



Coupling BFM with ocean models: the NEMO model V3.6

(Nucleus for the European Modelling of the Ocean)

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1 Introduction

1.1 Eulerian coupling

This introduction presents the major theoretical assumptions for the Eulerian coupling between a general circulation model of the ocean (NEMO, Nucleus for the European Modelling of the Ocean, <http://nemo-ocean.eu>) and a biogeochemical model of the pelagic system (BFM, Biogeochemical Flux Model, <http://bfm-community.eu>). The concepts presented in this section and partly in the more technical Chap. 2 are to be considered valid for any coupling of the BFM with an ocean general circulation model (OGCM).

The BFM is designed as a set of ordinary differential equations that resolve the fluxes of biogeochemical constituents in the marine environment. By construction, it assumes that biological and chemical variables are homogeneously distributed in the infinitesimal water volume, which is clearly a poor approximation for living cells and particulate organic matter in general. From a theoretical point of view, the biological components of the marine environment have always been casted in the Eulerian representation, using dissolved nutrients and unicellular plankton as models because they are sufficiently small and passive to be considered “parts” of the fluid. This theoretical formulation has been proposed initially by O’Brien and Wroblewski (1973), then Robinson (1997) and summarized in Hofmann and Lascara (1998) and Vichi et al. (2007b). It must be noted that all these formulations either neglected the role of turbulent diffusive processes or assumed that turbulent fluctuations in the biological fields are affected by the same Reynolds averaging used for the fluid properties.

We use the conceptual framework proposed by Vichi et al. (2007b), and we acknowledge that a similar theoretical formulation was previously proposed by Robinson (1997), who also provided a mathematical derivation of the analytical solutions. Passively transported variables can be basically described using concentrations of functional living and non-living components (the chemical functional families proposed by Vichi et al., 2007b), and we write the conservation equation for an infinitesimal volume of fluid containing the concentration C for a BFM variable. We apply the continuum hypothesis that the value of C is a continuous function of space and time. The basic equation in a fluid is thus:

$$\frac{\partial C}{\partial t} = -\vec{\nabla} \cdot \vec{F}, \quad (1.1.1)$$

where \vec{F} is the generalized flux of C_i through and within the basic infinitesimal element of mass of the fluid. By making the continuum approximation valid for biogeochemistry, we can further separate the flux in a physical part and a biological reaction term

$$\frac{\partial C}{\partial t} = -\vec{\nabla} \cdot \vec{F}_{phys} - \vec{\nabla} \cdot \vec{F}_{bio}. \quad (1.1.2)$$

The second term on the right hand side of (1.1.2) cannot be measured directly because living cells have finite dimensions, and therefore we assume that it can be approximated with the following eulerian approach:

$$\vec{\nabla} \cdot \vec{F}_{bio} = -w_B \frac{\partial C}{\partial z} + \frac{\partial C}{\partial t} \Big|_{bio}. \quad (1.1.3)$$

1 Introduction

Both terms in eq. (1.1.4) represent the biogeochemical divergence flux and parameterize the sinking of biological particulate matter and the local time rate of change due to biogeochemical transformation processes. The sinking velocity w_B is introduced for those state variables that have a mass-related vertical velocity other than the fluid vertical velocity.

This approximation brings us to the typical form of an advection-diffusion-reaction equation in an incompressible fluid:

$$\frac{\partial C}{\partial t} = -\mathbf{u} \cdot \nabla C + \nabla_H \cdot (A_H \nabla_H C) + \frac{\partial}{\partial z} A_V \frac{\partial C}{\partial z} - w_B \frac{\partial C}{\partial z} + \left. \frac{\partial C}{\partial t} \right|_{bio} \quad (1.1.4)$$

where $\mathbf{u} \equiv (u, v, w)$ is the three-dimensional current velocity and (A_H, A_V) are the horizontal and vertical turbulent diffusivity coefficient for tracers. To highlight the coupling between physical and biogeochemical processes, we may rewrite this equation in component forms, also indicating the ocean variables that are resolved by the OGCM and needed for the reaction term R :

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \nabla_H \cdot (A_H \nabla_H C) + \frac{\partial}{\partial z} A_V \frac{\partial C}{\partial z} - w_B \frac{\partial C}{\partial z} + R(T, S, W, E) \quad (1.1.5)$$

where the scalar symbols in the last term indicate water temperature (T), salinity (S), the intensity of wind (W), and shortwave irradiance (E).

1.2 Information flow and numerical integration

Equation (1.1.4) is one approximated form of a primitive equation for biogeochemical variables in the ocean and requires the knowledge of ocean physical variables to be solved. The time evolution of physical variables is carried out by the OGCM and transferred to the biogeochemical model. A typical, generic scheme of the information flow between the two models is presented in Fig. 1.1. The physical variables are used to compute the advection, diffusion and reaction terms in eq. (1.1.4) and then combined to obtain the forward in time biogeochemical states. This equation cannot be solved analytically but requires a numerical integration, just as it happens for temperature and salinity on OGCM. Usually, the same kind of numerical scheme is used. The sensitivity of the BFM to integration schemes has been tested by Butenschön et al. (2012), and it was concluded that the source splitting method is more accurate. Currently, NEMO uses a time integration based on source splitting with a leapfrog scheme for active tracers (Madec, 2008); in the case of BFM-NEMO the final integration is carried out with a simple Euler-forward step, but still with source splitting .

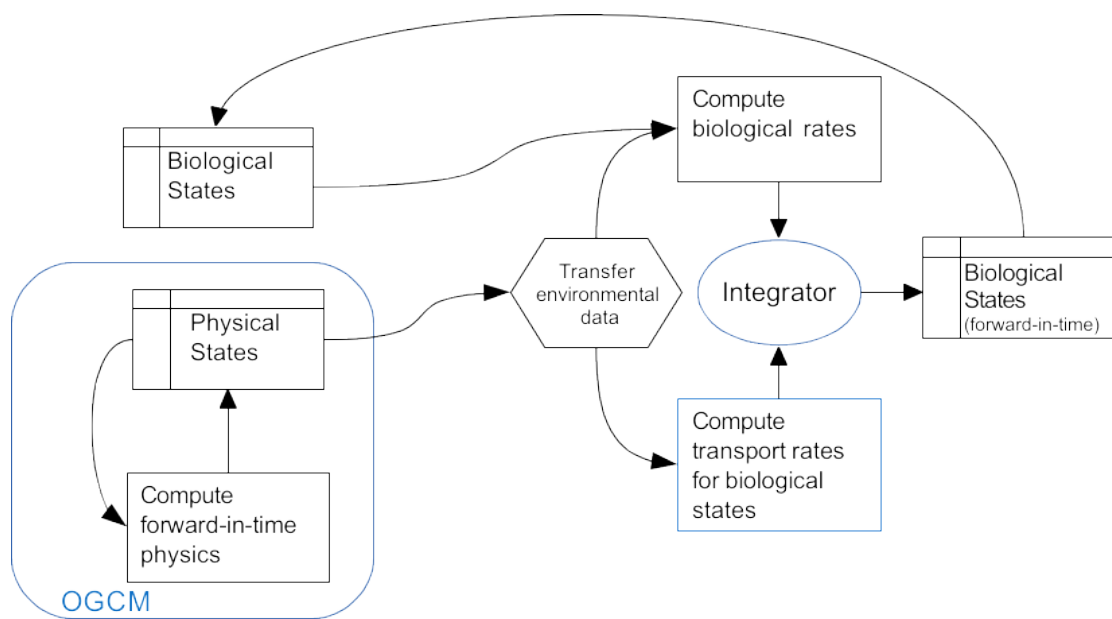


Figure 1.1: Scheme of the information flow between the ocean model and the biogeochemical state variables. The blue boxes indicate that the computation is carried out directly by the OGCM or using modified routines belonging to the OGCM. Integrator is a generic name for the solver used to advance in time the solution of the coupled physical-biogeochemical system.

2 Technical coupling with NEMO

2.1 Integration of BFM in the NEMO-TOP interface

BFM and NEMO are separated codes that are maintained by different groups of developers. The coupled configuration is therefore the result of a joint compilation of the two codes, where the BFM is a modular external library of NEMO. This document assumes that you are already familiar with NEMO and it does not substitute the NEMO documentation (Madec, 2008) which should be used as reference for the specific namelist parameters and code macros.

NEMO contains an interface for the computation of biogeochemical tracers named TOP (from the French *Traceurs Oceanographique Passives*) which is contained in the TOP_SRC directory of NEMO code. This interface allows to use all the same numerical schemes available for the active tracers to solve the advective and diffusive processes, as well as to prescribe surface, bottom and lateral boundary conditions. This is a crucial requirement for the inclusion of BFM in any OGCM, and it is possible because all NEMO routines have been written with explicit input-output arguments to pass either temperature or salinity or biogeochemical tracers.

The BFM has been integrated in this framework with the addition of a seamless software layer that uses the generic tracer interface called MY_TRC. In addition, the BFM source code provides all the ancillary routines that are required for the coupling in the directory \$BFMDIR/src/nemo. When a NEMO configuration containing the BFM is compiled, this generic tracer interface is activated and the external directory containing the BFM coupling interface is included, substituting some of the standard routines contained in TOP_SRC. The compilation of the coupled system is done with the BFM configuration script detailed in Sec. 3.2.

This is activated with the macro key_my_trc and the BFM is plugged into the NEMO flow chart during the initialization and stepping phases. It important to make clear that BFM still uses its own libraries for diagnostic output and restart files.

2.2 BFM and TOP parameters

The biogeochemical processes of the BFM are controlled by their own namelist files as described in the BFM core manual Vichi et al. (2020), but when run in coupled configuration there are some additional parameters derived from the NEMO TOP namelist that must be adjusted. Particularly, this occurs for the prescription of initial and boundary conditions because both rely on the NEMO facilities for reading and interpolating external files. The file namelist_top_cfg generated by the BFM configuration script (see Sec. 3.2) contains the namelist namtrc_dta which gives the information on the initial data values for the BFM variables:

```
!-----!  
!NAMELIST namtrc_dta  
!-----!  
!   Initialisation from data input file  
!   for each BFM variable set the structure sn_trcdta(VARNAME)  
!   and the conversion factor rn_trfac(VARNAME)  
!   Specifications for fld_read:  
!   !file name!frequency (hr)!variable!time interp.!clim !'yearly' or !weights !rotation!land/sea  
!   !   !(if <0 mon)   ! name ! (logical) !(T/F)! 'monthly' !filename ! pairing! mask  
!-----!
```

2 Technical coupling with NEMO

```
&namtrc_dta
sn_trcdta(O2o) = 'data_1m_O_nomask', -12, 'O2', .false., .true., 'yearly', '', '', ''
sn_trcdta(N1p) = 'data_1m_P_nomask', -1, 'P04', .false., .true., 'yearly', '', '', ''
rn_trfac(O2o) = 22.4 ! conversion factor from ml/l to mmol m3 (1 mol O2 = 22.4 l)
rn_trfac(N1p) = 1.0 ! no conversion
...
cn_dir = './' ! root directory for the location of the data files
/
```

The parameters of the `fld_read` structure `sn_trcdta` allow to specify the name of the file, the frequency of input data and the interpolation weights. Note that the interpolation is still two-dimensional only and the input data must already be on the vertical grid of the model. It is possible to give a conversion factor that may also be used to increase artificially the initial values of a uniform factor. The BFM named constants for the variables are substituted by the configuration script at compilation time and then copied to the running directory as fully detailed in Sec. 3.2.

In addition to this part that is common to other biogeochemical models in the TOP interface, the BFM allows to choose the specific mode of initialization for each variable in the namelist `bfm_init_nml`. This is the same namelist used for the STANDALONE model as described in BFM core manual (chap. 5), but when coupled with NEMO it also allows to specify if each variable should start from the initial file given in the namelist above, from a constant homogeneous value or from an analytical profile:

```
!-----!
! NAMELIST bfm_init_nml
!-----!
!Pelagic initialisation of standard variables
!<variablename>0 = <realvalue>
!
! Initialization with InitVar structure
!-----!
! NOTE:
! This part is still experimental and will be improved in the future
!-----!
! BFM variable information for data input
! available fields:
! integer init: select the initialization
!             0 = homogeneous
!             1 = analytical
!             2 = from file
! options for init==1
!   real anv1: value in the surface layer
!   real anz1: depth of the surface layer
!   real anv2: value in the bottom layer
!   real anz2: depth of the bottom layer
! options for init==2
! * Options currently used when coupled with NEMO
!   logical obc: variable has open boundary data
!   logical sbc: variable has surface boundary data
!   logical cbc: variable has coastal boundary data
! * Options not used when coupled with NEMO because
!   overridden by values in namelist_top_cfg
!   char filename: name of the input file
!   char varname: name of the var in input file
!-----!
&bfm_init_nml
  InitVar(O2o)%init = 0
  O2o0 = 300.0,
  InitVar(N1p)%init = 2
  InitVar(N1p)%sbc = .false.
  InitVar(N1p)%cbc = .false.
  InitVar(N1p)%obc = .false.
  InitVar(N1p)%init = 1
  InitVar(P1c)%anv1 = 5.0
  InitVar(P1c)%anz1 = 20.0
```

```

InitVar(P1c)%anv2 = 1.0
InitVar(P1c)%anz2 = 100.0
\

```

In the above example, oxygen is initialized with a constant value, phosphate is read from file and phytoplankton carbon is initialized with a stepwise analytical profile with higher concentration in the surface 20 m, a lower value in the adjacent 100 m and the background concentration in the reminder of the water column.

Surface, coastal and open boundary values for biogeochemical variables can also be switched on and off from this namelist and they are fully detailed in Sec. 2.4.

Another important parameter to be checked in coupled configurations is the sinking velocity of BFM variables. BFM computes a dynamical sinking velocity for phytoplankton that is dependent on nutrient stress (if activated) and a constant background sinking rate for phytoplankton and detritus. These are considered to be global variables and they are included in the namelist `PelGlobal_parameters`:

```

!-----!
!NAMELIST PelGlobal_parameters
!-----!
! Sinking rates of Pelagic Variables
! : for mem_PelGlobal filled by InitPelGlobal
! NAME          UNIT          DESCRIPTION
! p_rR6m         [m/d]        detritus sinking rate
! KSINK_rPPY      [m]          prescribe sinking rate for phytoplankton below this
!                               depth threshold to p_rR6m value. Use 0.0 to disable.
! AggregateSink   logic        use aggregation = true to enhance the sink rate
!                               below a certain depth and bypass the prescribed
!                               sinking
! depth_factor    [m]          depth factor for aggregation method
!-----!
&PelGlobal_parameters
  p_rR6m          = 10.0
  KSINK_rPPY      = 150.0
  AggregateSink   = .FALSE.
  depth_factor    = 2000.0
/

```

The coupling with NEMO adds three parameters that allow to parameterize the change in the sinking rate at depth. Below a certain depth, it is assumed that aggregation takes place. This is parametrized either by imposing the sinking rate of detritus to phytoplankton concentration below a fixed depth `KSINK_rPPy` (in meters), or by activating the enhancement of background velocity also found in the PISCES model of NEMO (`AggregateSink = .TRUE.`).

2.3 The flow chart

The BFM is zero-dimensional by construction and defined only in the ocean points. This implies that the BFM memory is one dimensional, with all the land points stripped out from the 3D domain and the remapping into the ocean grid is done only when dealing with transport processes (as shown in Fig. 2.1 taken from the BFM manual).

The flow of information between NEMO and the BFM is presented using “butterfly” graphs that show the main caller of the function of interest and the tree of calls. By convention, the routines of NEMO are indicated with blue boxes while the BFM routines are in green. Routines indicated with red boxes originally belong to NEMO TOP_SRC but are substituted by the ones provided in the BFM directory (`$BFMDIR/src/nemo`).

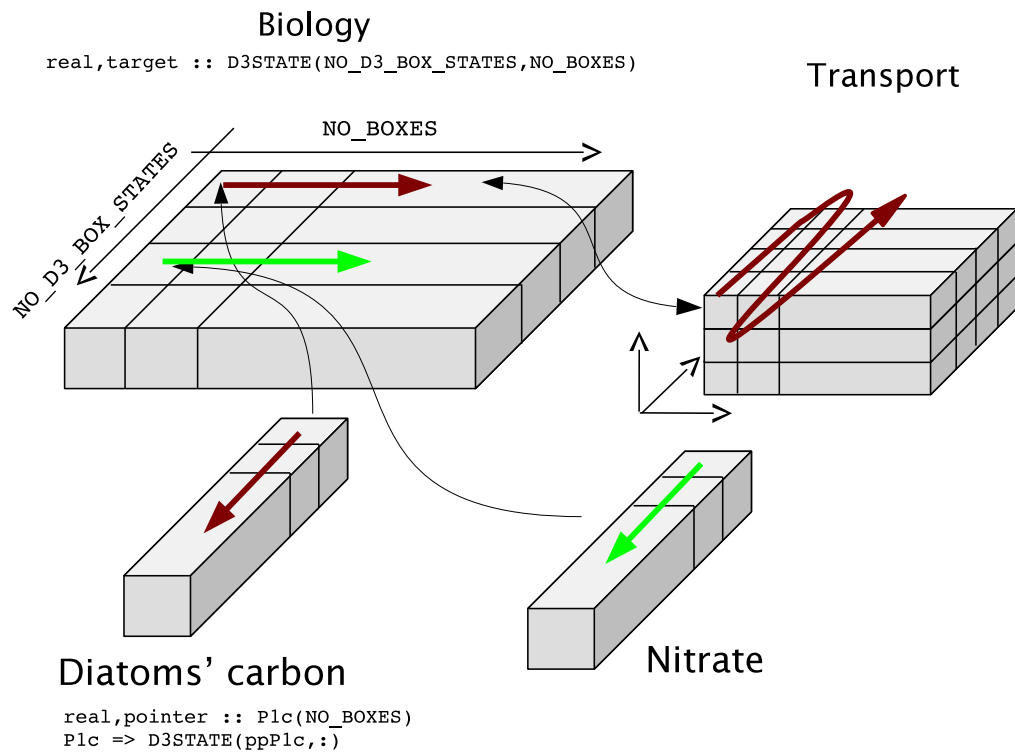


Figure 2.1: Layout of the main memory array for the pelagic variables and schematic of the remapping into the NEMO three-dimensional ocean grid for transport processes (see BFM core manual for a description of the code naming).

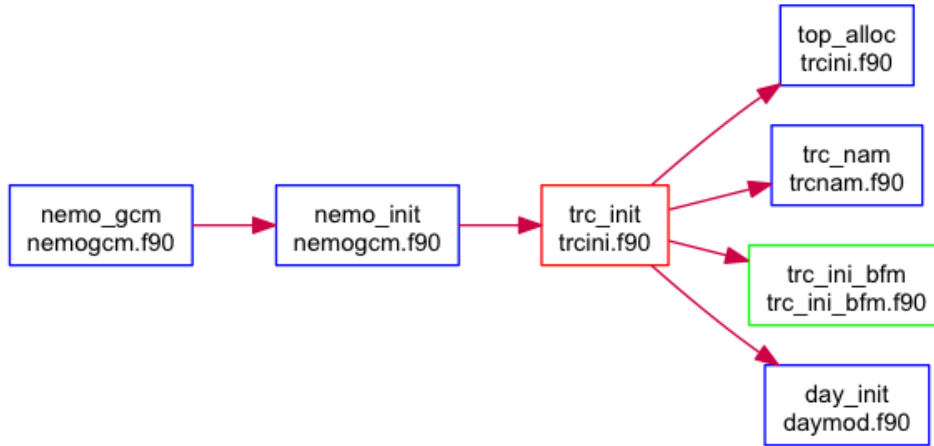


Figure 2.2: Graph of the initialization routine for passive tracers. This routine is not the default TOP routine but it is substituted by the version contained in \$BFMDIR/src/nemo that contains the call to the BFM routine `trc_ini_bfm`.

A scheme of the NEMO initialization of passive tracers is shown in Fig. 2.2, where a specific routine was designed to handle the information flow toward BFM (`trc_ini_bfm`). The initialization of BFM (Fig. 2.3) in the coupling is different from the STANDALONE configuration, because it includes also the transfer of grid parameters from NEMO and the reading of three-dimensional field data of initial conditions (see Sec. 2.4).

The time marching computation in NEMO are performed in the `stp` routine (Fig. 2.4) and the passive tracers are specifically addressed in `trc_stp`. A modified version of the latter subroutine was created to include three different routines for the solution of BFM core processes (`trc_bfm`), the advection and diffusion of state variables (`trc_trp_bfm`), and the computation of output data (`trc_dia_bfm`). In particular, the `trc_bfm` routine includes the retrieval of environmental conditions from NEMO (`envforcing_bfm`), like e.g., temperature, salinity, light, and the computation of BFM biogeochemical processes (EcologyDynamics).

The transport of BFM state variables is operated by `trc_trp_bfm` subroutine (Fig. 2.5), which is derived from the general one of NEMO for passive tracers (namely, `trc_trp`). In fact, this subroutine also handles the application of external boundary conditions (`trc_bc_bfm`), vertical sinking (`trc_set_bfm`) and it prepares the model variables to perform the Euler Forward integration (`trc_nxt_bfm`).

2.4 Boundary conditions in TOP

In version 3.6, NEMO allows to define different types of boundary conditions for biogeochemical tracers. For every single variable it is possible to define a field of surface boundary conditions, such as deposition of dust or nitrogen, which is then interpolated to the grid and timestep using the `fld_read` function. The same facility is available to include river inputs (coastal boundary conditions) and it is under development the treatment of open boundary conditions.

The namelist `namtrc_bc` is contained in file `namelist_top_cfg` (which in the BFM is generated during the first compilation, see Sec. 3.2) and allows to specify the name of the files, the frequency

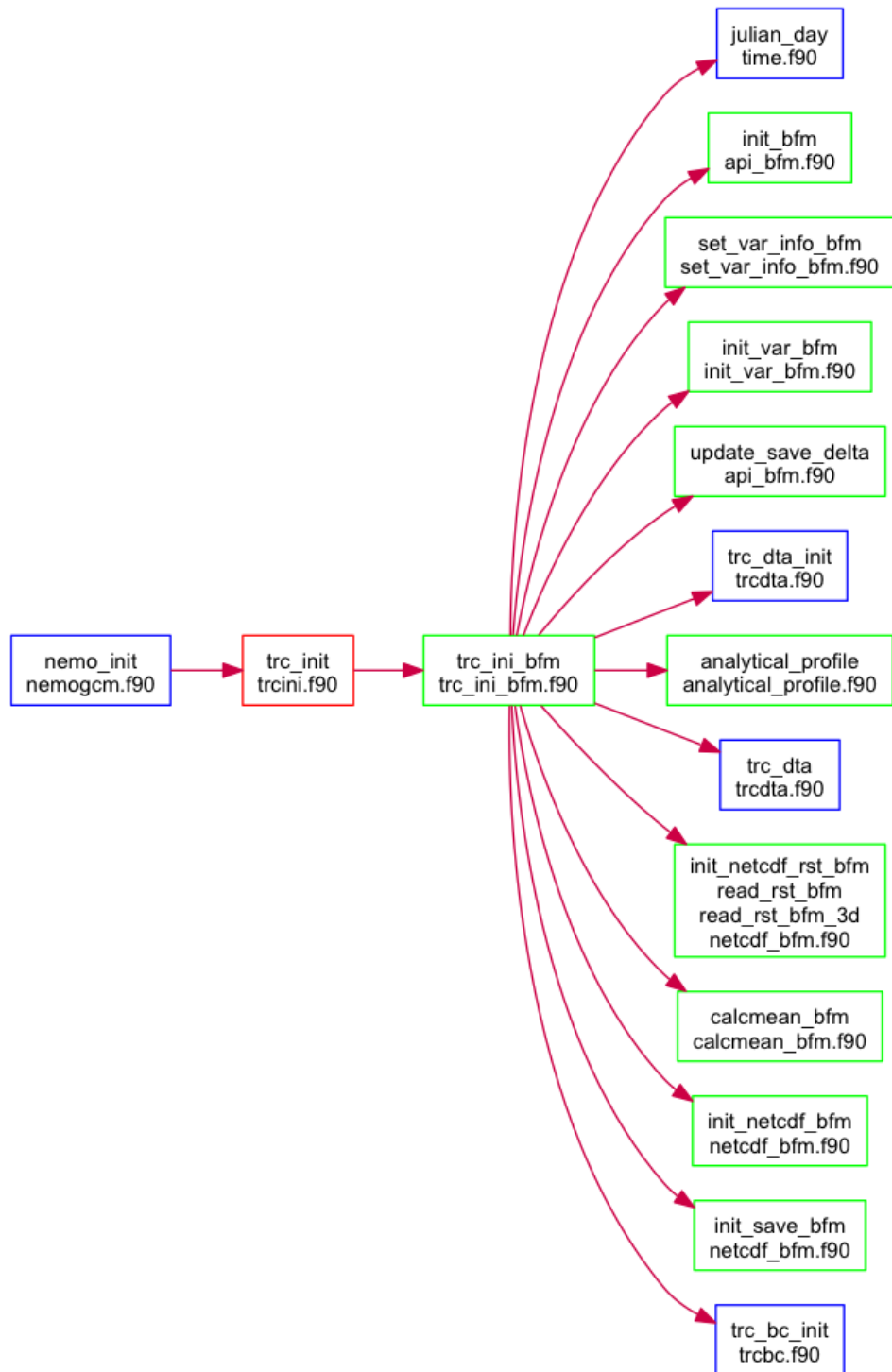


Figure 2.3: Butterfly graph of the BFM initialization within NEMO.

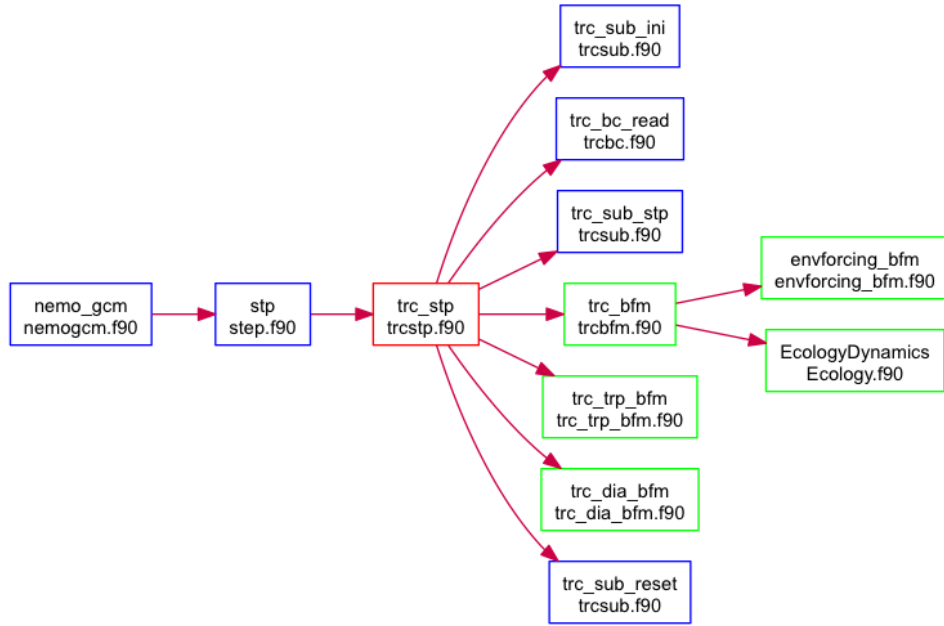


Figure 2.4: Graph of the stepping routine `trc_stp` for passive tracers. This routine is not the default TOP routine but it is substituted by the version contained in `$BFMDIR/src/nemo` that contains the calls to the BFM routines `trc_bfm`, `trc_trp_bfm` and `trc_dia_bfm`.

of the input and the time and space interpolation as done for any other field using the `fld_read` interface. It also allows to specify how freshwater fluxes from sea ice freezing and melting affect the concentration of tracers.

```

!-----!
!NAMELIST namtrc_bc
!-----!
! Set input files for surface (s), coastal (c) or open (o) boundary
! conditions for each variable
! sn_trc?bc(VARNAME): structure with file name and interpolation
! rn_tr?fac(VARNAME): conversion factor
! Specifications for fld_read:
! !file name!frequency (hr)!variable!time interp.!clim !'yearly' or !weights
!rotation!land/sea
! ! !!(if <0 mon) ! name ! (logical) !(T/F)! 'monthly'
!filename ! pairing! mask
!-----!
&namtrc_bc
  sn_trcsbc(N7f) = 'IRON_DEPOSITION', -12, 'fedep', .false., .true., 'yearly', '', '', ''
  rn_trsfac(N7f) = 5.0e-03 ! umol/m2/day, dissolution fraction 5o/oo
  sn_trccbc(N1p) = 'RIVER', -12, 'po4', .false., .true., 'yearly', '', '', ''
  rn_trcfac(N1p) = 8.8464e+10 ! 1 mol P = 30.97 g; 1.e12*1.e3/30.97/365
                        ! conversion factor from Tg/y to mmol/d
  ln_dynsiw = .false. ! parameterize the water flux from sea ice as virtual salt flux (T) on
  cn_dir = './' ! root directory for the location of the boundary condition files
/

```

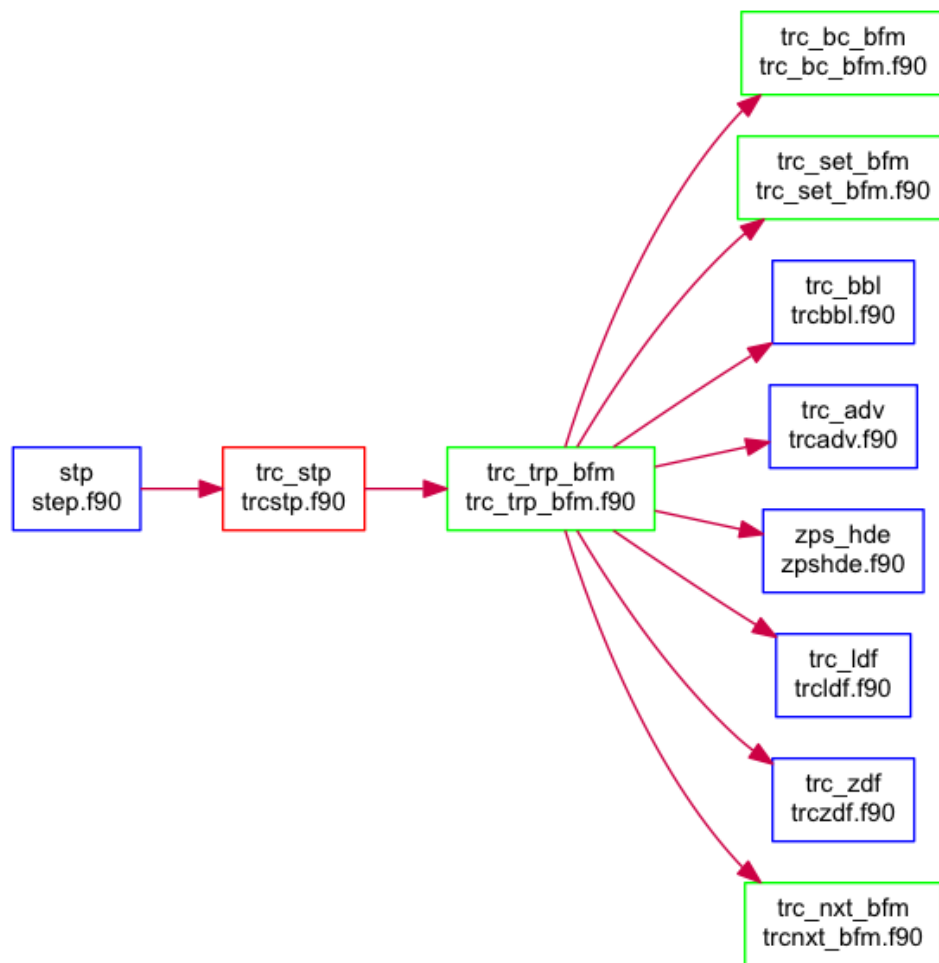


Figure 2.5: Call graph of the transport routine `trc_trp_bfm` for BFM tracers.

2.5 Coupling of the underwater shortwave irradiance

One of the largest coupling mechanism between ocean physics and biogeochemistry is the irradiance attenuation driven by suspended and dissolved components (e.g. Patara et al., 2012). In NEMO this is controlled by the namelist `namtra_qsr`, which is usually not modified in the configuration files and it is located in `namelist_ref`

```
!-----
&namtra_qsr      !   penetrative solar radiation
!-----
  sn_chl         ='chlorophyll',      .....
  cn_dir         = './'              !   root directory for the location of the runoff files
  ln_traqsr      = .true.             !   Light penetration (T) or not (F)
  ln_qsr_rgb     = .true.             !   RGB (Red-Green-Blue) light penetration
  ln_qsr_2bd     = .false.            !   2 bands                light penetration
  ln_qsr_bio     = .false.            !   bio-model light penetration
  nn_chldta      = 1                  !   RGB : Chl data (=1) or cst value (=0)
  rn_abs        = 0.58                !   RGB & 2 bands: fraction of light (rn_si1)
  rn_si0        = 0.35                !   RGB & 2 bands: shortest depth of extinction
  rn_si1        = 23.0                !   2 bands: longest depth of extinction
  ln_qsr_ice     = .true.             !   light penetration for ice-model LIM3
/
```

The coupling with a biogeochemical model is controlled by the parameter `ln_qsr_bio`. If this is set to false as in the default settings above, shortwave radiation penetrates the interior of the ocean according to a 4 waveband algorithm (`ln_qsr_rgb=.true.`), where the incident spectrum is decomposed in infrared, red, green and blue (RGB) portions that are attenuated differentially as a function of chlorophyll concentration. This approximated tabulated solution has been proposed by Lengaigne et al. (2007) using original data by Morel (1988) for 68 wavelengths. If available for the specific configuration, the chlorophyll field is read from a data file (given in the structure `sn_chl`) and used to compute the attenuation coefficients for RGB and the shortwave radiation that is absorbed at every level. This information is used to compute the trend of ocean temperature. The alternative uncoupled configuration is the standard formulation by Paulson and Simpson (`ln_qsr_2bd=.true.`) where light is attenuated according to a 2 waveband formulation, near-infrared and visible.

In both of the cases above the BFM is not coupled to NEMO, that is the evolution of BFM chlorophyll does not feedback into the physical model to determine the vertical divergence of the shortwave field. When `ln_qsr_bio=.true.`, the control of light propagation is completely passed to the BFM (`PAR_parameters` in `Pelagic_Environment.nml`) and the namelist above is not considered. The infrared attenuation depth is substituted by the attenuation coefficient (`p_epsIR=1/rn_si0`) and the fraction of visible light spectral energy is equivalent to `p_PAR=1-rn_abs`:

```
!-----
!   PAR_parameters
!-----
&PAR_parameters
...
  p_PAR          = 0.42
  p_epsIR        = 2.857
...
/
```

The difference between a coupled and uncoupled simulation depends on two factors: how different the chlorophyll seasonality is from the climatological dataset used to compute the attenuation coefficient and the vertical distribution of dynamical chlorophyll, because the satellite-derived chlorophyll is assumed to be homogeneous in the vertical. An example of the difference in the resulting shortwave flux at every depth is given in Fig. 2.6 for a station in the North Pacific (Station PAPA).

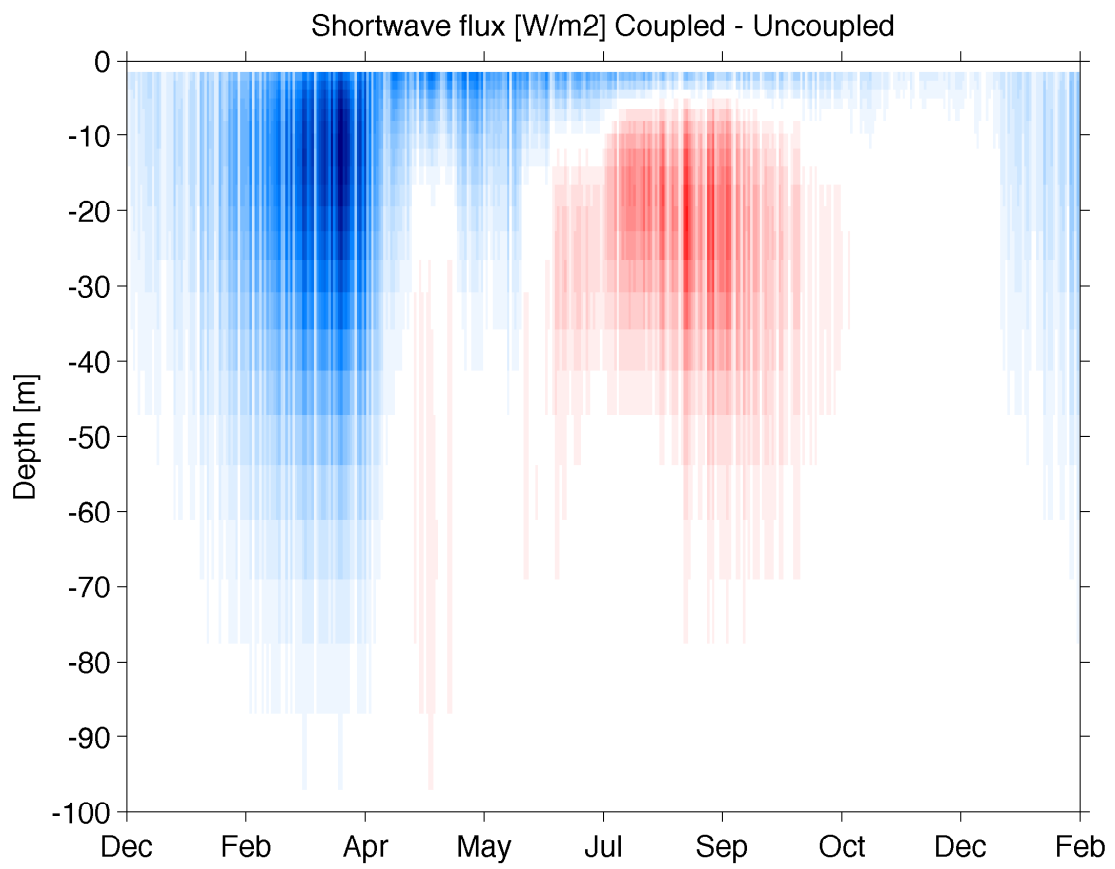


Figure 2.6: Difference of shortwave heat flux between an uncoupled and coupled simulation, where light attenuation is a function of the BFM chlorophyll.

3 Installation, configuration and compilation

3.1 Installation

Both the BFM and NEMO codes have to be downloaded from the respective distribution sites. The present coupling is officially distributed for NEMO version 3.6 and BFM version 5.2. Please contact the BFM System Team (bfm_st@cmcc.it) for information on the use of BFM with the stable version of NEMO 3.4.1. In the following, it is assumed that the NEMO code is found in a directory identified by the environmental variable `$NEMODIR` and the BFM in the directory `$BFMDIR`.

As it occurs for the NEMO compilation, it is necessary to select a configuration before doing the compilation of BFM-NEMO. The default basic configuration of BFM coupled with NEMO is `GYRE_BFM` (Chap. 4), which simulates the general circulation of a double gyre ideally located in the north-western Atlantic. The directory `GYRE_BFM` is already distributed with NEMO 3.6 in the directory `NEMOGCM/CONFIG`, while the global ocean configuration `PELAGOS` (see Chap. 5) is provided with the BFM and other coupled configurations can be added by the user.

Refer to the NEMO web site for how to obtain the code and how to install it. It is suggested to first compile and run the desired NEMO configuration without the BFM, in order to set up the necessary compilation environment. The same architecture file contained in the directory `NEMOGCM/ARCH` will in fact be used by the BFM configuration script. The same software required for running NEMO is necessary for the coupled configuration, with the only addition of `perl` (version 5.8.2 and above), which is used automatically during compilation time to generate the code.

Download the source code from the BFM website or through the git repository. In the example below it is assumed that you downloaded the tarball. The downloaded file may have a different name based on the version. As a final step create the required basic environmental variables pointing at the root directories as:

```
% mkdir $HOME/BFM
% cd $HOME/BFM
% gunzip bfm-release-<version>.tgz
% tar xvf bfm-release-<version>.tar
% export BFMDIR=$HOME/BFM
% export NEMODIR=$HOME/NEMO
```

3.2 Configuring BFM with NEMO

Configuration and deployment of the model is done automatically by the script *bfm_configure.sh* (see the BFM manual for more information or simply run `./bfm_configure.sh -h`). The default configuration (see Chap. 4) is generated, compiled and deployed with the command:

```
% cd $BFMDIR/build
% ./bfm_configure.sh -gcd -a ARCHFILENAME -p GYRE_BFM
```

where `ARCHFILENAME` must be substituted by the name of your specific architecture files that is found in `NEMOGCM/ARCH`. The generated namelists and model executable will be found in

3 Installation, configuration and compilation

`$BFMDIR/run/gyre_bfm` or in the directory indicated by the environmental variable `$BFMDIR_RUN` if set.

3.2.1 The GYRE_BFM preset

As it occurs for BFM STANDALONE, a configuration is defined by a model layout structure and initial input values. The GYRE_BFM preset is found in the `$BFMDIR/build/configurations/GYRE_BFM` folder and contains the following files:

configuration: **compilation and deployment options**

This file uses the F90 namelist format to set values and strings must be surrounded by the `'` character:

```
&BFM_conf
  MODE      = 'NEMO',
  CPPDEFS   = 'BFM_PARALLEL INCLUDE_PELCO2 INCLUDE_PELFE INCLUDE_DIAG',
  ARCH      = 'ARCHFILENAME',
  PROC      = 8,
  EXP       = 'gyre_bfm',
  QUEUE     = 'poe_short',
  EXPFILES  = 'iodef.xml namelist_cfg namelist_top_cfg'
/
```

These options prescribe that the GYRE_BFM configuration is a coupled MODE with NEMO, and it has the pre-compiler macros specified in CPPDEFS (parallel simulation, as it is in the standard NEMO GYRE configuration; inclusion of carbonate and iron dynamics and possibility to store the diagnostic output). In particular, the BFM_PARALLEL macro is used to enable the creation of a simulation log file when using parallel execution on multiple processors. Please refer to the BFM core manual for further details on the other macros.

The coupled configurations also require to include the parameters to run the OGCM in the running directory. This is done by means of the variable EXPFILES, that contains the name of the ancillary files (the configuration namelist for NEMO and TOP interface), as well as the the I/O definition that have to be copied to the running directory. The configuration script also copies the reference configurations from the CONFIG/SHARED directory of NEMO.

layout: **memory layout configuration file**

This file contains the list of state variables defined in the BFM. This is independent of the coupled configuration and it is fully detailed in the BFM core manual.

namelists_bfm: **template namelist file for BFM and NEMO-TOP with standard values**

This file contains all the standard values of the namelists used for the experiment. This file is processed by the configuration script and the BFM named constants are substituted by numerical constants both for BFM parameters and for the ones needed by NEMO-TOP, such as the boundary conditions (see Sec. 2.4), generating the configuration namelist file `namelist_top_cfg`. Namelists are checked for consistency against the source code at generation time and the files effectively used for the simulation are copied to the `$BFMDIR/run` directory. The regular user will generally work with generated namelists and usually there is no need to change any keyword in this file unless new boundary conditions are added or the layout is changed.

3.3 Compilation and interaction with makenemo

This section provides more details on the joint compilation and it is intended mostly for NEMO developers. The configuration script, when called with MODE option equal to NEMO, prepares the BFM code and make it compatible with the NEMO compilation using the FCM configuration manager (<http://www.metoffice.gov.uk/research/collaboration/fcm>). More specifically, `bfm_configure.sh` creates an fcm file for the BFM source code that is then included in the compilation process by means of the `NEMOGCM/CONFIG/GYRE_BFM/cpp_GYRE_BFM.fcm` file (or any other `cpp_*` file from a coupled BFM configuration, see for instance Chap. 5):

```
bld::tool::fppkeys key_dynspg_flt key_ldfslp key_zdftke key_vectopt_loop
               key_top key_my_trc key_mpp_mpi key_iomput
inc $BFMDIR/src/nemo/bfm.fcm
```

The file `bfm.fcm` does not exist initially in the BFM tree and it is generated from a template found in `$BFMDIR/build/scripts/proto` depending on the directory structure and model choices. The specific pre-compilation macro `BFM_NEMO` that is required by BFM to activate the NEMO-related parts of the code is also added to the list of macros.

Finally, the compilation with `makenemo` is launched by prescribing the use of an external directory (option `-e`, introduced since version 3.5) that allows the substitution of the `TOP_SRC` files with the ones containing the coupling with the BFM (see Chap. 2). After the first generation with the `bfm_configure.sh` script it is also possible to compile the model from the standard `NEMOGCM/CONFIG` directory with the command

```
./makenemo -n GYRE_BFM -m ARCHFILE -e ${BFMDIR}/src/nemo
```


4 Running GYRE_BFM

4.1 Description

GYRE_BFM is an analytical configuration of NEMO that simulates a warm and cold gyre ideally located in the North Atlantic. Only the pelagic system can be currently simulated with this configuration. The model is forced with analytical heat and momentum fluxes over a regular year of 360 days and starts from homogeneous initial conditions for biogeochemistry. The model output is in NetCDF. The default grid is 22 x 32 with 31 vertical levels.

4.2 Serial and parallel simulations

GYRE_BFM is the simplest example to run as a single process on a desktop computer because the grid is rather coarse. However, the default GYRE configuration in NEMO is set up to use parallel computation and the advanced XIOS library (see chap. 11 of NEMO v3.6 manual). To compile in serial mode it is necessary to remove the macro `key_mpp_mpi` for parallel computation that is found in `$NEMODIR/NEMOGCM/CONFIG/GYRE_BFM/cpp_GYRE_BFM.cpp`. It is also possible to use the standard NEMO output instead of the XIOS library by removing the macro `key_iomput` in the `cpp` file of the configuration.

Together with the BFM, the GYRE configuration increases substantially the computational burden, therefore it is also a good example to learn how to use the model with multiple processes. In this case, it is necessary to install an MPI library (like <http://www.open-mpi.org/>) and use a NEMO ARCH file with the `mpif90` compiler. When GYRE_BFM is run in parallel, the BFM netcdf output is produced for each sub-domain just like it happens for NEMO and the same naming convention is used. The output can be “rebuilt”, that is all the tiles are combined together, to obtain the full domain using the tool described in Sec 6.2.

4.3 Results

This example demonstrates the role of the major physical factors in driving the plankton response. The double gyre is characterized by a warm subtropical cell and a cold subpolar cell (Fig. 4.1) that are separated by a simplified current that should mimic the features of a western boundary current. Phytoplankton production is generally localized around the current bordering the gyres and in correspondence with the cold and less stratified parts of the sub-polar gyre.

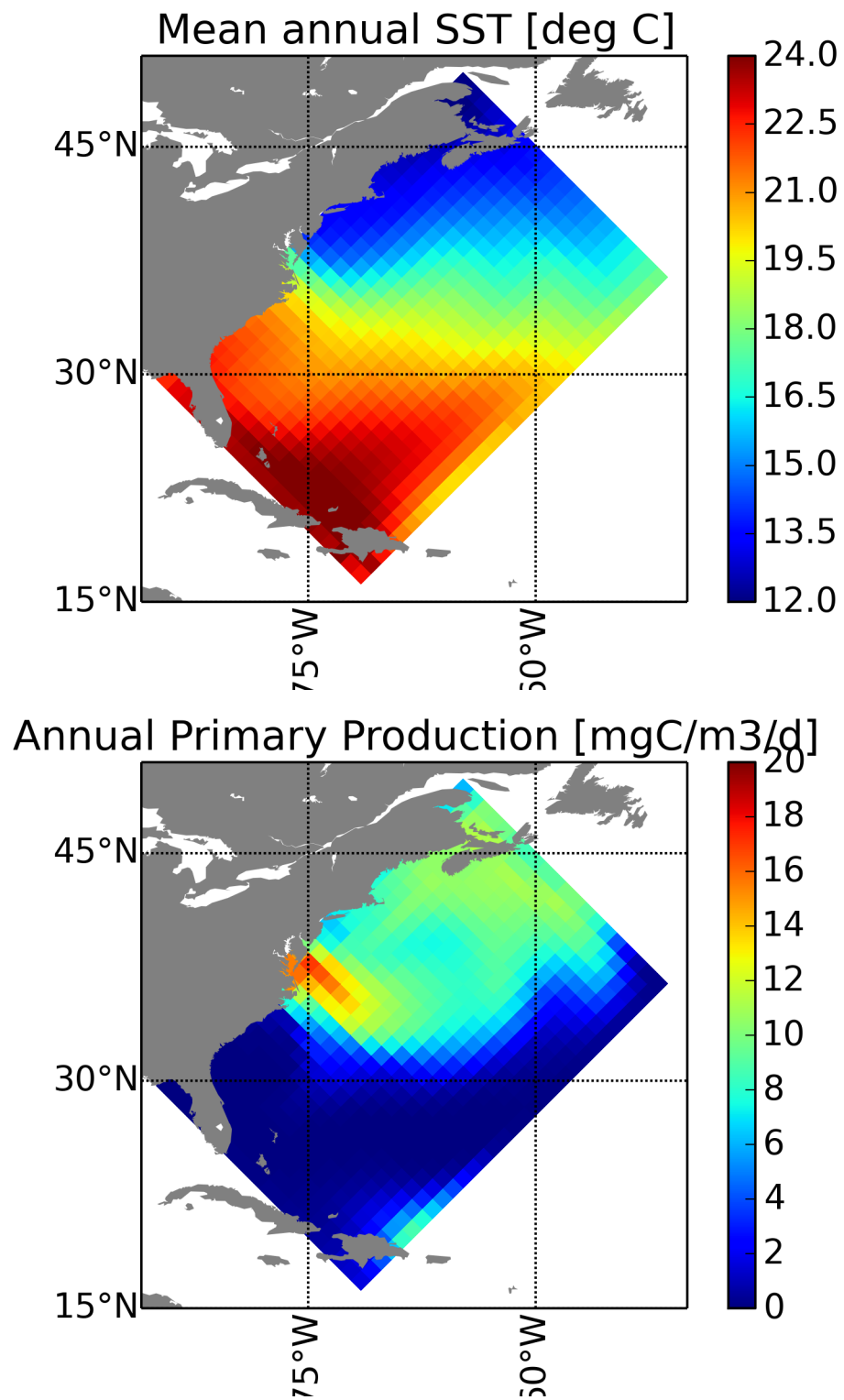


Figure 4.1: Example output from GYRE_BFM after 9 years of simulation. Mean annual sea surface temperature (top) and net primary production (bottom).

5 The PELAGOS global ocean configuration

5.1 Description

PELAGOS stands for PELAGic biogeochemistry for Global Ocean Simulations (Vichi et al., 2007a) and it is a global ocean implementation of the BFM with NEMO using the family of ORCA grids. It was originally designed as a specific sub-set and integration of functional parameterizations that were required to address global ocean dynamics (see Vichi et al. (2007b)), but it is now intended to be just another configuration of the BFM. This implies that any BFM feature can now be used with NEMO also in global ocean configurations. The PELAGOS family of configurations follows the ORCA family specifications, that is PELAGOS2 refers to the ORCA2 grid, PELAGOS1 to ORCA1 and so forth.

PELAGOS2 is the coarsest global ocean resolution but still requires a parallel computing environment for its usage. One needs to have a fully functioning implementation of the ORCA2_LIM reference configuration before attempting to run PELAGOS2. The default set up is the same as ORCA2_LIM with the following features:

- sea ice model LIM2 (`key_lim2`)
- filtered linear free surface (`key_dynspgflt`)
- Laplacian diffusion with isopycnal diffusion (`key_ldfslp`) and coefficients for horizontal diffusion with 2-D variation (`key_traldf_c2d`)
- eddy-induced velocity parameterization of enhanced diffusion (`key_traldf_eiv`) and related diagnostics (`key_diaeiv`)
- coefficients for horizontal viscosity with 3-D variation (`key_dynldf_c3d`)
- vertical turbulence TKE closure and vertical tidal mixing (`key_zdftke` and `key_zdftmx`)
- bottom boundary layer parameterization (`key_trabbl`)
- double diffusion (`key_zdfddm`)

with the addition of the pre-processing macros to turn on passive tracers and the BFM (`key_top` and `key_my_trc`)

By default, PELAGOS2 is compiled with the embedded I/O library XIOS (`key_iomput`) which must be compiled as an external library. On a modern super-computer, 1 month of simulation takes about 5 minutes using 128 processors.

5.2 The PELAGOS2 preset

This preset is not part of the official NEMO release but uses the `makenemo` tool to create the configuration PELAGOS2 in the `$NEMODIR/NEMOGCM/CONFIG` directory to allow the compilation with FCM.

5 The PELAGOS global ocean configuration

Users should know that the file `cpp_PELAGOS2.fcm` containing the preprocessing macros listed above is found in this directory, and once you have created the corresponding configuration directory in the NEMO tree it will be copied there and should be subsequently modified from there.

When the configuration script is called with the PELAGOS2 preset, `makenemo` is requested to create a new configuration and

```
% ./bfm_configure.sh -gcd -a ARCHFILE -p PELAGOS2
You are installing a new configuration
Creating PELAGOS2/WORK = OPA_SRC TOP_SRC LIM_SRC_2 for PELAGOS2
MY_SRC directory is : PELAGOS2/MY_SRC
....
```

The run directory is created in `$BFMDIR_RUN/pelagos2` just like all other BFM presets and the NEMO executable is linked to there.

5.3 Results

A 9 years-long simulation was performed with the PELAGOS2 configuration by using the normal year CORE II atmospheric forcing (Large and Yeager (2009)) and climatological river runoff (Dai and Trenberth (2002)) and nutrients loads (Cotrim da Cunha et al. (2007)). Input data can be retrieved from NEMO Reference configurations inputs NEMO Consortium (2017). The initial conditions of both physical and biogeochemical variables were set using the World Ocean Atlas 2009 climatological fields (NESDIS NOAA Atlas (2010)). In Fig. 5.1 are shown the mean annual fields for the sea surface temperature and the satellite-like chlorophyll concentration (using 1% light threshold for depth integration, see Sec. 6.3) computed in the last year of simulation. PELAGOS2 is capable to reproduce the main distribution patterns of primary producers across the different oceanic regions, by preserving also the minimum concentration within the subtropical oceanic gyres.

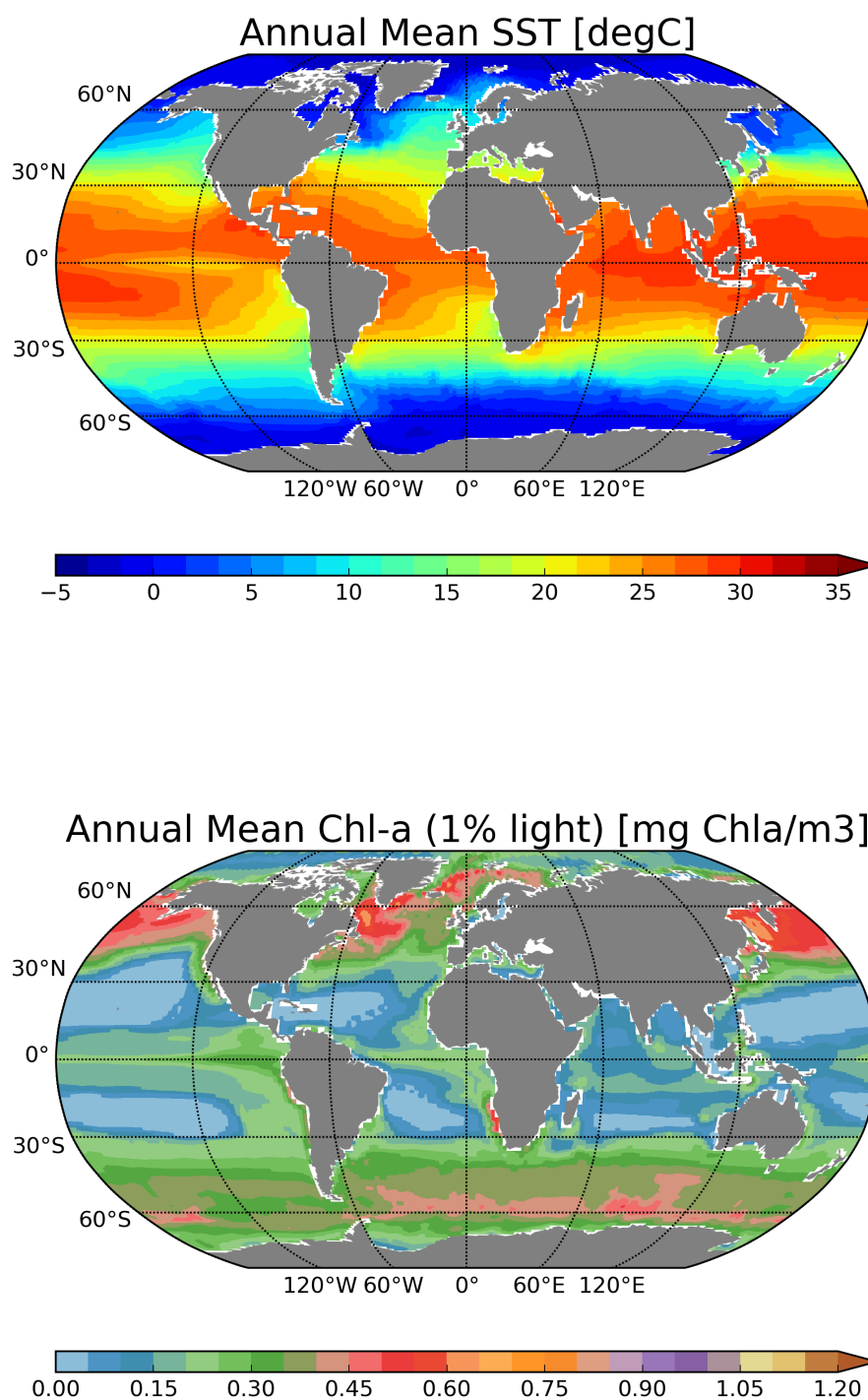


Figure 5.1: Example output from PELAGOS2 after 9 years of simulation. Mean annual surface temperature (top) and satellite-like chlorophyll at 1% light level (bottom). See Sec. 6.3 for satellite-like chlorophyll computation.

6 Output and diagnostics

6.1 Introduction

BFM uses its own libraries for NetCDF output that are specifically built to create diagnostic rates between the biogeochemical variables (see Chap. 8 in BFM core manual).

Since version 3.6 of NEMO, the external library XIOS can be used to distribute the computation and preparation of output over different processes and with a different domain decomposition.

The XIOS library functions can be used also with BFM, as a set of dedicated XML files are produced during code generation to setup required output files and fields as in NEMO. In particular, `field_def_bfm.xml` file contains the description of all accessible BFM variables and `file_def_bfm.xml` it is used to select the variables to be included in the output files. In order to be used by XIOS, these two files must be integrated in the general `general NEMO iodef.xml` file (using the `include` sentence).

6.2 Rebuilding the output and restart files

The BFM is by construction defined only in the ocean grid points and the output file consists of a one-dimensional vector. It is therefore required to post-process the output to obtain the three-dimensional fields on the ocean model grid.

This operation is done with the tool `bnmerge` found in the `$BFMDIR/tools` directory that allows to merge together the individual output files per domain containing a vector with the ocean grid points of that specific domain only into the full 3D domain.

The application is controlled with a `namelist` (see use details in `$BFMDIR/tools/README.md`), where it is possible to specify the list of variables to be remapped and the names of the files.

In the case of restart files, it is also possible to use the tool `bnmerge` to build a single restart file which may turn to be useful in the case a user want to restart an experiment but with a different number of parallel processes. The reading of restart input files is controlled by the option `bfm_init` in the `BFM_General.nml` `namelist` file, which can be set to 0 = no restart, 1 = multiple restart files (one per process), 2 = restart is a single merged file.

6.3 Diagnostic computation of satellite chlorophyll

This tool is available in directory `$BFMDIR/tools/chlsat` and computes the chlorophyll concentration as seen by satellite considering:

1. the optical depth and a tolerance level as described in eq. 2 of Vichi et al. (2007b);
2. the 1% light level;
3. the 0.1% light level

6 Output and diagnostics

Input files are the chlorophyll concentration (variable Chla) and the attenuation coefficient (variable xEPS), both with the same number of time stamps, and the mask file. It also allows to compute the attenuation coefficient using the BFM formula from total chlorophyll concentration, background attenuation and chlorophyll-specific absorption coefficient but neglecting the contribution from inorganic suspended matter and detritus.

This tool also computes the integrated primary production (gross and net) down to 1% and 0.1% light level by setting the flag `compute_intpp` and providing the paths to the files containing the BFM diagnostics `ruPPYc` (gross primary production) and `resPPYc` (respiration).

The input parameters are in the namelist `chlsat.nml`:

```
!-----!
!Main initialisation and output specifications
!NAME          KIND      DESCRIPTION
!out_fname      string      Name of output file
!inp_dir        string      Path to the input files
!out_dir        string      Path to the output file
!mask_fname     string      Full path to NEMO mesh_mask file
!chla_fname     string      Name of data file containing 3D Chl
!chla_name      string      Name of Chl variable in file
!compute_chlsat logical      Compute chlsat (true by default useful only for NPP)
!compute_eps    logical      Use attenuation coefficient from output
!               or computed using the BFM formula from Chl
!               concentration, neglecting ISM and detritus
!               The computation requires:
!   p_eps0      real          background attenuation of water (m-1)
!   p_epsChla   real          specific attenuation of Chla (m2/mg Chl)
!
!eps_fname      string      Name of data file containing 3D att. coeff.
!eps_name       string      Name of attenuation coeff. variable in file
!tolerance      real          multiplicative factor for optical depth
!
!compute_intpp  logical      Compute integrated GPP and NPP down to 1% and 0.1%
!gpp_fname      string      Name of data file containing 3D GPP
!gpp_name       string      Name of GPP variable in file
!rsp_fname      string      Name of data file containing 3D RSP
!rsp_name       string      Name of RSP variable in file
!-----!
&chlsat_nml
  out_fname='chlsat.nc'
  inp_dir='.'
  out_dir='.'
  mask_fname='ORCA2_chlmask.nc'
  chla_fname='bfm_output.nc'
  chla_name='Chla'
  compute_chlsat=.true.
  compute_eps=.false.
  p_eps0=0.0435
  p_epsChla=0.03
  eps_fname='bfm_output.nc'
  eps_name='xEPS'
  tolerance=0.0
  compute_intpp=.false.
  gpp_fname='bfm_output.nc'
  gpp_name='ruPPYc'
  rsp_fname='bfm_output.nc'
  rsp_name='resPPYc'
/
```

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