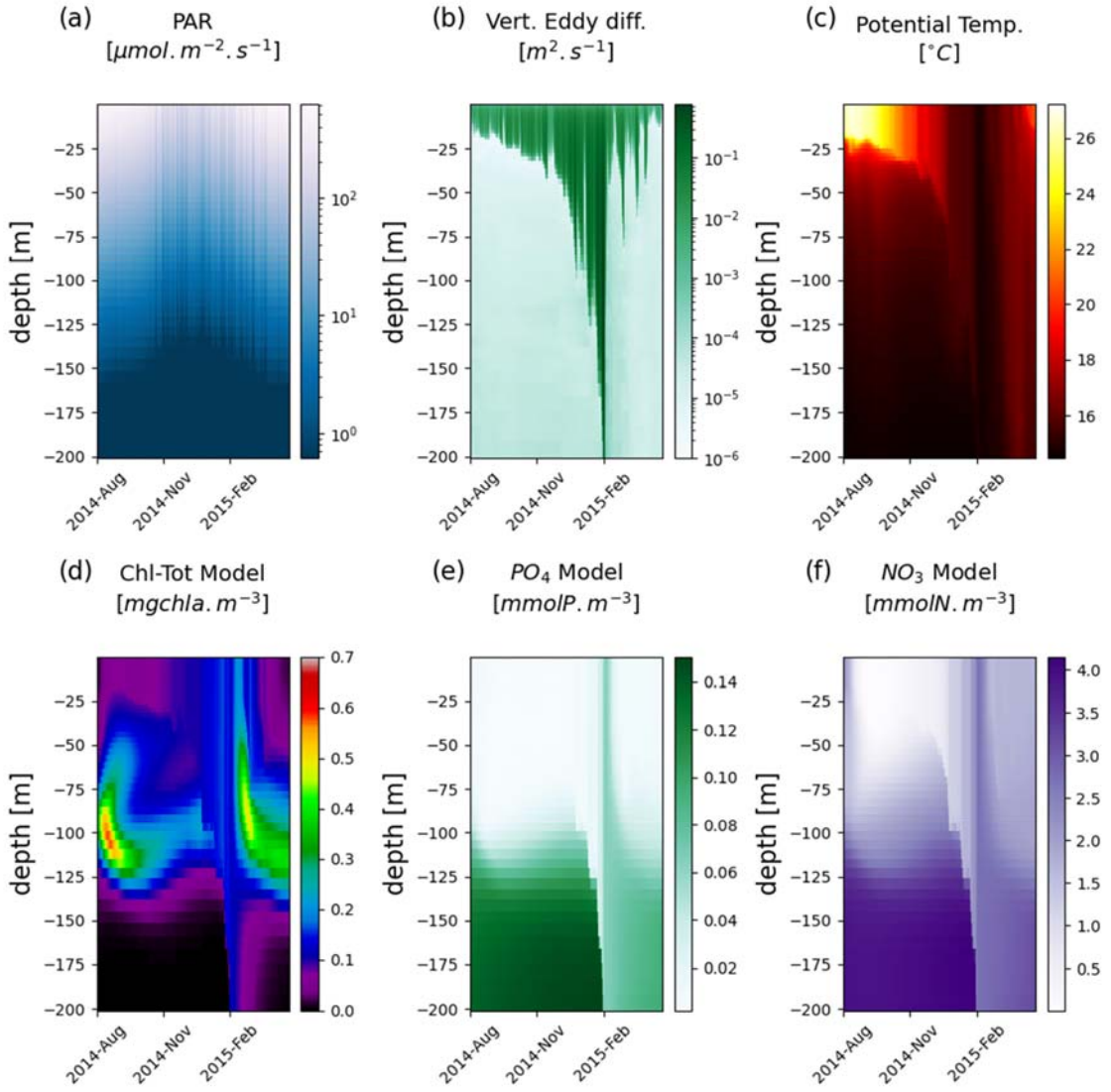

Figure 4.4.2 : Hovmöller diagrams of BGC-Argo float lovbio066d (WMO code 6901655) produced using GOTM-FABM-BFM. The six-image composite is organized as follows: panels (a), (b), and (c) show PAR, vertical eddy diffusivity, and potential temperature; panels (d), (e), and (f) show, chlorophyll, phosphate, and nitrate.

4.4.3 Model validation

The assessment of model results with respect to BGC-Argo data is presented in Figure 4.4.3 for vertical diffusivities (estimated from the BGC-Argo density profiles; following Terzić et al., 2019) and chlorophyll. Mixing events due to Etesian winds, as consistently shown in data and in model results

(Fig 4.4.3a and Fig.4.4.3b), are responsible for the nutrient uplift mechanism responsible for chlorophyll bloom. The mixing model of GOTM is consistent with the data-derived estimates both showing an intense mixing peak in winter 2015. The capability of the model to represent high frequency variability is also shown in Fig 4.4.3b. The visual comparison of the model results with BGC-Argo data of chlorophyll (Fig. 4.4.3c-d) corroborated the robustness of the model results and of the pseudo-lagrangian approach adopted. In particular, the formation of a deep chlorophyll maximum during summer and the occurrence of the surface bloom during winter are modelled behavior in agreement with the observations, with model underestimating surface bloom in late winter. The new implementation based on GOTM-FABM-BFM is consistent with previous results published in (Terzić et al., 2019) which used the BFM model coupled with another 1D physical model (i.e., the 1D-OGSTM).

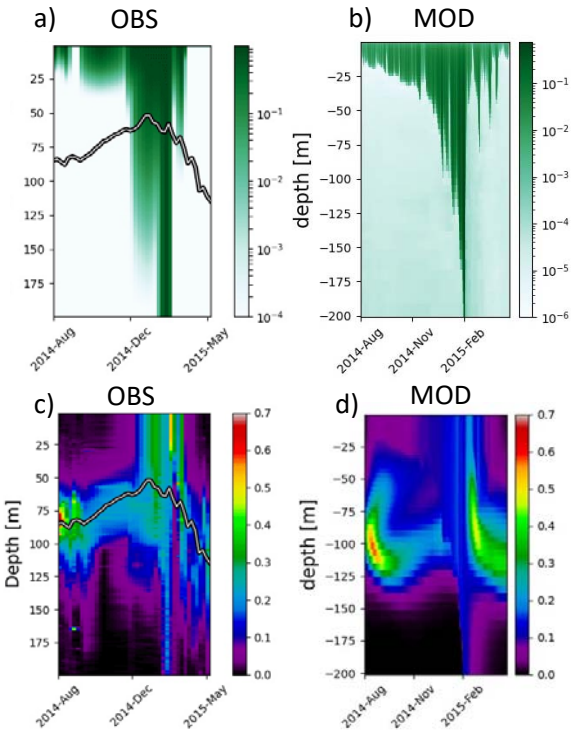

Figure 4.4.3: Hovmöller diagrams of BGC-Argo float lovbio066d (WMO code 6901655) comparing vertical mixing (m^2s^{-1} computed from T-S profiles (OBS, panel a) with the simulated mixing profile (MOD, panel b). Chlorophyll (mgchl m^{-3} derived from fluorescence measured by BGC-Argo float (OBS, panel c) is compared with total chlorophyll simulated by BGC-Argo (MOD, panel d).

4.5 GOTM-FABM-ERSEM at Station L4 (English Channel)

Authors: Josef Skakala and Stefano Ciavatta (PML)

4.5.1 Site description and input data

The station L4 is a mesotrophic location in the English Channel and is part the SmartSound Plymouth (www.smartsoundplymouth.co.uk; see Fig.4.5.1). The station provides weekly measurements for biogeochemical variables of interest (e.g. pigments, nutrients, optical data, data for phytoplankton, or zooplankton carbon biomass), as well as data for temperature and salinity. The measurements are typically taken in multiple vertical layers within the 50m L4 water-column depth (e.g see Fig.4.5.2-4.5.4).

The L4 observations for temperature and salinity have been used for GOTM spin-up initialization and also as monthly relaxation values for all GOTM simulations at L4. Similarly the ERSEM spin-up was annually relaxed towards the observed L4 nutrient climatologies, to prevent spurious trends in ERSEM nutrient variables (e.g. in nitrogen due to denitrification). Furthermore, the observed climatologies for nutrients and total chlorophyll were also used to initialize the ERSEM model spin-up.

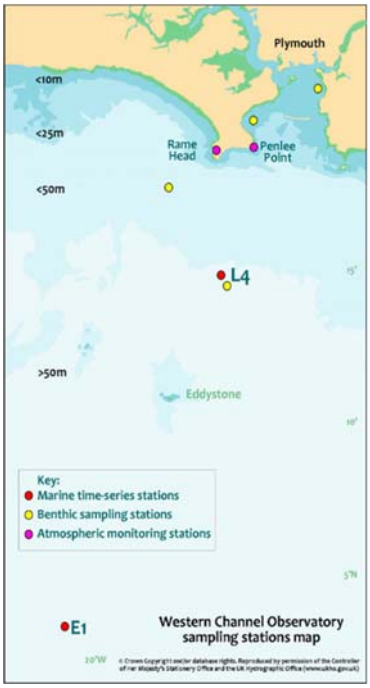

Fig.4.5.1: The L4 location as part of WCO facilities in the SmartSound region in the English Channel. The picture is taken from the WCO website (https://www.westernchannelobservatory.org.uk/).

4.5.2 Model implementation

The GOTM-FABM-ERSEM set-up for the L4 station used in this work has already been established in previous studies (Butenschön et al., 2016; Powley et al., 2020). The model configuration is based on

100 vertical layers with varying resolution between 6-87 cm and uses meteorological data derived from hourly ERA5 data-set of Copernicus Climate Change Service (C3S) Climate Data Store (CDS). The tidal forcing was generated using the FVCOM model in the Risks and Opportunities for Sustainable Aquaculture (ROSA) project. The physical initial values are typically based on the depth-varying observed temperature and salinity, whilst biogeochemistry is typically spun-up from a vertically constant values in the fully mixed period (e.g. in January). All the required atmospheric and observation physical data are available for the 2002-2020 period. We used in this study a 7.5 year spin-up starting from 01/01/2007, providing initialization for different simulations starting on, or after, 01/06/2014.

4.5.2 Model validation

The model configuration at L4 used here has been validated in the previous publications (Powley et al., 2020). However, we did some further assessment within this project, providing a visual comparison of model results with available observations (Fig. 4.5.2-4). In particular, the Fig.4.5.2 compares the 2011-2013 Hovmoeller diagrams for physical variables (temperature, salinity) with their corresponding L4 observations, Fig.4.5.3 shows the same for total chlorophyll-*a* and oxygen, and the last, Fig.4.5.4, compares three selected nutrient concentrations (from top-down: nitrate, phosphate and silicate). It should be noted that to fill the many observational gaps in the L4 observations, some of the data shown in the right-hand panels have been linearly interpolated. The three Fig.4.5.2-4.5.4 show that the model captures broadly correctly the existing seasonal cycles in all the physical and biogeochemical variables, with more pronounced seasonality in the simulated total chlorophyll than in the observed chlorophyll values (this is however a well-known feature of ERSEM, e.g Skakala et al, 2020). In case of some specific variables (temperature, nitrate) one can also observe some biases (differences in total mean values) between the model and the observations, but these are frequently present also in the 3D configuration (e.g Skakala et al, 2020) and are within an acceptable range. We conclude that a good quality L4 prototype has been established in WP2, ready to be used for further developments in SEAMLESS.

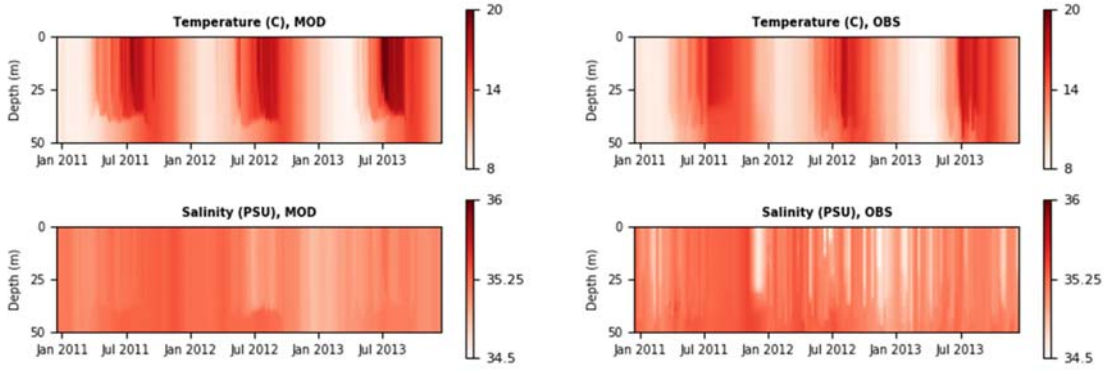

Fig.4.5.2: The 2011-2013 L4 model (MOD: left-hand) vs observations OBS: (right-hand) comparison for temperature (C) and salinity (PSU).

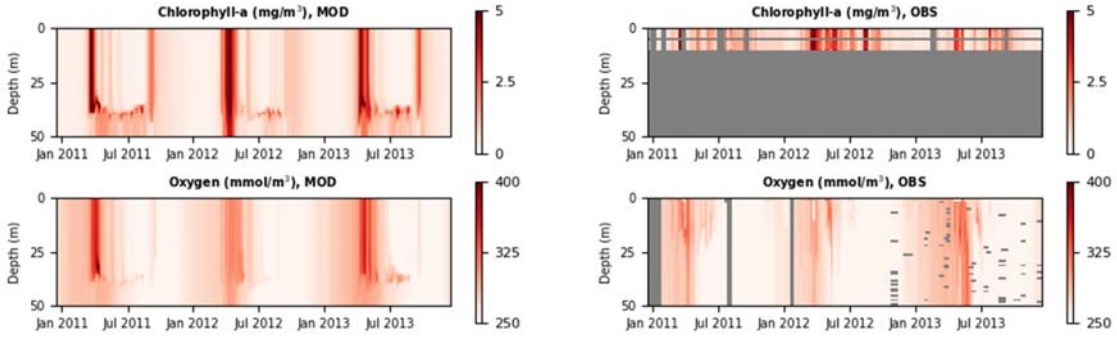

Fig.4.5.3: The 2011-2013 L4 model vs observations comparison for chlorophyll-a (mg/m3) and oxygen (mmol/m3). The grey color marks the areas and times far from any observations, where no values have been interpolated.

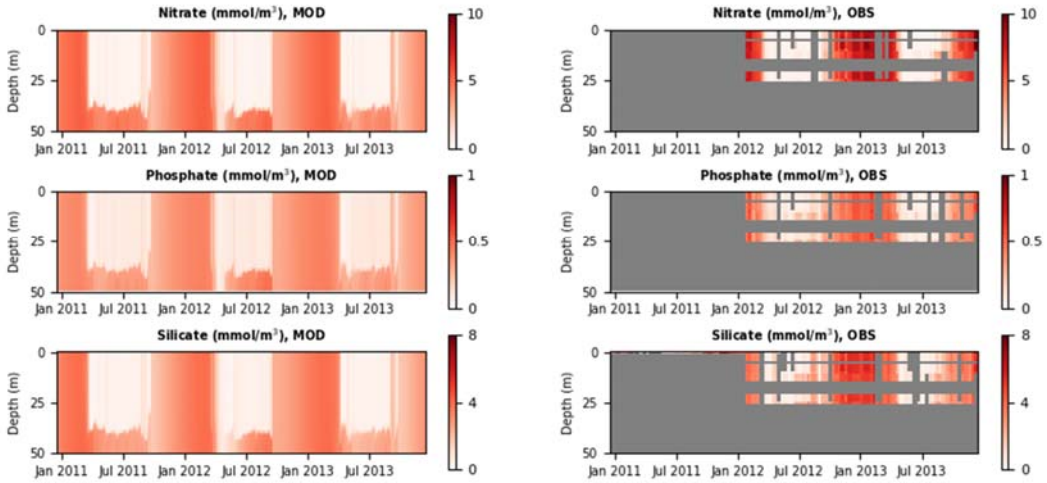

Fig.4.5.4: The 2011-2013 L4 model vs observations comparison for nutrients (nitrate, phosphate, silicate, all in mmol/m3).

4.6 GOTM-FABM-ECOSMO at station M (Norwegian Sea)

Authors: Tsuyoshi Wakamatsu and Çağlar Yumruktepe (NERSC)

In this section, we summarize our activities towards the SEAMLESS prototype system at Station M (66N, 02E) (St.M). Two updates are made to our reference GOTM-FABM-ECOSMO system for development of SEAMLESS prototype system. GOTM-FABM-ECOSMO coupled system is setup at Station M. The new configuration is used for SEAMLESS related observability and sensitivity experiments in WP3.

4.6.1 Site description and input data

The station M is located at the eastern periphery of the Norwegian Basin which represents pelagic biogeochemical dynamics of the Norwegian Sea. Station M is located in the western branch of the Norwegian Atlantic Current (NwAC) and its general water mass structure is relatively warm, nutrient rich Atlantic Water in the upper 300-400 m, cold Norwegian Atlantic Deep water below about 1200 m, and intermediate water between (Skjelvan et al., 2008). Surface nutrients are supplied from the subsurface water mass by vertical mixing.

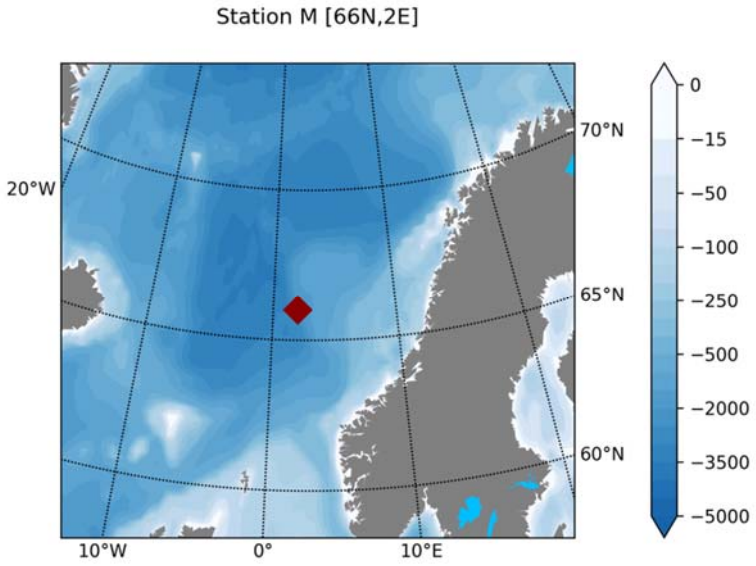

Fig.4.6.1 Station M location (red diamond) in the Norwegian Sea. Background contour is bottom bathymetry in meter.

4.6.2 Model implementation

The present FABM-ECOSMO model implementation includes also the upgrading ECOSMO to include light-limitation on phytoplankton growth rates as a function of chlorophyll:carbon ratio (Chl:C) following (Evans and Parslow, 1985) (EP85) using (Bagniewski et al., 2011) (B11) Chl-specific parameterization, which is tuned at southwest of Iceland. ECOSMO with its reference configuration (ECO-OLD) uses explicit Chl state variables for each functional type, diatoms and flagellates, and the

growth rate of Chl state variables takes into account PAR and Chl:C using (Geider et al., 1997) formulation following B11 parameterization. Such that the light limitation on growth rates is parameterized as the following, which does not include chlorophyll dependency:

$$\tanh(PAR * \alpha) \quad (1)$$

With this approach, simulated Chl concentration does not have a direct influence on primary productivity. During the process of upgrade, we have introduced, as in EP85 and B11, the control of Chl:C ratio on light-limitation into the phytoplankton growth rates as follows:

$$\frac{\left(\frac{Chl}{C} * \alpha * PAR\right)}{\sqrt{\mu_{max}^2 + \left(\frac{Chl}{C}\right)^2 * \alpha^2 * PAR^2}} \quad (2)$$

Eq.2 allows the model to simulate higher light-limited growth rates under low PAR conditions since the model will have a tendency to produce more Chl-a (Chl:C will increase), such that in early spring and deeper layers, the model increases productivity. Reverse effects are true for high PAR conditions.

Since the addition of Chl:C dependency to light-limited growth rate is a major change to the model formulation, other parameters that are directly related to growth and grazing dynamics have been modified as well, as such growth rates of phytoplankton were decreased because the model was too productive with the new approach using the old parameters. Too balance prey-predation relationship, while lowering phytoplankton growth rates, we also lowered the zooplankton grazing rates. The effects are shown in Fig. 4.6.2, where we present an example 1D simulation at station M for a year of high data availability (1991). Significant changes depicted in Fig.4.6.2 are:

(1) ECO-NEW simulates the surface Chl maximum earlier than the old configuration, whereas ECO-OLD configuration locates the Chl maxima late-June, with higher than observed concentration. Chl concentration prior to June is better resolved with the new configuration.
(2) ECO-NEW has an earlier bloom (April) in response to the added functionality of linking the modelled Chl to light-limitation formulation (Eq.2), such that the model is more productive during low-light conditions. We note that further tuning is required, as the ECO-NEW, though it improves the recurring late-bloom issue in ECOSMO, simulates higher Chl concentration.
(3) In relation to (2), ECO-NEW is also more productive in deeper layers where the light-limitation is an important factor on growth rates. The model produces a DCM layer (15 – 40 meters) during post-bloom period (June - September), where there is evidence of Chl presence in the in situ data. Likewise, during April, ECO-NEW simulates higher Chl concentrations deeper than 40 meters, which is also an improvement towards achieving better fit with the observations.

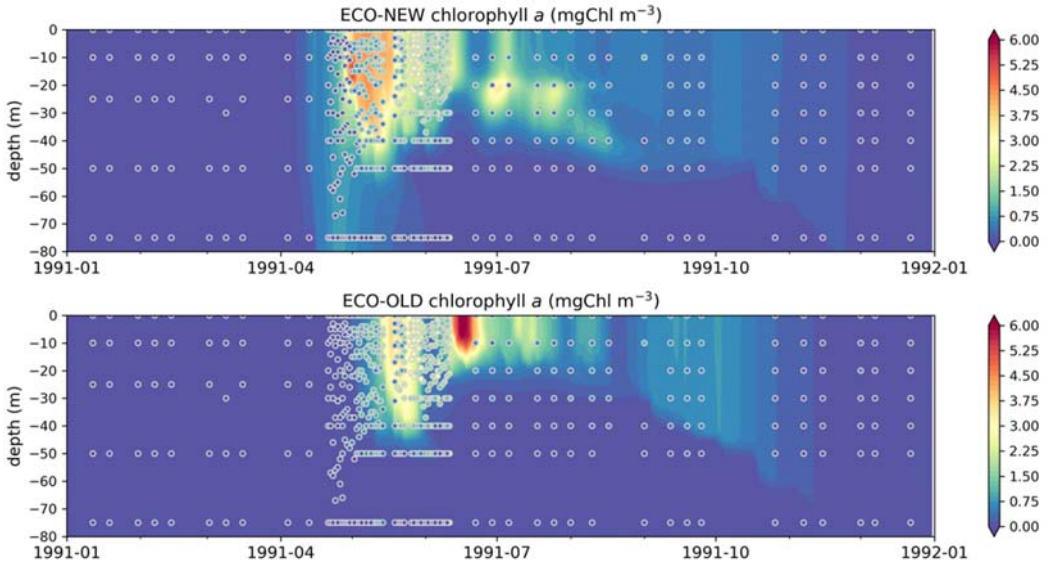

Figure 4.6.2. ECO-NEW (top) and ECO-OLD (bottom) configurations are compared to in situ chlorophyll a data at Station-M, where in situ data is depicted in markers matching the timing and depth of measurement.

4.6.3 Model validation

Being initialized with climatology nutrient at 2005 January 1st, GOTM-FABM-ECOSMO with ECO-NEW configuration was spun-up with ECMWF hourly atmospheric forcing for 9 years first. Since this sub-surface nutrient stream at station M is lacking in the one-dimensional settings of GOTM, we have introduced weak nudging towards climatological nutrients during the spinning-up run with 1 year relaxation time scale. After introducing the weak nutrient nudging, we confirmed that the sub-surface nutrients (Nitrate and Silicate in the figures) values are comparable to the observed data at station M. The impact of the nudged nutrient is visible in the surface Chl-a. Without the nutrient nudging, the surface Chl-a shows strong cyclic signal of about one month period, which is not confirmed from satellite ocean colour and Argo-float data in the Norwegian Sea. Result of 2014 simulation and its comparison with observation is plotted in Fig.4.6.3. Observation data are from bottle data collected by the Norwegian Institute of Marine Research. Overall, seasonal cycles of model nutrients (nitrate and silicate) are consistent with observation, but timing of surface silicate depletion in model is earlier than observation.

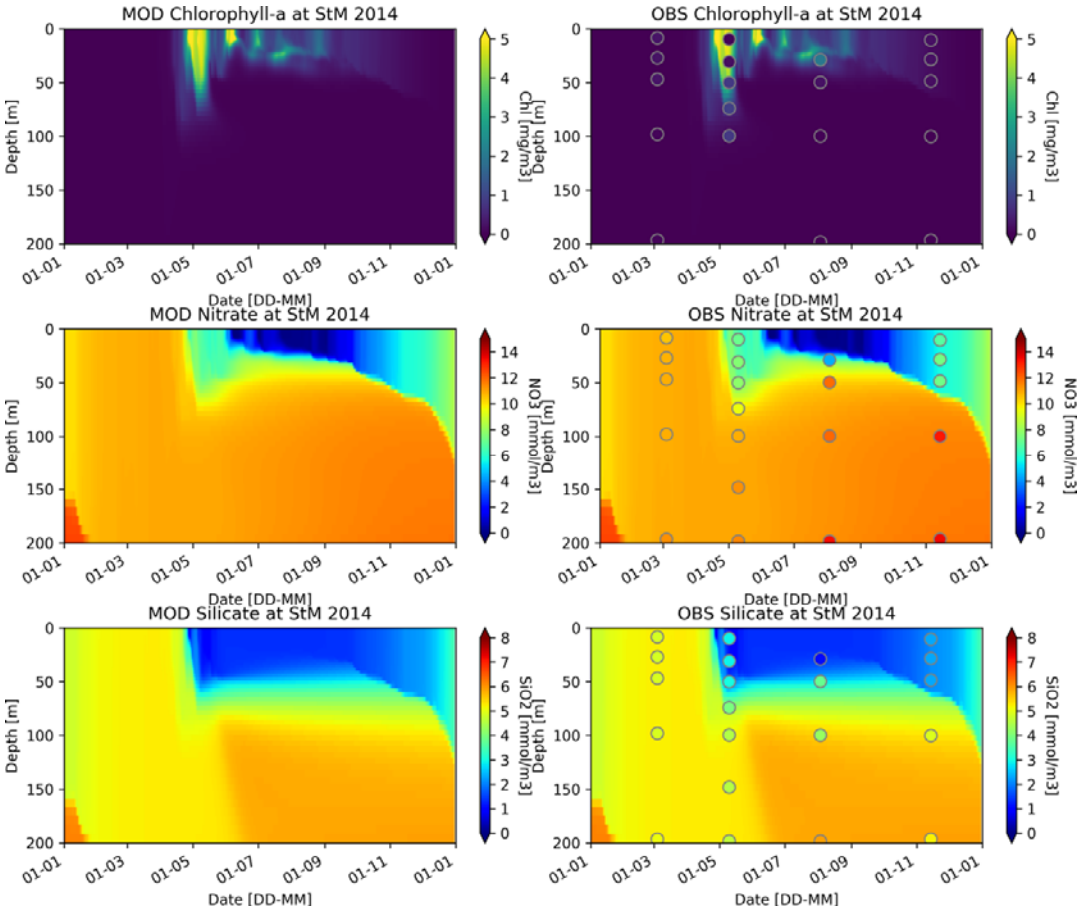

Figure 4.6.3. One year simulation of GOTM-FABM-ECOSMO at station M in 2014. Left column shows the model results (MOD). Right column shows the Observations (circles, OBS) overlapped on model data. Plotted variables are Chl-a (top), Nitrate (middle) and Silicate (bottom).

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