The Biogeochemical Flux Model (BFM)

Equation Description and User Manual

BFM version 5 (BFM-V5)

The BFM System Team
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Release 1.0, March 2013
—— BFM Report series N. 1 ——

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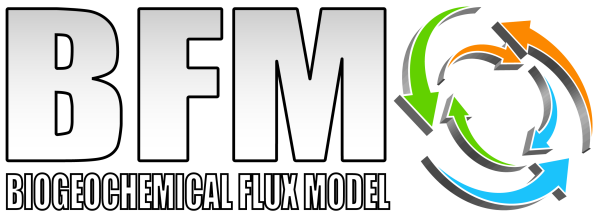

This document should be cited as:
Vichi M., Cossarini G., Gutierrez Mlot E., Lazzari P., Lovato T., Mattia G., Masina S., McKiver W., Pinardi N., Solidoro C., Zavatarelli M. (2013) The Biogeochemical Flux Model (BFM): Equation Description and User Manual. BFM version 5 (BFM-V5). Release 1.0; BFM Report series N. 1. March 2013, Bologna, Italy, http://bfm-community.eu, pp. 87

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Introduction

Synopsis

This report is divided in two main parts. The first part contains an extended description of the Biogeochemical Flux Model (BFM version 5) equations and as such it describes different parameterizations that can be used to simulate biogeochemical processes in the marine system. Part II describes the model set-up, compilation and execution of the standard test cases. It also provides the major technical implementation of the model and information to understand the code structure. This part gives examples of the possible diagnostics that can be activated and illustrates advanced features that allow the user to modify the model adding new state variables and components.

The BFM is a direct descendant of the European Regional Seas Ecosystem Model (ERSEM) and shares most of its characteristics with the original formulations (Baretta et al., 1995; Baretta-Bekker et al., 1997). The major difference is that BFM focuses more on the biogeochemistry of lower trophic levels in marine ecosystems than on trophic food webs, which is where it takes its name. The philosophy of the BFM and the mathematical formulation applied throughout the book are described in Vichi et al. (2007b). The users familiar with ERSEM will find that the code notation described by Blackford and Radford (1995) has not changed substantially and that the state variables are indicated with the same naming convention. Vichi et al. (2007b) have extended this notation making it formally consistent and additional variables have been named accordingly.

The structure of the code was instead extensively modified with respect to the original ERSEM code. The major reason for a full rewriting lied in the growing need to couple biogeochemical processes with hydrodynamical model of various forms and to allow a modular expansion of the number and type of state variables in modern coding standards. The necessity to have a flexible system which can be embedded in the existing state-of-the-art ocean general circulation models (OGCM) required a re-organization of the structure, yet the fundamentals of the coupling strategy are very similar to the first coupled implementations.

The BFM module

This report documents the BFM equations for the standalone pelagic configuration of the code that solves the reaction part of the general equations for biogeochemical tracers in the marine environment. The state variables presented in Part I are historically derived from the pelagic component of ERSEM and represent the standard set of transformations for the major chemical constituents. The BFM by construction solves the cycles of C, O, N, P, Si in the lower trophic levels of marine ecosystems and it also allows the inclusion of the Fe cycle and carbonate chemistry by means of user-controlled flags. Different parameterizations are proposed for the various functional groups as they have been demonstrated valid in certain model applications. Given the inherent empirical nature of biogeochemical modelling, the proposed parameterizations are given "as they are" and it is up to the user to decide which one to use given the specific application. The modular implementation of the BFM allows to implement new parameterizations and new state variables.

The BFM module can be easily coupled with different ocean models and some of these couplings will be illustrated in separate documents. The equations of Part I consider no vertical or horizontal processes and the system is solved as a set of ordinary differential equations. At the heart of the BFM module is the possibility to increase

the number of components, as for instance implementing any number of phytoplankton groups that share the same dynamical terms but differ in term of parameter and parameterization choices. The user interested in this feature, in the modification of the model layout and in the definition of specific diagnostics will find in Part II all the required information. The reference test cases will be presented in the STANDALONE implementation, which is a time-dependent box model with a given depth where pelagic processes are assumed homogeneous.

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Acknowledgments

The code support and development is currently done by the BFM System Team whose members are listed on the BFM web site (http://bfm-community.eu). The initial core of the BFM system software was developed by Piet Ruardij and Marcello Vichi. The BFM system team is grateful to Job Baretta, Hanneke Baretta-Bekker, Piet Ruardij and Wolfgang Ebenhoeh for their contribution to the science of biogeochemical modelling.

Part I.

The BFM Equations

1. The formalism of the BFM equations

The BFM equations are written following the notation proposed by Vichi et al. (2007b), which is briefly summarized in this section. The reader is referred to Vichi et al. (2007b) for a more theoretical viewpoint on the extension of the ERSEM approach to the system state variables of the plankton ecosystem. As shown in Tab. 1.1, each variable is mathematically expressed by a multi-dimensional array that contains the concentrations of reference chemical constituents. We use a superscript indicating the CFF for a specific living functional group and a subscript for the basic constituent. For instance, diatoms are LFG of producers and comprise 6 living CFFs written as

$$P_i^{(1)} \equiv \left(P_c^{(1)}, P_n^{(1)}, P_p^{(1)}, P_s^{(1)}, P_f^{(1)}, P_l^{(1)}\right).$$

The standard model resolves 4 different groups for phytoplankton $P^{(j)}$, $j = 1,2,3,4$ (diatoms, autotrophic nanoflagellates, picophytoplankton and large phytoplankton), 4 for zooplankton $Z^{(j)}$, $j = 3,4,5,6$ (carnivorous and omnivorous mesozooplankton, microzooplankton and heterotrophic nanoflagellates), 1 for bacteria, 7 inorganic variables for nutrients and gases (phosphate, nitrate, ammonium, silicate, reduction equivalents, oxygen, carbon dioxide) and 10 organic non-living components for dissolved and particulate detritus (cf.. Tab. 1.1 and Fig. 1.1). The state variable nitrate is assumed here to be the sum of both nitrate and nitrite. Reduction equivalents represent all the reduced ions produced under anaerobic conditions. This variable was originally used only in the benthic nutrient regeneration module of ERSEM (Ruardij and Van Raaphorst, 1995) but was extended to the water column in Vichi et al. (2004). In this approach, all the nutrient-carbon and chlorophyll-carbon ratios are allowed to vary within their given ranges and each component has a distinct biological time rate of change.

Following Vichi et al. (2007b) the dynamical equations are written in two forms: 1) rates of change form; and 2) explicit functional form. In "rates of change form", the biogeochemical reaction term a generic state variable C is written as:

$$\left.\frac{dC}{dt}\right|_{bio} = \sum_{i=1,n}\sum_{j=1,m}\left.\frac{dC}{dt}\right|_{V_i}^{e_j}, \qquad (1.0.1)$$

where the right hand side contains the terms representing significant processes for each living or non-living component. The superscripts e_j are the abbreviations indicating the process which determines the variation. In Table 1.2 we report the acronyms of the processes used in the superscripts. The subscripts V_i indicate the state variable involved in the process. If $V = C$, we refer to intra-group interactions such as cannibalism.

When a term is present as a source in one equation and as a sink in another, we refer to it following this equivalent notation:

$$\left.\frac{dC}{dt}\right|_{V}^{e} = -\left.\frac{dV}{dt}\right|_{C}^{e}. \qquad (1.0.2)$$

In "functional process form", the formulation of the dynamic dependencies on other variables is made explicit, *i.e.*: all the rates of change in (1.0.1) are given in the complete functional parameterization. Although this is the more complete mathematical form, it is more difficult to read and interpret at a glance, especially when trying to distinguish which processes affect the dynamics of which variable . All equations in this Part will be presented both in rate of change and in functional process forms.

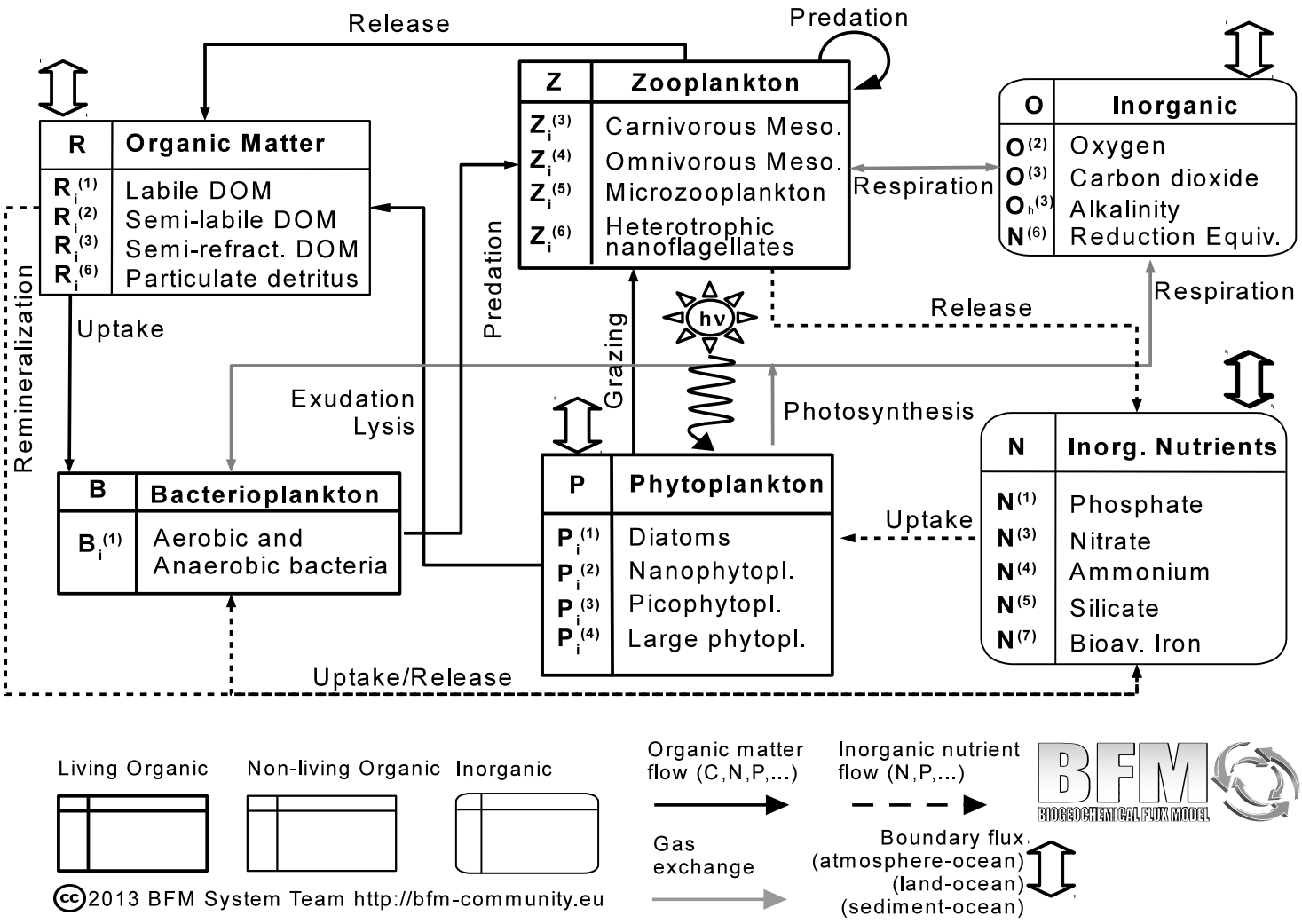

Figure 1.1.: Scheme of the state variables and pelagic interactions of the reference STANDALONE model. Living components are indicated with bold-line square boxes, non-living organic components with thin-line square boxes and inorganic components with rounded boxes (modified after Blackford and Radford (1995) and Vichi et al. (2007b)).

Variable	Code	Type	Const.	Units	Description
$N^{(1)}$	N1p	IO	P	mmol P m^{-3}	Phosphate ()
$N^{(3)}$	N3n	IO	N	mmol N m^{-3}	Nitrate ()
$N^{(4)}$	N4n	IO	N	mmol N m^{-3}	Ammonium ()
$N^{(5)}$	N5s	IO	Si	mmol Si m^{-3}	Silicate ()
$N^{(6)}$	N6r	IO	R	mmol S m^{-3}	Reduction equivalents, HS^-
$N^{(7)}$	N7f	IO	Fe	μmol Fe m^{-3}	Reduction equivalents, HS^- (mmol S m^{-3}r)
$O^{(2)}$	O2o	IO	O	mmol O_2 m^{-3}	Dissolved Oxygen
$O^{(3)}$	O3c	IO	C	mg C m^{-3}	Dissolved Inorganic Carbon
$O^{(5)}$	O3h	IO	-	mmol Eq m^{-3}	Total Alkalinity
$P_i^{(1)}$	P1[cnpslf]	LO	C N P Si Chl Fe	mg C m^{-3}, mmol N-P-Si m^{-3}, mg Chl-*a* m^{-3}, μmol Fe m^{-3}	Diatoms
$P_i^{(2)}$	P2[cnplf]	LO	C N P Chl Fe	mg C m^{-3}, mmol N-P m^{-3}, mg Chl-*a* m^{-3}, μmol Fe m^{-3}	NanoFlagellates
$P_i^{(3)}$	P3[cnplf]	LO	C N P Chl Fe	mg C m^{-3}, mmol N-P m^{-3}, mg Chl-*a* m^{-3}, μmol Fe m^{-3}	Picophytoplankton
$P_i^{(4)}$	P4[cnplf]	LO	C N P Chl Fe	mg C m^{-3}, mmol N-P m^{-3}, mg Chl-*a* m^{-3}, μmol Fe m^{-3}	Large phytoplankton
B_i	B1[cnp]	LO	C N P	mg C m^{-3}, mmol N-P m^{-3}	Pelagic Bacteria
$Z_i^{(3)}$	Z3[cnp]	LO	C N P	mg C m^{-3}, mmol N-P m^{-3}	Carnivorous Mesozooplankton
$Z_i^{(4)}$	Z4[cnp]	LO	C N P	mg C m^{-3}, mmol N-P m^{-3}	Omnivorous Mesozooplankton
$Z_i^{(5)}$	Z5[cnp]	LO	C N P	mg C m^{-3}, mmol N-P m^{-3}	Microzooplankton
$Z_i^{(6)}$	Z6[cnp]	LO	C N P	mg C m^{-3}, mmol N-P m^{-3}	Heterotrophic Flagellates
$R_i^{(1)}$	R1[cnpf]	NO	C N P Fe	mg C m^{-3}, mmol N-P m^{-3}, μmol Fe m^{-3}	Labile Dissolved Organic Matter
$R_c^{(2)}$	R2c	NO	C	mg C m^{-3}	Semi-labile Dissolved Organic Carbon
$R_i^{(3)}$	R3c	NO	C	mg C m^{-3}	Semi-refractory Dissolved Organic Carbon
$R_i^{(6)}$	R6[cnpsf]	NO	C N P Si Fe	mg C m^{-3}, mmol N-P-Si m^{-3}, μmol Fe m^{-3}	Particulate Organic Detritus

Table 1.1.: List of the reference state variables for the pelagic model. Type legend: IO = Inorganic; LO = Living organic; NO = Non-living organic. The subscript *i* indicates the basic components (if any) of the variable, e.g. $P_i^{(1)} \equiv \left(P_c^{(1)}, P_n^{(1)}, P_p^{(1)}, P_s^{(1)}, P_l^{(1)}, P_f^{(1)}\right)$.

Abbreviation	Process
gpp	Gross primary production
rsp	Respiration
prd	Predation
rel	Biological release: Egestion, Excretion
exu	Exudation
lys	Lysis
syn	Biochemical synthesis
nit/denit	Nitrification, denitrification
scv	Scavenging
rmn	Biochemical remineralization

Table 1.2.: List of all the abbreviations used to indicate the physiological and ecological processes in the equations

2. The pelagic plankton model

2.1. The environmental parameters affecting biological rates

This section describes the dependencies of the pelagic biogeochemical processes from the physical environment. The BFM has defined a set of environmental variables that are provided by external data or by a physical model (Tab.). The local coupling between physics and biogeochemistry is realized explicitly through surface irradiance and temperature. Temperature regulates all physiological processes in the model and its effect, denoted by f^T, is parameterized in this non-dimensional form

$$f^T = Q_{10}^{\frac{T-10}{10}} \tag{2.1.1}$$

where the Q_{10} coefficient is different for each functional process considered.

Light is fundamental for primary producers and the energy source for photosynthesis is the downwelling amount of the incident solar radiation at the sea surface. We assume that the Photosynthetic Available Radiation (PAR) E_{PAR} (the notation of Sakshaug et al., 1997, is used here) is parameterized according to the Lambert-Beer formulation with depth-dependent extinction coefficients

$$E_{PAR}(z) = \varepsilon_{PAR}\, Q_S\, e^{\lambda_w z + \int_z^0 \lambda_{bio}(z')dz'} \tag{2.1.2}$$

ε_{PAR} is the coefficient determining the fraction of PAR in Q_S. Light propagation takes into account the extinction due to suspended particles, λ_{bio}, and λ_w as the background extinction of water. The biological extinction is written as

$$\lambda_{bio} = \sum_{j=1}^{4} c_{_{P(j)}} P_l^{(j)} + c_{_{R(6)}} R_c^{(6)} \tag{2.1.3}$$

where the extinctions due to the concentration of phytoplankton chlorophyll and particulate detritus are considered (see Sec. 2.2 and 2.5). The c constants are the specific absorption coefficients of each suspended substance (Tab. 2.2 and 2.8), which may also include extinction by suspended sediments (not currently resolved by the BFM but can be included from an external model).

The short-wave surface irradiance flux Q_S is obtained generally from data or from an atmospheric radiative transfer model. Three types of forcings are allowed depending on the value of `LightPeriodFlag` in `Pelagic_Ecology.nml`:

1. Instantaneous irradiance (`LightPeriodFlag=1`)
2. Daily average (`LightPeriodFlag=2`)
3. Daylight average (with explicit photoperiod, `LightPeriodFlag=3`)

The discretized irradiance E_{PAR}^k is located at the top of each layer k, and three different choices are available according to the parameter `LightLocationFlag` in `Pelagic_Ecology.nml`: light at the upper interface $E_{PAR} = E_{PAR}^k$, light in the middle of the cell as in Lazzari et al. (2012),

$$E_{PAR} = E_{PAR}^k \exp\left(-\lambda^k \frac{\Delta z^k}{2}\right) \tag{2.1.4}$$

and integrated light over the level depth as in Vichi et al. (2007b):

$$E_{PAR} = \frac{E_{PAR}^k}{\lambda^k \Delta z^k}\left(1 - \exp\left(-\lambda^k \Delta z^k\right)\right) \tag{2.1.5}$$

When needed for physiological computations, the value is converted from W m^{-2} to the unit of μE m^{-2} s^{-1} with the constant factor 1/0.215 (Reinart et al., 1998).

Symbol	Code	Unit	**Description**
T	ETW	^{o}C	Sea water salinity
S	ESW	(-)	Sea water temperature
ρ	ERHO	Kg m^{-3}	Sea water density
E_{PAR}	EIR	μE m^{-2}s^{-1}	Photosynthetically available radiation
S_S	ESS	g m^{-3}	Suspended sediment load
W_{atm}	EWIND	m s^{-1}	Wind speed
F_{ice}	EICE	(-)	Sea ice fraction
Φ	SUNQ	hours	Daylight length

Table 2.1.: Mathematical and code symbols, units and description of the environmental state variables defined in the model.

2.2. Phytoplankton

Primary producers are divided in four principal sub-groups coarsely representing the functional spectrum of phytoplankton in marine systems. The operational model definitions of the phytoplankton groups are:

- diatoms ($P_i^{(1)}$), ESD = 20-200μ, unicellular eukaryotes enclosed by a silica frustule eaten by micro- and mesozooplankton;
- autotrophic nanoflagellates ($P_i^{(2)}$), ESD = 2-20μ, motile unicellular eukaryotes comprising smaller dinoflagellates and other autotrophic microplanktonic flagellates eaten by heterotrophic nanoflagellates, micro- and mesozooplankton;
- picophytoplankton ($P_i^{(3)}$), ESD = 0.2-2μ, prokaryotic organism generally indicated as non-diazotrophic autotrophic bacteria such as *Prochlorococcus* and *Synechococcus*, but also mixed eukaryotic species (Worden et al., 2004), mostly preyed by heterotrophic nanoflagellates;
- large, slow-growing phytoplankton ($P_i^{(4)}$), ESD > 100μ, that represents a wide group of phytoplankton species, also comprising larger species belonging to the previous groups (for instance dinoflagellates) but also those that during some period of the year develop a form of (chemo)defense to predator attack. This group generally has low growth rates and small food matrix values with respect to micro- and mesozooplankton groups.

The processes parameterized in the biological source term are gross primary production (*gpp*), respiration (*rsp*), exudation (*exu*), cell lysis (*lys*), nutrient uptake (*upt*), predation (*prd*) and biochemical synthesis (*syn*). All the phytoplankton groups share the same form of primitive equations, but are differentiated in terms of the values of the physiological parameters.

Phytoplankton in the model is composed of several constituents and the related dynamical equations (Box 2.1): some of them are mandatory (C, N, P), that is they are required to compute physiological terms, and some others are required for specific groups (like Si in diatoms) or they are optional such as the Chl and Fe constituents. The inclusion of Fe is a typical example of the model flexibility as it allows to have an additional multiple-nutrient limitation term without affecting the other parameterizations (see Sec. 2.2.8).

When Chl constituent is not used (see Sec. 2.2.7), light acclimation in phytoplankton can be described by means of the optimal light property as proposed by Ebenhöh et al. (1997). The notation remains mostly unchanged but in this case the variable $\hat{P}_l$ indicates the optimal light level to which phytoplankton is acclimated and the alternative equation to (2.2.1d) is given in Sec. 2.2.7.

Equation Box 2.1 Phytoplankton equations

$$\left.\frac{dP_c}{dt}\right|_{bio} = \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} - \left.\frac{dP_c}{dt}\right|_{R_c^{(2)}}^{exu} - \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{rsp} - \sum_{j=1,6} \left.\frac{dP_c}{dt}\right|_{R_c^{(j)}}^{lys} - \sum_{k=4,5,6} \left.\frac{dP_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.2.1a}$$

$$\left.\frac{dP_n}{dt}\right|_{bio} = \sum_{i=3,4} \left.\frac{dP_n}{dt}\right|_{N^{(i)}}^{upt} - \sum_{j=1,6} \left.\frac{dP_n}{dt}\right|_{R_n^{(j)}}^{lys} - \frac{P_n}{P_c} \sum_{k=4,5,6} \left.\frac{dP_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.2.1b}$$

$$\left.\frac{dP_p}{dt}\right|_{bio} = \left.\frac{dP_p}{dt}\right|_{N^{(1)}}^{upt} - \sum_{j=1,6} \left.\frac{dP_p}{dt}\right|_{R_p^{(i)}}^{lys} - \frac{P_p}{P_c} \sum_{k=4,5,6} \left.\frac{dP_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.2.1c}$$

$$\left.\frac{dP_l}{dt}\right|_{bio} = \left.\frac{dP_l}{dt}\right|^{syn} - \frac{P_l}{P_c} \sum_j \left.\frac{dP_c}{dt}\right|_{Z_c^{(j)}}^{prd} \tag{2.2.1d}$$

$$\left.\frac{dP_s}{dt}\right|_{bio} = \left.\frac{dP_s}{dt}\right|_{N^{(5)}}^{upt} - \left.\frac{dP_s}{dt}\right|_{R_s^{(6)}}^{lys} - \frac{P_s}{P_c} \sum_{k=4,5,6} \left.\frac{dP_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.2.1e}$$

$$\text{if } P_s\exists, \text{ otherwise } \left.\frac{dP_s}{dt}\right|_{bio} = 0$$

$$\left.\frac{dP_f}{dt}\right|_{bio} = \left.\frac{dP_f}{dt}\right|_{N^{(7)}}^{upt} - \left.\frac{dP_f}{dt}\right|_{R_f^{(6)}}^{lys} - \frac{P_f}{P_c} \sum_j \left.\frac{dP_c}{dt}\right|_{Z_c^{(j)}}^{prd} \tag{2.2.1f}$$

$$\text{if } P_f\exists, \text{ otherwise } \left.\frac{dP_f}{dt}\right|_{bio} = 0 \tag{2.2.1g}$$

Symbol	Code	Unit	Description
Q_{10_P}	p_q10	-	Characteristic Q10 coefficient
c_P^T	p_temp	-	Cut-off threshold for temperature regulating factor
r_{0_P}	p_sum	d^{-1}	Maximum specific photosynthetic rate
b_P	p_srs	d^{-1}	Basal specific respiration rate
d_{0_P}	p_sdmo	d^{-1}	Maximum specific nutrient-stress lysis rate
$h_P^{p,n,s}$	p_thdo	-	Nutrient stress threshold
d_P^x	p_seo	d^{-1}	Extra lysis rate
h_P^x	p_sheo	mg C m^{-3}	Half saturation constant for extra lysis
β_P	p_pu_ea	-	Excreted fraction of primary production
γ_P	p_pu_ra	-	Activity respiration fraction
	p_switchDOC	1-3	Switch for the type of DOC excretion. This choice must be consistent with bacteria parameterization in Sec. 2.3. 1. All DOC is released as $R_c^{(1)}$ (Vichi et al., 2007b), consistent with BACT1; 2. Activity DOC is released as $R_c^{(2)}$ as there is no nutrient-stress excretion in BACT2 parameterization (Vichi et al., 2004); 3. All DOC is released as $R_c^{(2)}$, consistent with BACT3 in Polimene et al. (2006)
	p_netgrowth	logical	Switch for parameterization of nutrient limited growth (T or F)
	p_limnut	0-2	Switch for parameterization of nutrient co-limitation
a_4	p_qun	m^3 mg C^{-1} d^{-1}	Specific affinity constant for N
h_P^n	p_lN4	mmol N-NH4 m^{-3}	Half saturation constant for ammonium uptake preference over ammonium
n_P^{min}, n_P^{opt}, n_P^{max}	p_qnlc, p_qnRc, p_xqn*p_qnRc	mmolN mgC^{-1}	Minimum, optimal and maximum nitrogen quota
a_1	p_qup	m^3 mg C^{-1} d^{-1}	Specific affinity constant for P
p_P^{min}, p_P^{opt}, p_P^{max}	p_qplc, p_qpRc, p_xqp*p_qpRc	mmolP mgC^{-1}	Minimum, optimal and maximum phosphorus quota
	p_switchSi	1,2	Switch for parameterization of silicate limitation (1=external, 2=internal)
h_P^s	p_chPs	mmol Si m^{-3}	Half saturation constant for Si-limitation
ρ_P^s	p_Contois	-	Contois parameter for variable half saturation constant for Si-limitation (reverts to Monod if 0)
a_5	p_qus	m^3 mg C^{-1} d^{-1}	Specific affinity constant for Si
s_P^{min},s_P^{opt}	p_qsRc	mmolSi mg C^{-1}	Standard Si:C ratio in silicifiers
ω_P^{sink}	p_res	m d^{-1}	Maximum sedimentation rate
l_P^{sink}	p_esNI	-	Nutrient stress threshold for sinking
	p_ChlSynthesis		Choice of the Chl synthesis parameterization
α_{chl}^0	p_alpha_chl	mgC $(mg\ chl)^{-1}$ μE^{-1} m^2 s	Maximum light utilization coefficient
θ_{chl}^0	p_qchlc	mg chl mg C^{-1}	Maximum chl:C quotum
c_P	p_epsChla	m^2 $(mg\ chl)^{-1}$	Chl-specific light absorption coefficient
d_P^{chl}	p_sdmo	d^{-1}	Chlorophyll turn-over rate
ε^{opt}	p_EpEk_or	-	Optimal value of E_{PAR}/E_K
τ^{opt}	p_tochl_relt	d^{-1}	Relaxation rate toward the optimal Chl:C value

Table 2.2.: Mathematical and code symbols, units and description of the phytoplankton parameters (namelist `Pelagic_Ecology.nml: Phyto_parameters`).

2.2.1. Photosynthesis and carbon dynamics

Photosynthesis is primarily controlled by light by means of the non-dimensional light regulation factor proposed by Jassby and Platt (1976)

$$f_P^E = 1 - \exp\left(-\frac{E_{PAR}}{E_K}\right) \tag{2.2.2}$$

where E_K is the optimal irradiance, defined as

$$\begin{aligned} E_k &= P_m^*/\alpha^* \\ P_m^* &= f_P^T\, f_P^{PP}\, r_P^0\, \frac{P_c}{P_l} \\ \alpha^* &= f_P^T\, f_P^{PP}\, \alpha_{chl}^0 \end{aligned} \tag{2.2.3}$$

The maximum chl-specific photosynthetic rate P_m^* is controlled by the non-storable nutrients that control primary production f_P^{PP} (Sec. 2.2.2). It is assumed that both α^* and P_m^* are controlled by the same regulating factors (Jassby and Platt, 1976; Behrenfeld et al., 2004). When instantaneous light is used, the equation is written in the following form:

$$f_P^E = 1 - \exp\left(-\frac{\alpha_{chl}^0 E_{PAR} P_l}{r_P^0 P_c}\right) \tag{2.2.4}$$

while in case the length of the photoperiod is considered, this is implicitly done in P_m^* that becomes.

$$P_m^* = f_P^T\, f_P^{PP}\, r_P^0\, \frac{P_c}{P_l}\, \frac{\Phi}{24} \tag{2.2.5}$$

where Φ is the daylight length in hours (Lazzari et al., 2012). The final form of gross primary production also depends on the choice of the daylight availability. In the case of instantaneous or average daily irradiance (Vichi et al., 2007a), it is written as

$$\left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} = f_P^T\, f_P^E\, f_P^{PP}\, r_P^0 P_c. \tag{2.2.6}$$

Note that it is possible to further control temperature limitation with a cut-off value c_P^T applied to the temperature regulating factor as done in (Vichi et al., 2007a) to control the growth of picophytoplankton at high latitudes:

$$f^T = \max\left(0, f^T - c_P^T\right). \tag{2.2.7}$$

Respiration is defined as the sum of the basal respiration, which is independent of the production rate, and the activity respiration:

$$\left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{rsp} = b_P f_P^T P_c + \gamma_P \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp}. \tag{2.2.8}$$

Basal respiration is only a function of the carbon biomass, temperature (through the regulating factor f_P^T) and the specific constant rate b_P. The activity respiration is a constant fraction (γ_P) of the total gross primary production.

The term lysis includes all the non-resolved mortality processes that disrupt the cell membrane, such as mechanical causes, virus and yeasts. It is assumed that the lysis rate is partitioned between particulate and dissolved detritus and tends towards the maximum specific rate d_P^0 with a saturation function of the nutrient stress as:

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(6)}}^{lys} = \varepsilon_P^{n,p}\left(\frac{h_P^{p,n}}{f_P^{p,n} + h_P^{p,n}} d_P^0 P_c + \chi^{lys}\right) \tag{2.2.9}$$

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(1)}}^{lys} = \left(1 - \varepsilon_P^{n,p}\right) \left(\frac{h_P^{p,n}}{f_P^{p,n} + h_P^{p,n}} d_P^0 P_c + \chi^{lys}\right) \tag{2.2.10}$$

The lysis of cells generates both dissolved and particulate detritus; the structural parts of the cell are not as easily degradable as the cytoplasm, therefore the percentage going to DOC is inversely proportional to the internal nutrient content and constrained by the minimum structural content in the following way:

$$\varepsilon_P^{n,p} = \min\left(1, \frac{p_P^{min}}{P_p/P_c}, \frac{n_P^{min}}{P_n/P_c}\right). \tag{2.2.11}$$

This equation ensures that the carbon and nutrients in the supportive structures, which are assumed to have p_P^{min} and n_P^{min} nutrient ratios, are always released as particulate components.

The model also implements and extra lysis rate in the last term of eq. (2.2.9-2.2.10), which is dependent on the population density. This term is controlled by an optional specific lysis rate

$$\chi^{lys} = d_P^x \frac{P_c}{P_c + h_P^x} P_c \tag{2.2.12}$$

which is usually included for those phytoplankton population that are indedible and therefore acts as an additional mortality term to regulate the population dynamics.

2.2.2. Multiple nutrient limitation

The BFM inherits the treatment of nutrient limitation from the original work by Baretta-Bekker et al. (1997) which has similarities to the Caperon and Meyer equation, with some specific extensions. Nutrients are divided in two main groups, the ones that directly control carbon phosynthesis (as silicate, since duplication can only occur with Si deposition) and the ones that are decoupled from carbon uptake because of the existence of cellular storage capabilities. Limiting factors for nutrients can be both internal (i.e. based on the internal nutrient quota) or external (based on dissolved inorganic concentration). The internal limitation is only partly based on Droop (1973), with the concepts of nutrient surge and storage by Baretta-Bekker et al. (1997) and the possibility to apply the parameterization of net growth described in Vichi et al. (2004) by means of the parameter `p_netgrowth` in the namelist (Tab. 2.2). The regulating factors for internal limitation are controlled by the optimal and minimum values for the existence of structural components ($n_P^{opt}, n_P^{\min}$), and they are implemented for N, P and Fe (Sec. 2.2.8) and also for Si (Lazzari et al., 2012), although in this case it is not possible to have luxury uptake because there is no storage for dissolved silicate in the cell:

$$f_P^n = \min\left(1, \max\left(0, \frac{P_n/P_c - n_P^{min}}{n_P^{opt} - n_P^{min}}\right)\right) \tag{2.2.13}$$

$$f_P^p = \min\left(1, \max\left(0, \frac{P_p/P_c - p_P^{min}}{p_P^{opt} - p_P^{min}}\right)\right) \tag{2.2.14}$$

$$f_P^f = \frac{P_f/P_c - \phi_P^{min}}{\phi_P^{opt} - \phi_P^{min}} \tag{2.2.15}$$

$$\hat{f}_P^s = \frac{P_s/P_c - s_P^{\min}}{s_P^{opt} - s_P^{\min}} \tag{2.2.16}$$

$$f_P^p = \min\left(1, \max\left(0, \frac{P_p/P_c - p_P^{min}}{p_P^{opt} - p_P^{min}}\right)\right) \tag{2.2.17}$$

Note that the ratios between brackets can be larger than 1 because the nutrient quota are allowed to reach the maximum values (cf. Sec. 2.2.3) but the regulating factor has to be limited to 1 because above the optimal quotum there is no limitation to physiological processes.

There is a flag (Tab. 2.2) for the choice of external and internal silicon limitation in case of diatoms. External dissolved silicate control should be preferable (Flynn, 2003) and it implements a Monod regulation with variable half-saturation constant h_P^s, modified according to Contois (1959):

$$\begin{aligned} f_{P^{(1)}}^s &= \frac{N^{(5)}}{N^{(5)} + (h_P^s + \rho_P^s P_s^{(1)})} \\ f_{P^{(j)}}^s &= 1, \quad j \neq 1 \end{aligned} \tag{2.2.18}$$

The Contois formulation implements a control on dissolved nutrient uptake that is dependent on the size of the population, in this case it is applied to biogenic silica as suggested by Tsiaras et al. (2008). If the Contois parameter is zero a classical Monod function is obtained, while if $\rho_P^s \neq 0$ the half-saturation constant is increased and the resulting silicate control factor is smaller.

Multiple nutrient limitation is different for nutrients that can be stored in the cell and nutrients that cannot. The threshold combination (Liebig-like) is usually preferred to the multiplicative approach (Flynn, 2003): the BFM allows the three alternative ways implemented in ERSEM-II to combine N and P limitation (that can be selected

differently for each phytoplankton group, Tab. 2.2),

$$f_P^{n,p} = \min\left(f_P^n, f_P^p\right) \quad (2.2.19)$$

$$f_P^{n,p} = \frac{2}{1/f_P^n + 1/f_P^p} \quad (2.2.20)$$

$$f_P^{n,p} = \sqrt{f_P^n f_P^p} \quad (2.2.21)$$

and a simple multiplicative approach for the effect of nutrients that directly control photosynthesis (eq. 2.2.6), such as $f^{PP} = \hat{f}_P^s$ as done by Lazzari et al. (2012) or $f^{PP} = f_P^f f_P^s$ when iron dynamics is included (Sec. 2.3) as in Vichi et al. (2007b). The co-limitation from all nutrients is always done with a threshold method

$$f_P^{nut} = \min\left(f_P^{n,p}, f_P^f, f_P^s\right) \quad (2.2.22)$$

and it is considered in the parameterization of some processes such as chlorophyll synthesis and sinking (Secs. 2.2.6 and 2.2.9).

2.2.3. Nutrient uptake

A major problem in modelling nutrient uptake is to deal with unbalanced growth conditions, and any realistic application is expected to produce transient environmental conditions resulting in uncoupled assimilation rates of carbon and nutrients. The Droop (intracellular quota approach) and Monod (external concentration approach) equations produce consistent results when applied in balanced growth conditions (Morel, 1987). The BFM approach, largely derived from Baretta-Bekker et al. (1997), combines both mechanisms with a threshold control.

2.2.3.1. Nitrogen

The uptake of DIN is the sum of the uptake of dissolved nitrate and ammonium and is the minimum between a diffusion-dependent uptake rate (when internal nutrient quota are low and nutrients are only structural), and a rate based on considerations of balanced growth and luxury uptake:

$$\sum_{j=3,4} \left.\frac{dP_n}{dt}\right|_{N^{(j)}}^{upt} = \min\left(\left(a_P^n \frac{h_P^n}{h_P^n + N^{(4)}} N^{(3)} + a_P^n N^{(4)}\right) P_c, \; n_P^{opt} G_P + \nu_P \left(n_P^{\max} - \frac{P_n}{P_c}\right) P_c\right) \quad (2.2.23)$$

A preference for ammonium is parameterized through a saturation function that modulates the affinity constant for dissolved nitrate. Balanced uptake is a function of the net primary production G_p, which is computed as:

$$G_P = \max\left(0, \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} - \left.\frac{dP_c}{dt}\right|_{R_c^{(i)}}^{exu} - \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{rsp} - \left.\frac{dP_c}{dt}\right|_{R_c^{(i)}}^{lys}\right) \quad (2.2.24)$$

and

$$\nu_P = \max\left(0.05, \frac{G_P}{P_c}\right).$$

When the nitrogen uptake rate in (2.2.23) is positive, the partitioning between $N^{(3)}$and $N^{(4)}$uptake is done by multiplying the rate by the fractions:

$$\varepsilon_P^{(3)} = \frac{a_P^n \frac{h_P^n}{h_P^n + N^{(4)}} N^{(3)}}{a_P^n N^{(4)} + a_P^n \frac{h_P^n}{h_P^n + N^{(4)}} N^{(3)}} \quad (2.2.25)$$

$$\varepsilon_P^{(4)} = \frac{a_P^n N^{(4)}}{a_P^n N^{(4)} + a_P^n \frac{h_P^n}{h_P^n + N^{(4)}} N^{(3)}} \quad (2.2.26)$$

When it is negative, the whole flux is directed to the DON pool $R_n^{(1)}$.

2.2.3.2. Phosphorus

Phosphate uptake is simpler than N uptake as one single species is considered:

$$\left.\frac{dP_p}{dt}\right|_{N^{(1)}}^{upt} = \min\left(a_P^{(1)} N^{(1)} P_c, \; p_P^{opt} G_P + \nu_P \left(p_P^{\max} - \frac{P_p}{P_c}\right) P_c\right) \quad (2.2.27)$$

2.2.3.3. Silicate

Silicate is not stored in the cell and therefore the uptake is directly proportional to the net carbon growth (2.2.24):

$$\left.\frac{dP_s}{dt}\right|_{N^{(5)}}^{upt} = s_P^{opt} G_P \quad (2.2.28)$$

2.2.4. Nutrient loss associated with lysis

Nutrients in the cell are not evenly distributed between cytoplasm and structural parts. When the cell wall is disrupted, part of the nutrients are released as dissolved organic matter (the nutrients in the cytoplasm) and part as particulate organic matter (the nutrients in the structural parts, such as the cell wall).

The redistribution of the cellular elements C, N and P over the excretion variables reflects the preferential remineralization of P and to a lesser extent of N, with respect to C. This parameter values are based on the ERSEM-II parameterizations (Baretta-Bekker et al., 1997).

$$\left.\frac{dP_p}{dt}\right|_{R_i^{(6)}}^{lys} = \varepsilon_P^i \frac{h_P^{p,n}}{f_P^{p,n}+h_P^{p,n}} d_P^0 P_i \quad i=n,p \tag{2.2.29}$$

$$\left.\frac{dP_p}{dt}\right|_{R_i^{(1)}}^{lys} = \left(1-\varepsilon_P^i\right) \frac{h_P^{p,n}}{f_P^{p,n}+h_P^{p,n}} d_P^0 P_i \quad i=n,p \tag{2.2.30}$$

In the case of Si, the release is always in particulate form and thus is a constant fraction of the particulate carbon lysis

$$\left.\frac{dP_s^{(1)}}{dt}\right|_{R_s^{(6)}}^{lys} = s_P^{opt} \left.\frac{dP_c^{(1)}}{dt}\right|_{R_c^{(6)}}^{lys} \tag{2.2.31}$$

2.2.5. Exudation of carbohydrates

In the case of intra-cellular nutrient shortage, not all photosynthesized carbon can be assimilated into biomass, and the non-assimilated part is released in the form of dissolved carbohydrates. The model considers three different types of DOC (Tab. 1.1, Sec. 2.3) and phytoplankton excretion must be consistent with the bacteria parameterization. Carbohydrates are excreted when phytoplankton cannot equilibrate the fixed C with sufficient nutrients to maintain the minimum quotum needed for the synthesis of new biomass. The choice of the parametrization for DOC exudation is controlled by the flag parameters `p_netgrowth` and `p_switchDOC` in the phytoplankton namelist (Tab. 2.2), which can be set differently for each sub-group. There is a runtime check that controls the consistency between the two parameters. When the flag is false, the ERSEM-II parameterization (Baretta-Bekker et al., 1997) as implemented in Vichi et al. (2007b) is used,

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(1)}}^{exu} = \left[\beta_P + (1-\beta_P)\left(1-f_P^{n,p}\right)\right] \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} \tag{2.2.32}$$

where exudation (and thus carbon biomass loss) increases when phytoplankton has low nutrient:carbon ratios. The nutrient-stress excretion can also be partly directed to semi-refractory DOC ($R_c^{(2)}$) by setting the parameter `p_switchDOC=3`:

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(1)}}^{exu} = \beta_P \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} \tag{2.2.33}$$

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(2)}}^{exu} = (1-\beta_P)\left(1-f_P^{n,p}\right) \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} \tag{2.2.34}$$

However, the ERSEM-II parameterization not only leads to the desired extra release of C-enriched DOM but also to a decrease of the population biomass. It has been shown by Vichi et al. (2004) that the use of a different parameterization results in the maintenance of higher standing stocks in the post bloom period with a consequently enhanced consumption of the non-limiting nutrients. This parameterization is also used by Lazzari et al. (2012) to allow the consumption of N species in a P-depleted environment.

When the `p_netgrowth` flag is true, total exudation is directed to the state variable $R_c^{(2)}$ (see also Sec. 2.3 for a detailed explanation of DOM in the BFM), and it is written as the sum of an activity exudation linked to the gross primary production and a balance term

$$\left.\frac{dP_c}{dt}\right|_{R_c^{(2)}}^{exu} = \beta_P \left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp} + G_P - G_P^{bal} \tag{2.2.35}$$

where

$$G_P^{bal} = \max\left(0, \min\left(G_P, \frac{1}{n_P^{min}} \sum_{j=3,4} \left.\frac{dP_n}{dt}\right|_{N^{(j)}}^{upt}, \frac{1}{p_P^{min}} \left.\frac{dP_p}{dt}\right|_{N^{(1)}}^{upt}\right)\right) \tag{2.2.36}$$

2.2.6. Chlorophyll synthesis and photoacclimation

The chl equation in (2.2.1d) is composed of two terms. The first one is net chlorophyll synthesis, which is mostly derived from Geider et al. (1996, 1997) with some adaptations, and the second one represents the losses due to grazing.

Net chl synthesis is namely a function of acclimation to light conditions, nutrient availability and turnover rate. The former process is taken into account by Geider's parameterization, while the latter is generally parameterized with different formulations, for instance by assuming a dependence on gross carbon uptake (Geider et al., 1997; Blackford et al., 2004) and/or on nitrogen assimilation (Geider et al., 1998; Flynn et al., 2001). To integrate the variety of processes into our formulations, we consider three different parameterizations presented in 2.2 that have been used in different applications of the BFM (Vichi and Masina, 2009), (Lazzari et al., 2012) (Clementi et al., in preparation). The synthesis part is rather similar as it is controlled by the dynamical chl:C ratio ρ_{chl} proposed by Geider et al. (1997) which regulates the amount of chl in the cell according to a non-dimensional ratio between the realized photosynthetic rate in (2.2.6) and the maximum potential photosynthesis:

$$\rho_{chl} = \theta_{chl}^0 \frac{\left.\frac{dP_c}{dt}\right|_{O^{(3)}}^{gpp}}{\alpha^* E_{PAR} P_l} \tag{2.2.38}$$

and multiplying by a maximum chl:C ratio θ_{chl}^0 which is different for each phytoplankton functional group (Tab. 2.2). The major difference in eq. (2.2.37b) proposed by Lazzari et al. (2012) is the presence of the combined nutrient regulating factor, which implies that chl synthesis is reduced in regions limited by phosphorus like for instance the Mediterranean.

Following the notation shown in Sec. 2.2.3, Geider's original formulation is rewritten after some algebra as:

$$\rho_{chl} = \theta_{chl}^0 \frac{f_P^E r_P^0 P_c}{\alpha_{chl}^0 E_{PAR} P_l} \tag{2.2.39}$$

The ratio is down-regulated when the rate of light absorption (governed by the quantum efficiency and the amount of light-harvesting pigments) exceeds the rate of utilization of photons for carbon fixation, as explained in detail in Geider et al. (1996). Also here it is assumed that both α^* and P_m^* are controlled by the same regulating factors (Jassby and Platt, 1976; Behrenfeld et al., 2004).

The formulation of the lysis term is still unknown and this is reflected in the diversity of parameterizations that are available in the model and controlled by the namelist parameter `p_switchChl` (Tab. 2.2). The user should consider the different assumptions and use them accordingly. A different parameterization can be used for each phytoplankton group to allow their testing. In eq. (2.2.37a) it is assumed that chl lysis is simply linked to the carbon term, while in eq. (2.2.37b) there is a relaxation to the optimal chl:C ratio with an additional lysis term linked to background mortality. The parameterization proposed in eq. (2.2.37c) is slightly more elaborated as it considers an optimal cell acclimation to light that corresponds to an optimal value $E_{PAR}/E_K = \varepsilon^{opt}$ of the exponential in eq. (2.2.4).

The theoretical chl concentration corresponding to optimal light acclimation in eq. (2.2.37c) is computed as follows:

$$\begin{aligned} \frac{r_P^0 P_c}{P_l^{opt} \alpha_{chl}^0} &= \frac{E_{PAR}}{\varepsilon^{opt}} \\ P_l^{opt} &= \varepsilon^{opt} \frac{r_P^0 P_c}{\alpha_{chl}^0 E_{PAR}} \end{aligned} \tag{2.2.40}$$

and the chl content in (2.2.37c) is relaxed to this optimal value with a specific time scale parameter τ_{chl}.

Equation Box 2.2 Different parameterizations for the chlorophyll synthesis.

$$\left.\frac{dP_l}{dt}\right|^{syn} = \rho_{chl}\, G_P - \frac{P_l}{P_c}\left.\frac{dP_c}{dt}\right|^{lys} \tag{2.2.37a}$$

$$\left.\frac{dP_l}{dt}\right|^{syn} = f_P^{p,n}\rho_{chl}\, G_P - \max\left(0, d_P^{\circ}(1-f_P^{p,n})\right) P_l - \min\left(0, G_P\right) * \max\left(0, P_l - \theta_{chl}^0 P_c\right) \tag{2.2.37b}$$

$$\left.\frac{dP_l}{dt}\right|^{syn} = \rho_{chl}\, G_P - \theta_{chl}\left(\left.\frac{dP_c}{dt}\right|^{lys} + \left.\frac{dP_c}{dt}\right|^{rsp}\right) - \max\left(0, P_l - P_l^{opt}\right)\,\tau_{chl} \tag{2.2.37c}$$

$$\left.\frac{dP_l}{dt}\right|^{syn} = \rho_{chl}\, G_P - d_P^{chl} P_l\left(h_P^{p,n,s} - f_P^{nut}\right) - \frac{P_l}{P_c}\frac{1}{1+E_{PAR}}\left.\frac{dP_c}{dt}\right|^{rsp} \tag{2.2.37d}$$

The parameterization presented in eq. (2.2.37d) has instead an explicit term for the turn-over rate of chl d_P^{chl} and includes . The losses of chl are not considered as mass losses in the model because we have currently not implemented a chl component in detritus and dissolved organic matter. The same consideration applies to the ingested chl fraction in zooplankton. All these terms are presently collected into a generic sink term used for mass conservation purposes, which can be easily split into its major components once it is deemed necessary to follow the degradation products of chl (phaeopigments).

2.2.7. Light limitation and photoacclimation based on optimal light

This parameterization is alternative to the one above and is consistent with the one originally implemented in ERSEM-II (Ebenhöh et al., 1997). It assumes that phytoplankton is acclimated to the prevailing light in a few days and that the C:chl ratio is constant.

The state variable I_{opt} in the original ERSEM-II formulation represented the light intensity at which production saturated for the whole phytoplankton community. We consider here an optimal light for each phytoplankton group indicated with $\hat{P}_l^{(j)}$, which has the same meaning as the light saturation parameter E_k used in the alternative formulation of chlorophyll dynamics (Sec. 2.2.3).

A note of caution on the application of this parameterization: the model was formulated to simulate the daily production, therefore it is suggested to apply it with the daylight-averaged irradiance, possibly modulated by the duration of the daylight period. Several forms of the P-E curve are available:

$$prod = f_P^T f_P^s r_{0P} \min\left(1, \frac{E_{PAR}}{\hat{P}_l}\right) \quad \text{(ramp)}$$

$$prod = f_P^T f_P^s r_{0P} \frac{E_{PAR}}{\hat{P}_l} e^{1-\frac{E_{PAR}}{\hat{P}_l}} \quad \text{(Steele)}$$

The light regulating factor is computed by integrating the P-E curve over the depth of the considered layer, therefore the irradiance at the top of the layer is used

$$f_P^E = \frac{1}{f_P^T f_P^s r_{0P} D}\int_{-D}^{0} prod\left(\frac{E_{PAR}}{\hat{P}_l}\right) dz \tag{2.2.41}$$

The time rate of change of $\hat{P}_l$ is computed with a relaxation term

$$\left.\frac{d\hat{P}_l}{dt}\right|_{bio} = \nu_P^I\left(E_P^{opt} - \hat{P}_l\right) \tag{2.2.42}$$

where E_P^{opt} is the reference light saturation parameter to which the phytoplankton adapt with frequency ν_P^I (generally 4 days for a full acclimation).

The irradiance level to which phytoplankton may adapt is

$$E_P^{opt} = \min\left(E_P^{max}, \max\left(E_P^{min}, E_{PAR}\right)\right)$$

which is a constrained ramp function over the range of saturating irradiance.

2.2.8. Iron in phytoplankton

The iron (Fe) constituent in phytoplankton shown in eq. (2.2.1f) is not activated by default in the model. It is available as a compilation key `INCLUDE_PELFE` and implements the iron dynamics proposed by Vichi et al. (2007b) described by the parameters of Tab. 2.3. The iron cycle involves a phytoplankton, particulate and dissolved component (Sec.), while the zooplankton and bacteria fraction is neglected.

The equation (2.2.1f) for iron in phytoplankton P_f contains a term for the uptake of [Fe'], a loss term related to turnover/cell lysis and a predation term. Similarly to N and P content, intracellular Fe:C quota are allowed to vary between a maximum and a minimum thresholds (ϕ_P^{max} and ϕ_P^{min}, Tab. 2.3), and the realized quotum is used to derive a non-dimensional regulating factor as in eq. (2.2.19). The allowed minimum ratio ϕ_P^{min} represents the evolutive adaptation of each functional group at the prevailing iron concentrations, and the optimal value ϕ_P^{opt} indicates the cellular requirement for optimal growth. This regulating factor modulates the actual photosynthetic rate in eq. (2.2.6) since there is a clear decrease in the activity of PSUs due to insufficient cellular Fe (Sunda and Huntsman, 1997).

The regulating factor inhibits carbon fixation, but iron can still be taken up in the cell, progressively increasing the internal quotum. Iron uptake from dissolved pools is computed as for N and P (Sec. 2.2.3) by taking the minimum of two rates, a linear function of the ambient concentration simulating the membrane through-flow at low external Fe concentration, and the balancing flux according to the carbon assimilation:

$$\left.\frac{\partial P_f}{\partial t}\right|_{N^{(7)}}^{upt} = \min\left(a_P^7 N^{(7)} P_c, \phi_P^{opt} G_P + f_P^T r_P^0 \left(\phi_P^{max} - \frac{P_f}{P_c}\right) P_c\right) \quad (2.2.43)$$

It is assumed that the only physiological iron loss from phytoplankton is linked to cell disruption, computed according to carbon lysis and assuming that particulate material has the minimum structural Fe:C ratio:

$$\left.\frac{\partial P_f}{\partial t}\right|_{R_f^{(6)}}^{lys} = \phi_P^{min} \left.\frac{\partial P_c}{\partial t}\right|_{R_c^{(6)}}^{lys}. \quad (2.2.44)$$

2.2.9. Phytoplankton sinking

The sinking of biogenic material is a fundamental process for the simulation of carbon sequestration in the interior of the ocean. However, the estimation of the sinking velocity w_B is still parameterized in a very simplified way in the model. Any phytoplankton group is allowed to have a sinking velocity using the original ERSEM formulation (Varela et al., 1995). This is generally valid only for diatoms, which reach their maximum velocity ω^{sink} as a function of the total nutrient stress (2.2.22) as follows:

$$w_{P^{(1)}} = \omega^{sink} \max\left(0, l^{sink} - f_P^{nut}\right) \quad (2.2.45)$$

where l^{sink} is the nutrient regulating factor value below which the mechanism is effective.

2.3. Bacterioplankton

Bacterioplankton is included in the standard BFM with one single state variable representing a wide group of aerobic and anaerobic bacteria. The user can eventually expand the number of bacteria group using the modular facilities described in Part II of this document by providing new dynamical equations.

In addition to the original ERSEM parameterization (Baretta-Bekker et al., 1995) further expanded in Vichi et al. (2007b), the code contains also two alternative parameterizations proposed by Vichi et al. (2004) and Polimene et al.

Symbol	Code	Unit	**Description**
a_7	p_quf	m^{-3} mg C^{-1} d^{-1}	Specific affinity constant for Fe in phytoplankton
ϕ_P^{min}, ϕ_P^{opt}, ϕ_P^{max}	p_qflc, p_qfRc, p_xqf*p_qfRc	μmol Fe mgC^{-1}	Minimum, optimal and maximum iron quota in phytoplankton
$\Lambda 1_f^{rmn}$	p_sR1N7	d^{-1}	Specific remineralization rate of dissolved biogenic iron
$\Lambda 6_f^{rmn}$	p_sR6N7	d^{-1}	Specific remineralization rate of particulate biogenic iron
Q_{10_f}	p_q10R6N7	(-)	Characteristic Q10 coefficient for Fe remineralization
φ_f^{scv}	p_N7fsol	μmol Fe m^{-3}	Solubility concentration
Λ_f^{scv}	p_scavN7f	d^{-1}	Specific scavenging rate of dissolved iron
Λ_f^{dep}	p_qflc	(-)	Specific dissolution fraction of dust iron

Table 2.3.: Mathematical and code symbols, units and description of the iron cycle parameters (namelist `Pelagic_Ecology.nml:Phyto_parameters_iron` `Pelagic_environment.nml:PelChem_parameters_iron`).

(2006). We will refer to BACT1 when indicating the standard most simple parameterization and to BACT2 and BACT3 for theVichi et al. (2004) and Polimene et al. (2006) parameterizations, respectively. BACT1 set of equations is the default choice but all parameterizations are deemed equal and can be activated at run time.

The different parameterizations consider that dissolved organic matter (DOM) available to pelagic bacteria may have different degrees of lability/refractivity. The lability/refractivity characteristics of DOM are dependent on two factors: the C:N and C:P ratios of bacteria and the structure of organic molecules constituting the DOM matrix. DOM is assumed to be partitioned into three broad and distinct state variables, each of them corresponding to different degrees of lability/refractivity and having different production pathways. The parameterizations described below consider only 1, 2 or all of the three classes. It is important to remark that the DOC fraction considered by the model covers only the labile and the semi-labile DOC part. Therefore, in the following we define, as "semi-refractory" the DOC fraction more slowly remineralized by bacteria only to avoid confusion with the truly refractory DOC (with turnover time of 100-1000 years) that is not considered at all in the model.

The most labile fraction of the total DOM pool $R_i^{(1)}$, $i = c,n,p$ is produced by phytoplankton, zooplankton and bacteria via the lysis, mortality and sloppy feeding (mesozooplankton only) processes. This DOM variable is characterized by C:N and C:P ratios identical to those of the producing functional groups. The characteristic turnover time-scale is assumed to be 1 day. The semi-labile DOM fraction $R_c^{(2)}$ is produced by excretion by phytoplankton and bacteria in order to achieve/maintain their internal "optimal" stoichiometry (this part is considered only in BACT2 and BACT3 parameterizations). The production process of semi-labile DOM can be thought as release of excess carbon and, therefore, negligible N and P pools are assumed. The characteristic turnover time-scale is assumed to be 10 days. DOM released by bacteria as capsular material $R_c^{(3)}$ is also introduced in BACT2 and BACT3, and it represents the semi-refractory fraction of the DOM, but it is only considered a source of carbon in BACT3 (Polimene et al., 2006). This component of the DOM pool is also assumed (as for the semi-labile fraction) to be DOC only and to be formed by high molecular weight substances such as

polysaccharid fibrils (Heissenberger et al., 1996), which are quite resistant to enzymatic attack (Stoderegger and Herndl, 1998). Therefore, the characteristic turnover time-scale is assumed to be longer (100 days) as this material is only degradable by bacteria at time-scales of 2-3 orders of magnitude longer with respect to the labile DOC (Stoderegger and Herndl, 1998).

Bacteria have 3 free-varying constituents C, N, P, and the fundamental equations shown in Eq. Box 2.3 are common to all parameterizations. In all versions, pelagic bacteria behave as remineralizers or phytoplankton competitors depending on their internal nutrient quota, taking up inorganic nutrients directly from the water. Before providing a detailed description of the three versions the common processes are described.

2.3.1. Regulating factors

The oxygen non dimensional regulating factor f_B^o (eq. 2.3.2) is parameterized with a type III control formulation as:

$$f_B^o = \frac{\left(O^{(2)}\right)^3}{\left(O^{(2)}\right)^3 + \left(h_B^o\right)^3} \tag{2.3.2}$$

where the dissolved oxygen concentration $O^{(2)}$ is considered, and h_B^o is the oxygen concentration at which metabolic functionalities are halved. This steep sigmoid has been proposed by Vichi et al. (2004) to efficiently switch between bacteria metabolism under aerobic conditions and anaerobic metabolism.

The non dimensional regulating factor based on the nutritional content of bacterial cells is given by:

$$f_B^{n,p} = \min\left(1, \frac{B_p/B_c}{p^{opt}}, \frac{B_n/B_c}{n^{opt}}\right); \tag{2.3.3}$$

n_B^{opt} and p_B^{opt} are the "optimal" $N:C$ and $P:C$ bacterial internal quota (Goldman and McCarthy, 1978).

2.3.2. Respiration

The respiration sink term is composed of basal and activity respiration as:

$$\left.\frac{dB_c}{dt}\right|_{O^{(3)}}^{rsp} = b_B f_B^T B_c + \left[\gamma_B^a + \gamma_B^o\left(1 - f_B^o\right)\right] \sum_{j=1,2,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} \tag{2.3.4}$$

The basal respiration is parameterized as for phytoplankton with a constant specific respiration rate b_B and the regulating factor for temperature given in eq. (2.1.1). γ_B^a and γ_B^O are the fraction of production that is used for activity respiration under oxic and low oxygen conditions respectively. Since the BFM pelagic bacteria parameterization encompasses both aerobic and anaerobic bacterial activities, we consider here the differences in the energetics of the metabolic pathways in relation to oxygen availability. Anaerobic bacteria have a lower efficiency because they need to consume (respire) more carbon in order to produce the same amount of energy.

2.3.3. Mortality

The mortality (lysis) process is given by

$$\left.\frac{dB_c}{dt}\right|_{R_i^{(1)}}^{lys} = \left(d_{0_B} f_B^T + d_B^d B_c\right) B_c \quad i = c,n,p \tag{2.3.5}$$

where d_{0_B} is a temperature enhanced background mortality specific rate and d_B^d is a density dependent mortality specific rate assumed to be dependent on virus infection.

2.3.4. BACT1 parameterization

In this parameterization labile $R_{c,n,p}^{(1)}$ is the only class of dissolved organic matter resolved by the model and, together with $R_{c,n,p}^{(6)}$, constitute the organic substrate available to bacteria. This parameterization requires that phytoplankton

Symbol	*Code*	*Units*	**Description**	**Parameterization**
Q_{10_B}	p_q10	(-)	Characteristic Q10 coefficient	All
h_B^o	p_chdo	mmolO_2 m^{-3}	Half saturation value for oxygen limitation	All
r_{0_B}	p_sum	d^{-1}	Potential specific growth rate	All
b_B	p_srs	d^{-1}	Basal specific respiration rate	All
γ_B^a	p_pu_ra	(-)	Activity respiration fraction	All
γ_B^o	p_pu_ra_o	(-)	Additional respiration fraction under anoxic conditions	All
d_{0_B}	p_sd	d^{-1}	Specific mortality rate	All
d_B^d	p_sd2	d^{-1} mgC^{-1} m^3	Density-dependent specific mortality rate	All
$v_B^{R^{(2)}}$	p_suR2	d^{-1}	Specific potential $R^{(2)}$ uptake (semi-labile)	BACT2,BACT3
$v_B^{R^{(3)}}$	p_suR3	d^{-1}	Specific potential $R^{(3)}$ uptake (semi-refractory)	BACT3
$v_B^{R^{(6)}}$	p_suR6	d^{-1}	Specific potential $R^{(6)}$ uptake (particulate)	All
$v_B^{R^{(1)}}$	p_suhR1	d^{-1}	Specific quality-dependent potential $R^{(1)}$ uptake (nutrient-rich labile)	All
$v_{0_B}^{R^{(1)}}$	p_sulR1	d^{-1}	Specific quality-independent potential $R^{(1)}$ uptake (nutrient-poor labile)	BACT1
$a1_B$	p_qup	m^{-3} mg C^{-1} d^{-1}	Specific affinity constant for P	BACT2
$a4_B$	p_qun	m^{-3} mg C^{-1} d^{-1}	Specific affinity constant for N	BACT2
v_B^n, v_B^p	p_ruen, p_ruep	d^{-1}	Relaxation time scales for N and P uptake or remineralization	All
v_B^c	p_rec	d^{-1}	Relaxation time scale for semi-labile carbon release	BACT3
n_B^{opt}, p_B^{opt}	p_qnc, p_qpc	mmolN mgC^{-1}, mmolP mgC^{-1}	Optimal nutrient quota	All
n_B^{min}, p_B^{min}	p_qlnc, p_qlpc	mmolN mgC^{-1}, mmolP mgC^{-1}	Minimum nutrient quota	BACT2
h_B^n, h_B^p	p_chn, p_chp	mmolN mgC^{-1}, mmolP mgC^{-1}	Half saturation for nutrient uptake	All
β_B	p_pu_ea_R3	(-)	Fractional excretion of $R^{(3)}$ (semi-refractory)	BACT3
-	p_version		Switch for bacteria parameterization: 1=BACT1; 2=BACT2; 3=BACT3	

Table 2.4.: Mathematical and code symbols, units and description of the bacterioplankton parameters (namelist `Pelagic_Ecology.nml: PelBac_parameters`).

Equation Box 2.3 Bacteria equations

$$\left.\frac{dB_c}{dt}\right|_{bio} = \sum_{j=1,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} - \left.\frac{dB_c}{dt}\right|_{O^{(3)}}^{rsp} - \left.\frac{dB_c}{dt}\right|_{R_c^{(1)}}^{lys} - \sum_{k=5,6} \left.\frac{dB_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.3.1a}$$

$$\left.\frac{dB_n}{dt}\right|_{bio} = \sum_{j=1,6} \frac{R_n^{(j)}}{R_c^{(j)}} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} + \sum_{i=3,4} \left.\frac{dB_n}{dt}\right|_{N^{(i)}}^{upt} - \left.\frac{dB_n}{dt}\right|_{N^{(4)}}^{rel} - \frac{B_n}{B_c} \left.\frac{dB_c}{dt}\right|_{R_c^{(1)}}^{lys} + \tag{2.3.1b}$$

$$- \frac{B_n}{B_c} \sum_{k=5,6} \left.\frac{dB_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.3.1c}$$

$$\left.\frac{dB_p}{dt}\right|_{bio} = \sum_{j=1,6} \frac{R_p^{(j)}}{R_c^{(j)}} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} + f_B^p \left.\frac{dB_p}{dt}\right|_{N^{(1)}}^{upt,rel} - \frac{B_p}{B_c} \left.\frac{dB_c}{dt}\right|_{R_c^{(1)}}^{lys} - \frac{B_p}{B_c} \sum_{k=5,6} \left.\frac{dB_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.3.1d}$$

2.3.4.1. Substrate uptake

The total carbon uptake rate of organic substrate in (2.3.1a) is regulated by environmental factors and substrate availability with a threshold formulation:

$$\sum_{j=1,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} = \min\left(f_B^{n,p} f_B^T r_{0_B} B_c, \sum_{j=1,6} \nu_B^{R^{(j)}} f_{R^{(j)}}^{n,p} R_c^{(j)} + \nu_{0_B}^{R^{(1)}} \left(1 - f_{R^{(1)}}^{n,p}\right) R_c^{(1)}\right) \tag{2.3.6}$$

where r_{0_B} is the maximum potential specific growth rate, $\nu_B^{R^{(j)}}$ is the specific quality-dependent uptake rate for substrate, $\nu_{0_B}^{R^{(1)}}$ is the specific, quality-independent uptake rate for semi-labile organic matter and $f_{R^{(j)}}^{n,p}$ is the non-dimensional regulating factor based on the of organic substrate

$$f_{R^{(j)}}^{n,p} = \min\left(1, \frac{R_p^{(j)}/R_c^{(j)}}{p^{opt}}, \frac{R_p^{(j)}/R_c^{(j)}}{n^{opt}}\right) \; j = 1,6 f_{R^{(j)}}^{n,p} \tag{2.3.7}$$

The uptake of the nutrient components in the dissolved and particulate fractions is then derived from the actual nutrient ratios in the organic matter as:

$$\left.\frac{dB_i}{dt}\right|_{R_i^{(j)}}^{upt} = \frac{R_i^{(j)}}{R_c^{(j)}} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt}, \quad i = n,p; \; j = 1,6 \tag{2.3.8}$$

2.3.4.2. Nutrient release and uptake

The mineralizers/phytoplankton competitors behavior is controlled by the non-dimensional factors f_B^p and f_B^n and by the specific relaxation rates ν_B^p and ν_B^n towards the optimal internal quota. The process it involves only phosphate and ammonium components:

$$\left.\frac{dB_p}{dt}\right|_{N^{(1)}}^{upt,rel} = f_B^p \nu_B^p \left\| \frac{B_p}{B_c} - p_B^{opt} \right\| B_c \tag{2.3.9}$$

$$\left.\frac{dB_n}{dt}\right|_{N^{(4)}}^{upt,rel} = f_B^n \nu_B^n \left\| \frac{B_n}{B_c} - n_B^{opt} \right\| B_c \tag{2.3.10}$$

$$\left.\frac{dB_n}{dt}\right|_{N^{(3)}}^{upt} = 0 \tag{2.3.11}$$

In the case of phosphorus as in eq. (2.3.9), for instance, if there is an excess of nutrients in the cell, $\frac{B_p}{B_c} - p_B^{opt} > 0$, the non-dimensional parameter $f_B^p = -1$, and if $\frac{B_p}{B_c} - p_B^{opt} < 0$ there is direct uptake from the water as a function of the nutrient concentration in a Michaelis-Menten form, $f_B^p = \frac{N^{(1)}}{N^{(1)} + h_B^p}$. The same applies to nitrogen, and the direct uptake is regulated by the factor $f_B^n = \frac{N^{(4)}}{N^{(4)} + h_B^n}$.

2.3.4.3. Excretion

In this parameterization the release term appearing in eq. (2.3.1a) is nil.

2.3.5. BACT2 parameterization

In this parameterization originally proposed by Vichi et al. (2004), the substrate available for uptake is composed of $R_{c,n,p}^{(1,6)}$ and $R_c^{(2)}$.

2.3.5.1. Substrate uptake

The $R_c^{(1,6)}$ uptake is parameterized as in BACT1 (see eq.2.3.6) and the $R_c^{(2)}$ uptake is added.

$$\sum_{j=1,2,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} = \min\left(f_B^{n,p} f_B^T r_{0_B} B_c, \quad (2.3.12)\right.$$
$$\left.\sum_{j=1,6} \nu_B^{R^{(j)}} f_{R^{(j)}}^{n,p} R_c^{(j)} + \nu_{0_B}^{R^{(1)}} \left(1 - f_{R^{(1)}}^{n,p}\right) R_c^{(1)} + \nu_B^{R^{(2)}} R_c^{(2)}\right)$$

where $\nu_B^{R^{(2)}}$ is the $R_c^{(2)}$ specific uptake rate. The uptake of the nutrient components in the dissolved and particulate fractions is the same defined for BACT1 in eq. (2.3.8).

2.3.5.2. Nutrient release and uptake

The uptake dynamics is similar to the one for phytoplankton, with affinity constants for phosphate and ammonia ($a1_B$ and $a4_B$ respectively) and also nitrate with a inhibition factor due to ammonium. This flux regulates the direct uptake and the activity uptake based on the optimal quota and the net carbon uptake

$$G_B = \sum_{j=1,2,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} - \left.\frac{dB_c}{dt}\right|_{O^{(3)}}^{rsp}. \quad (2.3.13)$$

Remineralization dynamics occur only when internal quotas are in excess with respect to the "optimal" value and the dissolved nutrient uptake is linearly dependent on the membrane affinity as follows:

$$\left.\frac{dB_p}{dt}\right|_{N^{(1)}}^{upt} = \quad (2.3.14)$$
$$\min\left[a_B^1 N^{(1)} B_c, \max\left(0, p_B^{opt} G_B - \sum_{j=1,6} \left.\frac{dB_p}{dt}\right|_{R_p^{(j)}}^{upt}\right)\right]$$

$$\left.\frac{dB_p}{dt}\right|_{N^{(1)}}^{rel} = \max\left(0, \sum_{j=1,6} \left.\frac{dB_p}{dt}\right|_{R_p^{(j)}}^{upt} - p_P^{opt} G_B\right) \quad (2.3.15)$$

$$\left.\frac{dB_n}{dt}\right|_{N^{(4)}}^{rel} = \max\left(0, \sum_{j=1,6} \left.\frac{dB_n}{dt}\right|_{R_n^{(j)}}^{upt} - n_B^{opt} G_B\right) \quad (2.3.16)$$

$$\sum_{i=3,4} \left.\frac{dB_n}{dt}\right|_{N^{(i)}}^{upt} = \min\left(a4_B \frac{h_B^n}{h_B^n + N^{(4)}} N^{(3)} + a4_B N^{(4)}\right) B_n, \max\left(0, n_B^{opt} G_B - \sum_{j=1,6} \left.\frac{dB_n}{dt}\right|_{R_n^{(j)}}^{upt}\right)\Bigg) \quad (2.3.17)$$

2.3.6. BACT3 parameterization

2.3.6.1. Substrate uptake

The organic substrate uptake differs from the BACT1 and BACT2 parameterizations not only for the wider resolution of the DOM lability/refractivity characteristics given in the introduction, but also because the DOC uptake is not constrained by the nutritional content of bacterial cells (see eq. 2.3.3)

$$\sum_{j=1,2,3,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} = \min\left(f_B^T f_B^o r_{0_B} B_c, \sum_{j=1,2,3,6} \nu_B^{R^{(j)}} R_c^{(j)}\right) \quad (2.3.18)$$

The uptake of the nutrient components in the dissolved and particulate fractions is instead the same defined for BACT1 (eq. 2.3.8).

2.3.6.2. Nutrient release and uptake

The Nutrient release and uptake parameterization is the same described for the BACT1 version (see Sec. 2.3.4.2)

2.3.6.3. Excretion

This version also defines a bacterial first-order excretion of carbohydrates

$$\left.\frac{dB_c}{dt}\right|_{R_c^{(2)}}^{rel} = \max\left(0, 1-\frac{B_p/B_c}{p_B^{opt}}, 1-\frac{B_n/B_c}{n_B^{opt}}\right) \nu_B B_c \tag{2.3.19}$$

based on the optimal nutrient content and the constant relaxation time scale ν_B. The release of semi refractory DOC is assumed to be at constant rate (d^{-1}), assumed to be proportional to the activity respiration rates:

$$\left.\frac{dB_c}{dt}\right|_{R_c^{(3)}}^{rel} = \beta_B \sum_{j=1,2,3,6} \left.\frac{dB_c}{dt}\right|_{R_c^{(j)}}^{upt} \tag{2.3.20}$$

where β_B is the constant fraction of renewal of capsular material, usually equivalent to about 1/4 of the respiration rate (Stoderegger and Herndl, 1998). Note that this parameter must be set by the user and a warning is issued if the resulting bacterial growth efficiency is too low.

2.4. Zooplankton

Zooplankton is subdivided into microzooplankton and mesozooplankton with 2 sub-groups defined for each component:

- carnivorous mesozooplankton $Z_i^{(3)}$;
- omnivorous mesozooplankton $Z_i^{(4)}$, mainly comprising calanoid copepods ;
- microzooplankton $Z_i^{(5)}$, representing the biomass concentration of microzooplankton with a ESD in the range 20- 200 μm, excluding flagellates and naupliar/larval stages of multicellular zooplankton or meroplanktonic larvae of benthic organisms;
- heterotrophic nanoflagellates $Z_i^{(6)}$, protozoa with dimensions between 2 and 20 μm, mainly grazing upon picophytoplankton and bacteria.

Mesozooplankton is operationally defined in the model as any zooplankter between 200 μm and 3 to 4 cm long as an adult, also embracing many species that are traditionally considered part of the microzooplankton when in juveniles stages (Broekhuizen et al., 1995). The BFM core contains a specific parameterization for microzooplankton and mesozooplankton but the formal description is presented for the generic zooplankton as in Vichi et al. (2007b). The zooplankton parameterization is modified from Baretta-Bekker et al. (1995) and Broekhuizen et al. (1995) and it includes the processes of growth due to ingestion and the loss terms due to excretion/egestion, mortality, respiration and predation. Each zooplankton group comprises 3 constituents for C, N and P content as shown in Eq. Box 2.4, however the model is constructed to reduce the parameterizations to C-based dynamics assuming constant nutrient to carbon ratios (see Sec. 6.2.3).

Si and chl are currently not included as constituents for zooplankton, because biogenic silica in the form of frustules is directly egested by zooplankters and chl is a negligible part of C and N in the total biomass of preys.

2.4.1. Food availability

The total amount of food available to zooplankton is computed considering the set of possible preys $X_i \in \left\{P_i^{(j)}, B_i, Z_i^{(j)}\right\}$ as the vector $F_i = \sum_X \delta_{Z,X} e_{Z,X} X_i$, where $\delta_{Z,X}$ is the availability of prey X_i for predator Z and $e_{Z,X}$ is the capture efficiency. The product of the latter terms gives the total preference. There are many definitions of preferences in the literature, and we have used concepts from Gentleman et al. (2003) and Gibson et al. (2005) to combine the parameterizations described in Baretta-Bekker et al. (1995) for microzooplankton and in Broekhuizen et al. (1995) for mesozooplankton. Availability represents the suitability of the prey and is assumed to be mostly dependent on the prey's nominal dimensions. Capture efficiency (or relative preference) is also a non-dimensional factor which is set to 1 for mesozooplankton and it is density-dependent in microzooplankton, $e_{Z,X} = \frac{X_c}{X_c+\mu_Z}$, according to the threshold

Equation Box 2.4 Zooplankton equations.

$$\left.\frac{dZ_c}{dt}\right|_{bio} = \sum_{X=P,Z} \left.\frac{dZ_c}{dt}\right|_{X_c}^{prd} - \sum_{j=1,6} \left.\frac{dZ_c}{dt}\right|_{R_c^{(j)}}^{rel} - \left.\frac{dZ_c}{dt}\right|_{O^{(3)}}^{rsp} - \sum_{k=4,5,6} \left.\frac{dZ_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.4.1a}$$

$$\left.\frac{dZ_n}{dt}\right|_{bio} = \frac{F_n}{F_c} \sum_{X=P,Z} \left.\frac{dZ_c}{dt}\right|_{X_c}^{prd} - \sum_{j=1,6} \left.\frac{dZ_n}{dt}\right|_{R_n^{(j)}}^{rel} - \left.\frac{dZ_n}{dt}\right|_{N^{(4)}}^{rel} - \frac{Z_n}{Z_c} \sum_{k=4,5,6} \left.\frac{dZ_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.4.1b}$$

$$\left.\frac{dZ_p}{dt}\right|_{bio} = \frac{F_p}{F_c} \sum_{X=P,Z} \left.\frac{dZ_c}{dt}\right|_{X_c}^{prd} - \sum_{j=1,6} \left.\frac{dZ_p}{dt}\right|_{R_p^{(j)}}^{rel} - \left.\frac{dZ_p}{dt}\right|_{N^{(1)}}^{rel} - \frac{Z_p}{Z_c} \sum_{k=4,5,6} \left.\frac{dZ_c}{dt}\right|_{Z_c^{(k)}}^{prd} \tag{2.4.1c}$$

Symbol	Code	Units	Description
Q_{10_Z}	p_q10	(-)	Characteristic Q10 coefficient
h_Z^F	p_chuc	mg C m^{-3}	Michaelis constant for total food ingestion
μ_Z	p_minfood	mg C m^{-3}	Feeding threshold
r_{0_Z}	p_sum	d^{-1}	Potential specific growth rate
$\delta_{Z,B}$	p_paPBA(z,p)	(-)	Availability of pelagic bacteria B to zooplankton Z
$\delta_{Z,P}$	p_paPPY(z,p)	(-)	Availability of phytoplankton P to zooplankton Z
$\delta_{Z,Z}$	p_paMIZ(z,p)	(-)	Availability of microzooplankton P to zooplankton Z
b_Z	p_srs	d^{-1}	Basal specific respiration rate
η_Z	p_pu	(-)	Assimilation efficency
β_Z	p_pu_ea	(-)	Excreted fraction of uptake
ε_Z^c	p_pe_R1c	(-)	Partition between dissolved and particulate excretion of C
ε_Z^n	p_pe_R1n	(-)	Partition between dissolved and particulate excretion of N
ε_Z^p	p_pe_R1p	(-)	Partition between dissolved and particulate excretion of P
n_Z^{opt}, p_Z^{opt}	p_qncMIZ, p_qpcMIZ	mmolN mgC^{-1}, mmolP mgC^{-1}	Maximum nutrient quota
ν_Z	1	d^{-1}	Specific rate of nutrients and carbon excretion
d_{0_Z}	p_sd	d^{-1}	Specific mortality rate
d_Z^o	p_sdo	d^{-1}	Oxygen-dependent specific mortality rate

Table 2.5.: Mathematical and code symbols, units and description of the microzooplankton parameters (namelist `Pelagic_Ecology.nml: MicroZoo_parameters`).

Symbol	Code	Units	Description
Q_{10_Z}	p_q10	(-)	Characteristic Q10 coefficient
r_{0_Z}	p_sum	d^{-1}	Potential specific growth rate
v_Z	p_vum	m^3 mg C $^{-1}d^{-1}$	Specific search volume
$\delta_{Z,P}$	p_paPPY(z,p)	(-)	Availability of phytoplankton P to zooplankton Z
$\delta_{Z,Z}$	p_paMIZ(z,p)	(-)	Availability of microzooplankton P to zooplankton Z
$\delta_{Z,Z}$	p_paMEZ(z,p)	(-)	Availability of mesozooplankton P to zooplankton Z
b_Z	p_srs	d^{-1}	Basal specific respiration rate
η_Z	p_puI	(-)	Assimilation efficency
β_Z	p_peI	(-)	Excreted fraction of uptake (faeces production)
n_Z^{opt}, p_Z^{opt}	p_qncMEZ, p_qpcMEZ	mmolN mgC^{-1}, mmolP mgC^{-1}	Maximum nutrient quota
ν_Z	1	d^{-1}	Specific rate of nutrients and carbon excretion
d_{0_Z}	p_sd	d^{-1}	Specific mortality rate
d_Z^{dns}	p_sdo	m^3 mgC^{-1} d^{-1}	Density-dependent specific mortality rate
γ_Z	p_sds	(-)	Exponent for density dependent mortality

Table 2.6.: Mathematical and code symbols, units and description of the mesozooplankton parameters (namelist `Pelagic_Ecology.nml: MesoZoo_parameters`).

half-saturation density μ_Z ($\mu_Z = 0$ for mesozooplankton).

2.4.2. Ingestion

The first term on the right hand side of eq. (2.4.1a) is the total carbon ingestion, which corresponds to the sum of all the predation loss terms in the carbon equations of the other functional groups preyed by zooplankton. Applying the inter-functional group conversion defined in (1.0.2), the rate term for each predation processes is parameterized with a Type 2 formulation (Gentleman et al., 2003),

$$\left.\frac{dZ_c}{dt}\right|_{X_c}^{prd} = -\left.\frac{dX_c}{dt}\right|_{Z_c}^{prd} = f_Z^T\, r_Z^0 \frac{\delta_{Z,X} e_{Z,X} X_c}{F_c} \frac{F_c}{F_c + h_Z^F} Z_c \tag{2.4.2}$$

which is traditionally rewritten in terms of the specific search volume in the case of mesozooplankton ($h_Z^F = \frac{r_{0_Z}}{v_Z}$), because this parameter is generally available in the literature. For brevity, in the zooplankton equations we will use the following notation to indicate the total ingestion rate in units of each constituent:

$$I_j = \sum_X \left.\frac{dZ_j}{dt}\right|_{X_j}^{prd} \quad j = c,n,p. \tag{2.4.3}$$

2.4.3. Excretion/egestion

Metabolic rates in zooplankton are assumed to be closely coupled to growth, therefore total ingested carbon is used part for net production, part for respiration and the remainder is egested/excreted. The parameters that can be measured in laboratory experiments are net growth efficiency η_Z and the egested portion of ingested material β_Z . The ingestion rate in eq. (2.4.3) is not directly affected by prey quality in our present formulation, although this process appears to modulate zooplankton feeding rates substantially (cf. Mitra and Flynn, 2005). Nevertheless, the definition of constant (optimal) nutrient quota in zooplankton (Baretta-Bekker et al., 1997), equivalent to the Threshold Elemental Ratios of Andersen et al. (2004, TER), implies that the ingestion of low-quality (i.e. nutrient-poor) food lead to the disposal of the ingested carbon in excess, thus effectively limiting biomass growth.

On the other hand, an excess of nutrients, as for instance due to the ingestion of phytoplankton under "luxury uptake" conditions, leads to an

increase of the nutrient remineralization rates as shown below in eqs. (2.4.14-2.4.15). The release of extra C is parameterized as an increase of the egestion rates of organic carbon compounds or, alternatively, by increasing the respiration rates. Both processes are well documented in freshwater zooplankton (Frost et al., 2004; Anderson, 2005) and we have decided to parameterize increased excretion rates. The two pathways are equivalent from the point of view of internal element regulation in zooplankton, but the consequences of one choice or another on the biogeochemical cycling of carbon are still to be investigated both experimentally and in model studies.

The carbon loss term in (2.4.1a) thus represents the sum of the activity excretion/egestion (higher for mesozooplankton because of sloppy feeding), the mortality rates and the nutrient-limited excretion of organic carbon. For the microzooplankton the carbon loos term reads:

$$\sum_{j=1,6} \left.\frac{dZ_c}{dt}\right|_{R_c^{(j)}}^{rel} = \beta_Z I_c + (d_{0_Z} + d_Z^o(1-f_Z^o))\, f_Z^T\, Z_c \tag{2.4.4}$$

for mesozooplankton the carbon loss term reads:

$$\left.\frac{dZ_c}{dt}\right|_{R_c^{(6)}}^{rel} = \beta_Z I_c + (d_{0_Z} + doxy_{0_Z}(1-f_Z^o))\, f_Z^T\, Z_c + d_Z^{dns} Z_c^2 + Q_Z^c \tag{2.4.5}$$

The released fraction is further divided into particulate (faecal pellets) and dissolved organic forms using a constant percentage ε_Z^c (mesozooplankton is assumed to have no dissolved products). Mortality is parameterized as senescence with a first-order rate based on a constant d_{0_Z}, as oxygen regulated component $doxy_{0_Z}$, and as a grazing closure by higher trophic levels not resolved in the model, which is a power function of density valid only for mesozooplankton ($d_Z^{dns} = 0$ for microzooplankton).

The balancing flows of C, N, P, $Q_Z^{c,n,p}$ are computed from the actual elemental ratios of ingested material:

$$\Gamma_Z^i = \frac{(1-\beta_Z)\, I_i}{\eta_Z I_c}, \quad i = n, p \tag{2.4.6}$$

the $(1-\beta_Z)$ factor is the assimilation fraction of element uptake. The SWITCH indicates which is the limiting element, default is carbon, if the $\Gamma_Z^i$is lower than the internal quota Z_i/Z_c indicates that i is limiting. The ratios between theΓ_Z^i and the respective zooplankton internal elemental quota of Z_i/Z_c are cross-compared, the lowest defines the most limiting element i. For example in the case of nitrogen limitation (N column Tab.2) the correction on carbon (Q_Z^c) is the difference between effective ingestion of carbon $(\eta_Z I_c)$ and the effective ingestion of nitrogen scaled by the nitrogen TER (n_Z^{opt}):

$$Q_Z^c = \eta_Z I_c - \frac{(1-\beta_Z)}{n_Z^{opt}} I_n, \tag{2.4.7}$$

2.4.4. Respiration

Taking into account the energy cost of ingestion (1 - assimilation - egestion) and basal metabolism the total respiration rate can be written as:

$$\left.\frac{dZ_c}{dt}\right|_{O^{(3)}}^{rsp} = (1-\eta_Z-\beta_Z) I_c + b_Z\, f_Z^T\, Z_c \tag{2.4.8}$$

where the constant basal respiration rate b_Z is also considered. The energy cost of ingestion is computed considering the following metabolic balance:

$$I_c = G_c + E_c + R_c \tag{2.4.9}$$

where Ingestion (I) is partitioned in Growth (G), Excretion (E) and Respiration (R). Assimilation efficiency η_Z is:

$$\eta_Z = \frac{G_c}{I_c} \tag{2.4.10}$$

and excretion is:

$$E_c = \beta_Z I_c \tag{2.4.11}$$

after some algebra we can express R in term of I:

$$R_c = (1-\eta_Z-\beta_Z) I_c \tag{2.4.12}$$

Limiting Element ->	C	N	P
SWITCH	default	if $\frac{\Gamma_Z^n}{Z_N/Z_C} < \frac{\Gamma_Z^p}{Z_p/Z_C}$ and $\frac{\Gamma_Z^n}{Z_N/Z_C} < 1$	if $\frac{\Gamma_Z^p}{Z_p/Z_C} < \frac{\Gamma_Z^n}{Z_n/Z_C}$ and $\frac{\Gamma_Z^p}{Z_p/Z_C} < 1$
Q_Z^c	0	$\eta_Z I_c - \frac{(1-\beta_Z)}{n_Z^{opt}} I_n$	$\eta_Z I_c - \frac{(1-\beta_Z)}{p_Z^{opt}} I_p$
Q_Z^n	$(1-\beta_Z) I_n - n_Z^{opt} \eta_Z I_c$	0	$(1-\beta_Z) I_n - n_Z^{opt} \eta_Z (I_c - Q_Z^c)$
Q_Z^p	$(1-\beta_Z) I_p - p_Z^{opt} \eta_Z I_c$	$(1-\beta_Z) I_p - p_Z^{opt} \eta_Z (I_c - Q_Z^c)$	0

Table 2.7.: Mesozooplankton formulation to eliminate the excess of the non-limiting constituent. The SWITCH control determines whether C, P or N is the limiting element. η_Z is the net growth efficiency factor, β_Z is the egested portion of ingested material, n_Z^{opt} and p_Z^{opt} are the optimal Threshold Elemental Ratios (TERs).

2.4.5. Excretion/egestion of organic nutrients

The nutrient dynamics for zooplankton given in eqs. (2.4.1b) and (2.4.1c) are mainly derived from carbon dynamics taking into account the nutrient content of the total food uptake. The excretion/egestion rate of organic nutrients is obtained from eq. (2.4.4):

$$\sum_{j=1,6} \left.\frac{dZ_i}{dt}\right|_{R_i^{(j)}}^{rel} = \frac{Z_i}{Z_c}\left(\beta_Z I_c + d_{0_Z} f_Z^T Z_c + d_Z^{dns} Z_c^{\gamma_Z}\right) \qquad i = n, p \tag{2.4.13}$$

for microzooplankton is subsequently partitioned between particulate and dissolved matter according to the non-dimensional fraction ε_Z^i which parameterizes the different distribution of nutrients between structural parts and cytoplasm. Mesozooplankton only releases particulate organic detritus.

2.4.6. Inorganic nutrients

The third terms on the right hand side of eq. (2.4.1b) and (2.4.1c) parameterize the zooplankton excretion of inorganic nutrients, which occur only when the internal nutrient quota exceed the optimal quota for P and N, p_Z^{opt} and n_Z^{opt}, respectively. The following formulation is applied to microzooplankton:

$$\left.\frac{dZ_p}{dt}\right|_{N^{(1)}}^{rel} = v_Z^p \max\left(0, \frac{Z_p}{Z_c} - p_Z^{opt}\right) Z_c \tag{2.4.14}$$

$$\left.\frac{dZ_n}{dt}\right|_{N^{(4)}}^{rel} = v_Z^n \max\left(0, \frac{Z_n}{Z_c} - n_Z^{opt}\right) Z_c \tag{2.4.15}$$

and the time scales of excretion are controlled by the specific constant rates v_Z^p and v_Z^n (see Appendix). The excretion is in the form of phosphate and urea, but the latter in the model is assumed to be as labile as the ammonium, therefore the rate is directed to the $N^{(4)}$ pool. In the case of mesozooplankton the inorganic excretion is congruent with the formulation for carbon excretion (Tab.2):

$$\left.\frac{dZ_p}{dt}\right|_{N^{(1)}}^{rel} = d_{0_Z} f_Z^o f_Z^T Z_p + Q_Z^p \tag{2.4.16}$$

$$\left.\frac{dZ_n}{dt}\right|_{N^{(4)}}^{rel} = d_{0_Z} f_Z^o f_Z^T Z_n + Q_Z^n \tag{2.4.17}$$

2.5. Non-living components

2.5.1. Oxygen and anoxic processes

The dynamics of dissolved oxygen and carbon dioxide are important closures of global biogeochemical cycles. We do not describe here the exchange of gases at the air sea interface which is assumed to be a purely physical process and has been thoroughly investigated elsewhere, especially for CO_2 (Olsen et al., 2005).

Anaerobic processes and denitrification dynamics are a consequence of oxygen dynamics and are described here for completeness, although they are of limited impact in the well-oxygenated euphotic zones of the open ocean. Nevertheless, these processes are important for the sulfur cycle and for the fate of exported carbon in the meso- and bathypelagic layers of the ocean where bacteria are the major drivers of these processes. To account for hypoxic and anoxic remineralization in the water, the original ERSEM parameterization of anaerobic processes in the sediments proposed by Ruardij and Van Raaphorst (1995) was extended to the pelagic system by Vichi et al. (2004). The state variable "reduction equivalents" $N^{(6)}$ (Table 1.1 and Fig. 1.1) is an inorganic state variable containing all the reduced chemical species and assumed to be chemically equivalent to the sulphide ion HS^-. The basic constituent is indicated with the letter R because this variable account for all the reduced biochemical products, although it should be mostly regarded as sulphur S. Reduction equivalents are produced as a result of bacterial anoxic respiration and are partly used for the parameterization of denitrification processes and partly for direct sulphide production.

The pelagic net production of oxygen is derived from the sum of gross primary production and community respiration rates from phytoplankton, zooplankton and bacteria, also subtracting the losses due to pelagic chemical reactions:

$$\begin{aligned}\left.\frac{dO^{(2)}}{dt}\right|_{bio} = & \ \Omega^o_c \sum_{j=1}^{3}\left(\left.\frac{dP^{(j)}_c}{dt}\right|^{gpp}_{O^{(3)}} - \left.\frac{dP^{(j)}_c}{dt}\right|^{rsp}_{O^{(3)}}\right) + \\ & -\Omega^o_c f^o_B \left.\frac{dB_c}{dt}\right|^{rsp}_{O^{(3)}} + \\ & -\Omega^o_c \sum_{j=4}^{6}\left.\frac{dZ^{(j)}_c}{dt}\right|^{rsp}_{O^{(3)}} + \\ & -\Omega^o_n \left.\frac{dN^{(4)}}{dt}\right|^{nit}_{N^{(3)}} - \frac{1}{\Omega^r_o}\left.\frac{dN^{(6)}}{dt}\right|^{reox}_{sink_r}\end{aligned} \tag{2.5.1}$$

All the rates are converted into oxygen units by means of constant stoichiometric coefficients. Since bacteria are active both under aerobic and anaerobic conditions the bacterial oxygen demand (2.3.4) is partitioned into oxygen consumption and reduction equivalent production by using the oxygen regulating factor f^o_B in (2.3.2). The nitrification rate is a source term of the nitrate equation (2.5.6b), and a sink term for ammonium (2.5.6c) and oxygen (2.5.1). Nitrification is not explicitly resolved but parameterized with a simple first-order dependence on ammonium and oxygen concentrations:

$$\left.\frac{dN^{(4)}}{dt}\right|^{nit}_{N^{(3)}} = \Lambda^{nit}_{N^{(4)}} f^T_n \frac{O^{(2)}}{O^{(2)}+h_o} N^{(4)} \tag{2.5.2}$$

where Λ^{nit}_{N4} is the constant specific nitrification rate and f^T_n a temperature regulating factor with the Q10 formulation shown in (2.1.1).

The formation of reduction equivalents is parameterized converting the biological oxygen demand of bacteria (under low oxygen conditions) into sulphide ions by using the stoichiometric coefficient Ω^r_o (see Appendix) as:

$$\begin{aligned}\left.\frac{dN^{(6)}}{dt}\right|_{bio} = & \ \Omega^r_o \Omega^o_c \left(1-f^o_{B1}\right)\left.\frac{dB_c}{dt}\right|^{rsp}_{O^{(3)}} + \\ & -\Omega^r_o \widetilde{\Omega}^o_n \left.\frac{dN^{(3)}}{dt}\right|^{denit}_{sink_n} - \left.\frac{dN^{(6)}}{dt}\right|^{reox}_{sink_r}\end{aligned} \tag{2.5.3}$$

The utilization of nitrate as an electron acceptor in microbial metabolic reactions is parameterized in an indirect way. Firstly, when the oxygen level falls below the threshold level and $f^o_B < 1$ (eq. (2.3.2)), the metabolic formation of reduction equivalents begins according to the carbon

mineralization rate (2.3.4). The denitrification reaction is favored with respect to the strictly anaerobic sulphate reduction, therefore a portion of this oxygen demand is redirected towards the denitrification process. In order to achieve this net effect, the changes in the redox conditions enhance the denitrification flux in the following way:

$$\left.\frac{dN^{(3)}}{dt}\right|^{denit} = \Lambda^{denit}_{N^{(3)}} f^T_n \left[\frac{1}{\mathscr{M}^*_o}\Omega^o_c\left(1-f^o_B\right)\left.\frac{dB_c}{dt}\right|^{rsp}_{O^{(3)}}\right] N^{(3)}. \tag{2.5.4}$$

where $\Lambda^{denit}_{N^{(3)}}$ is the specific denitrification rate at a reference anoxic mineralization $\mathscr{M}^*_o$. If nitrate is still present in the water, the bacterial rate of production of reduction equivalents $N^{(6)}$ is converted to nitrate consumption, mimicking the bacteria-mediated denitrification reactions. This chemical rate leads to a direct production of gaseous N_2 in the water, which is the only time rate of change for state variable $O^{(4)}$ in the model.

Furthermore, as long as there is some oxygen left, reduction equivalents are also quickly re-oxidized at the following rate:

$$\left.\frac{dN^{(6)}}{dt}\right|^{reox}_{sink_r} = \Lambda^{reox}_{N^{(6)}} \frac{O^{(2)}}{O^{(2)}+h_o} N^{(6)} \tag{2.5.5}$$

where $\Lambda^{reox}_{N^{(6)}}$ is the (constant) specific daily re-oxidation rate, and h_o is the half-saturation oxygen concentration. When oxygen and nitrate are completely depleted the last two terms in (2.5.3) become zero and the process turns to a strict anaerobic formation of sulphide ions coupled to the availability of the organic substrate.

2.5.2. Dissolved inorganic nutrients

The pelagic cycles of dissolved inorganic nutrients are essential components of any biogeochemical model of the marine ecosystem. Five inorganic CFFs for dissolved compounds are considered here (Fig. 1.1): phosphate, nitrate (nitrate + nitrite), ammonium and silicate with the equations shown in Box 2.5 and derived from the processes described in the previous sections.

The pelagic cycle of phosphate $N^{(1)}$ in (2.5.6a) is affected by phytoplankton uptake (2.2.23), bacterial uptake/release (2.3.9) and excretion from zooplankton groups (2.4.14).

The pelagic processes for nitrate $N^{(3)}$ shown in (2.5.6b), involve phytoplankton uptake described in (2.2.1b) and the nitrification and denitrification process parameterizations described in (2.5.2) and (2.5.4), respectively.

Ammonium (eq. (2.5.6c)) is consumed by phytoplankton as described in (2.2.23) and remineralized (or utilized) by bacteria according to the quality of the substrate and their internal content of nitrogen according to eq. (2.3.10). Zooplankton participates in the ammonium dynamics through the excretion of urea, which is assumed to be directly available in the form of ammonium, as shown in eq. (2.4.15).

The pelagic cycle of silicate is quite simple in the model because of the many uncertainties linked to the complex dynamics of this element in the water. Silicate concentration was originally only affected by diatom uptake (2.2.1e), but a simple first-order reaction parameterizing bacterial dissolution (e.g. Bidle and Azam, 2001) has been introduced accounting for the dissolution of silicate frustules as:

$$\left.\frac{dR^{(6)}_s}{dt}\right|^{rmn}_{N^{(5)}} = \Lambda^{rmn}_s f^T_{R^{(6)}} R^{(6)}_s \tag{2.5.7}$$

where Λ^{rmn}_s is the constant specific dissolution rate and $f^T_{R^{(6)}}$ is the temperature regulating factor as in eq. (2.1.1), mimicking bacterial activity enhancement at higher temperatures.

Iron is made available in dissolved form through remineralization of biogenic particles produced by phytoplankton and zooplankton. The biochemical pathways of the remineralization process are not completely clear and involve both siderophores and photochemical reactions. Since all these processes are primarily bacterial-mediated, it is assumed here that dissolved Fe is released from detritus according to a first-order relationship as for silicate (2.5.7):

$$\left.\frac{dR^{(6)}_f}{dt}\right|^{rmn}_{N^{(5)}} = \Lambda^{rmn}_f f^T_{R^{(6)}} R^{(6)}_f \tag{2.5.9}$$

Symbol	Code	Units	Description
Ω_c^o	MW_C	mmolO_2 mgC^{-1}	Unit conversion factor and stoichiometric coefficient
Ω_n^o	p_qon_nitri	mmolO_2 mmolN^{-1}	Stoichiometric coefficient for nitrification reaction
$\widetilde{\Omega}_n^o$	p_qon_dentri	mmolO_2 mmolN^{-1}	Stoichiometric coefficient for denitrification reaction
Ω_o^r	p_qro	mmolHS $^-$ mmol$O_2{}^{-1}$	Stoichiometric coefficient for oxic-anoxic reaction
Ω_n^r	p_qro * p_qon_dentri	mmolHS $^-$ mmolN^{-1}	Stoichiometric coefficient nitrogen-anoxic reaction
Λ_{N4}^{nit}	p_sN4N3	d^{-1}	Specific nitrification rate at 10^oC
Q_{10_n}	p_q10N4N3	(-)	Q10 factor for nitrification/denitrification reaction
h_o	p_clO2o	mmolO_2 m^{-3}	Half saturation for chemical processes
h_r	p_clN6r	mmolHS $^-$ m^{-3}	Half saturation oxygen concentration for anoxic processes
Λ_{N3}^{denit}	p_sN3O4n	d^{-1}	Specific denitrification rate
$\mathscr{M}_o^*$	p_rPAo	mmol O_2 m^{-3} d^{-1}	Reference anoxic mineralization rate
Λ_{N6}^{reox}	p_rOS	d^{-1}	Specific reoxidation rate of reduction equivalents
$Q_{10_{N5}}$	p_q10R6N5	(-)	Q10 factor for dissolution of biogenic silica
Λ_s^{rmn}	p_sR6N5	d^{-1}	Specific dissolution rate of biogenic silica
ε_{PAR}	p_PAR	(-)	Fraction of Photosynthetically Available Radiation
λ_W	p_eps0	m^{-1}	Background attenuation coefficient
$c_{\substack{R^{(6)} \\ sed}}$	p_epsR6	m^2 mg C^{-1}	C-specific attenuation coefficient of particulate detritus
v_{R6}	p_sediR6	m d^{-1}	Settling velocity of particulate detritus

Table 2.8.: Chemical stoichiometric coefficients and general parameters involving pelagic components.

Equation Box 2.5 Dissolved inorganic nutrient equations.

$$\left.\frac{dN^{(1)}}{dt}\right|_{bio} = -\sum_{j=1}^{4}\left.\frac{dP_p^{(j)}}{dt}\right|_{N^{(1)}}^{upt} + f_B^p\left.\frac{dB_p}{dt}\right|_{N^{(1)}}^{upt,rel} + \sum_{k=4,5,6}\left.\frac{dZ_p^{(k)}}{dt}\right|_{N^{(1)}}^{rel} \tag{2.5.6a}$$

$$\left.\frac{dN^{(3)}}{dt}\right|_{bio} = -\sum_{j=1}^{4}\left.\frac{dP_n^{(j)}}{dt}\right|_{N^{(3)}}^{upt} + \left.\frac{dN^{(3)}}{dt}\right|_{N^{(4)}}^{nit} - \left.\frac{dN^{(3)}}{dt}\right|_{sink_n}^{denit} \tag{2.5.6b}$$

$$\left.\frac{dN^{(4)}}{dt}\right|_{bio} = -\sum_{j=1}^{4}\left.\frac{dP_n^{(j)}}{dt}\right|_{N^{(4)}}^{upt} + f_B^p\left.\frac{dB_n}{dt}\right|_{N^{(4)}}^{upt,rel} + \sum_{k=4,5,6}\left.\frac{dZ_n^{(k)}}{dt}\right|_{N^{(4)}}^{rel} - \left.\frac{dN^{(4)}}{dt}\right|_{N3}^{nit} \tag{2.5.6c}$$

$$\left.\frac{dN^{(5)}}{dt}\right|_{bio} = -\left.\frac{dP_s^{(1)}}{dt}\right|_{N^{(5)}}^{upt} + \left.\frac{dR_s^{(6)}}{dt}\right|_{N^{(5)}}^{rmn} \tag{2.5.6d}$$

Equation Box 2.6 Dissolved organic matter equations

$$\left.\frac{dR_c^{(1)}}{dt}\right|_{bio} = \sum_{j=1}^{3} \left.\frac{dP_c^{(j)}}{dt}\right|_{R_c^{(1)}}^{exu} - \left.\frac{dB_c}{dt}\right|_{R_c^{(1)}}^{upt} + \sum_{k=5,6} \left.\frac{dZ_c^{(k)}}{dt}\right|_{R_c^{(1)}}^{rel} \tag{2.5.8a}$$

$$\left.\frac{dR_i^{(1)}}{dt}\right|_{bio} = \sum_{j=1}^{3} \left.\frac{dP_i^{(j)}}{dt}\right|_{R_i^{(1)}}^{exu} - \frac{R_i^{(1)}}{R_c^{(1)}} \left.\frac{dB_c}{dt}\right|_{R_c^{(1)}}^{upt} + \sum_{k=5,6} \frac{Z_i^{(k)}}{Z_c^{(k)}} \left.\frac{dZ_c^{(k)}}{dt}\right|_{R_c^{(1)}}^{rel} \quad i = n, p \tag{2.5.8b}$$

$$\left.\frac{dR_c^{(2)}}{dt}\right|_{bio} = \left.\frac{dP_c}{dt}\right|_{R_c^{(2)}}^{exu} - \left.\frac{dB_c}{dt}\right|_{R_c^{(2)}}^{upt} \left(+ \left.\frac{dB_c}{dt}\right|_{R_c^{(2)}}^{rel} \right) \tag{2.5.8c}$$

where Λ_f^{rmn} is a constant specific dissolution rate and $f^T_{R^{(6)}}$ is the temperature dependence. Both numbers are currently unknown, and therefore they need to be adjusted by trial-and-error for balancing the iron cycle in the ocean. The inclusion of iron as an explicit component of zooplankton and bacteria may link this process to the direct excretion of organisms and bacterial regeneration activity, once the important pathways and timescales have been properly assessed by laboratory and in situ experiments.

Dissolved inorganic iron species are scavenged onto particle surfaces owing to hydroxide precipitation. Since the concentration of iron ligands is about 0.6 nM in the deep ocean, Johnson et al. (1997) suggested that iron scavenging can be parameterized with a constant rate when the [Fe'] is above this threshold. Ligand dynamics have been further investigated by Archer and Johnson (2000); Parekh et al. (2004); Lefevre and Watson (1999), but the simplest approach as proposed by Johnson et al. (1997) and Aumont et al. (2003) has been used here:

$$\left.\frac{dN^{(7)}}{dt}\right|_{sink_f}^{scv} = \Lambda_f^{scv} \min\left(0, N^{(7)} - 0.6\right) \tag{2.5.10}$$

with a given time constant $\Lambda_f^{scv} = \frac{1}{40}$ years^{-1} and with the further assumption that scavenging results in adsorption onto sinking particles and consequently sequestration in the deeper layers.

2.5.3. Dissolved and particulate organic matter

The state variables describing dissolved organic matter shown in Box 2.6 have been introduced in Sec. 2.3 because they are tightly linked to the parameterizations of pelagic bacteria. 3 biogeochemical basic constituents C, N and P and are thus described by 3 equations shown in. DOM is produced by phytoplankton, bacteria and microzooplankton and used as organic substrate by bacteria. The different degrees of lability of DOM are reflected in the nutrient content of $R_j^{(1)}$, which regulates bacterial uptake as shown in eq (2.3.18), while variables $R_c^{(2)}$ and $R_c^{(3)}$ only contains the carbon constituent. The equation (2.5.8c) for semi-labile DOC (carbohydrates) is derived from the production terms implemented in the different bacteria parameterizations (Secs. 2.3.4, 2.3.5 and 2.3.6). Bacteria are allowed to release carbohydrates only in BACT2 and BACT3 parameterizations.

Particulate detritus is instead described by 4 equations, one for each biogeochemical basic constituent C, N, P, Si as in Box 2.7. The carbon, nitrogen and phosphorus component of particulate detritus in (2.5.11a) and (2.5.11b) respectively) are produced by all the members of the planktonic community except bacteria, which are the only utilizers of this component according to (2.3.18).

The pelagic cycle of biogenic silica is instead restricted to the release of diatom frustules through mortality and other lysis processes as in (2.2.28) and via micro/mesozooplankton preda-

tion (including sloppy feeding) with the addition of the chemical dissolution shown in (2.5.7).

Particulate iron dynamics are the consequence of processes described in (2.2.9), (2.5.9) and (2.5.10). Particulate organic Fe is also derived from zooplankton egestion and mortality. It is assumed that zooplankton is never iron-limited and the iron fraction of the ingested phytoplankton is directly egested as particulate detritus.

2.5.4. The carbonate system

The aquatic chemistry of CO_2 and carbonates (dissolved inorganic carbon forms, DIC, state variable $O^{(3)}$) is a further extension to the original ERSEM formulation and it is activated with the key `INCLUDE_PELCO2`. The theory of DIC chemical reactions is well understood (Zeebe and Wolf-Gladrow, 2001) and we propose here a slightly revised formulation with respect to Blackford and Burkill (2002) which also takes into account the algorithms proposed by the Ocean Carbon Model Intercomparison Project (Doney et al., 2004).

In the ocean, DIC exists in three different forms: free carbon dioxide ($[CO_2] = [CO_2]_{aq} + [H_2CO_3]$), bicarbonate ion ($HCO_3^-$) and carbonate ion ($CO_3^{2-}$). The carbonate species reach the following equilibrium:

$$CO_2 + H_2O \rightleftharpoons HCO_3^- + H^+ \rightleftharpoons CO_3^{2-} + 2H^+ \tag{2.5.12}$$

defined by the equilibrium constants K_1 and K_2 for the first and second reaction, respectively. The carbonate system in seawater is described in terms of 7 chemical species, i.e., free carbon dioxide (CO_2), bicarbonate ion (HCO_3^-), carbonate ion (CO_3^{2-}), carbon dioxide partial pressure in seawater (pCO_2), hydrogen ion concentration ($pH = -log_{10}([H^+])$), total carbon concentration (DIC) and total alkalinity (TA). These species are governed by the following relations:

$$K_1 = \frac{[HCO_3^-]\cdot[H^+]}{[CO_2]} \tag{2.5.13}$$

$$K_2 = \frac{[CO_3^{2-}]\cdot[H^+]}{[HCO_3^-]} \tag{2.5.14}$$

$$DIC = [CO_2] + [HCO_3^-] + [CO_3^{2-}] \tag{2.5.15}$$

$$pCO_2 = \frac{[CO_2]}{K_0} \tag{2.5.16}$$

$$\begin{aligned} TA \;=\; & [HCO_3^-] + 2[CO_3^{2-}] + [B(OH)_4^-] + \\ & + [OH^-] + [HPO_4^{2-}] + 2[PO_4^{3-}] + \\ & + [H_3SiO_4^-] - [H^+]_F - [HSO_4^-] + \\ & - [HF] - [H_3PO_4] \end{aligned} \tag{2.5.17}$$

The species appearing in this latter equation are expressed in terms of their equilibrium constants and of their total elemental concentrations. Total alkalinity is therefore computed as a function of:

$$\begin{aligned} TA = f\,([H^+], DIC, K_1, K_2, K_w, K_b, \\ K_{1p}, K_{2p}, K_{3p}, K_{si}, K_s, K_f, bt, st, ft, \\ O^{(3)}, O^{(5)}, N^{(5)}, N^{(1)}) \end{aligned} \tag{2.5.18}$$

where $K_1$and K_2 are the previously seen equilibrium constants for carbonic acid (H_2CO_3) and bicarbonate ion (HCO_3^-), K_0 is the Henry's constant which regulates CO_2 solubility in seawater, K_w is the ion product of water, K_b is the dissociation constant for boric acid ($B(OH)_3$), K_{1p}, K_{2p} and K_{3p} are the dissociation constants for phosphoric acid (H_3PO_4), di-hydrogen phosphate ion ($H_2PO_4^-$) and hydrogen phosphate ion (HPO_4^{2-}) respectively, K_{si} is the dissociation constant for silicic acid ($Si(OH)_4$), K_s is the dissociation constant for bisulfate ion (HSO_4^-), K_f is the dissociation constant for hydrogen fluoride (HF), bt is the total boron concentration ($[B(OH)_3 + [B(OH)_4^-]$), st is the total sulfate concentration ($[HSO_4^-] + [SO_4^{2-}]$), ft is the total fluoride concentration ($[HF] + [F^-]$), and $O^{(3)}$, $O^{(5)}$, $N^{(1)}$ and $N^{(5)}$ are the model state variables for DIC, total alkalinity, total phosphorus concentration ($[H_3PO_4] + [H_2PO_4^-] + [HPO_4^{2-}] + [PO_4^{3-}]$), and total silica concentration ($[Si(OH)_4] + [H_3SiO_4^-]$), respectively. Note that total fluoride, sulfate and

Equation Box 2.7 Particulate organic detritus equations.

$$\left.\frac{dR_c^{(6)}}{dt}\right|_{bio} = \sum_{j=1}^{4} \left.\frac{dP_c^{(j)}}{dt}\right|_{R_c^{(6)}}^{lys} - \left.\frac{dB_c}{dt}\right|_{R_c^{(6)}}^{upt} + \sum_{k=4}^{6} \left.\frac{dZ_c^{(k)}}{dt}\right|_{R_c^{(6)}}^{rel} \tag{2.5.11a}$$

$$\left.\frac{dR_i^{(6)}}{dt}\right|_{bio} = \sum_{j=1}^{4} \left.\frac{dP_i^{(j)}}{dt}\right|_{R_i^{(6)}}^{lys} - \frac{R_i^{(6)}}{R_c^{(6)}} \left.\frac{dB_c}{dt}\right|_{R_c^{(6)}}^{upt} + \sum_{k=4}^{6} \frac{Z_i^{(k)}}{Z_c^{(k)}} \left.\frac{dZ_c^{(k)}}{dt}\right|_{R_c^{(6)}}^{rel} \quad i = n, p \tag{2.5.11b}$$

$$\left.\frac{dR_s^{(6)}}{dt}\right|_{bio} = \left.\frac{dP_s^{(1)}}{dt}\right|_{R_s^{(6)}}^{lys} + \frac{P_s^{(1)}}{P_c^{(1)}} \sum_{j=4}^{6} \left.\frac{dP_c^{(1)}}{dt}\right|_{Z_c^{(j)}}^{prd} - \left.\frac{dR_s^{(6)}}{dt}\right|_{N^{(5)}}^{rmn} \tag{2.5.11c}$$

boron concentrations (ft, st and bt) are given as dependent on the temperature and salinity only. Currently, the model does not take into account changes of alkalinity due to calcification.

The effects of biogeochemical processes on alkalinity linked to the N cycle are taken into account with a correction to the total alkalinity value after Wolf-Gladrow et al. (2007). The uptake of 1 mole of N leads to (i) an increase of alkalinity by 1 mole when nitrate is the source, (ii) to a decrease of alkalinity by 1 mole when ammonia is used. Nitrification leads to a decrease of TA by 2 moles per mole of nitrate formed and denitrification leads to an increase of TA by 1 mole per mole of nitrate converted. Thus, considering the equations in (2.5.6b) and (2.5.6c), the source form equation for TA reads:

$$\left.\frac{dO^{(5)}}{dt}\right|_{bio} = \sum_{j=1}^{4} \left.\frac{dP_n^{(j)}}{dt}\right|_{N^{(3)}}^{upt} - \sum_{j=1}^{4} \left.\frac{dP_n^{(j)}}{dt}\right|_{N^{(4)}}^{upt} + -2 \left.\frac{dN^{(3)}}{dt}\right|_{N^{(4)}}^{nit} + \left.\frac{dN^{(3)}}{dt}\right|_{sink_n}^{denit} \tag{2.5.19}$$

The equilibrium constants are also computed from temperature and salinity according to the methods described in Zeebe and Wolf-Gladrow (2001) where the total pH scale is used. The carbonate equilibrium calculation is done in units of $mol \cdot kg^{-1}$, therefore conversions from model units are done by taking into account the actual seawater density.

This is a five equation system with seven unknown variables: the system is therefore determined when two of the seven variables are known, which in this case are DIC and TA. Total alkalinity equation is used to compute $[H^+]$ by means of the Newton-Raphson convergence method. A new state variable is also introduced to store the total hydrogen ions and to allow the restart of the model from previous simulations. The other carbon species are eventually computed from the carbonate equilibrium equations.

Alternatively, the model allows the usage of a simplified computation of DIC equilibria as suggested by Follows et al. (2006), which does not imply an iterative procedure. This solution is suggested for coupled configurations because in that case the inaccuracy of the computation is less important due to the presence of advective and diffusive processes.

Finally, the biological production and consumption of CO_2 considered in the model can be easily derived by collecting the first 4 terms on the right hand side of eq. (2.5.1) without considering the stoichiometric factor Ω_c^o and taking the total bacterial respiration as

$$\left.\frac{dO^{(3)}}{dt}\right|_{bio} = \sum_{j=1}^{3} \left(\left.\frac{dP_c^{(j)}}{dt}\right|_{O^{(3)}}^{gpp} - \left.\frac{dP_c^{(j)}}{dt}\right|_{O^{(3)}}^{rsp} \right) + - \left.\frac{dB_c}{dt}\right|_{O^{(3)}}^{rsp} - \sum_{k=4,5,6} \left.\frac{dZ_c^{(k)}}{dt}\right|_{O^{(3)}}^{rsp} \tag{2.5.20}$$

The parameters of the carbonate system are controlled with a specific namelist found in file

CO2.nml and listed in Tab. 2.9. The namelist also allows to read an external file containing data for atmospheric concentration of inorganic carbon or to set it constant to a certain value of the mixing ratio. Atmospheric partial pressure can also be computed or read from an external file.

Parameter	Units	Description
pCO2Method	Integer Switch	Methods for computing pCO2 1 = AtmCO20* sea level pressure (slp0 in Param.nml or external input AtmSLP_N), 2 = Compute the pCO2 using the Magnus formula: Sea Level Pressure and Dew Point Temperature have to be provided
AtmCO20	ppmv	Set constant atmospheric CO2 concentration (ppm), also referred as the CO2 mixing ratio
calcAtmpCO2	Logical	Compute the atmospheric pCO2
phstart	pH	Initial guess of the seawater pH.
K1K2	Integer Switch	Acidity constants parameterization 1- Roy et al. (1993); DOE (1994); pH on total scale; 2- Mehrbach et al. (1973) refit by Dickson & Millero (1987); pH on Sea Water Scale; 3 - Mehrbach et al.(1973) refit by Lueker et al. (2000), pH on total scale; 4 - Hansson (1973b) data as refitted by Dickson and Millero (1987), pH on Sea Water Scale.
MethodCalcCO2	Integer Switch	Method for Carbonate System computation: 1 - Approximate static solution; 2 - Standard OCMIP iteration; 3 - Approximation by Follows et al. (2006).
CalcBioAlkFlag	Logical	Compute the corrections of alkalinity due to biogeochemical processes
M2XACC	Threshold	Accuracy of the iterative scheme for OCMIP (with MethodCalcCO2=2)
M2PHDELT	pH	pH range for the root search in the OCMIP scheme (with MethodCalcCO2=2)
M2MAXIT	Integer	maximum number of iterations for OCMIP (with MethodCalcCO2=2)
Caconc0	mol m^{-3}	Calcium ion concentration (In "Seawater : Its composition, properties and behaviour", Open University Course Team, 1995)
Canorm	Logical	Normalize Calcium ion concentration by sea water salinity
AtmCO2_N	ppmv	Read external file with atmospheric CO_2 mixing ratio data.
AtmSLP_N	Pa	Read external file with Sea Level Pressure data (with pCO2Method=1 and 2).
AtmTDP_N	^{o}C	Read external file with atmospheric Dew Point Temperature data (with pCO2Method = 2).

Table 2.9.: Parameters controlling the carbonate system (from namelist CO2.nml)

Part II.

BFM code description

3. Installation, configuration and compilation

The default basic configuration of BFM is the STANDALONE model, which simulates the biogeochemistry of a water volume with given depth. The typical example is a micro- or mesocosm batch culture. Only the pelagic system can be currently simulated with this configuration. The model is forced with prescribed or analytical functions of temperature, salinity and light and can be integrated for any desired period with three different numerical schemes. The model output is in NetCDF.

3.1. Installation

After downloading the tarball from the website, create a directory for the BFM and cd into that directory. Uncompress and extract the contents of the tarball. The downloaded file will have a different name based on the version. For example:

```
% mkdir $HOME/BFM
% cd $HOME/BFM
% gunzip bfm-release-<version>.tgz
% tar xvf bfm-release-<version>.tar
```

This operation will create and populate the directory `bfm` containing the source files and the directory `run` for running the various test cases which are described in Sec. 4.4. The full directory tree of the BFM core is given in Fig. 3.1.

3.2. System Requirements

The currently supported architectures are

- linux
- Mac OSX (Darwin)
- AIX

The software requirements are:

- PERL (version 5.8.2 and above), used automatically during compilation time to generate the code from the model template (see Sec. 6.2).
- FORTRAN 90/95 compiler. Under linux and Mac OSX the model can be currently compiled with gfortran (version 4.5 and above) and ifort. For AIX xlf90 is required.
- NetCDF library (http://www.unidata.ucar.edu/software/netcdf) . It is mandatory that the library has been compiled with the same compiler used for the model compilation since the F90 netcdf module is used.

```
|-- bin
|-- build
|   |-- configurations
|   |-- logs
|   `-- scripts
|       `-- conf
|-- compilers
|-- doc
|-- include
|-- run
|-- src
|   |-- BFM
|   |   |-- CO2
|   |   |-- Forcing
|   |   |-- General
|   |   |-- Light
|   |   |-- Oxygen
|   |   |-- Pel
|   |   |-- PelBen
|   |   |-- include
|   |   `-- proto
|   |-- share
|   `-- standalone
`-- tools
    |-- bnmerge
    |-- bnremap
    |-- matlab
    `-- scripts
```

Table 3.1.: Source directory tree and description of the directory contents.

3.3. Configuring the BFM STANDALONE

Configuration and deployment of the model is done automatically by the script *bfm_configure.sh*. The minimal user local settings for compilation is provided by means of the environmental shell variable:

- BFMDIR The root directory of the BFM model (the path to the installed bfm-<version> directory).

After setting-up $BFMDIR variable in your shell environment you can go to *$BFMDIR/build* directory and execute *bfm_configure.sh* using default values:

```
./bfm_configure.sh -gcd
```

An execution without errors[1] will show the output directory for running the experiment and the command to execute. Output after successful compilation should end with:

```
...
Go to .../bfm/run/standalone.pelagic and execute command:
./bfm_standalone.x
...
```

bfm_configure.sh generates, compiles and/or deploys files needed for the BFM model. There are three different steps to have an executable model (see Fig. 3.1): *Generation* (generate .h , .f90 needed for compilation and .nml files needed for execution), *Compilation* (compile and create the executable file) and *Deployment* (create experiment folder and copy namelists for execution).

For a full description of the script usage and available options, see Tab. 3.2 or execute the following command:

```
./bfm_configure.sh -h
```

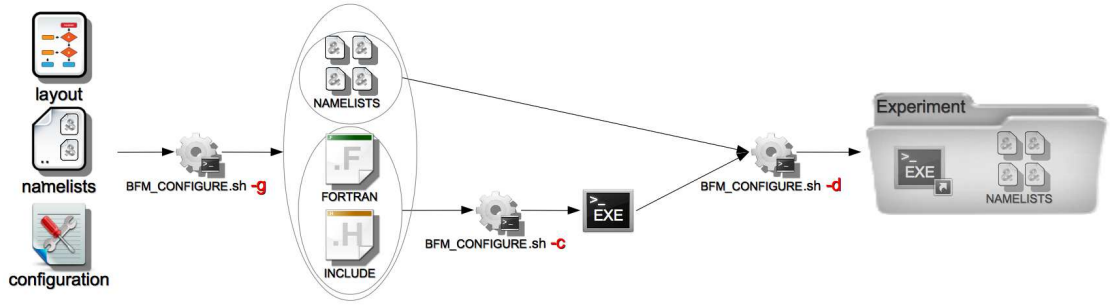

Figure 3.1.: Steps for experiment deployment

[1] If you experience problems during the generation or compilation, visit `http://bfm-community.eu/documentation` for help

Option	Argument	Description
		Compilation options
VERBOSE	-v	Verbose mode to print all messages
PRESET	-p	Preset to generate the configuration
MODE	-m	Mode for compilation and deployment
CPPDEFS	-k	Key options to configure the model
BFMDIR	-b	path to root directory of BFM
NEMODIR	-n	path to root directory of NEMO
ARCH	-a	Specify compilation Architecture file
PROC	-r	Number of procs used for compilation (and execution)
FAST	-f	Fast mode. Dont execute "clean" command in compilation
NETCDF	-t	Path to netcdf library and header files
		Deployment options
EXP	-x	Name of the experiment for generation of the output folder
NMLDIR	-l	Input dir where are the namelists to run the experiment
PROC	-r	Number of procs used for running (same as compilation)
QUEUE	-q	Name of the queue number of procs used for running

Table 3.2.: List of optional arguments for bfm_configure

3.3.1. Presets

An experiment is defined by a model layout structure and initial input values. These definitions put together with compilation and run options is what is called a PRESET. A preset is contained together in a folder and it is all you need to execute a particular experiment.

The folder containing presets is *${BFMDIR}/build/configurations/*. Execute the following command to show a list of all available presets:

```
./bfm_configure.sh -P
```

Presets are loaded using option “-p” followed by the preset name, eg.:

```
./bfm_configure.sh -p STANDALONE_PELAGIC
```

Presets are composed of three different main files:

`configuration`: compilation and deployment options

This file uses the F90 namelist format to set values. Below a schematic view of the configuration file format:

```
&BFM_conf
        <option>=<value>,
        ...
        <option>=<value>
/
```

Not all the options available in Tab. 3.2 can be specified in the configuration file and all the values are overridden by the command line options. Available options are: MODE, CPPDEFS, BFMDIR, NEMODIR, ARCH, CLEAN, PROC, NETCDF, EXP, NMLDIR, PROC and QUEUE. Do not use the character " to surround values, but use ’ instead.

`layout:` memory layout configuration file

This file is the template for the memory model. For a detailed description of the memory layout content goes to Sec. 5.2.

`namelists:` namelist file with standard values

This file contains all the standard values of the namelists[2] used for the experiment. Namelists are checked for consistency against the source code at generation time and the files effectively used for the simulation will be copied in the *$BFMDIR/run* directory. This check will guarantee an executable file compatible with the namelists provided. The regular user will generally work with generated namelists and usually there is no need to change any keyword in this file besides the values in case there is the willingness to generate a new standard set of values.

[2] BFM input namelists follows F90 namelist standard

4. Running the STANDALONE model

4.1. Description

The execution of the configuration script described in the previous section creates the executable and the running environment for the default preset of the STANDALONE model (called STANDALONE_PELAGIC). The list of the available presets is obtained with the command `bfm_configure.sh -P` and the results of the test cases are detailed in Sec. 4.4. The generated namelists are copied to the directory `$BFMDIR/run/standalone.pelagic` and the model is run by executing `./bfm_standalone.x` or `./bfm_standalone.x &> outputfile` to redirect the output messages to a file in bash. Most of the BFM settings can be controlled via namelists. The STANDALONE model behaviour is controlled with 2 major namelist files `BFM_General.nml` and `Standalone.nml`. The first file contains the namelist to control the model setup (Tab. 4.1), model formulation (Tab. 4.2) and the parameters for all the functional groups described in Part I. The second fie contains

4.2. Numerical integration

Three integration schemes are implemented in the STANDALONE model. They can be chosen by the parameter `method` in the namelist file `standalone.nml`. They are all explicit and use a time step cutting approach to avoid negative concentrations. In detail, indicating with $S(c_n)$ the right-hand-side source term computed with concentration c_n, they are written as:

- the Euler scheme (`method=1`):

  $c_{n+1} = c_n + S(c_n)\Delta t$

- the Runge-Kutta scheme of 2$^{\text{nd}}$ order (`method=2`):

  $c_{n+1} = c_n + \frac{1}{2}\left[S(c_n) + S(c_n + S(c_n)\Delta t)\right]\Delta t$

- the leap-frog scheme (`method=3`):

  $c_{n+1} = c_{n-1} + S(c_n)2\Delta t$ with the Asselin-filter: $c_n = c_n + \gamma(c_{n-1} - c_n + c_{n+1})$

4.3. Forcing functions

The STANDALONE model can be forced with different kind of forcing functions to provide the physical information for the aquatic system (e.g. temperature, irradiance, etc.). Two options are currently available: analytical forcing functions and data from an external file. All external data formats and time interpolations are derived from the code provided by GOTM under the GPL.

name	*kind*	*description*
bio_setup	integer	STANDALONE configuration: 1. pelagic 2. benthic (not yet available) 3. pelagic and benthic (not yet available)
bfm_rstctl	string	Save initial state in the output file
out_fname	string	Name of NetCDF output file
out_dir	string	Path to the output file
out_title	string	Name of the experiment in NetCDF file
out_delta	integer	Output is saved every out_delta timesteps

Table 4.1.: Parameters that control the model setup and output file (bfm_nml in BFM_General.nml)

4.3.1. Analytical forcing functions

This option is activated by setting forcing_method=1 in the namelist forcings_nml (Tab. 4.4). The simple analytical forcing functions give the user a easily accessible and quickly usable basic setup of the physical forcing fields. The basic concept behind all forcing functions is the interpolation of some (northern hemisphere) summer and winter values by a sine wave, considering them as the two extreme values. This simple case is used for salinity forcing data (sw and ss in Table 4.5), while for temperature, in addition to the sine wave, it is possible to superimpose a daily excursion (constant all over the year).

Light forcing is interpolated with a sine wave from a winter minimum value to a summer maximum value (lw and sw in Table 4.5) to obtain the actual value of average daylight for each day of the year. These variables are as well intended as the placeholders for instantaneous light values and average daylight, i. e. the mean value of light energy over the light period:

$$\frac{1}{daylength}\int_{\tau_{dawn}}^{\tau_{dusk}} light(t)dt$$

The daylength is computed by the model as a function of the latitude value given in the namelist . In case of the instantaneous light option (ltype=1) the average daylight is distributed in a sine wave over the daylight period reaching thus a maximum of twice the average daylight while being zero at the beginning and in the end of the light period. In the case of constant light (ltype=2) the mean daylight is smoothed out over the whole day by the factor daylength/24. In the case of rectangular light distribution (ltype=3) the light equals the average daylight value over the whole daylight period and is zero at night time. In order to setup a constant-light experiment, it is sufficient to put the winter value equal to the summer value and set ltype=2.

4.3.2. Boundary forcing for atmospheric CO_2

The STANDALONE model (but also any other coupled configuration that does not provide a connection with the atmosphere) has the possibility to turn on the prescription of an atmospheric CO_2 concentration for computing the surface fluxes. A time series can be specified as input to the atmospheric

name	*kind*	*description*
CalcPelagic	logical	Switch on off the pelagic system
CalcBenthicFlag	integer	Switch for the benthic model (only option 1. is currently allowed) 1. no benthic model; 2. simple benthic return; 3. benthic organisms and intermediate complexity nutrient regeneration; 4. benthic organisms and full nutrient regeneration (early diagenesis)
CalcPhytoplankton(P)	logical	Switch for phytoplankton (P=1,2,3,4)
CalcPelBacteria(B)	logical	Switch for pelagic bacteria (B=1)
CalcMesoZooplankton(Z)	logical	Switch for mesozooplankton (Z=1 for Z3, Z=2 for Z4)
CalcMicroZooplankton(Z)	logical	Switch for microzooplankton (Z=1 for Z5, Z=2 for Z6)
CalcPelChemistry	logical	Switch for pelagic chemistry
AssignPelBenFluxesInBFMFlag	logical	Switch to turn on/off the fluxes between the pelagic and the benthic system. Fluxes are always computed but not integrated if the flag is false
AssignAirPelFluxesInBFMFlag	logical	Switch to turno on/off the fluxes between the atmosphere and the pelagic system. Fluxes are always computed but not integrated if the flag is false
ChlDynamicsFlag	integer	Switch for chlorophyll parameterization in phytoplankton 1. constant chl:C ratio and acclimation through optimal light (ERSEM-II). Note: the variable for chl content P1l is used to store optimal irradiance in W m^{-2} 2. Chlorophyll is a phytoplankton constituent and variable chl:C ratio. Note: P1l is in mg chl m^{-3}
LightPeriodFlag	integer	Provide the light averaging period of the external irradiance: 1. Instantaneous irradiance 2. Daylight average with explicit photoperiod 3. Daily average
LightLocationFlag	integer	Choose the parameterization of light location in the discrete grid: 1. Light at the top of the cell 2. Light in the middle of the cell 3. Average Light in the cell

Table 4.2.: Parameters that control model formulation in BFM_General.nml

name	*kind*	*description*
nboxes	integer	Number of water volumes (boxes)
indepth	real	Depth of each box (m)
latitude	real	Latitude of each box
longitude	real	Longitude of each box
maxdelt	real	Maximum timestep duration (s)
mindelt	real	Minimum timestep duration (s)
method	integer	Integration method 1. Euler forward 2. Runge-Kutta 2nd order 3. Leap-frog

Table 4.3.: Main parameters for controlling time marching and integration in the STANDALONE (standalone_nml in Standalone.nml)

name	*kind*	*description*
timefmt	integer	Format of the time limits and loop: 1. MaxN only. Give number of iterations, fake start time is used. 2. start and stop dates. MaxN calculated. 3. start and MaxN. stop time calculated. 4. simdays only. Give number of simulation days, fake start time used and MaxN calculated.
MaxN	integer	Number of iterations in time-loop
simdays	integer	Number of simulation days
start	string "yyyy-mm-dd hh:mm:ss"	Start date
stop	string "yyyy-mm-dd hh:mm:ss"	Stop date

Table 4.4.: Main parameters for time management and integration length (time_nml in Standalone.nml))

name	*kind*	*description*
forcing_method	integer	Choice of the external forcing functions 1. analytical forcings 2. from file 3. interactive fluxes (not yet implemented)
ltype	integer	Light forcing options: 1. instantaneous light description 2. constant light over 24h 3. rectangular light distribution (on/off) according to photoperiod 4. Constant light averaged over the photoperiod
lw	real	Sinusoidal light intensity (boreal winter) W m^{-2}
ls	real	Sinusoidal light intensity (boreal summer) W m^{-2}
sw	real	Sinusoidal salinity (boreal winter)
ss	real	Sinusoidal salinity (boreal summer)
tw	real	Sinusoidal temperature (boreal winter) degC
ts	real	Sinusoidal temperature (boreal summer) degC
tde	real	Sinusoidal temperature daily excursion degC
ww	real	Sinusoidal wind (boreal winter) m s^{-1}
ws	real	Sinusoidal wind (boreal summer) m s^{-1}
CO2inc	real	Linear increase in CO_2 air partial pressure [% per year]
forcing_file	char	Filename for external forcings (forcing_method = 2)
use_external_data	logical	Read external data (user defined)
data_file	char	Filename for external data

Table 4.5.: Parameters for the external forcing functions (forcings_nml in Standalone.nml

mixing ratio by setting the file name in `Carbonate_Dynamics.nml` parameters listed in Tab. 2.9. This is activated only if pelagic CO_2 is turned on in the model with the macros `INCLUDE_PELCO2` in the file `configuration`. The atmospheric value found in `Carbonate_Dynamics.nml` is given in units of partial pressure (μatm) and not in ppm. A simple annual increase of this initial value can be turned on by giving a percentage constant rate in the variable `CO2inc` found in `Standalone.nml` (Table 4.5, set to 0 by default, if set to 1.0 gives the typical 1% annual increase).

4.3.3. Environmental data from file

The `forcing_method=2` option allows the user to input the environmental data directly from a file. The required input data are seawater temperature (variable `ETW`, ^oC), salinity (`ESW`), irradiance (in W m^{-2}, converted directly into the model variable `EIR`) and wind velocity (`EWIND`, m s^{-1}). Any other parameter can be included by modifying the file `standalone/external_forcing.F90`. This file is a template for the input of external forcing data and must be modified by the user. The data input file format is an ASCII file with a first column indicating the date (`yyyy-mm-dd hh:mm:ss`) and one column for each parameter separated by space(s).

4.3.4. External event data

The model allows to input event data that force the state variables to certain values. This is useful in the case of a laboratory experiment when for instance phytoplankton is inoculated at given time interval or nutrients are restored to certain values. The syntax of the input file is the same as the environmental data file above and the template file `standalone/external_data.F90`. must be modified by the user according to the state variables that have to be modified. The subroutine is implemented to overwrite any obtained value of the selected state variable(s) with the input value(s) at the prescribed time(s).

4.4. Test cases

4.4.1. CO2TEST: carbonate system model

The most simple test case is `CO2TEST` that generates the run directory `run/co2test`. if the BFM is configured with `bfm_configure.sh -gcd -p CO2TEST`. It simulates a simple carbonate system equilibrium using the routines developed by OCMIP (`CalcCO2Method=2` in `Carbonate_Dynamics.nml`). Initial conditions are set for a Mediterranean station with high alkalinity value and output is created every 60 days. The system is forced with observed atmospheric CO_2 increase over the period 1979-2009. The default simulation prescribes a constant temperature value and it is interesting to note the differences shown in Fig. 4.1 when seasonal variability of temperature is turned on. The seasonal cycle in temperature can be prescribed by changing the winter and summer temperature minima and maxima of the analytical forcing functions (Sec. 4.5).

4.4.2. STANDALONE_PELAGIC: the full pelagic BFM

The standard test case for the full BFM is created in directory `run/standalone.pelagic` and it is the default preset when the code is generated and compiled without any option. It simulates the seasonal cycle of a well-mixed temperate coastal sea, with mean depth 5 m. This example is to be considered as a template for other applications, as it is not meant to describe any real-world

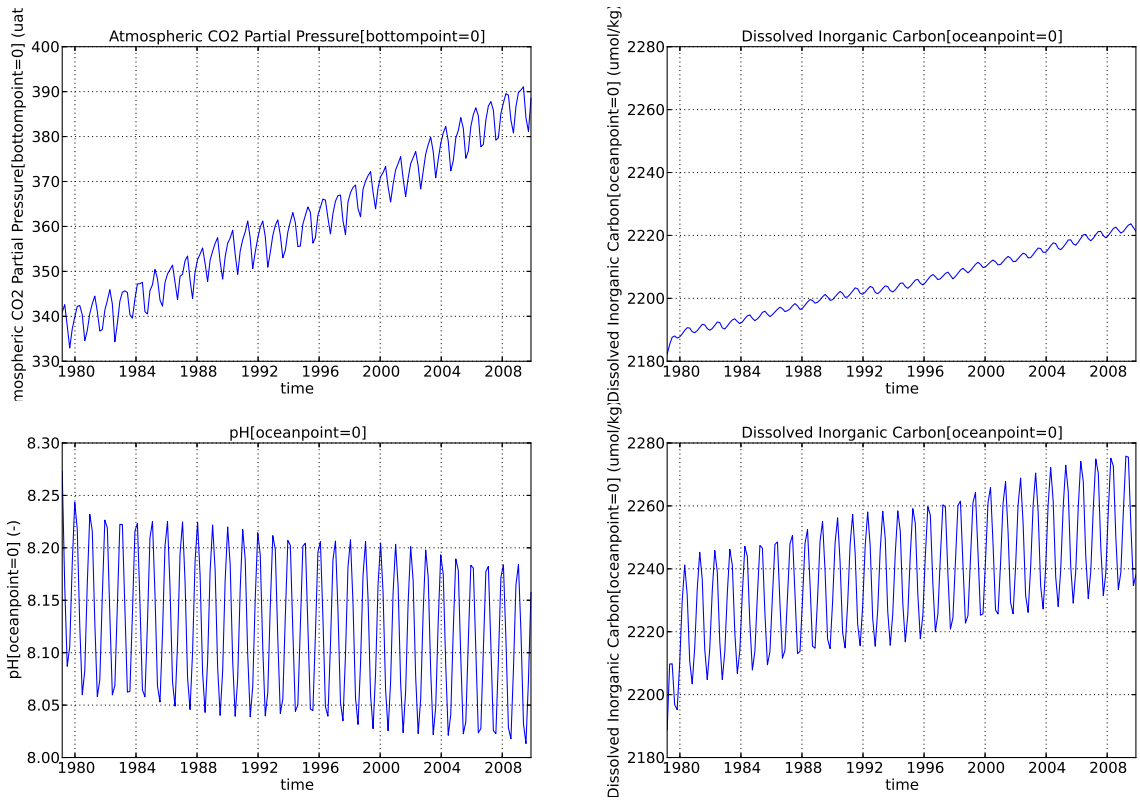

Figure 4.1.: Examples from the `CO2TEST` simulation. Top panels: atmospheric CO_2 partial pressure from the NOAA marine boundary layer data at 33N () and DIC with temperature set to the constant value of 25 ^oC (default run). Bottom panels) pH and DIC with seasonally varying temperature (`tw=14, ts=27` in `Standalone.nml`)

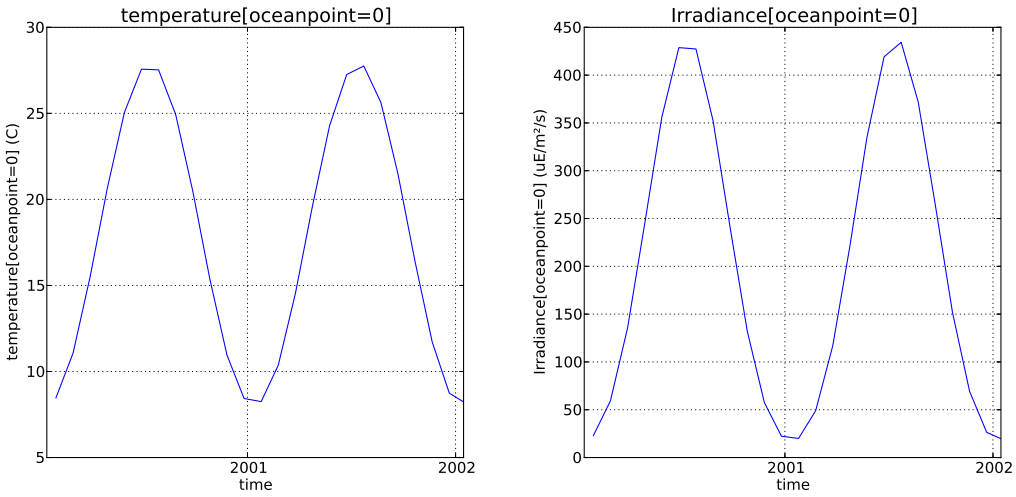

Figure 4.2.: Sample output of the STANDALONE test case temperate.pelagic. a) temperature; b) irradiance

application. The simulation starts in January 2000 and terminates in 2010 with a maximum time step of 8640 s in the adaptive Runge-Kutta solver and with the output stored every 30 days (see namelists in Tab. 4.4, 4.3 and 4.1). The time evolutions of temperature, irradiance, nutrients (the system is sustained with regenerated nutrients only, therefore nitrate plot is logarithmic and goes very close to 0), chlorophyll and gross primary production are shown in Figs. 4.2-4.4 for comparison.

4.5. Output visualization

Output values are stored in netCDF according to the CF convention (`http://www.cgd.ucar.edu/cms/eaton/cf-metadata/`). The STANDALONE output can be visualized with the all-round `ncview` software (`http://meteora.ucsd.edu/~pierce/ncview_home_page.html`), with the Python utility PyNcview `https://sourceforge.net/projects/pyncview/` or with `ncbrowse`. Matlab users can use the `bfm_ncload.m` utility available in the tools directory. The figures presented in Sec. 4.4 have been produced with pyncview.

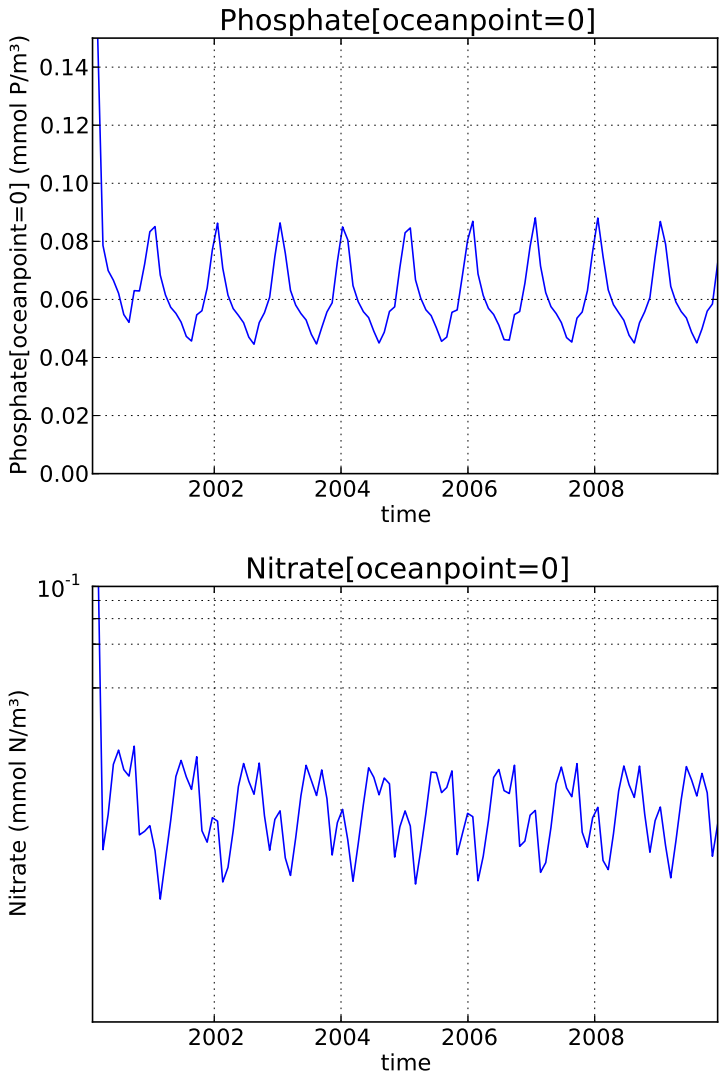

Figure 4.3.: Sample output of the STANDALONE test case standalone.pelagic. a) phosphate; b) nitrate

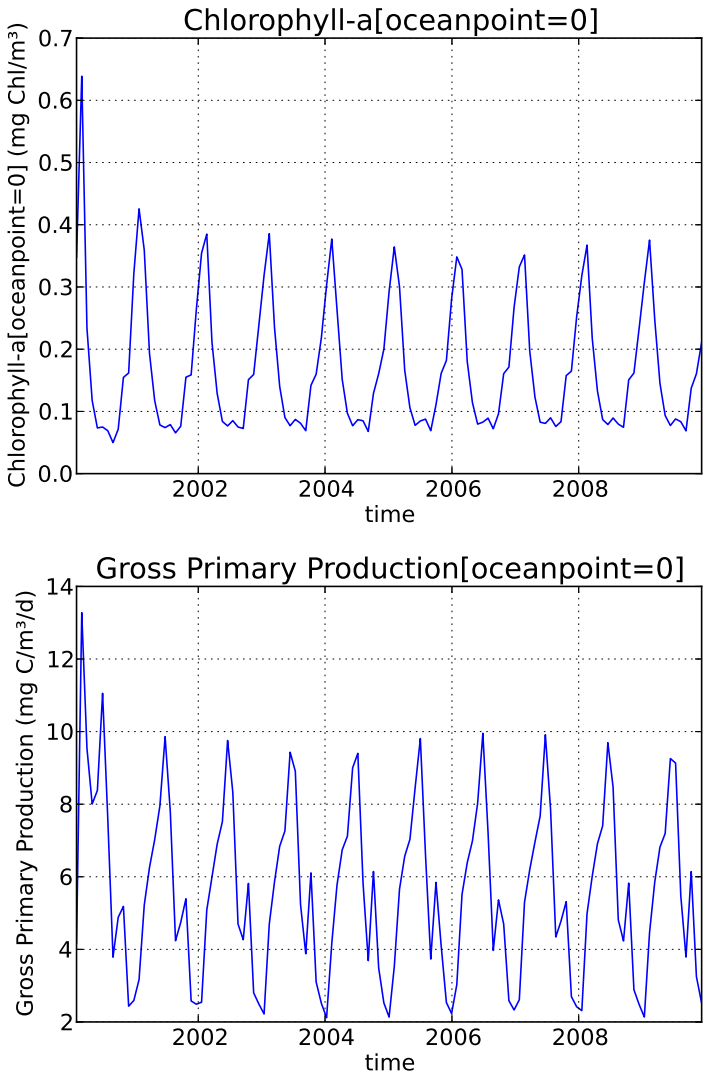

Figure 4.4.: Sample output of the STANDALONE test case temperate.pelagic. a) Chlorophyll-a; b) gross primary production

5. Structure of the code

5.1. Coding rules

The BFM is written in plain F90 and it can generally be compiled with any F90 (and above) compiler. There are no fixed coding rules apart from standard clean programming. For historical reasons, the subroutine and symbols of the BFM biogeochemistry module are indicated with C-style capitalized long-names (e.g. EcologyDynamics), even if F90 does not distinguish capital letters. Constants and main memory arrays are generally indicated with capital names, to highlight their global static behavior. It is recommended to follow this style when possible.

5.2. Memory layout and variable definition

The BFM is structured similarly as the original ERSEM used to be. Pelagic variables are defined as virtually 3-dimensional, while benthic and sea ice variables are 2-dimensional. Only the sea-points are stored in memory, and thus the BFM has no knowledge of any land-sea mask or spatial relationships between grid-points in general. The number of bottom points is the same as the number of surface points, therefore the 2-D arrays can also be used for the surface variables and/or surface fluxes. These definitions are also maintained when the model is applied to a 1-D vertical setup. In that case, the pelagic variables have the spatial dimension of the number of vertical layers while the benthic and surface variables have dimension 1 (the bottom and surface levels, with the index depending on the definitions of the physical model). In a 0-D setup (as in the STANDALONE test case described in Chap. 4), the same grid-point is at the same time a bottom, surface and ocean layer.

Fig. 5.1 illustrates the memory layout of pelagic variables. They are gathered in a single 2-dimensional array holding the number of different variables and the number of ocean grid-points:

```
D3STATE(NO_D3_BOX_STATES,NO_BOXES)
```

and the same is done for the 2-dimensional variables (defined for the benthic and sea ice ecosystem models):

```
D2STATE(NO_D2_BOX_STATES,NO_BOXES_XY)
```

Each variable memory is accessed by means of a pointer to the corresponding row containing all the grid-point values. This pointer array has the same naming convention of ERSEM. The rows are numbered with named constants starting with the letters `pp` (`ppP1c` for phytoplankton carbon, `ppN1n` for nitrate or `ppR1p` for dissolved organic phosphorus, etc.). When the BFM is coupled to a 3-D model, then a mapping function must be taken into account as shown in Fig. 5.1 in order to compute the transport terms.

In addition to this direct mechanism, the memory can be accessed by means of *group functions*. These functions have been created to allow the addition of any number of sub-groups in the same trophic compartment, such as diatoms, nanoflagellates, picoplankton, etc. in the group of phytoplankton. The group function is in this case called `PhytoPlankton(no_of_subgroups, no_of_components)`, and allows to access the memory `P1c` by writing

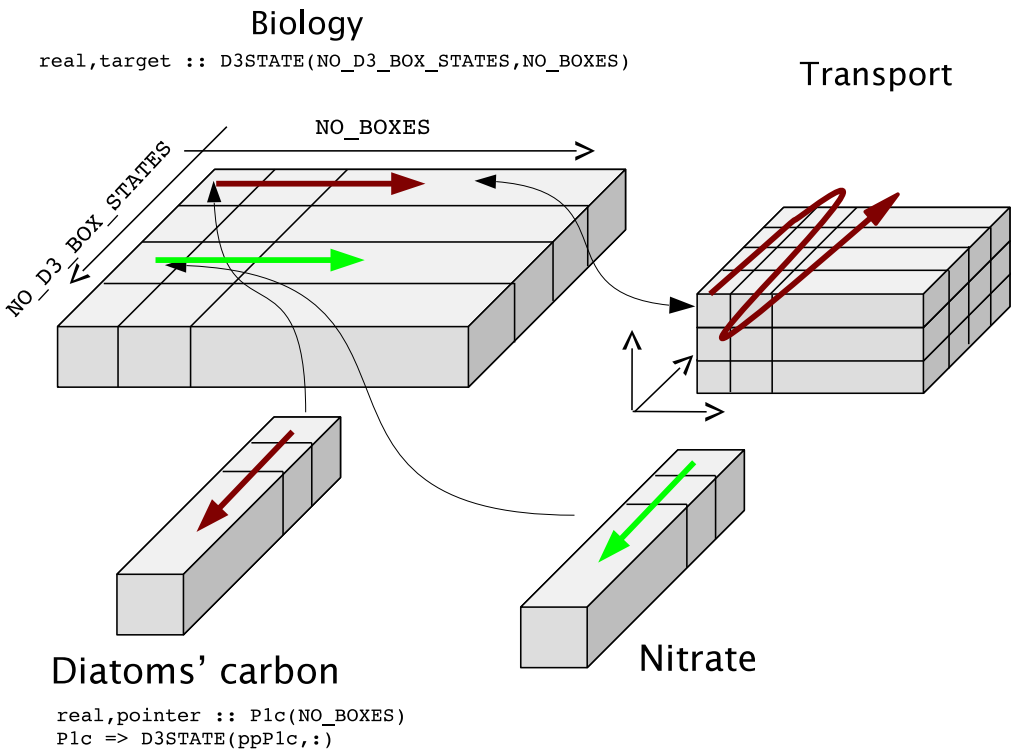

Figure 5.1.: Layout of the main memory array for the pelagic variables (`D3STATE`) and schematic of the remapping into a three-dimensional ocean grid for transport processes.

`PhytoPlankton(iiP1,iiC)`

The model state variables and components are defined in the model layout file of each preset (Sec. 3.3.1) which will be detailed in Chap. 6. It is now only sufficient to list the constants indicating the constituents, namely `iiC`, `iiN`, `iiP` and `iiSi`. For each defined group there is a named constant starting with the letters `ii` which holds the total number of existing subgroups (e.g. `iiPhytoPlankton`).

A typical example of the use of groups is to compute the total amount of food available to microzooplankton (from `MicroZoo.F90`):

```
do i = 1 ,iiPhytoPlankton
    PPYc(:,i) = p_paPPY(zoo,i)*PhytoPlankton(i,iiC)* &
                MM_vector(PhytoPlankton(i,iiC), p_minfood(zoo))
    rumc = rumc + PPYc(:,i)
    rumn = rumn + PPYc(:,i)*qncPPY(i,:)
    rump = rump + PPYc(:,i)*qpcPPY(i,:)
 end do
```

Compare this code with the equation for food availability and capture efficiency presented in Sec. 2.4.1 of the BFM description and it will show how it is simple to cycle over all the phytoplankton variables, independently of the number and type of the defined subgroups.

The other basic arrays of the memory are the ones containing the time rates of change due to each physiological or ecological interaction. The rate of mass exchange between two state variables is an element of an array D3SOURCE, if it is a production term, and D3SINK if it is a loss term, both with dimensions NO_D3_BOX_STATES × NO_D3_BOX_STATES × NO_BOXES (Fig. 5.2). It is clear that the two matrices are symmetrical and a predation (negative) rate from variable P1c to Z4c is equivalent to an ingestion rate (positive) of Z4c over P1c. All the rates are defined positive by convention, so that to obtain the net rate of change for variable of row j, it is sufficient to compute

```
sum(D3SOURCE(j,:,:)-D3SINK(j,:,:))
```

This separation between positive and negative terms allow to use more sophisticated positive-definite integration schemes although it may result in excessive memory usage. It is therefore possible to combine the two symmetrical matrices into one (D3SOURCE), that contains all the source terms in the upper-left part and the sink terms in the lower-right part. It is finally allowed to further shrink the memory by adding all the terms

Fluxes which involve a variable not defined in the model, such as oxygen production from water during photosynthesis can be taken into account by using the diagonal of the matrix. There is a positive flow from O2o to itself computed stoichiometrically from the gross carbon production rate and inserted in (D3SOURCE(O2o,O2o,:), cf. Fig. 5.2).

The same definitions apply for the 2-dimensional system, and the arrays are called D2SOURCE and D2SINK with dimensions NO_D2_BOX_STATES × NO_D2_BOX_STATES × NO_BOXES_XY.

No direct mass exchanges are allowed between variables from different realms (like for instance between pelagic and benthic variables), and therefore those fluxes are defined as diagonal fluxes each one within its own realm taking into account any change of units. Specialized functions have been written to take into account all the possible kind of exchanges and are collected in General/FluxFunctions.F90.

5.3. The BFM flow-chart

The BFM core will be described in its STANDALONE configuration. The main program (Fig. 5.3) consists of 3 subroutines, one for initialization, one for the time-loop and one for closing all active processes. The same structure is likely to be maintained also for all the coupled configurations, but the calls are going to be distributed differently according to the structure of the general circulation model.

5.3.1. Initialization procedures

The initialization of the BFM requires 4 different phases:

1. Initialization of geometric domain (number of boxes/gridpoints). This part depends on the configuration: in the STANDALONE case, this is done in standalone/standalone.F90[init_standalone] while in the other coupled configuration there are specific interface subroutines;
2. Initialization of the set-up via namelist and definition of variable information (share/api_bfm.F90[init_bfm] for the STANDALONE case);
3. Definition of variable information and allocation/initialization of variables;
4. Initialization of the NetCDF output.

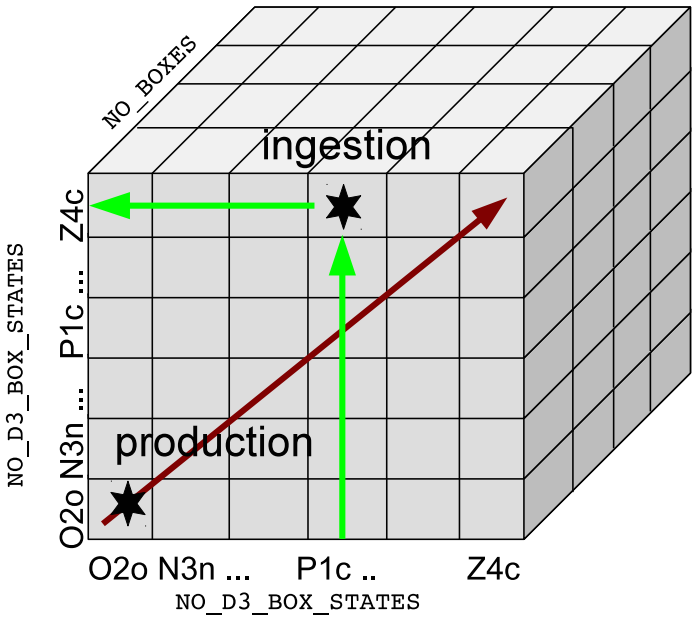

Figure 5.2.: Schematic of the `D3SOURCE` array collecting the source terms.

5.3.2. Time marching

The time marching is driven by the host hydrodynamical model, or in the case of the STANDALONE model, by a specific built-in routine. The phases of the time stepping shown in Fig. 5.3 are the following:

1. update of the physical forcing functions needed by the biogeochemical model (temperature, irradiance, wind, etc.). This is done by subroutine `envforcing_bfm`, which in the case of the STANDALONE model computes the analytical values based on the time of the day/year. When coupled with an ocean model, this routine is the contact point between the two models. Note that information may flow in two directions because the light attenuation coefficient might also be passed back to the physical model via this routine.

2. computation of the reaction term for the BFM module. This is done in `EcologyDynamics`, which is further explained in the next section.

3. numerical integration of the biogeochemical terms. In the Standalone model there are three different numerical schemes that can be used (see the quickstart guide for the specific namelist values). Note that `EcologyDynamics` can be called more than one time by this routine when the integration scheme is of higher-order.

4. preparation and writing of the NetCDF output, routines `calcmean_bfm` and `save_bfm` (the names of the routines can be different for each coupling according to the ocean model structure and naming conventions).

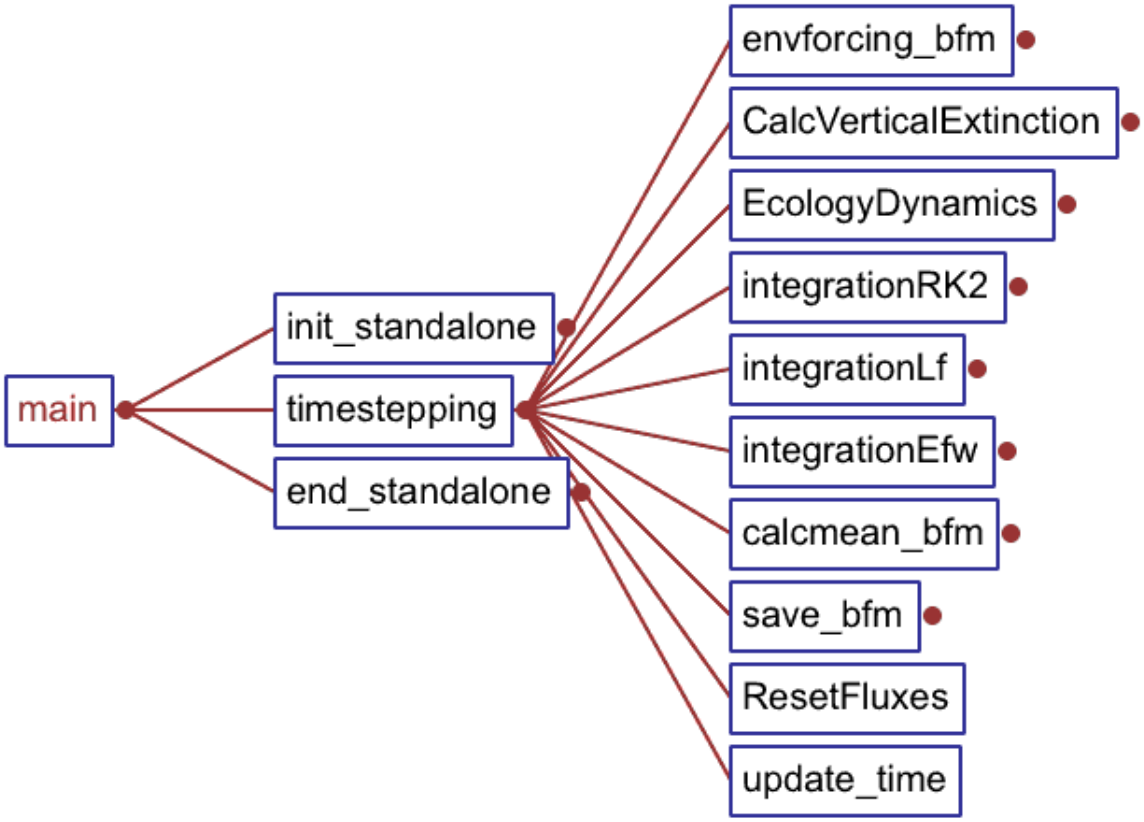

Figure 5.3.: Invocation tree of the Standalone main.

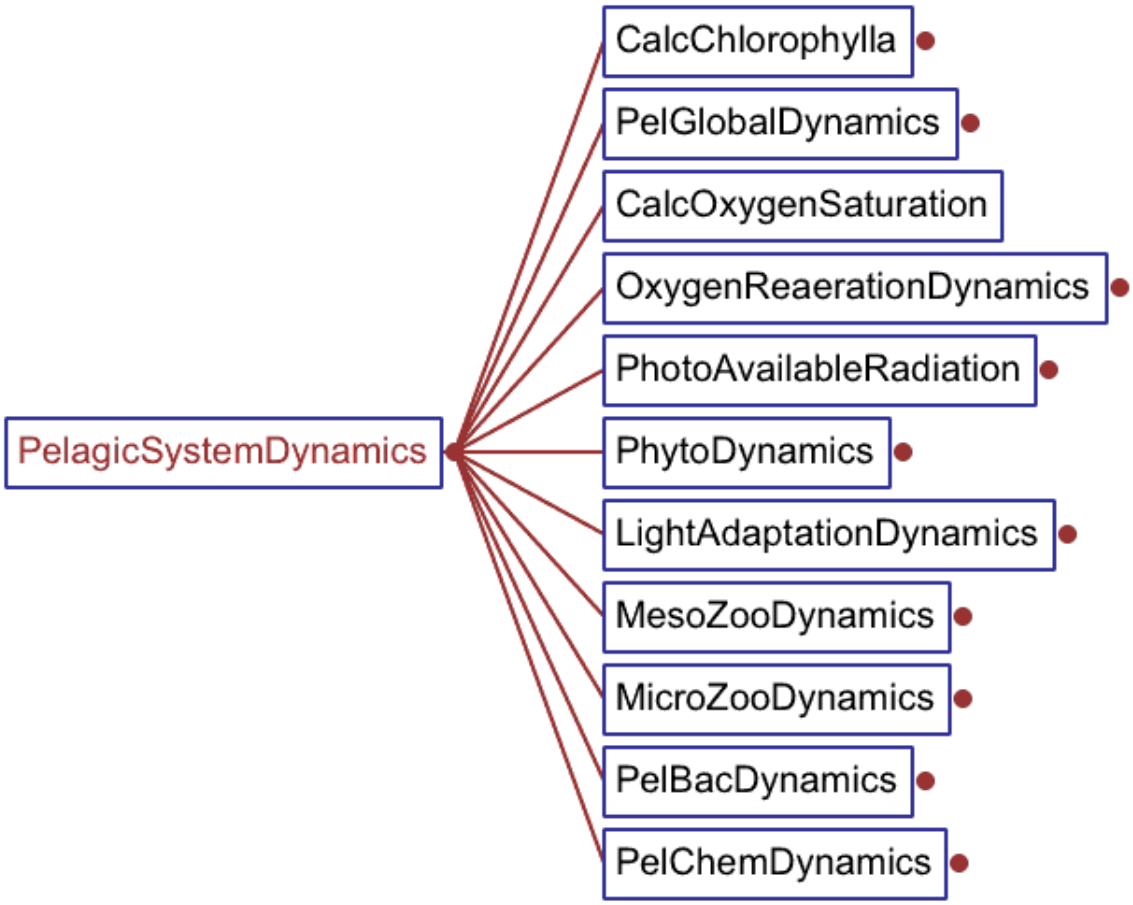

Figure 5.4.: Invocation tree for PelagicSystemDynamics

5.3.3. Computation of pelagic reaction terms

The pelagic components are computed in `PelagicSystemDynamics`, which invokes the routines shown in Fig. 5.4. It first sets the diagnostic values for total chlorophyll (sum of all the chlorophyll components in phytoplankton) and for the nutrient:carbon ratios in all the components (`PelGlobalDynamics`) and for oxygen saturation and surface fluxes with the atmosphere.

The routines for the computation of light availability are only used when the parameterization of optimal irradiance is activated (as in ERSEM-II, Ebenhöh et al., 1997), see Sec. 2.2.7, which is done in `Param_parameters` (Tab. 4.2) by setting `ChlDynamicsFlag=1`.

The standard groups, phytoplankton, meso- micro-zooplankton and bacteria are computed in `PhytoDynamics`, `Meso- MicroZooDynamics` and `PelBacDynamics`, respectively. The same routine is modularly used for each sub-group, as

```
!-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
! Compute phytoplankton dynamics
!-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
do i =1,iiPhytoPlankton
   if ( CalcPhytoPlankton(i)) call PhytoDynamics( i )
end do
```

...

```
!-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
! Compute MesoZooPlankton dynamics
!-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
do i =1,iiMesoZooPlankton
   if ( CalcMesoZooPlankton(i)) call MesoZooDynamics( i )
end do
```

`PhytoDynamics` has the declaration structure depicted in Fig. 5.5. This is an example of how the memory layout presented in Sec. 5.2 is accessed by each submodel of the BFM. To refer to the pointer of each phytoplankton component, one can use the placeholder function `ppPhytoPlankton(i,j)`, where *i* is the phytoplankton subgroup number (up to 4 in the reference model) and *j* is the component (c, n, p, etc). Using `ppPhytoPlankton(1,iiC)` is equivalent to writing `ppP1c`.

The function `flux_vector` is invoked many times by `PhytoDynamics` (Fig. 5.5) because it is used to fill in the source/sink term arrays described in Sec. 5.2. This function is used throughout the BFM modules. In case of a mass exchange term such as the excretion of dissolved carbon we have

```
call flux_vector(iiPel,ppphytoc,ppR1c,rr1c)
```

where the flux is pelagic (`iiPel`), from phytoplankton carbon to dissolved organic carbon (`ppphytoc, ppR1c`) and the value is `rr1c`, which will be assigned both to `D3SINK` and `D3SOURCE` in the appropriate element. The oxygen production rate is instead assigned as

```
call flux_vector(iiPel,ppO2o,ppO2o,rugc/MW_C)
```

which concerns a pelagic flux (`iiPel`), on the oxygen diagonal (from `ppO2o` to `ppO2o`) and `MW_C` is the mass weight of carbon to convert gross primary production (`rugc`). Since the last term is positive, this flux will be assigned to `D3SOURCE`.

The same methodology is applied for all the other pelagic fluxes and also in the benthic and sea ice system. After the computation of all the reaction terms for pelagic organisms, there is the call

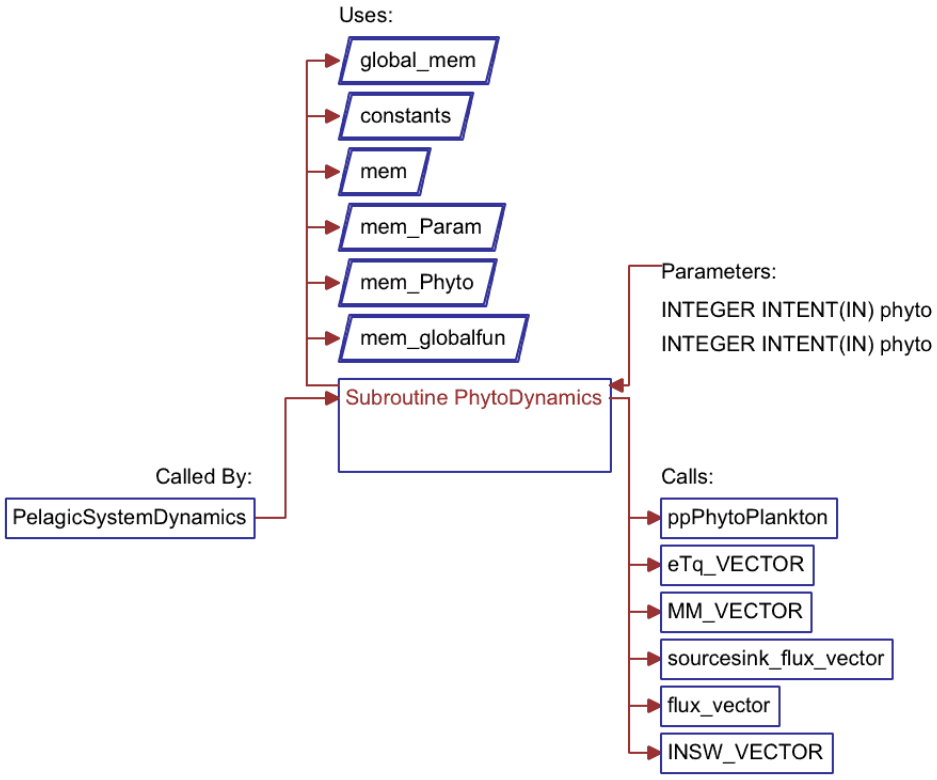

Figure 5.5.: Declaration scheme of PhytoDynamics.

to pelagic chemistry (`PelChemDynamics`, see Fig. 5.4). This part computes all the parameterized bacteria-mediated biochemical processes such as nitrification and denitrification, reoxidation of reduction equivalents and dissolution of biogenic silica.

6. Advanced features

The BFM is conceived in a modular way and the number of state variables and biogeochemical basic components can be modified according to the modelling needs. This section addresses the advanced features that are useful to change the structure of the model and to optimize some behaviour at compilation.

6.1. Compilation macros

There are 2 major macros that belong to the core of the BFM source code and additional compilation keywords that activates model components. The first 2 macros are "negative", which means that their options are activated by default and needs to be deactivated when desired.

NOT_STANDALONE: This macro controls the main memory structure of the BFM. In default configuration the BFM allocates its own memory array. When the macro is defined at compilation (`-DNOT_STANDALONE`) all the variables belonging to the main memory are defined as pointers and are not allocated during the initialization phase. This is the configuration used in combination with hydrodynamical models that already defines a memory array for biogeochemical variables.

BFM_NOPOINTERS: by default, all the F90 symbols of the BFM state variables are defined as pointers to the main memory (cf. Sec. 5.2). By defining the macro `-DBFM_NOPOINTERS`, it is possible to substitute all the pointers with the actual memory location. For instance, all the occurrences of the keyword `P1c(:)` which are pointers to the memory address of phytoplankton carbon content, are substituted with the name `D3STATE(ppP1c,:)`. To facilitate this feature, it is requested that all the references to the pointers in the code are written with the indication of the number of dimensions: `P1c` should always be indicated as `P1c(:)`, otherwise a precompiler error is generated when `BFM_NOPOINTERS` is defined.

ONESOURCE: Join together the elements of `D3(D2)SOURCE` and `D3(D2)SINK` arrays to reduce memory storage

D1SOURCE: Further reduce memory storage by defining one source matrix `D3(D2)SOURCE(NO_BOX_STATES,NO_BOXES)` where all the right-hand side terms are summed when computed (this is incompatible with macro `INCLUDE_DIAG3D`)

INCLUDE_PELCO2: Define and activate the pelagic variables of the carbonate system;

INCLUDE_PELFE: Add iron dynamics to the system

INCLUDE_DIAG3D: Activate the customizable diagnostics described in Sec. (this is incompatible with macro `D1SOURCE`)

```
...

#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
#       PELAGIC STATE VARIABLES (volume)
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
3d-state

  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
  #     State Variable(s) for Nutrients
  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
   N1p  :       Phosphate : mmol P/m3
   N3n  :       Nitrate  : mmol N/m3
   N4n  :       Ammonium : mmol N/m3


  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
  #     State Variable(s) for Phytoplankton
  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
   group PhytoPlankton[cnpls] (PPY) :  mg C/m3 : mmol N/m3 : mmol P/m3 :
                                       mg Chl/m3 : mmol Si/m3
           P1           : Diatoms
           P2[-s]       : Flagellates
           P3[-s]       : PicoPhytoplankton
           P4[-s]       : Large Phytoplankton
   end

  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
  #     State Variable(s) for Mesozooplankton
  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
   group MesoZooPlankton[cnp] (MEZ) : mg C/m3 : mmol N/m3 : mmol P/m3
                Z3      : Carnivorous Mesozooplankton
                Z4      : Omnivorous Mesozooplankton
   end

end
```

Table 6.1.: Example of the model template file `layout` with the definition of pelagic state variables.

6.2. Model layout changes

BFM is built in a modular and flexible way because each state variable is not defined directly in the code but through a model template `layout` found in the PRESET directories (Sec. 3.3.1, `$BFMDIR/build/configurations`). All the ancillary F90 memory layout files (`AllocateMem.F90, INCLUDE.h, ModuleMem.f90, set_var_info_bfm.f90`) are automatically generated from this meta-data structure by way of a perl script (`$BFMDIR/build/script`). The prototypes of these files are found in directory `$BFMDIR/BFM/proto` and filled in with the user-defined state variables and diagnostics.

The structure of the model template given in Tab. 6.1 is divided in sections with specific headings. Sections can be repeated many times in the file. For clarity, it is suggested to follow a conceptual construction of the model, by grouping all the state variables and diagnostics as done in the standard released structure.

3d-state: this section is used for all the state variables, which are defined as being virtually three-dimensional. This means that they exist in the whole domain, be it 0-, 1- or 3-dimensional. An example of state variable definition is shown in Box 6.1.
According to the theoretical model description, variables are defined as functional families and identified by their main biochemical components, which are indicated according to the classical ERSEM syntax (Blackford and Radford, 1995). State variable definitions require 3 pieces of information, separated by colons: code symbol with components, long name and units. Components are indicated by one single letter and currently the following are reserved: c=carbon, n=nitrogen, p=phosphorus, s=silica, l=chlorophyll, f=iron. Any other new component (either atomic or molecular) can be added, provided that the user include the relative dynamics in an appropriate piece of code. The syntax for a multi-component variable is detailed below `varname[cnp...]`, and it is also possible to define group of state variables, such as `PhytoPlankton` or `PelDetritus` as shown in Box 6.1. This feature gives the advantage to cycle over all the group components with one single index (see the example in Sec. 5.2).

2d-state: all the features described above are also valid for the state variables belonging to the benthic or sea ice 2-D system.

1d-variable: this section defines the variable without a spatial component (more appropriately defined as 0-D variables). These are only function of time and defined as scalars.

2d-variable: this section includes the surface variables, originally identified as benthic variables. However, this section is also used to define surface variables such as wind velocity. In a 1D coupled model, this is a scalar, while it is a one-dimensional array holding all the surface (bottom) points in a coupled 3D model.

3d-variable: this section is used for all the ancillary diagnostic variables defined in the whole domain. Typically, this section is used for temperature, salinity, and other environmental or diagnostic variables. Environmental variables obtained from external data files or hydrodynamical models are indicated with capital symbols starting with E (e.g. `ETW` = environmental temperature of water).

The syntax of the allowed layout elements is the following

```
[dim]d-state [-if-exist]
        GROUP
```

```
        VARNAME
end

[dim]d-variable [-if-exist]
        VARNAME
        ARRAYNAME
        QUOTUM
end

[dim]d-flux [-if-exist]
        FLUXNAME
end
```

- GROUP, like `PhytoPlankton`

  ```
  group name[constituents] (acronym) : constituent_units
          VARNAME
  end
  ```

- VARNAME, like `N1p` or `P2[-s]` (if present, the constituent within brackets are removed from the group list of elements)

  ```
  name[-constituents] : description : units
  ```

- ARRAYNAME, a variable that is defined for each element of a group, like the specific uptake for each phytoplankton `suPPY(PhytoPlankton)`

  ```
  name(groupname) : description : units
  ```

- QUOTUM, like `qncPPY(PhytoPlankton)` (quotum N:C for each phytoplankton group)

  ```
  q+constituent+constituent+acronym() : description : units
  ```

- FLUXNAME, the named entity for a user-defined flux like `ruPPYc` (Sec. 7.3)

  ```
  name = FLUX : description : units
  ```

- FLUX, an expression combining several variables to store fluxes between components (Sec. 7.3)

  ```
  (var[+|-]var)[<-|->](var[+|-]var)
  ```

with the following fundamental elements

- **`name`**: an alphanumeric string starting with a non-numeric character
- **`constituents`**: one or several from the list: *c* (Carbon), *n* (nitrogen), *p* (phosphorus), *s* (silicon), *f* (iron), *l* (chlorophyll). They have to be written in lower case and without any separation
- **`description`**: phrase describing the variable, quota or flux
- ***`units`***: units in which the variable, quota or flux are measured
- ***`constituents_units`***: units separated by ":". Have to be same number of units as constituents have been specified

- ***groupname***: name of a group, also name of the function to access the group components
- ***var***: variable name (e.g. *R6c*) or first letter of group with constituents for naming all (e.g. *P.c*)
- ***acronym***: acronym representing the group. Currently accepted acronyms are: *PPY* (PhytoPlankton), *PBA* (PelBacteria), *MEZ* (MesoZooPlankton), *MIZ* (MicroZooPlankton), *OMT* (PelDetritus), *CAR* (Inorganic)
- ***dim***: dimension of the layout elements inside. Allowed values are: *1*, *2* and *3*

The configuration can be also modified at compilation time by means of the set of macros listed in Sec. 6.1. The statement `-if-exist` found after one of the layout declarations indicates that the following set of variables will be defined only when the macro is included in the compilation:

```
3d-variable -if-exist INCLUDE_PELCO2
  DIC        : Dissolved Inorganic Carbon : umol/kg
  CO2        : CO2(aq) : umol/kg
  pCO2       : Oceanic pCO2 : uatm
  HCO3       : Bicarbonate :  umol/kg
  CO3        : Carbonate : umol/kg
  Ac         : Alkalinity : umol eq/kg
  pH         : pH : -
end
```

6.2.1. Example 1. Adding a subgroup

This is the most simple example, because it involves a small number of changes. Let us assume we want to add another mesozooplankton component to the zooplankton group , such as macrozooplankton (as done for instance by Berline et al., 2011). It is also assumed that this group will have exactly the same dynamics as the other two subgroups, but different parameter values. It is first suggested to create a new preset by copying the directory `STANDALONE_PELAGIC` to a new name

```
cd $BFMDIR/build/configurations
cp -r STANDALONE_PELAGIC STANDALONE_PELAGIC_Z
```

and then edit the appropriate line in the template file `layout` by adding the new variable name and long name:

```
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
#     State Variable(s) for Mesozooplankton
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
   group MesoZooPlankton[cnp] (MEZ) : mg C/m3 : mmol N/m3 : mmol P/m3
               Z3      : Carnivorous Mesozooplankton
               Z4      : Omnivorous Mesozooplankton
               Z2      : Macrozooplankton
   end
```

It is also suggested to edit the name of the run directory where the namelists will be copied. This is done in the configuration file $BFMDIR/build/configurations/configuration and change

```
EXP     = 'standalone.macrozoo'
```

Now the configuration can be generated by compiling the new preset

```
cd $BFMDIR/build
./bfm_configure.sh -gcd -p STANDALONE_PELAGIC_Z
```

and the script will take care of the automatic generation of the new memory layout with the required named constants, pointers, initial value, run directory and namelists. A new Z2 element will be added to the group `MesoZooPlankton` (in this case `Z2` will be the third element as it comes after `Z3` and `Z4`). Particularly, a new column will be added in the mesozooplankton namelist and filled in with zero. A warning is issued for each added column or row of parameters:

```
WARNING: (2 < 3) adding zero values to element p_q10 in namelist MesoZoo
WARNING: (2 < 3) adding zero values to element p_srs in namelist MesoZoo
WARNING: (2 < 3) adding zero values to element p_sum in namelist MesoZoo
...
WARNING: (2 < 3) adding new predator term p_paMIZ(3,:) in namelist MesoZoo
WARNING: (2 < 3) adding new predator term p_paPPY(3,:) in namelist MesoZoo
```

Check the updated file `tmp/STANDALONE_PELAGIC_Z/ModuleMem.F90` and search for the new variable `Z2` to see the added pieces of code.

The final steps before running the new model are the addition of the proper parameter values in place of zeros in the new column/rows corresponding to Z2 of `MesoZoo_parameters` in `run/STANDALONE_PELAGIC_Z/Pelagic_Ecology.nml`

```
&MesoZoo_parameters
!                        Z3        Z4        Z2
    p_q10            =  2.0       2.0       0.0
    p_srs            =  0.01      0.02      0.0
    p_sum            =  2.0       2.0       0.0
    p_vum            =  0.025     0.025     0.0
    p_puI            =  0.6       0.6       0.0
    p_peI            =  0.3       0.35      0.0
    p_sdo            =  0.01      0.01      0.0
    p_sd             =  0.02      0.02      0.0
    p_sds            =  2.0       2.0       0.0
    p_qpcMEZ         =  1.67d-3   1.67d-3   0.0
    p_qncMEZ         =  0.015     0.015     0.0
    p_clO2o          =  30.0      30.0      0.0
!                        P1        P2        P3    P4
!   Z3
    p_paPPY(1,:)     =  0.0       0.0       0.0   0.0
!   Z4
    p_paPPY(2,:)     =  1.0       0.0       0.0   0.7
!                        Z5        Z6
!   Z3
    p_paMIZ(1,:)     =  0.0       0.0
!   Z4
    p_paMIZ(2,:)     =  1.0       0.0
!                        Z3        Z4        Z2
!   Z3
    p_paMEZ(1,:)     =  1.0       1.0       0.0
!   Z4
    p_paMEZ(2,:)     =  0.0       1.0       0.0
!                        Z5        Z6
!   Z2
    p_paMIZ(3,:)     =  0.0       0.0
```

```
!                       P1        P2        P3   P4
!   Z2
    p_paPPY(3,:)      =  0.0       0.0       0.0  0.0
!                       Z3        Z4        Z2
!   Z2
    p_paMEZ(3,:)      =  0.0       0.0       0.0
/
```

and to turn on the flag `CalcMesoZooPlankton(3)=.TRUE.` in Param_parameters and add initial value(s) by adding a line `Z2c0=<value>` in `bfm_init_nml`, both found in file `run/STANDALONE_PELAGIC_Z/BFM_General.nml`.

6.2.2. Example 2. Adding a biochemical component and a group

The BFM application in the global ocean is called PELAGOS (PELAgic biogeochemistry for Global Ocean Simulations) and the climatological simulations were described in Vichi et al. (2007a). A major requirement to simulate the global ocean ecosystem is the introduction of iron control on phytoplankton growth (Sec. 2.2.8), particularly to capture the high-nutrient low-chlorophyll regions. The example below shows how the iron component of phytoplankton and detritus have been added to the model structure template. Additional coding from the user is then required to parameterize the fluxes between these components and the regulations of plankton physiology (this is already included in the `GYRE_BFM` preset that requires the usage of the NEMO model and activated with the keyword `INCLUDE_PELFE`).

To add an iron constituent to a group, it is sufficient to specify a unique single-character constant between the square brackets in the `layout` file as shown below:

```
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
#      State Variable(s) for Phytoplankton
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=
group PhytoPlankton[cnplsf] (PPY) : mg C/m3 : mmol N/m3 : mmol P/m3 :
                                  mg Chl/m3 : mmol Si/m3 : umol Fe/m3
        P1      : Diatoms
        P2[-s]  : Flagellates
        P3[-s]  : PicoPhytoPlankton
end
```

It is also necessary to provide units separated by colons, in this case μmol Fe m^{-3}. Remember that the `[-s]` syntax in some phytoplankton groups indicates that this constituent, although being a component of the group vector, is not computed for that specific sub-group.

The preprocessing script will take care during compilation to generate an adequate entry in the main memory module and the definitions of the named constants (`ppP1f`, ...) and pointers (`P1f`, ...) to access the new variables from the model code.

New groups can also be defined in order to use the facilities shown in Sec. 5.3.3. All the detritus variables can be grouped together with the following syntax:

```
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
  #      State Variable(s) for Detritus (Biogenic Organic Material)
  #-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
    group PelDetritus[cnpsf] (OMT) : mg C/m3 : mmol N/m3: mmol P/m3:
                                   mmol Si/m3 : umol Fe/m3
      R1[-s]     : Labile Dissolved Organic Matter
      R2[-npsf]  : Semi-labile Dissolved Organic Carbon
```

```
    R3[-npsf]  : Semi-refractory Dissolved Organic Carbon
    R6        : Particulate Organic Matter
  end
```

6.2.3. Example 3. Removing components from zooplankton

For certain purposes it is not needed to carry out the computation of variable nutrient:carbon quota in selected Functional Groups (for instance, in the case of the new macrozooplankton group added in example 1). This can be done to save computational resources in the case of low-resolution long-term global ocean simulations or with high-resolution coastal models. A possible example is the assumption of a fixed quota in zooplankton which allows one to reduce the number of standard components of up to 8 state variables. The zooplankton group definitions are equal to the one shown in the code of Box 6.1 for MesoZooplankton but with the removal of the `n` and `p` constituents:

```
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
#      State Variable(s) for Mesozooplankton
#-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
   group MesoZooPlankton[cnp] (MEZ) : mg C/m3 : mmol N/m3 : mmol P/m3
              Z3[-np]      : Carnivorous Mesozooplankton
              Z4[-np]      : Omnivorous Mesozooplankton
   end
```

The additional requirement is the change of value in parameter `check_fixed_quota` from 0 to 1 in the `Param_parameters` namelist. Test experiments have shown that the simulation times can be reduced up to 30%. The physiological assumption is that zooplankton release in inorganic form the nutrients in excess of the given fixed quota.

6.2.4. Example 4. Creating new presets from experiments

After running the experiments, common behavior is to modify generated namelists in the deployed experiment folder (`$BFMDIR/run/$EXP`). If you want to preserve these changes into a "preset" you can use the tool "`nmlcreator`". This is for instance desired when a new group is added as in Sec. 6.2.1 and the parameters of the new group have to become default for the preset. To execute this tool do the following steps

```
cd $BFMDIR/build/scripts/conf
./nmlcreator.pl -i NAMELIST_IN -o NAMELIST_OUT
```

where

- `NAMELIST_IN`: Complete path of the file containing namelist/s to read (eg. $BFMDIR/run/standalone.pelagic/Pelagic_Ecology.nml)
- `NAMELIST_OUT`: Complete path of the "namelist" file of the preset where to append at the end of the input (eg: `$BFMDIR/build/configurations/STANDALONE_PELAGIC_Z/namelists`).

Basically, `nmlcreator` adds the "`filename_nml_conf`" key with the name of the file at the end of each namelist read. It is important to note that it will not delete the existing namelists in the target preset, it will only append the new namelist at the end.

7. Diagnostics

7.1. Output

The variables that can be stored in the output file are the ones defined in file `layout`. All the state variables can be stored (provided that they have a long name and units), both as instantaneous values and as means over the chosen output period. This behavior is controlled via the namelist `BFM_General.nml` when running the STANDALONE model. Other couplings may have different names. Additionally, a set of other variables can be saved, such as the ones obtained from the physical model and other diagnostics such as total chlorophyll and the nutrient quota.

7.2. Restart

The length of each BFM simulation is controlled by the physical transport model except for the STANDALONE model which has its own time marching. It is common practice in modelling to split the simulation in several chunks and to continue the simulation from the end values of each state variable at the end of a previous run. The BFM stores this information in a NetCDF file which is always generated at the end of each simulation. There is no automatic control on the date (neither it is stored as an attribute inside the NetCDF file), so it is totally up to the user to check that the initial restart file is the proper one.

7.3. Aggregated diagnostics and rates

All the ancillary 2D and 3D variables and diagnostics are grouped in two memory arrays, `D3DIAGNOS` and `D2DIAGNOS`, accessed by means of pointers. The dimensions of these arrays change according to the number of model elements in the `layout` file, and any diagnostic rate can be easily defined thanks to the automatic generation of the memory layout. Some fluxes are already defined by default, such as the gross/net primary production rates, total respiration rates and (de)nitrification rates. Any exchange of mass between every state variable can be tracked by means of a special syntax that access and combines the elements of the `D3(D2)SOURCE` and `D3(D2)SINK` arrays where all the rates are stored. Some examples are already present at the end of the `STANDALONE_PELAGIC/layout` file and are activated with the compilation macros `INCLUDE_DIAG3D` and `INCLUDE_DIAG2D`:

```
fP1Z4c=P1c->Z4c: diatom grazing by omnivorous zooplankton: mg C/m3/d
ruPTc=P.c<-*: gross primary production: mg C/m3/d
ruZTc=(Z.c<-P.c+B1c+Z.c)-(Z.c->R1c+R6c): gross secondary production: mg C
    /m3/d
```

The first line defines a diagnostic storing the carbon flux between diatoms and mesozooplankton. This diagnostic also defines the long_name and units attributes of the NetCDF and it can thus be included in the output just by adding it to the `bfm_save_nml` section in `BFM_General.nml`.

The second line defines the combined rate gross primary production, which is the sum of all the carbon fluxes to all the phytoplankton groups (notice the syntax without the subgroup number). The last example is the gross secondary production, which is defined as the difference between the carbon ingestion by all zooplankton groups and the carbon loss to dissolved and particulate detritus.

Boundary fluxes are defined by default for each pelagic state variable. The variables

```
PELSURFACE(NO_D3_BOX_STATES,NO_BOXES_XY)
PELBOTTOM(NO_D3_BOX_STATES,NO_BOXES_XY)
```

are themselves pointers to the main diagnostic memory `D2DIAGNOS`. They can be accessed by means of specific pointers allocated in the generated subroutine `BFM/General/AllocateMem.F90` (notice that the integer constants change at every code generation and are only reported here as an example of the code):

```
PELSURFACE => D2DIAGNOS(17+1:17+50,:); PELSURFACE=ZERO
jsurO2o => D2DIAGNOS(17+ppO2o,:); jsurO2o=ZERO
jsurN1p => D2DIAGNOS(17+ppN1p,:); jsurN1p=ZERO
jsurN3n => D2DIAGNOS(17+ppN3n,:); jsurN3n=ZERO
jsurN4n => D2DIAGNOS(17+ppN4n,:); jsurN4n=ZERO
```

The boundary rates (always in units per day) are accessed in the code by means of the `PELSURFACE(ppO2o,:)` or `jsurO2o(:)` names.

7.4. Mass conservation

The total mass in the system (mass units m^{-2}) can be checked by means of built-in diagnostic variables. There is a variable for each biogeochemical component (C, N, P, Si, etc.) both for the pelagic and the benthic systems. To activate the diagnostic it is necessary to add the following lines to the output namelist in the `var_save` section:

```
var_save = 'totpeln',
           'totpelp',
           'totpels'
```

The actual computation is done in `General/CheckMassConservation.F90`. Note that for technical reasons the total mass variables are multidimensional but the value is stored in the first element of the array. When checking a coupling with an OGCM, it is also important to turn off any additional boundary flux (e.g. dilution, atmospheric deposition, river input, etc.) because they are not taken into account by the standard BFM.

Bibliography

Andersen, T., Elser, J. J., Hessen, D. O., 2004. Stoichiometry and population dynamics. Ecol. Lett. 7, 884–900.

Anderson, T. R., 2005. Plankton functional type modelling: running before we can walk? J. Plankt. Res. 27, 1073–1081.

Archer, D. E., Johnson, K. S., 2000. A Model of the iron cycle in the ocean. Glob. Biogeochem. Cy. 14, 269–279.

Aumont, O., Maier-Reimer, E., Monfray, P., Blain, S., 2003. An ecosystem model of the global ocean including Fe, Si, P co-limitations. Glob. Biogeochem. Cy. 17 (2), 1060.

Baretta, J., Ebenhöh, W., Ruardij, P., 1995. The European Regional Seas Ecosystem Model, a complex marine ecosystem model. J. Sea Res. 33 (3-4), 233–246.

Baretta-Bekker, J., Baretta, J., Ebenhoeh, W., 1997. Microbial dynamics in the marine ecosystem model ERSEM II with decoupled carbon assimilation and nutrient uptake. J. Sea Res. 38 (3/4), 195–212.

Baretta-Bekker, J., Baretta, J., Rasmussen, E., 1995. The microbial food web in the European Regional Seas Ecosystem Model. J. Sea Res. 33 (3-4), 363–379.

Behrenfeld, M. J., Prasil, O., Babin, M., Bruyant, F., 2004. In search of a physiological basis for covariations in light-limited and light-saturated photosynthesis. J. Phycol. 40, 4–25.

Berline, L., Stemmann, L., Vichi, M., Lombard, F., Gorsky, G., 06 2011. Impact of appendicularians on detritus and export fluxes: a model approach at dyfamed site. J. Plankt. Res. 33 (6), 855–872.

Bidle, K. D., Azam, F., 2001. Bacterial control of silicon regeneration from diatom detritus: Significance of bacterial ectohydrolases and species identity. Limnol. Oceanogr. 46 (7), 1606–1623.

Blackford, J., Radford, P., 1995. A structure and methodology for marine ecosystem modelling. J. Sea Res. 33 (3-4), 247–260.

Blackford, J. C., Allen, J. I., Gilbert, F. J., 2004. Ecosystem dynamics at six contrasting sites: a generic modelling study. J. Mar. Sys. 52, 191–215.

Blackford, J. C., Burkill, P. H., 2002. Planktonic community structure and carbon cycling in the Arabian Sea as a result of monsoonal forcing: the application of a generic model. J. Mar. Sys. 36 (3), 239–267.

Broekhuizen, N., Heath, M., Hay, S., Gurney, W., 1995. Modelling the dynamics of the North Sea's mesozooplankton. J. Sea Res. 33 (3-4), 381–406.

Contois, D., 1959. Kinetics of bacterial growth: relationship between population density and specific growth rate of continuous cultures. Journal of general microbiology 21 (1), 40–50.

Doney, S. C., Lindsay, K., Caldeira, K., Campin, J. M., Drange, H., Dutay, J. C., Follows, M., Gao, Y., Gnanadesikan, A., Gruber, N., Ishida, A., Joos, F., Madec, G., Maier-reimer, E., Marshall, J. C., Matear, R. J., Monfray, P., Mouchet, A., Najjar, R., Orr, J. C., Plattner, G. K., Sarmiento, J., Schlitzer, R., Slater, R., Totterdell, I. J., Weirig, M. F., Yamanaka, Y., Yool, A., 2004. Evaluating global ocean carbon models: The importance of realistic physics. Glob. Biogeochem. Cy. 18, 3017.

Droop, M., 1973. Some thoughts on nutrient limitation in algae. J. Phycol. 9, 264–272.

Ebenhöh, W., Baretta-Bekker, J., Baretta, J., 1997. The primary production module in the marine ecosystem model ERSEM II with emphasis on the light forcing. J. Sea Res. 38, 173–193.

Flynn, K. J., 2 2003. Modelling multi-nutrient interactions in phytoplankton; balancing simplicity and realism. Prog. Oceanogr. 56 (2), 249–279.

Flynn, K. J., Marshall, H., Geider, R. J., 2001. A comparison of two N-irradiance interaction models of phytoplankton growth. Limnol. Oceanogr. 46, 1794–1802.

Follows, M. J., Ito, T., Dutkiewicz, S., 2006. On the solution of the carbonate chemistry system in ocean biogeochemistry models. Ocean Modelling 12 (3-4), 290–301.

Frost, P. C., Xenopoulos, M. A., Larson, J. H., 2004. The stoichiometry of dissolved organic carbon, nitrogen, and phosphorus release by a planktonic grazer, Daphnia. Limnol. Oceanogr. 49, 1802–1808.

Geider, R., MacIntyre, H., Kana, T., 1996. A dynamic model of photoadaptation in phytoplankton. Limnol. Oceanogr. 41 (1), 1–15.

Geider, R., MacIntyre, H., Kana, T., 1997. A dynamic model of phytoplankton growth and acclimation: responses of the balanced growth rate and chlorophyll *a*:carbon ratio to light, nutrient limitation and temperature. Mar. Ecol. Prog. Ser. 148, 187–200.

Geider, R., MacIntyre, H., Kana, T., 1998. A dynamic regulatory model of phytoplanktonic acclimation to light, nutrients, and temperature. Limnol. Oceanogr. 43 (3), 679–694.

Gentleman, W., Leising, A., Frost, B., Strom, S., Murray, J., 2003. Functional responses for zooplankton feeding on multiple resources: a review of assumptions and biological dynamics. Deep-Sea Res. Pt. II 50, 2847–2875.

Gibson, G. A., Musgrave, D. L., Hinckley, S., 2005. Non-linear dynamics of a pelagic ecosystem model with multiple predator and prey types. J. Plankt. Res. 27, 427–447.

Goldman, J., McCarthy, J., 1978. Steady state growth and ammonium uptake of a fast-growing marine diatom. Limnology and oceanography 23 (4), 695–703.

Heissenberger, A., Leppard, G. G., Herndl, G. J., 1996. Relationship between the intracellular integrity and the morphology of the capsular envelope in attached and free-living marine bacteria. Applied and environmental microbiology 62 (12), 4521–4528.

Jassby, A., Platt, T., 1976. Mathematical formulation of the relationship between photosynthesis and light for phytoplankton. Limnol. Oceanogr. 21, 540–547.

Johnson, K. S., Gordon, R. M., Coale, K. H., 1997. What controls dissolved iron concentrations in the world ocean? Mar. Chem. 57, 137–161.

Lazzari, P., Solidoro, C., Ibello, V., Salon, S., Teruzzi, A., Béranger, K., Colella, S., Crise, A., 2012. Seasonal and inter-annual variability of plankton chlorophyll and primary production in the mediterranean sea: a modelling approach. Biogeosciences 9 (1), 217–233.

Lefevre, N., Watson, A. J., 1999. Modeling the geochemical cycle of iron in the oceans and its impact on atmospheric CO2 concentrations. Global Biogeochem Cy 13, 727–736.

Mitra, A., Flynn, K. J., 2005. Predator-prey interactions: is 'ecological stoichiometry' sufficient when good food goes bad? J. Plankt. Res. 27, 393–399.

Morel, F., 1987. Kinetics of uptake and growth in phytoplankton. J. Phycol. 23, 137–150.

Olsen, A., Wanninkhof, R., Trinanes, J. A., Johannessen, T., 2005. The effect of wind speed products and wind speed-gas exchange relationships on interannual variability of the air-sea CO2 gas transfer velocity. Tellus B 57, 95–106.

Parekh, P., Follows, M. J., Boyle, E., 2004. Modeling the global ocean iron cycle. Glob. Biogeochem. Cy. 18, GB1002.

Polimene, L., Allen, J. I., Zavatarelli, M., Jun 2006. Model of interactions between dissolved organic carbon and bacteria in marine systems. Aquat. Microb. Ecol. 43 (2), 127–138.

Reinart, A., Arst, H., Blanco-Sequeiros, A., Herlevi, A., 1998. Relation between underwater irradiance and quantum irradiance in dependence on water transparency at different depths in the water bodies. J. Geophys. Res. 103 (C4), 7759–7752.

Ruardij, P., Van Raaphorst, W., 1995. Benthic nutrient regeneration in the ERSEM ecosystem model of the North Sea. J. Sea Res. 33 (3-4), 453–483.

Sakshaug, E., Bricaud, A., Dandonneau, Y., Falkowski, P. G., Kiefer, D. A., Legendre, L., Morel, A., Parslow, J., Takahashi, M., 1997. Parameters of photosynthesis: definitions, theory and interpretation of results. J. Plankt. Res. 19, 1637–1670.

Stoderegger, K., Herndl, G., 1998. Production and release of bacterial capsular material and its subsequent utilization by marine bacterioplankton. Limnol. Oceanogr. 43 (5), 877–884.

Sunda, W. G., Huntsman, S. A., 1997. Interrelated influence of iron, light and cell size on marine phytoplankton growth. Nature 390, 389–392.

Tsiaras, K. P., Kourafalou, V. H., Davidov, A., Staneva, J., 2008. A three-dimensional coupled model of the western black sea plankton dynamics: Seasonal variability and comparison to seawifs data. J. Geophys. Res. 113 (C7), C07007.

Varela, R., Cruzado, A., Gabaldon, J., 1995. Modelling primary production in the North Sea using the European Regional Seas Ecosystem Model. J. Sea Res. 33 (3-4), 337–361.

Vichi, M., Masina, S., 11 2009. Skill assessment of the PELAGOS global ocean biogeochemistry model over the period 1980-2000. Biogeosciences 6 (11), 2333–2353.

Vichi, M., Masina, S., Navarra, A., 2007a. A generalized model of pelagic biogeochemistry for the global ocean ecosystem. Part II: numerical simulations. J. Mar. Sys. 64, 110–134.

Vichi, M., Pinardi, N., Masina, S., 2007b. A generalized model of pelagic biogeochemistry for the global ocean ecosystem. Part I: theory. J. Mar. Sys. 64, 89–109.

Vichi, M., Ruardij, P., Baretta, J. W., 2004. Link or sink: a modelling interpretation of the open Baltic biogeochemistry. Biogeosciences 1, 79–100.

Wolf-Gladrow, D. A., Zeebe, R. E., Klaas, C., Körtzinger, A., Dickson, A. G., 2007. Total alkalinity: The explicit conservative expression and its application to biogeochemical processes. Marine chemistry 106 (1), 287–300.

Worden, A. Z., Nolan, J. K., Palenik, B., 2004. Assessing the dynamics and ecology of marine picophytoplankton: The importance of the eukaryotic component. Limnol. Oceanogr. 49, 168–179.

Zeebe, R. E., Wolf-Gladrow, D. A., 2001. CO_2 in Seawater: Equilibrium, Kinetics, Isotopes. Vol. 65 of Oceanography Book Series. Elsevier, Amsterdam.