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Report on the prototype BGC models and their 1D simulations in CMEMS MFC sites (M11)

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1. Scope

The present deliverable illustrates results from *Task 2.1a, Task 2.1b, Task 2.1c* and results from *Task2.3a*. These Tasks, whose objective is to include all biogeochemical models and their case site setups into the 1D prototype, are a prerequisite for all the SEAMLESS activities based on the 1D prototype and allow to carry out data assimilation experiments consistently throughout the CMEMS systems.

2. Introduction

The SEASMLESS 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. The physical component is GOTM has been chosen here because of its widespread use, large number of mixing schemes and user friendliness, so that it provides a widely usable prototype system that can be representative for the different physical models used in CMEMS.

The tasks 2.1 and 2.3 concern the porting of the CMEMS biogeochemical models PISCES, BFM and ERGOM into FABM making them readily available for the 1D physical model component. In particular, the activity is subdivided in porting and initial model setup (*Task 2.1a, Task 2.1b, Task 2.1c*) and testing the models at fixed stations (*Task 2.3a*).

The three subtasks of Task 2.1 were devoted to debugging and testing on 0D (or 1D setups) of the three biogeochemical models PISCES, BFM and ERGOM:

- *Task 2.1a*: BB ported the PISCES model to FABM; then integrate and test it within the prototype system and compare it with NEMO-PISCES
- *Task 2.1b*: OGS ported the BFM model to FABM with support by BB and will implement a setup for BFM in the prototype system.
- *Task 2.1c*: AWI prepared a setup of GOTM-FABM with ERGOM in the prototype system for the Baltic Sea as a blueprint for the DA implementation.

The Tasks 2.3 is related to the configuration of the 1D prototype system for the different CMEMS regional sea sites. The partners configured their own biogeochemical model systems at the different representative sites (see Figure 2.1). All the partners prepared the first 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) and for Lagrangian data (BGC-Argo float). All the implementations performed in this activity are developed in git-based versioning system platforms[1,2]. As a main outcome of the Task, the GOTM-FABM version of the biogeochemical models used by each

[1] https://github.com/BoldingBruggeman/seamless-notebooks

[2] https://github.com/inogs/bfmforfabm

partner was correctly set up and produced consistent results with respect to the observed dynamics in all the selected sites.

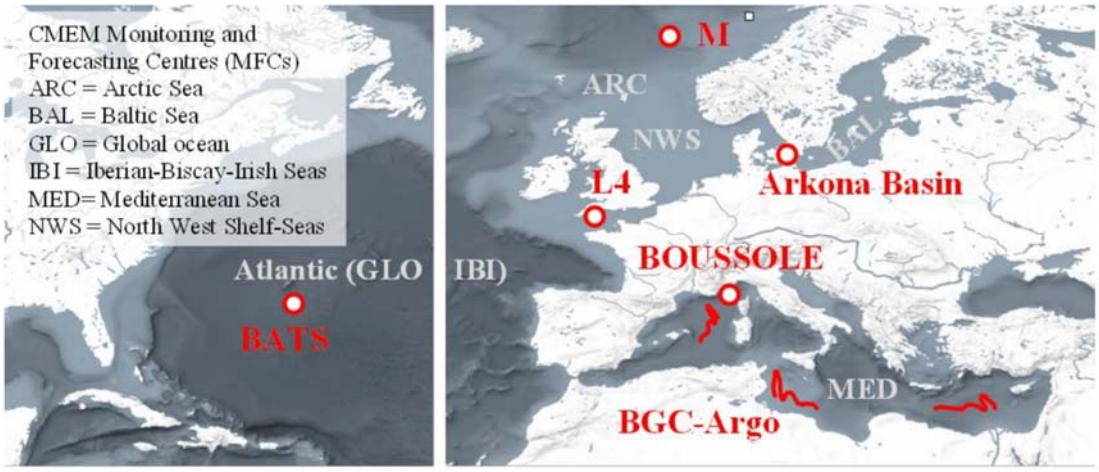

Figure 2.1 Sites (red circles) of the CMEMS Monitoring and Forecasting Centres (MFC) used for reference simulation of the 1D prototype. The red lines represent the trajectories of the biogeochemical-Argo floats (BGC-Argo) simulated with the pseudo-Lagrangian configurations of the prototype.

3. Procedures

3.1 Task 2.1a: Porting the PISCES model to FABM; integration and testing within the prototype system and compare it with NEMO-PISCES

Jorn Bruggeman (BB)

3.1.1 Background and availability

The FABM port of the PISCES biogeochemical model is based on the code that comes with the r4.0-HEAD.r13720 version of NEMO. 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

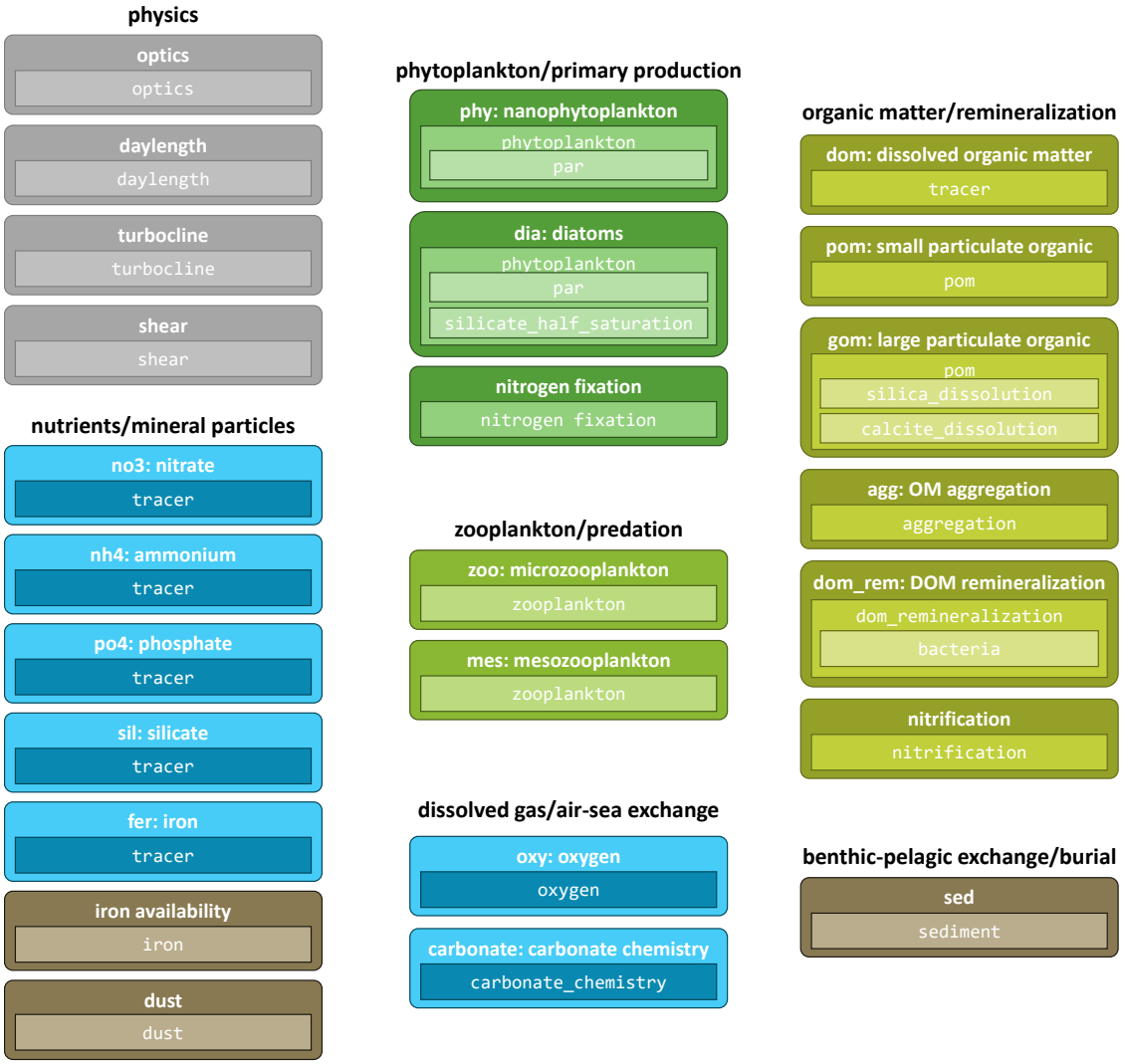

Figure 3.1.1. Overview of the default set of modules of the FABM port of the PISCES biogeochemical model. Rounded rectangles correspond to the modules defined at runtime by the user in the fabm.yaml configuration file. The contained rectangles indicate the underlying Fortran types that describe the relevant 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

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 original 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 Oliver 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 Oliver Aumont, 2021-07-15)
- The time scaling of the pdust diagnostic has been corrected (issue confirmed by Oliver 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.

3.1.3 Compilation and use

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.

3.1.4 Quality control

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 Task 2.1b: Porting of the BFM model into FABM and implementation of a 0D setup for FABM-BFM prototype system.

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

Jorn Bruggeman (BB)

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. 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 .

In FABM each modular component is *per se* defined as a model. The models we introduced in the framework are rjv2Sk|wr/#rjv2ShdEdf/#rjv2P lfur]rr/#rjv2P hvr]rr/#rjv2ShdF khp /#rjv2F ddflhG lvvroxwrq/# rjv2ShdR{|jhq, rjv2ShdljlfFV\V/#rjv2ljkwbvshfwudland also the general routines#rjv2eip bshdljlfbedvh#and vkduhgII<3.#To manage the multispectral code a number of python scripts to create diagnostic variables for arbitrary number of channels has been developed, see AUX_SCRIPTS folder[3].

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.

3.2.1 FABM/BFM biogeochemical model

The new FABM biogeochemical models that reproduce BFM, have been developed starting by 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). 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). We started including the header for type extension based on type_ogs_bfm_pelagic_base defined in ogs/bfm_pelagic_base.

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

models	Module name	Type extension
Phyto.F90	eip bSk|wr	w|shbrjvbeip bsulp du|bsurgxfhu
PelBac.F90	eip bShdEdf	w|shbrjvbeip bshdljlfbedfwhuld
MicroZoo.F90	eip bP lfur]rr	w|shbrjvbeip bp lfur}rr
MesoZoo.F90	eip bP hvr}rr	w|shbrjvbeip bp hvr}rr#
PelChem.F90	eip bShdF khp #	w|shbrjvbeip bShdF khp #
CalciteDissolution.F90	eip bF ddflhG lvvroxwrq	w|shbrjvbeip bF ddflhG lvvroxwrq
PelOxygen.F90	eip bShdR{|jhq	w|shbrjvbeip bShdR{|jhq#
PelagicCSYS.F90#	eip bShdljlfFV\V#	w|shbrjvbeip bShdljlfFV\V#

[3] https://github.com/inogs/bfmforfabm/tree/master/AUX_SCRIPTS

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;

3.2.2 Multispectral model

The FABM/BFM can run in two configurations with a simple mono spectral configuration (rjv2djkw) and a multispectral configuration (rjv2djkwbovshfwudo. 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 rjv2djkwbovshfwudd 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 Testing the BFM porting in FABM

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.

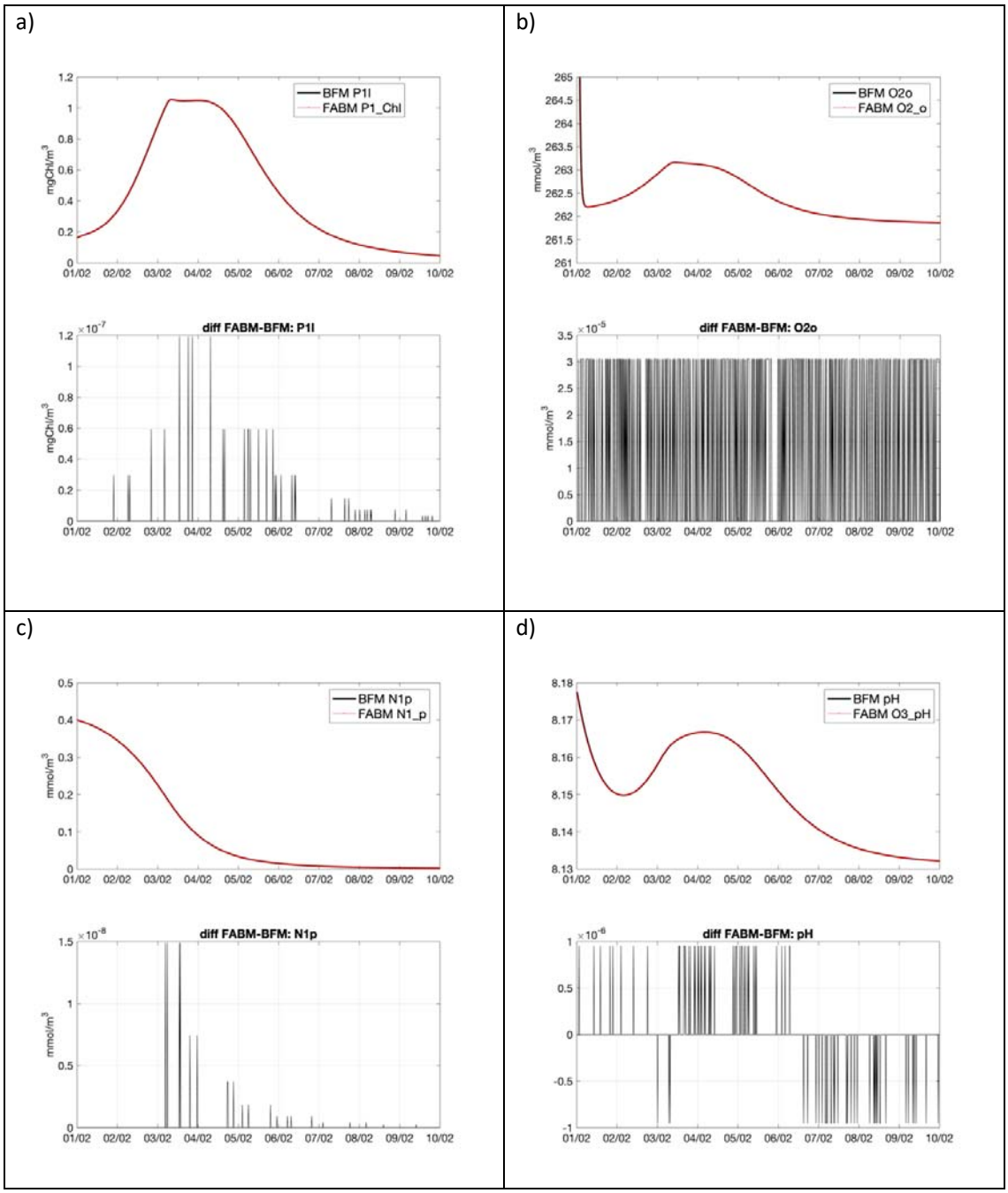

Figure 3.2.1 Results for the comparison between BFM official configuration and FABM coupled BFM. All state variables have been checked and here a subset is proposed, chlorophyll content in Diatoms a), Oxygen b), PO_4 c) and pH d). Each panel shows a 10 days timeseries of BFM standalone (black line) with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

3.3 Task 2.1c: Setup of GOTM-FABM with ERGOM in the prototype system for the Baltic Sea as a blueprint for the DA implementation.

Farshid Daryabor and Lars Nerger (AWI)

3.3.1 Introduction

The one-dimensional ecosystem model GOTM-ERGOM was configures for the prototype system for the Baltic Sea as a blueprint for the data assimilation (DA) implementation. The setup will be used to study the sensitivity of BGC observable variables and parameters to BGC indicators (e.g., chlorophyll, dissolved oxygen, pH, and etc.) as well as in data assimilation experiments to understand the ocean response to future climate change and its effects on marine ecosystems. For these studies, GOTM resolves the vertical distribution of water temperature, salinity, and density, and ERGOM simulates biogeochemical processes and variables. ERGOM model GOTM version ported to FABM by (Lessin et al., 2014).

3.3.2 ERGOM Biogeochemical model

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 blue-green algae (cyanobacteria). Diatoms represent larger cells which grow fast in nutrient-rich conditions. Flagellates represent smaller cells with an advantage at lower nutrients concentrations especially during summer conditions. The cyanobacteria group is able to fix and utilise atmospheric nitrogen and therefore, the model assumes phosphate to be the only limiting nutrient for cyanobacteria. Due to the ability of nitrogen fixation, cyanobacteria are a nitrogen source for the system. A dynamically developing bulk zooplankton variable provides grazing pressure on phytoplankton. Dead particles are accumulated in a detritus state variable. The detritus is mineralised 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, mineralised 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.

Table 3.3.1: Model state variables perturbed in sensitivity analysis and calibration.

No	State variables	Notation	Units
1	diatoms	pp	mmol n/m^3
2	flagellates	ff	mmol n/m^3
3	cyanobacteria	bb	mmol n/m^3
4	zooplankton	zz	mmol n/m^3
5	detritus	dd	mmol n/m^3
6	ammonium	aa	mmol n/m^3
7	nitrate	nn	mmol n/m^3
8	phosphate	po	mmol p/m^3
9	oxygen	O2	mmol o2/m^3
10	fluff	fl	mmol n/m^2

11	PFe_s	pb	mmol p/m^2
12	PFe_w	pw	mmol p/m^3

3.3.3 Model input and implementation

GOTM-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−1), 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 implementation is described in section 3.4 related to task 2.3a.

3.4 Task 2.3a: Setup of the prototype system for reference simulations at Arkona Basin.

Farshid Daryabor and Lars Nerger (AWI)

3.4.1 Setup of the prototype system for reference simulations at Arkona Basin

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. 3.4.1). The station is located in the Baltic Sea at Longitude 13.86 °E and Latitude of 54.8 °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.

For this study the diagnostic hydrographic and biogeochemical data for the model initialization, validation, and assimilation are derived from the German Marine Monitoring Network (MARNET). In addition, satellite data will be used for the assimilation.

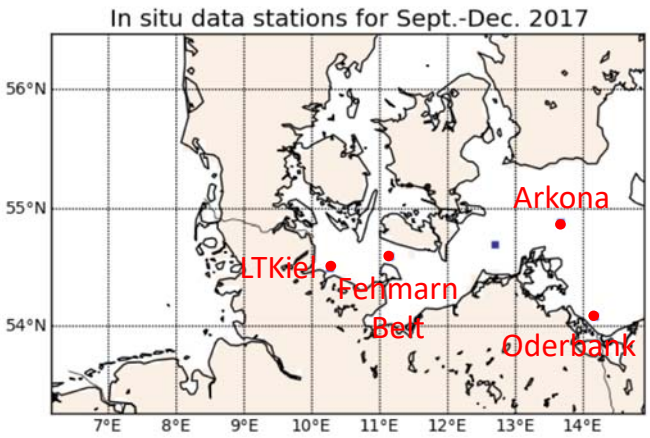

Figure 3.4.1 Overview of measurement stations of the MARNET network in the Baltic Sea. Here, the model is configured for the station 'Arkona'.

3.4.2 Model input and implementation

The GOTM-ERGOM physical and biogeochemical variables, e.g., temperature, salinity, air temperature, humidity, 10-meter horizontal eastward and northward wind components, oxygen, phosphate, nitrate, are derived from the German Marine Monitoring Network (MARNET). The model was implemented for a period of the four years with relaxation to climatology temperature and salinity observation and biogeochemical observation data. The model spin-up (equilibrium state) for the winter (January - March) and summer (June - August) seasons initialized to the model climatology restart file (the period of 2010-2015).

3.4.2 Model output

The figure 3.4.2 shows Hovmoller diagrams of temperature and salinity for year 2015. The upper row shows observed values, while the lower row shows the simulation. The simulated temperature and salinity are consistent with the observations. Figures 3.4.3 and 3.4.4, respectively, show the simulated biogeochemical parameters from the GOTM-ERGOM at the reference station, Arkona. As shown the simulated oxygen (Fig. 3.4.3a) is consistent with the observed derived from MARNET dataset (Fig. 3.4.3b), while the simulated phosphate (Fig. 3.4.3c) is overestimated from the middle of February to July in comparison with the observed (Fig. 3.4.3d).

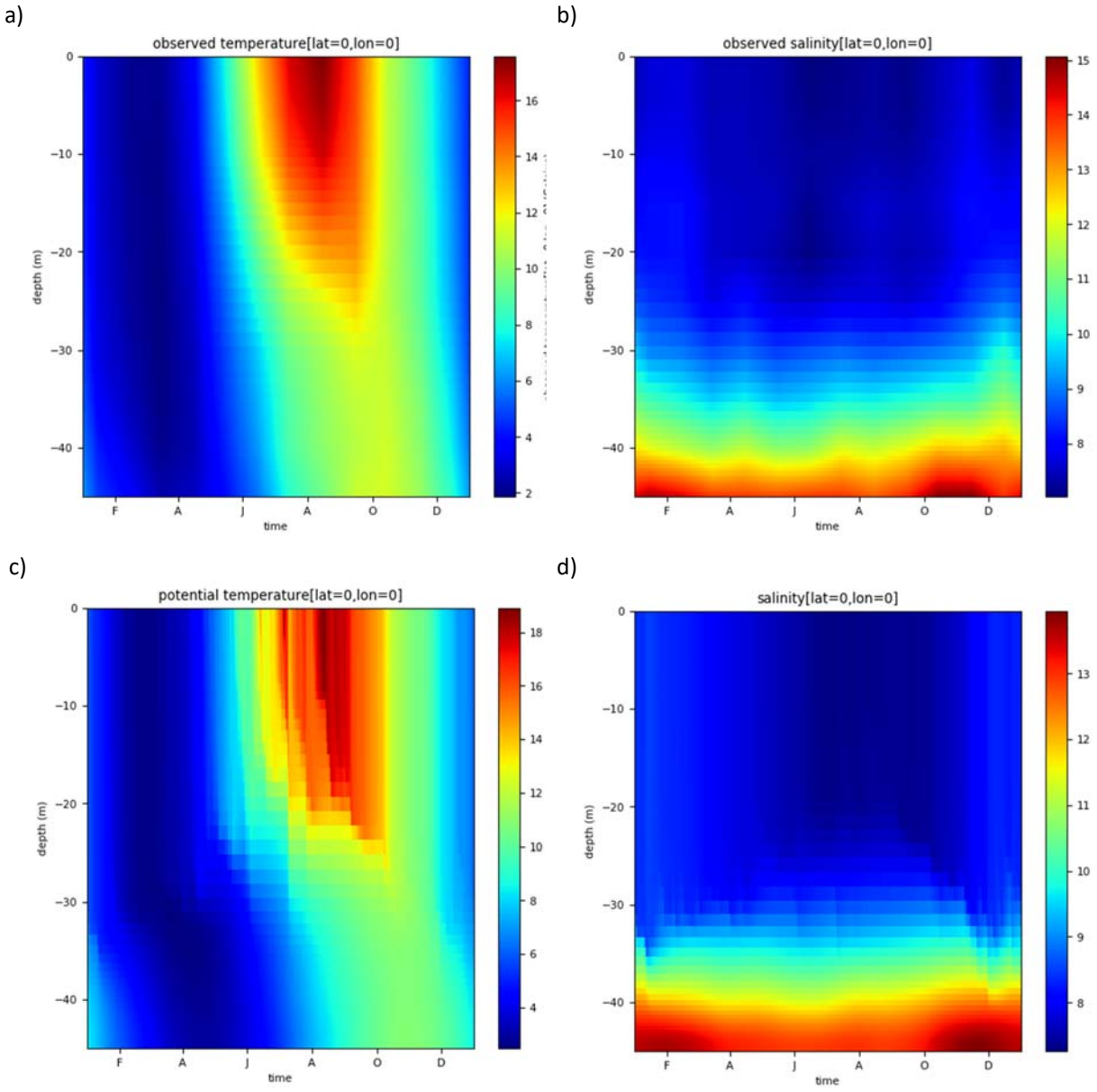

Figure 3.4.2: Hovmoller diagram for temperature (°C) and Salinity (g/kg) at the station Arkona for the period of January – December 2015. (a) Observed temperature and (c) the model, respectively, as well as observed Salinity (b) and the model (d).

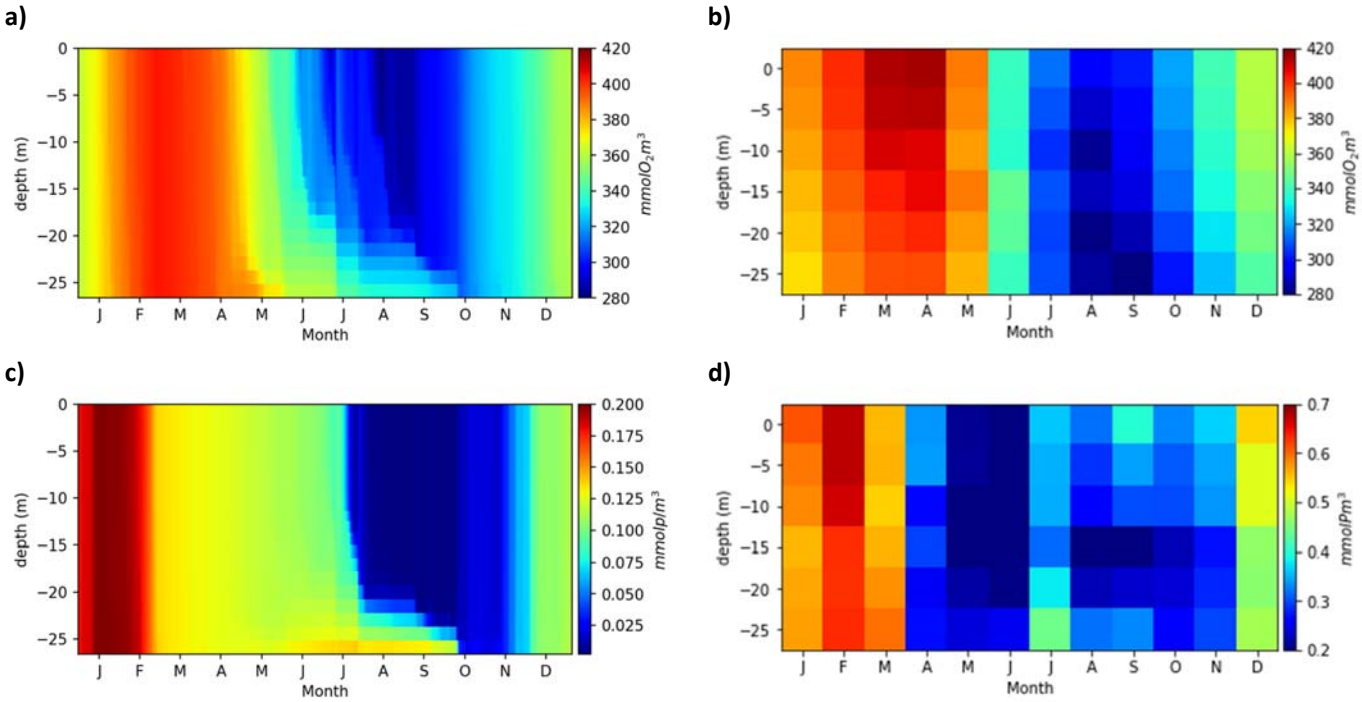

Figure 3.4.3: Hovmoller diagram for (a) simulated Oxygen (mmol o2/m^3) and (c) simulated phosphate (mmol p/m^3), while (b) and (d), respectively, indicate observed phosphate and Oxygen at the station Arkona for the period of January – December 2015.

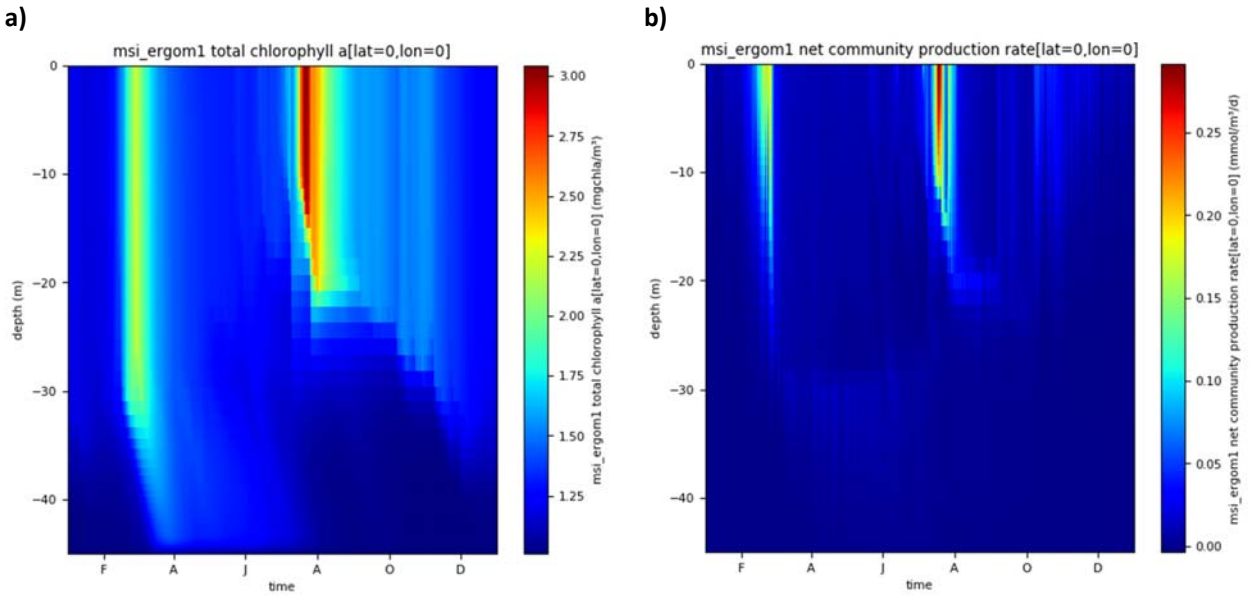

Figure 3.4.4: Hovmoller diagram for (a) total chlorophyll-a (mg chla/m^3) and (b) net primary production (mmol/m^3/d) at the station Arkona for the period of January – December 2015.

3.5 Task 2.3a: Setup of the prototype system for reference simulations at BATS.

Arthur Capet and Pierre Brasseur (IGE)

3.5.1 BATS case site

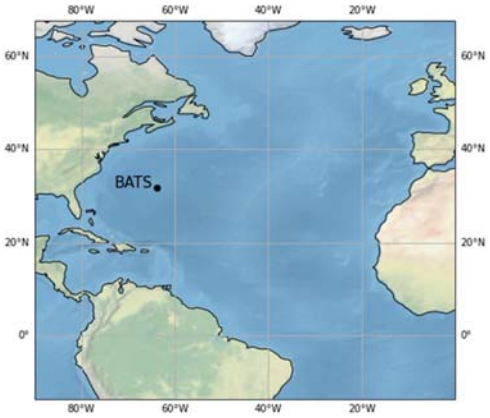

Figure 3.5.1 BATS station situation.

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 3.5.1), 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.

3.5.2 Setup of GOTM-FABM-PISCES at BATS

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 T.3.1a[4]. 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). Real-time forcing conditions were extracted from ECMWF ERA5 datasets for the simulation period (Hersbach et al., 2020). This framework can be obtained from documented testcase[5].

In-situ data were obtained from the ascii data file freely accessible for the BATS website[6]. 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.[7]

Oxygen, nitrate, phosphate, silicate, dissolved inorganic carbon, alkalinity, temperature and salinity were initialized for Jan 1st 2014, using the January climatology. A factor of 10% was applied to initialize

[4] https://github.com/BoldingBruggeman/fabm-pisces, last accessed Oct 15th 2021

[5] https://github.com/BoldingBruggeman/seamless-notebooks/tree/master/setups/bats, last accessed Oct 15th 2021

[6] http://bats.bios.edu/bats-data/, last accessed Oct 15th 2021

[7] https://github.com/plazzari/FABM_BATS, last accessed Oct 15th 2021

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 (eg. 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

3.5.3 Validation of PISCES at BATS

We favoured here visual assessment and discussion to systematic skill metrics, by comparing the 5 years of simulations to the repeated observed climatology for physics (Fig 3.5.2), oxygen (Fig.3.5.3), nutrients (Fig.3.5.4) and chlorophyll (Fig.3.5.5). The physical environment appears as well constrained, although winter mixing seems to reach excessive depths, in particular for 2016, 2017.

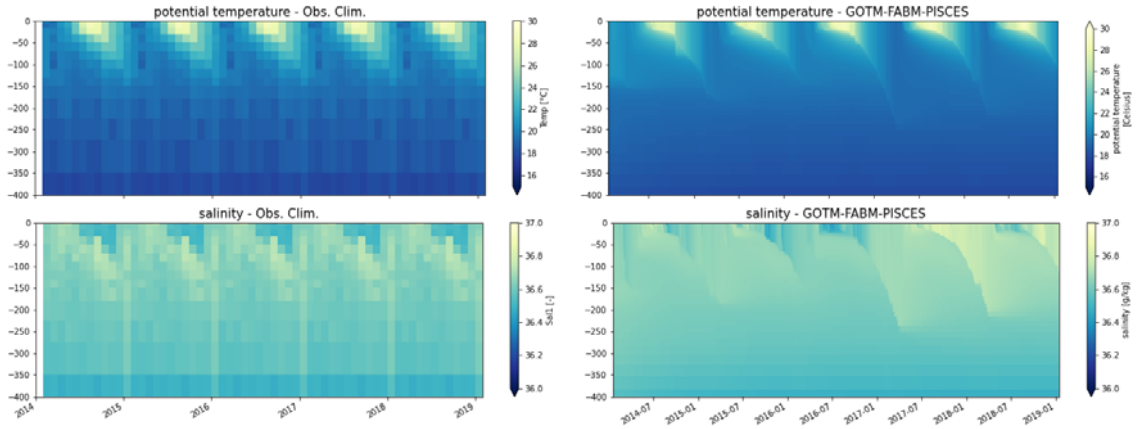

Figure 3.5.2 (Left) repeated climatology and (right) model results for potential temperature and salinity.

The general range of nutrients availability in the surface layer 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.

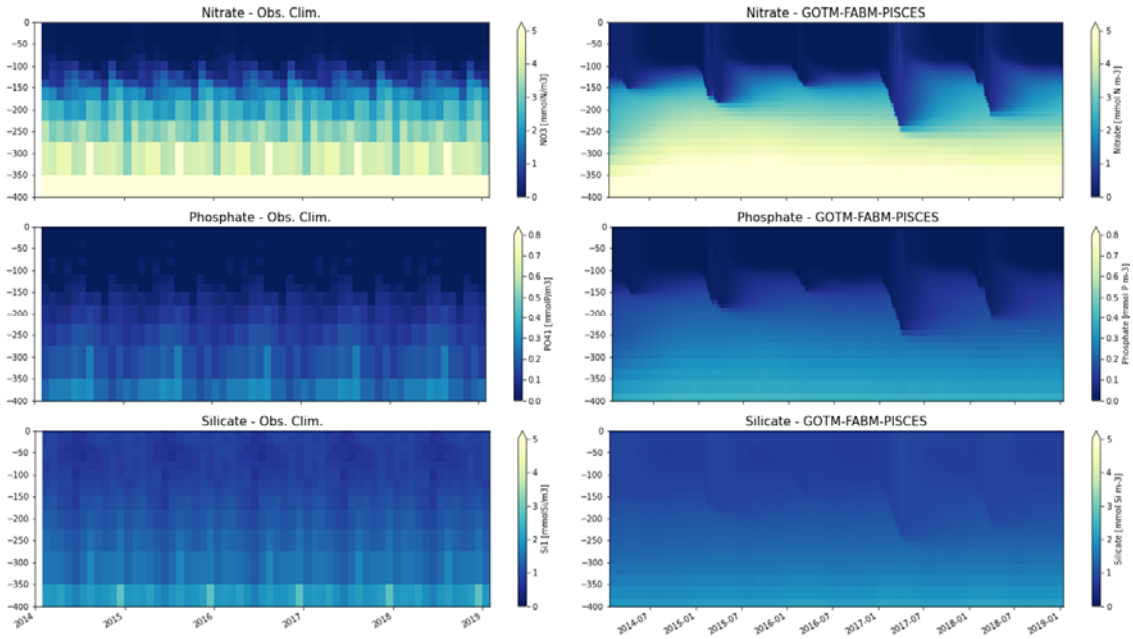

Figure 3.5.3 (Left) repeated climatology and (right) model results for nitrate, phosphate and silicate.

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. 3.5.4), which is also a maximum layer for CO2, is stable and does not increase nor decrease in its vertical extent.

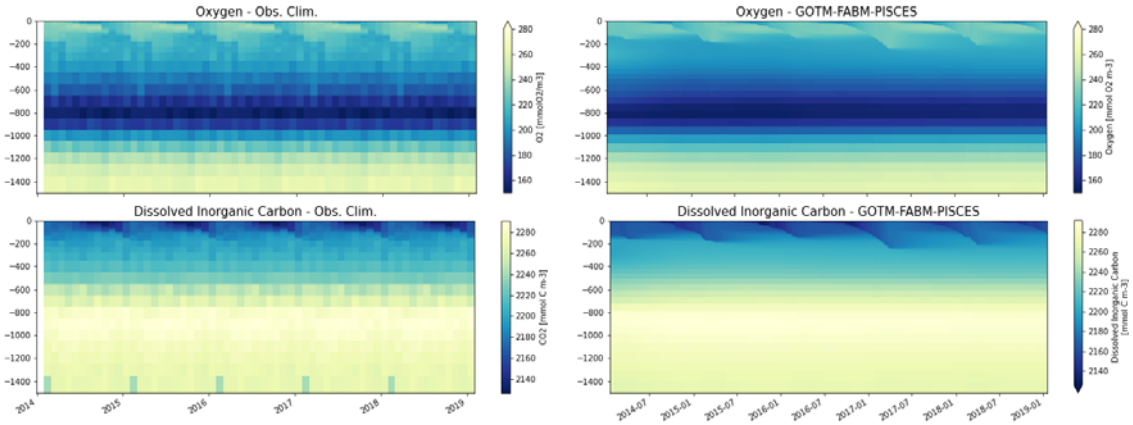

Figure 3.5.4 (Left) repeated climatology and (right) model results for oxygen and dissolved inorganic carbon.

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.

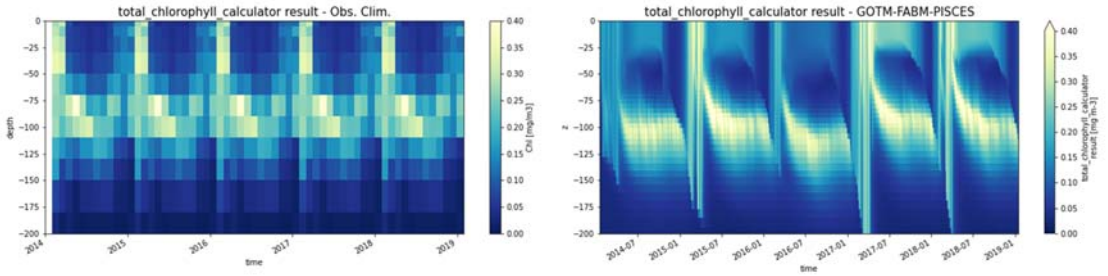

Figure 3.5.5 (Left) repeated climatology and (right) model results for chlorophyll.

Yet, net primary production seems in agreement, but rather on the lower side, with former in-situ estimates obtained in 2000 (but considered as representative of multi year average conditions, Bermuda Institute of Ocean Science, Fig. 3.5.6).

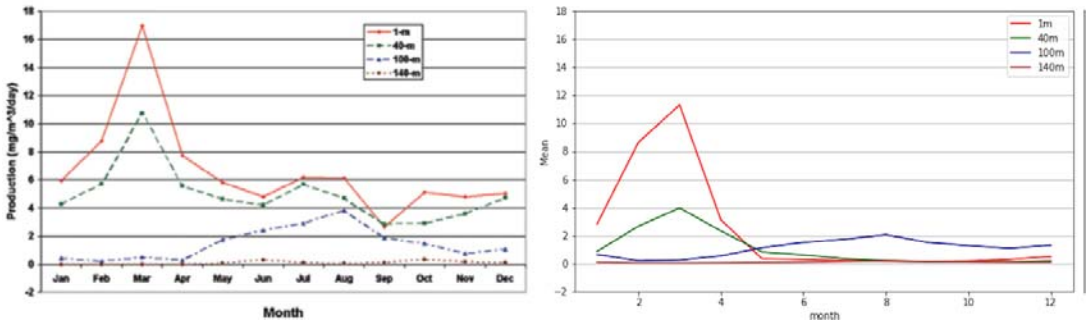

Fig 3.5.6 : Net primary production at BATS for different depths. (Left) As obtained from in-situ measurements [Bermuda Institute of Ocean Sciences], (Right) Mean 2015-2018 of the GOTM-FABM-PISCES simulation.

Analyses – To complete this overview, several diagnostics are depicted in Fig. 3.5.7, which were considered as relevant to characterize biogeochemical regimes and to compare various biogeochemical models of the prototype system (WP3).

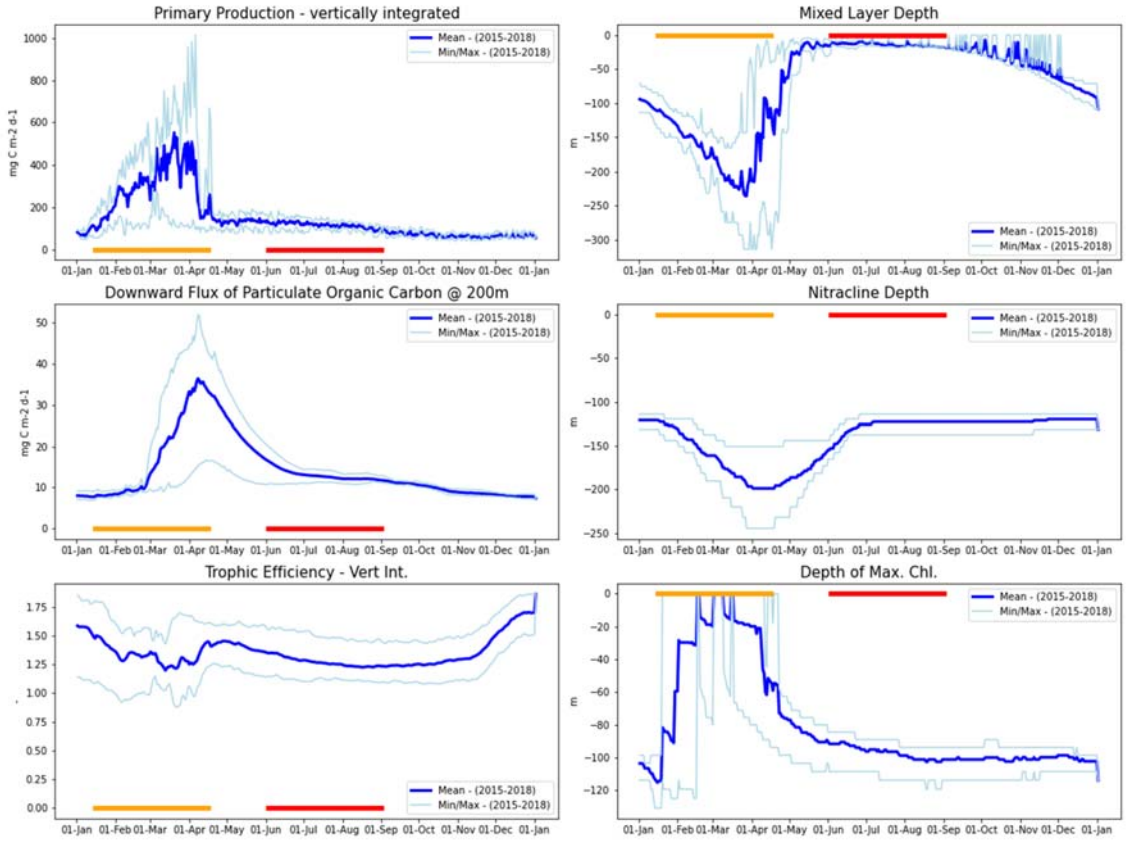

Figure 3.5.7 : Diagnostics are given as mean, min, and max value of the period 2015-2018. Yellow and red lines highlight the 3-months mixed and stratified regimes identified for T3.2 analyses. Nitracline depth is the depth where [NO3]>1µM. Trophic Efficiency is estimated as the ratio between vertically integrated (0-200m) zooplankton and phytoplankton carbon content.

3.6 Task 2.3a: Setup of the prototype system for reference simulations at BOUSSOLE and or Lagrangian data (BGC-Argo float).

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

The Mediterranean case study consists of two sites: BOUSSOLE buoy and pseudo-lagrangian BGC-Argo float. BOUSSOLE buoy data are complemented by DYFAMED data due to the proximity of the two mooring. Among all the possible BGC-Argo floats deployed in the Mediterranean Sea we selected as a test a BGC-Argo deployed in the oligotrophic eastern Mediterranean Sea as a contrasting site with respect to BOUSSOLE that is located in the mesotrophic north western Mediterranean Sea.

3.6.1 Description of the BOUSSOLE/DYFAMED site

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 area is located in the Ligurian sea, one of the sub-basins of the Western Mediterranean sea (Fig. 3.6.1a). 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.

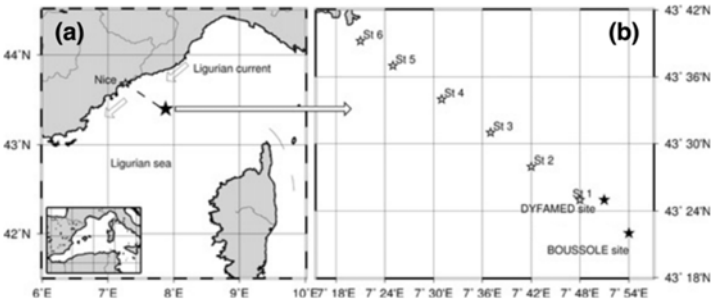

Figure 3.6.1 (a) The Northwestern Mediterranean Sea, with indication (black star) of the location of the work area. (b) Zoom from the general map, showing the position of the BOUSSOLE and the DYFAMED sites.

3.6.2 GOTM-FABM-BFM simulation at BOUSSOLE/DYFAMED

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 3.6.2 shows a general overview of model behaviour in terms of daily available irradiance at ocean surface (Fig. 3.6.2a), stratification and mixing (Fig. 3.6.2b-c) and the formation of a deep chlorophyll maximum (DCM)(Fig. 3.6.2d).

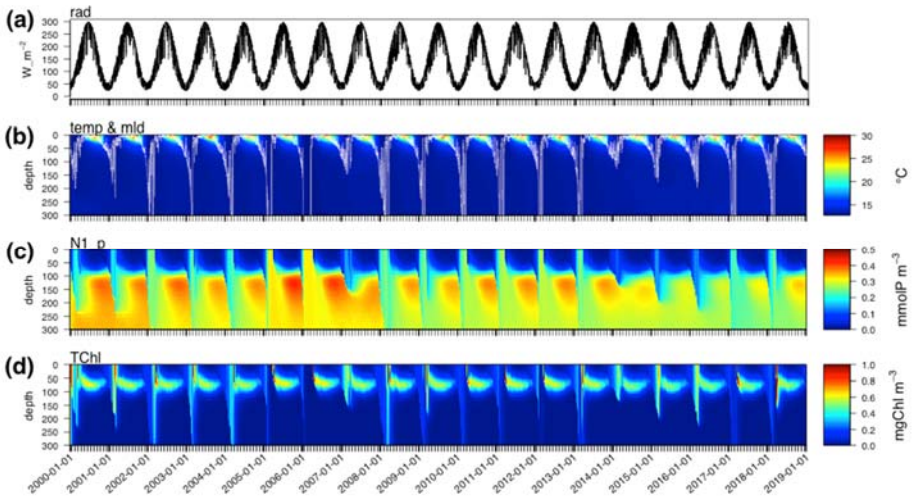

Figure 3.6.2 GOTM-FABM-BFM run at the BOUSSOLE location from 2000 to 2019: (a) Irradiance at ocean surface, and depth profiles of (b) temperature, (c) phosphate and (d) total chlorophyll.

Nutrients: comparison to the DYFAMED site (1991-2007).

Fig. 3.6.3 shows distribution of 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 period 2002-2007. Climatologies are computed by averaging observation at the 10 days basis and a common vertical discretization. Simulated values are consistent with the typical seasonal evolution and vertical gradients shown by the annual climatology of nutrients.

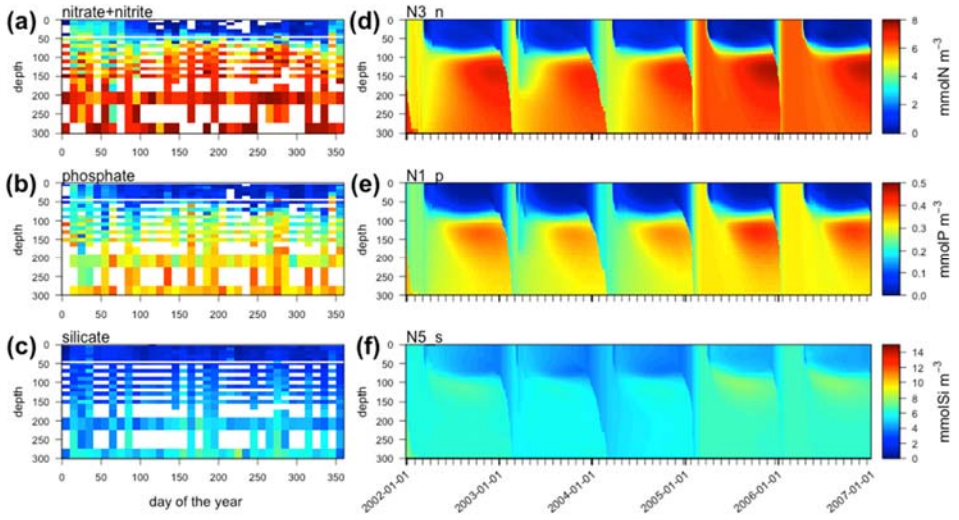

Figure 3.6.3 Hovmöller plots at Dyfamed site (left) and simulated by BFM (right) of (a, d) nitrate, (b, e) phosphate and (c, f) silicate.

Chlorophyll: comparison to the BOUSSOLE site (2001-2017).

Figure 3.6.4 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.

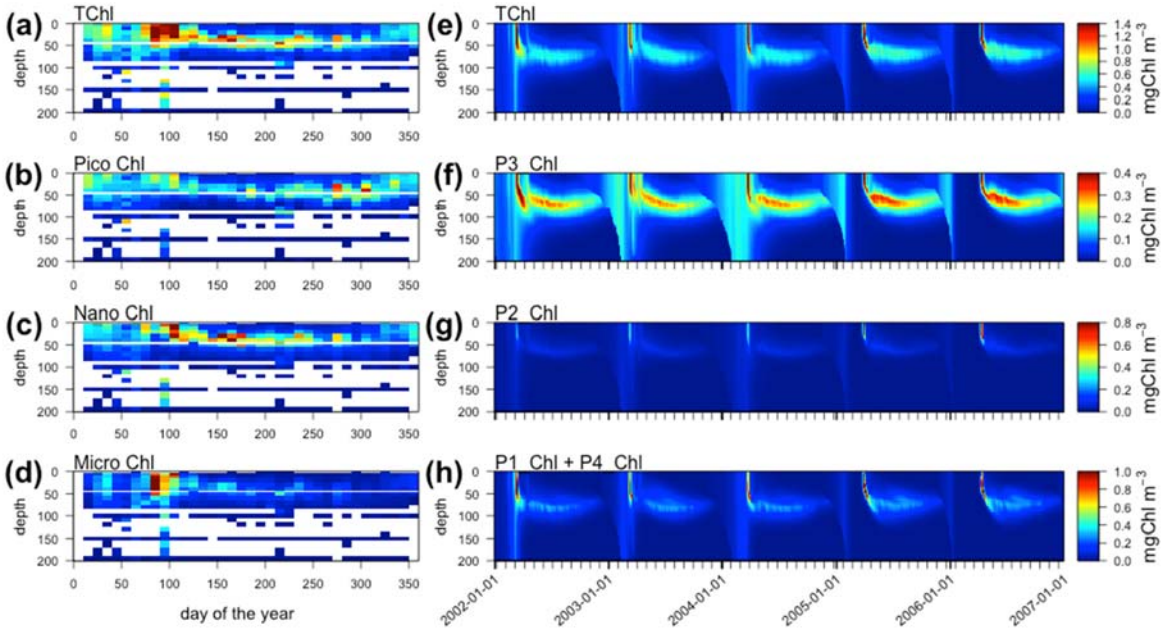

Figure 3.6.4 Hovmöller plots at Boussole site (left) and simulated by BFM (right) of (a, e) total chlorophyll, and chlorophyll of (b, f) pico- (c, g) nano- and (d, h) microphytoplankton.

3.6.3 GOTM-FABM-BFM simulation at the pseudo-lagrangian BGC-Argo

The second Mediterranean case study consists of the pseudo-Lagrangian simulations to reconstruct the biogeochemistry along BGC-Argo float data. 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, which 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.

We used the monochromatic light model for these tests accounting only for chlorophyll self-shading.

As an example of the BGC-Argo float implementation and in order 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 area tracked by the BGC-Argo float is typically characterized by lower nutrient content with respect to the BOUSSOLE site. However, mixing events due to Etesian winds, as shown in the model results (Fig 3.6.5b and Fig.3.6.6b), produced injections of nutrients from the deep layer (Fig. 3.6.5f and Fig 3.6.6ef) that clearly affected model chlorophyll (Fig. 3.6.5d and Fig. 3.6.6e). The comparison of the model results with BGC-Argo data of chlorophyll (Fig. 3.6.6e) corroborated the robustness of the model results and of the pseudo-lagrangian approach adopted. The new implementation based on GOTM-FABM-BFM is consistent with published results (Terzić et al., 2019). It is worth to note that BGC-Argo chlorophyll is not assimilated in the pseudo-lagrangian simulations, indeed it is a totally independent dataset.

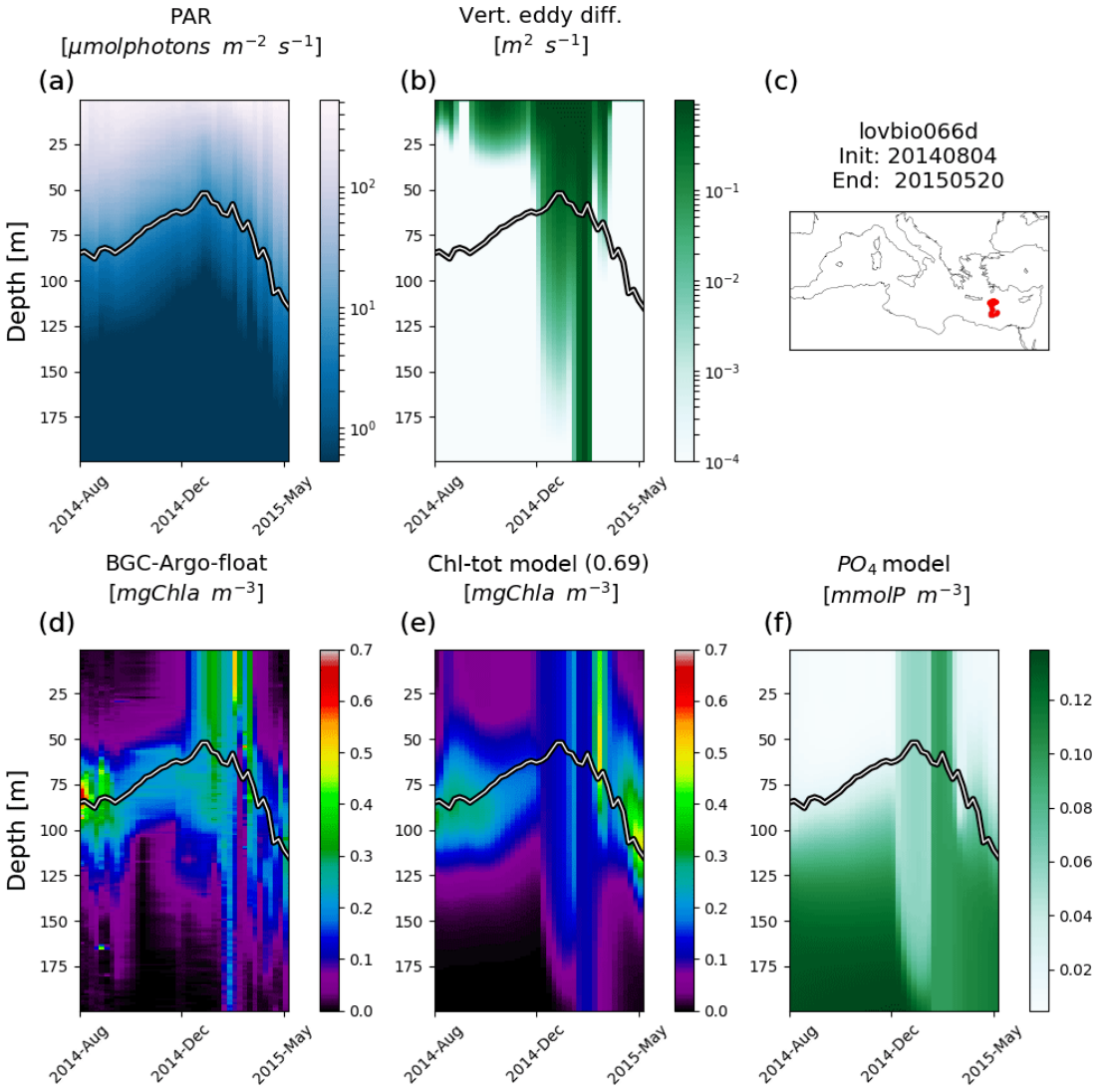

Figure 3.6.5: Hovmöller diagrams of BGC-Argo float lovbio066d (WMO code 6901655) comparing measured chlorophyll results and simulated ones. The six-image composite is organized as follows: panels (a), (b), and (c) show PAR, vertical eddy diffusivity, and the float trajectory; panels (d), (e), and (f) show Chl derived from fluorescence measurements, simulated Chl, and phosphate. The thick black–white line indicates the depth where PAR equals 5.8 µmol photons m^{-2} s^{-1} (Mignot et al., 2014). The Figure has been copied from the open access source (Terzić et al., 2019).

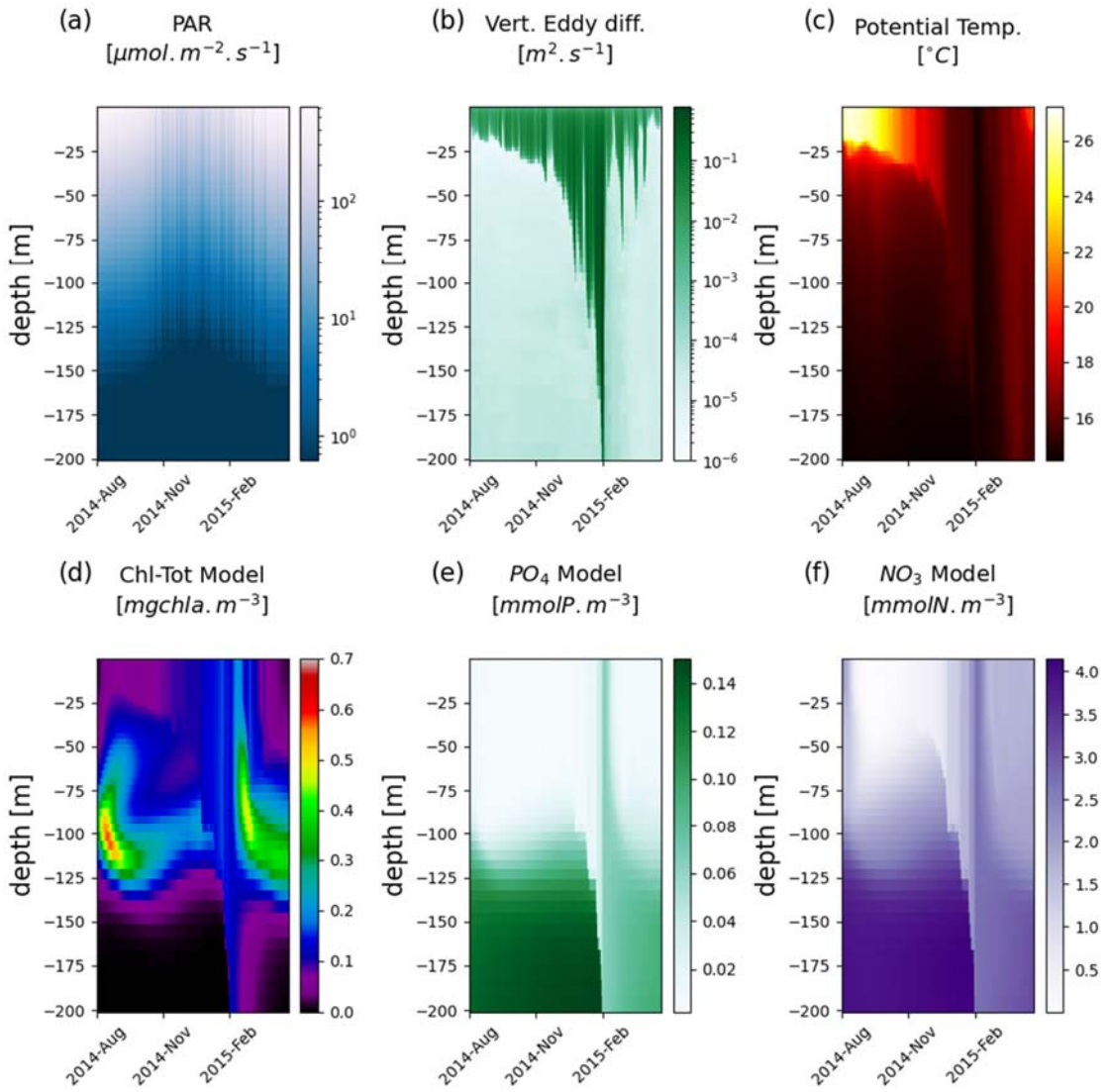

Figure 3.6.6: Hovmöller diagrams of BGC-Argo float lovbio066d (WMO code 6901655) produced using GOTM-FABM-BFM comparing measured chlorophyll results and simulated ones. The six-image composite is organized as follows: panels (a), (b), and (c) show PAR, vertical eddy diffusivity, and potential temperature; panels (d), (e), and (f) show, chlorophyll, phosphate, and nitrate.

3.7 Task 2.3a: Setup of the prototype system for reference simulations at Station L4

Josef Skakala and Stefano Ciavatta (PML)

L4 is a mesotrophic location in the SmartSound region in the English Channel (see Fig.3.7.1). The location is operated as part of Western Channel Observatory (WCO) and provides weekly measurements for biogeochemical variables of interest (e.g. pigments, nutrients, optical data, data for phytoplankon, 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 (for the surface chlorophyll see Fig.3.7.2).

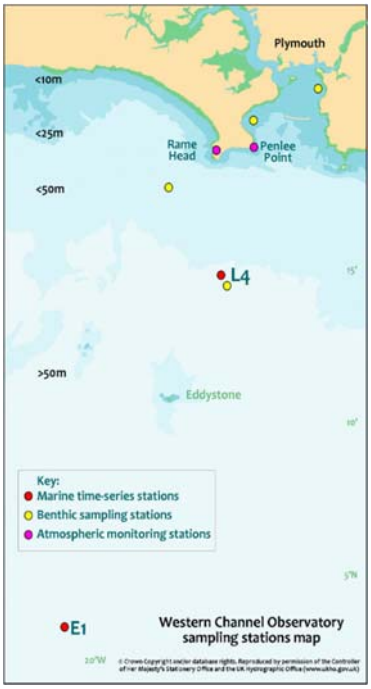

Fig.3.7.1: The L4 location as part of WCO facilities in the SmartSound region in the English Channel. The picture is taken from the WCO website (https://www.westernchannelobservatory.org.uk/).

The GOTM set-up for the L4 station has already been largely established in previous studies (Butenschön et al., 2016; Powley et al., 2020). The current set-up is based on 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 observed temperature and salinity, whilst biogeochemistry is typically spun up from a vertically constant values in the fully mixed period (e.g. in January). Some of the biogeochemical initial values are supplemented from the observed climatology. The physics (temperature and salinity) is relaxed to the observed data obtained from the Western Channel Observatory (for the simulated values, see Fig.3.7.3). To prevent

spurious trends in nutrient variables (e.g. in nitrogen due to denitrification) the longer term simulations are also being relaxed towards the observed L4 nutrient climatologies. All the required atmospheric and observation physical data are available for the 2002-2020 period. The configuration used here has been validated in the previous literature (Powley et al., 2020), but it has also been carefully verified within this project that it produces realistic simulations, when combined with specific biogeochemical models (see Fig.3.7.2). Furthermore, we have demonstrated (not shown here) that the methodology established at L4, including a 7 year spin-up time, is sufficient to provide the required-quality initialization for the sensitivity and observability analysis in WP3.2. In more general terms, a good quality L4 prototype has been established in WP2, ready to be used for further developments in SEAMLESS.

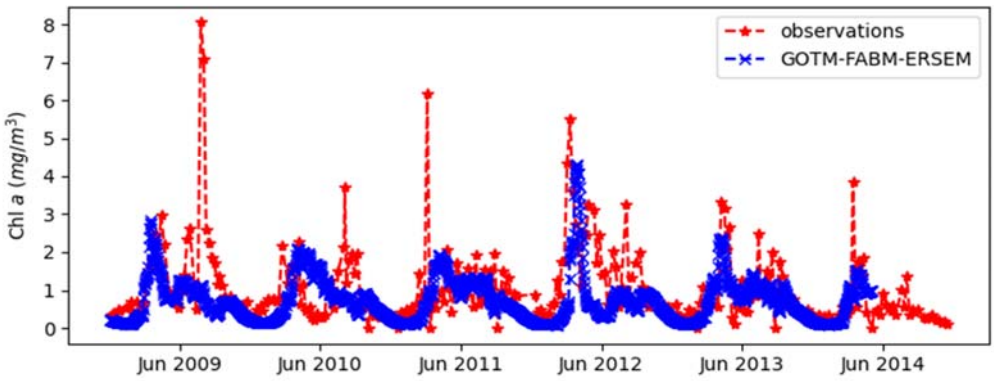

Fig.3.7.2: The 2012-2018 L4 observations for total surface chlorophyll a (in mg/m3).

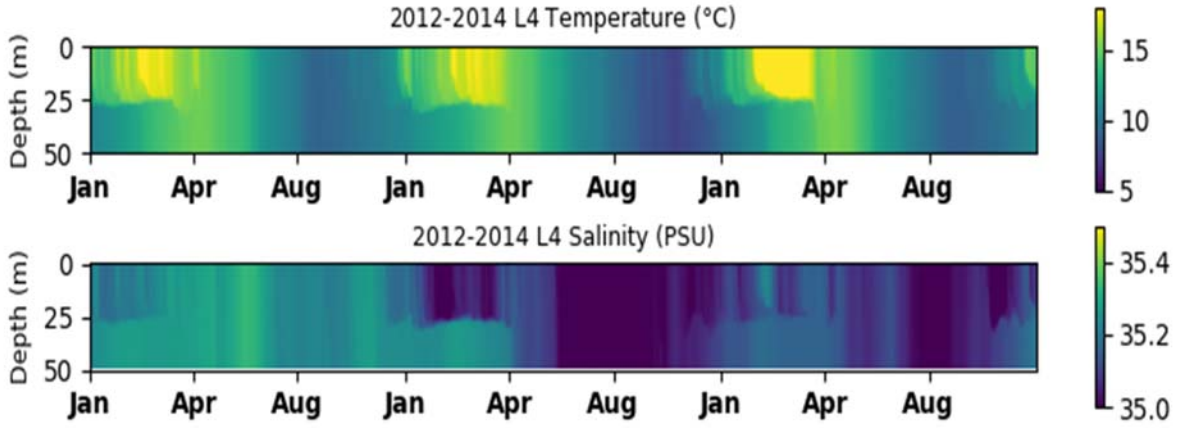

Fig.3.7.3: The temperature and salinity GOTM simulations for L4 in 2012-2014 period.

3.8 Task 2.3a: Setup of the prototype system for reference simulations at M station

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.

3.8.1 About Station M

St.M is located at the eastern periphery of the Norwegian Basin which represents pelagic biogeochemical dynamics of the Norwegian Sea. St.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.

3.8.2 ECOSMO setup updates for Station M

a. upgrading phytoplankton growth rate parameterization

We are at the process of 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-REF) 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 light limitation on growth rates is parameterized as the following, which does not include chlorophyll dependency:

$$\tanh(PAR * \alpha) \tag{1}$$

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

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

Eq2 allows the model to simulate higher light-limited growth rates under low PAR conditions, 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. The effects are summarized in Fig.3.8.1, where we present an example 1D simulation at St.M at a year of high data availability (1991). Significant changes depicted in Fig.3.8.1 are (1) ECO-NEW has earlier bloom, (2) earlier surface Chl maximum and (3) deeper chlorophyll production. All of these changes are in better agreement with the in-situ data. In the case of ECO-NEW, a deep chlorophyll maxima layer is evident in summer period.

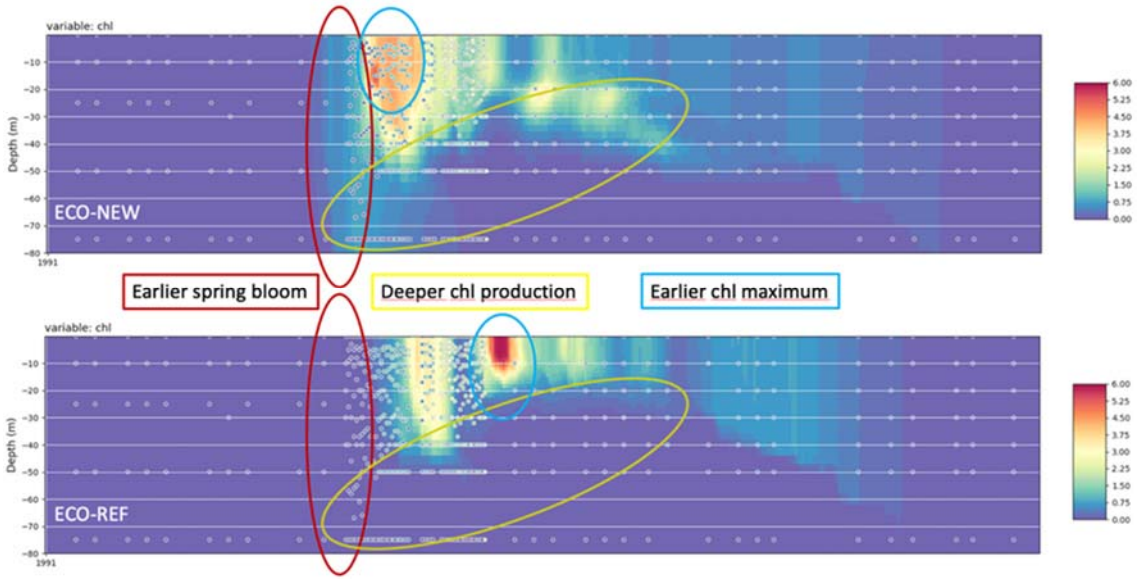

Figure 3.8.1. ECO-NEW (top) and ECO-REF (bottom) configurations are compared to in situ chlorophyll a data at Station-M, where in situ data is depicted in markers matching the timing and depth of measurement. The major differences between the configurations are highlighted.

b. Impact of nutrient stream by the Norwegian Atlantic Current (NAC)

Being initialized with climatology nutrient at 2010 January 1st, GOTM-FABM-ECOSMO with ECO-NEW configuration was spinned-up with ECMWF hourly atmospheric forcing for 9 years first. Result of 2019 simulation is plotted in Fig.3.8.2. We have observed that the sub-surface (100m-400m) nutrients during the pre-bloom period are drifted to lower values compared to their climatological values. Since this sub-surface nutrient stream at St.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 St.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 color and Argo-float data in the Norwegian Sea.

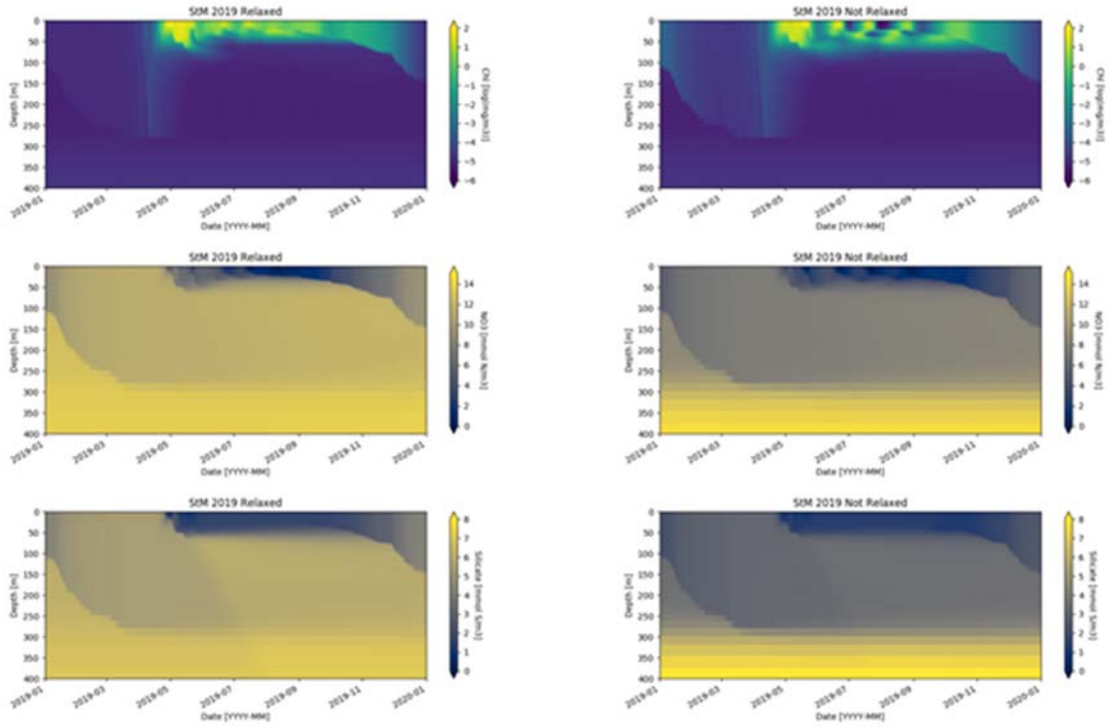

Figure 3.8.2. One year simulation of GOTM-FABM-ECOSMO at St.M in 2019. Left column) with nutrient nudging during spinning up run. Right column) without nutrient nudging. Plotted variables are Chl-a (top), Nitrate (middle) and Silicate (bottom).

References

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