

Nucleus for European Modelling of the Ocean











Tracers in Ocean Paradigm (TOP) The NEMO passive tracers engine

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Abstract

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"Tracers in Ocean Paradigm" (TOP) is the passive tracers engine of the NEMO ocean model ("Nucleus for European Modelling of the Ocean"). It is intended to be a flexible tool for studying the on/offline oceanic tracers transport and the biogeochemical processes ("green ocean"), as well as its interactions with the other components of the Earth climate system over a wide range of space and time scales. TOP is directly interfaced with the NEMO ocean engine, and, via the OASIS coupler, with several atmospheric general circulation models. This component provides the physical constraints and boundaries conditions for oceanic tracers transport and represents a generalized, hardwired interface toward biogeochemical models to enable a seamless coupling. In particular, transport dynamics are supplied by the ocean dynamical core thus enabling the use of all available advection and diffusion schemes in both on- and offline modes. TOP is designed to handle multiple oceanic tracers through a modular approach and it includes different sub-modules: ocean water age, inorganic carbon (CFCs) & radiocarbon (C14b), built-in biogeochemical model (PISCES), and prototype for user-defined cases or coupling with alternative biogeochemical models (e.g., BFM).











Disclaimer

Like all components of the modelling framework, the TOP core engine is developed under the CECILL license, which is a French adaptation of the GNU GPL (General Public License). Anyone may use it freely for research purposes, and is encouraged to communicate back to the development team its own developments and improvements.

The model and the present document have been made available as a service to the community. We cannot certify that the code and its manual are free of errors. Bugs are inevitable and some have undoubtedly survived the testing phase. Users are encouraged to bring them to our attention.

The authors assume no responsibility for problems, errors, or incorrect usage of NEMO.

Other resources

Additional information can be found on:

- Whith the website of the project detailing several associated applications and an exhaustive users bibliography
- \$\mathcal{V}\$ the development platform of the model with the code repository for the shared reference and some main resources (wiki, ticket system, forums, ...)
 - the repository of the demonstration cases for research or training
- 4 the online archive delivering the publications issued by the consortium (manuals, reports, datasets, ...)
- we two mailing lists: the newsletter for top-down communications from the project (announcements, calls, job opportunities, ...) and the forge updates (commits, tickets and forums)

Citation

Reference for papers and other publications is as follows:

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Introduction

TOP (Tracers in the Ocean Paradigm) handles oceanic passive tracers in NEMO. At present, this component provides the physical constraints and boundaries conditions for oceanic tracers transport and represents a generalized, hardwired interface toward biogeochemical models to enable a seamless coupling.

It includes three independent components:

- a transport code TRP sharing the same advection/diffusion routines with the dynamics, with specific treatment of some features like the surface boundary conditions or the positivity of passive tracers concentrations
- sources and sinks SMS models that can be typically biogeochemical, biological or radioactive
- an offline transport interface, which is a simplified version of the NEMO core workflow that read a set of physical fields previously stored on disk

There are two ways of coupling TOP to the dynamics:

- online coupling : the evolution of passive tracers is computed along with the ocean physical dynamics
- offline coupling: the physical variable fields are read from files and interpolated at each model time step, with no constraints on the temporal sampling in the input files

TOP is designed to handle multiple oceanic tracers through a modular approach and includes different submodules :

- the ocean water age module (AGE) tracks down the time-dependent spread of surface waters into the ocean interior
- inorganic (e.g., CFCs, SF6) and radiocarbon (C14) passive tracers can be modeled to assess ocean absorption timescales of anthropogenic emissions and further address water masses ventilation
- a built-in biogeochemical model (PISCES) to simulate lower trophic levels ecosystem dynamics in the global ocean
- a prototype tracer module (MY_TRC) to enable user-defined cases or the coupling with alternative biogeochemical models (e.g., BFM, MEDUSA, ERSEM, ECO3M)

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TOP structure and workflow

TOP is the NEMO hardwired interface toward biogeochemical models, which provides the physical constraints/boundaries for oceanic tracers (Fig. 1.1).

Based on a modular structure, this component allows one to exploit available built-in modules and further develop a range of applications, spanning from the implementation of a dye passive tracer to evaluate dispersion processes (by means of MY_TRC), track water masses age (AGE module), assess the ocean interior penetration of persistent chemical compounds (e.g., gases like CFC or even PCBs), up to the full set of equations to simulate marine biogeochemical cycles.

TOP interface has the following location in the code repository : <nemo-repository>/src/TOP/ and the following modules are available:

- TRP : Interface to NEMO physical core for computing tracers transport
- CFC: Inert tracers (CFC11,CFC12, SF6)
- C14: Radiocarbon passive tracer
- AGE: Water age tracking
- MY_TRC: Template for creation of new modules and external BGC models coupling
- PISCES: Built in BGC model. See Aumont et al. (2015) for a complete description

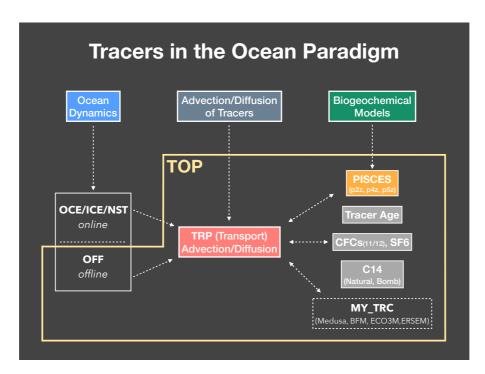


Figure 1.1.: Schematic view of the TOP interface within NEMO framework

The workflow of the TOP interface within the NEMO framework is organized around two main blocks of the code, the initialization (figure 1.2) and time marching or "stepping" (figure 1.3) procedures.

The initialization (trc_init) of passive tracers variables and parameters include reading namelist, set initial tracer fields (either read restart or read data), and specific initialisation for each SMS module.

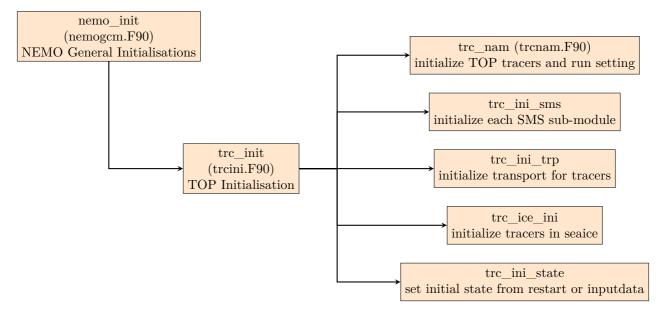


Figure 1.2.: TOP interface initialization workflow

In the time-marching procedure of the model (trc_stp), trends are computed for all tracers in relation to biogeochemical processes (source minus sinks of each TOP sub-module), physical transport (advective & diffusive, forcing and boundary conditions) and output is managed using the I/O library XIOS.

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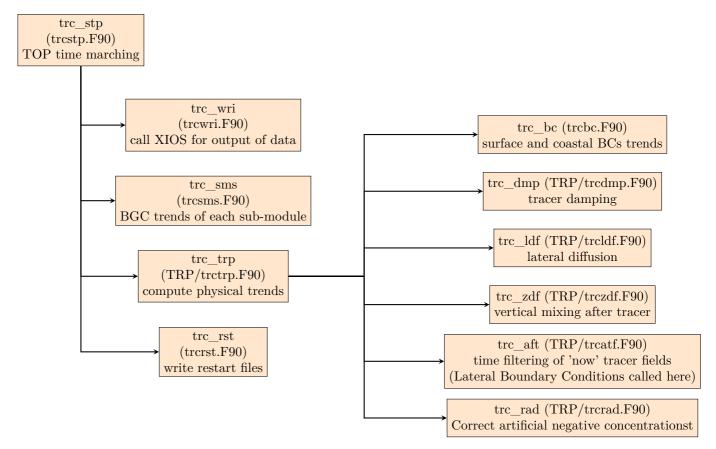


Figure 1.3.: TOP interface time-marching workflow (called by stp in OCE/step.F90 $\,$

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2.1. The transport-reaction equation

The time evolution of any passive tracer C is given by the transport equation, which is similar to that of active tracer - temperature or salinity:

$$\frac{\partial C}{\partial t} = S(C) - \frac{1}{b_t} \left[\frac{\partial e_{2u} \, e_{3u} \, u \, C}{\partial i} + \frac{\partial e_{1v} \, e_{3v} \, uv, C}{\partial i} \right] + \frac{1}{e_{3t}} \frac{\partial w \, C}{\partial k} + D^{lC} + D^{vC}$$

$$(2.1)$$

where expressions of D^{lC} and D^{vC} depend on the choice for the lateral and vertical subgrid scale parameterizations (see sections 4.2 and 4.3 in NEMO manual).

S(C), the first term on the right hand side of equation 2.1, is the SMS - Sources Minus Sinks - inherent to the tracer. In the case of a biological tracer such as phytoplankton, S(C) is the balance between phytoplankton growth and its loss through mortality and grazing. In the case of a tracer comprising carbon, S(C) accounts for gas exchange, river discharge, flux to the sediments, gravitational sinking and other biogeochemical processes. In the case of a radioactive tracer, S(C) is simply the loss due to radioactive decay.

The second term (within brackets) represents the advection of the tracer in three dimensions. It can be interpreted as the budget between the incoming and outgoing tracer fluxes in a volume T-cells $b_t = e_{1t} e_{2t} e_{3t}$

The third term represents the change due to lateral diffusion.

The fourth term denotes the change due to vertical diffusion, parameterized as eddy diffusion to represent vertical turbulent fluxes :

$$D^{vC} = \frac{1}{e_{3t}} \frac{\partial}{\partial k} \left[A^{vT} \frac{\partial C}{\partial k} \right] \tag{2.2}$$

where A^{vT} is the vertical eddy diffusivity coefficient of active tracers.

2.2. Physical transport component (TRP)

The passive tracer transport component shares the same advection/diffusion routines with the dynamics, with specific treatment of some features like the damping or the positivity of passive tracers concentrations.

2.2.1. Advection

The advection schemes used for the passive tracers are the same as those used for T and S. They are described in section 4.1 of the NEMO manual. The choice of an advection scheme can be selected independently and can differ from the ones used for active tracers. This choice is made in namelist_top (ref or cfg) in the namelist block namtrc_adv, by setting to true one and only one of the logicals $ln_tracers_t$, as it is done for the active tracers counterparts.

Note that Centred (cen), Flux Corrected Transport (fct), Upstream-Biased (ubs), and QuiCKest (qck) parameterizations are not positive schemes meaning that negative values can appear in an initially strictly positive tracer field which is advected, implying that artificial extrema are permitted. Their use is not recommended for passive tracers.

```
(default: NO selection)
&namtrc adv
                    ! advection scheme for passive tracer
  \label{ln_treadv_OFF} \begin{array}{ll} ln\_trcadv\_OFF = .false. ! No passive tracer advection \\ ln\_trcadv\_cen = .false. ! 2nd order centered scheme \\ \end{array}
                                        =2/4, horizontal 2nd order CEN / 4th order CEN
     nn_cen h = 4
                                        =2/4, vertical 2nd order CEN / 4th order COMPACT
     nn_cen_v
  ln\_trcadv\_fct = .false.! FCT scheme
                                    ! =2/4, horizontal 2nd / 4th order
! =2/4, vertical 2nd / COMPACT 4th order
     nn\_fct\_h = 2
     nn fct v = 2
  ln\_trcadv\_mus = .false. \ ! \ MUSCL \ scheme
     ln mus ups = .false.
                                        use upstream scheme near river mouths
  ln_trcadv_ubs = .false. ! UBS scheme
     nn_ubs_v = 2
                                     ! = 2 , vertical 2nd order FCT
  ln\_trcadv\_qck = .false. \ ! \ QUICKEST \ scheme
```

2.2.2. Lateral diffusion

After NEMO v4.0, the lateral diffusion of passive tracers uses exactly the same form of active tracers, meaning that the numerical scheme is inherited from the physical setup and forced to be the same. However the passive tracer mixing coefficient can be chosen as a multiple of the active ones by changing the value of rn_ldf_multi in namelist namtrc_ldf. The choice of the numerical scheme is then set in the &namtra_ldf namelist section for the dynamic described in section 4.2 of NEMO manual.

rn_fact_lap is a factor used to increase zonal equatorial diffusion for depths beyond 200 m. It can be useful to achieve a better representation of Oxygen Minimum Zone (OMZ) in some biogeochemical models, especially at coarse resolution (Getzlaff and Dietze, 2013).

2.2.3. Vertical sinking of particles

The module trc_sink computes the vertical flux of tracers that undergo to gravitational sinking (e.g., particulated matter). It also offers a temporary solution for the problem that may arise in specific situation where the CFL criterion is broken for vertical sedimentation of particles. To avoid this, a time splitting algorithm has been coded. The number of iterations (niter) necessary to respect the CFL criterion is dynamically computed. A specific maximum number of iterations (nitermax) can be specified in the namelist. This allows to avoid a very large number of iterations when explicit free surface is used, for instance. If niter is larger than the prescribed nitermax, sinking speeds are clipped so that the CFL criterion is respected. The numerical scheme used to compute sedimentation is based on the MUSCL advection scheme.

2.2.4. Tracer damping

The use of newtonian damping to climatological fields or observations is also coded, sharing the same routine as that of active tracers. Boolean variables are defined in namelist_top_ref to specify which tracers are affected by the restoring procedure. Options are defined through the &namtrc_dmp namelist variables. The restoring term is added when the namelist parameter ln_trcdmp is set to true. The restoring coefficient is a three-dimensional array read in a file, whose name is specified by the namelist variable cn_resto_tr. This netcdf file can be generated using the DMP_TOOLS tool.

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2.2.5. Tracer positivity

Some numerical schemes can generate negative values of passive tracers concentration, thus leading to unrealistic features. For example, isopycnal diffusion can created local extrema, meaning that negative concentrations are allowed to generate.

The trcrad routine artificially corrects negative concentrations with a very crude solution that either sets negative concentrations to zero without adjusting the tracer budget (CFCs or C14 chemical coumpounds), or by removing negative concentrations while computing the corresponding tracer content that is added and then, adjusting the tracer concentration using a multiplicative factor so that the total tracer concentration is preserved (e.g., in PISCES). The treatment of negative concentrations is an option and can be selected in the namelist &namtrc_rad by setting the parameter ln_trcrad to true.

2.2.6. Offline transport mode

Coupling passive tracers offline with NEMO requires a set of physical fields computed in a previous ocean simulation. Those fields are read in files and interpolated on-the-fly at each model time step. There are two sets of fields to perform offline simulations:

• linear free surface (ln_linssh = .true.) where the vertical scale factor is constant with time. At least, the following dynamical parameters should be absolutely passed to transport : the effective ocean transport velocities (eulerian plus the eddy induced plus all others parameterizations), vertical diffusion coefficient and the freshwater flux .

```
(OFF SRC only)
&namdta dvn ! offline ocean input files
                = './'
                         ! root directory for the ocean data location
  cn dir
               file name
                                        ! frequency (hours) ! variable ! time interp.! clim ! 'yearly'
                                                                         ! (logical) ! (T/F) ! 'monthly' !
                                       (if < 0 months) !
                                                               name
  sn\_tem
                 = 'dyna\_grid\_T
                                                       120.
                                                                   , 'vosaline' , .true. , .true. , 'yearly' , .true. , .true. , 'somixhgt' , .true
                                                                      'votemper', .true.
                                                                                                , .true. , 'yearly
  sn\_sal
                = \, 'dyna\_grid\_T'
                                                      120.
  sn_mld
                 = 'dyna_grid_T
                                                       120.
                                                                                   , .true. , .true. , 'yearly
                                                                     , 'sowaflup' , .true. , .true. , 'yearly 'iowaflup' , .true. , .true. , 'yearly
                 = 'dyna_grid_
  \begin{array}{c} sn\_emp \\ sn\_fmf \end{array}
                                                        120.
                                                                                                          'vearly
                = 'dyna_grid_T'
                                                       120.
                                                                  , 'soicecov' , .true. , .true. , 'yearly
, 'soshfldo' , .true
  sn\_ice
                = 'dyna\_grid\_T'
                                                                   , 'sowindsp' , true,
  sn\_qsr
                = 'dyna_grid_
                                                       120.
                                                                                             , .true. , 'yearly
                                                                    , 'sowindsp' , .true.
, 'uocetr_eff', .true.
, 'vocetr_eff', .true.
                                                                                               , .true. , 'yearly
                 = 'dyna_grid_T
                                                        120.
  sn_wnd
                 = 'dyna\_grid\_U'
  sn\_uwd
                                                        120.
                                                                                               , .true. , 'yearly
                 = 'dyna_grid_V'
                                                                                               , .true. , 'yearly
  sn vwd
                                                        120.
                                                                       'wocetr_eff', .true.
                  = 'dyna_grid_
                                                                      , 'wocetr_eff', .true. , .true. , 'yearly' voddmays' , .true. , .true. , 'yearly'
                                                         120.
  sn wwd
                = 'dyna_grid_W'
                                                        120.
  sn_avt
                = 'dyna_grid_U'
  sn\_ubl
                                                       120.
                                                                      'sobblcox', .true., .true., 'yearly
  sn_vbl
                = 'dyna_grid_V'
                                                       120.
                                                                   , 'sobblcoy' , .true. , .true. , 'yearly
```

• non linear free surface (ln_linssh = .false. or key_qco): the same fields than the ones in the linear free surface case. In addition, the horizontal divergence transport is needed to recompute the time evolution of the sea surface height and the vertical scale factor and depth, and thus the time evolution of the vertical transport velocity.

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```
(OFF_SRC only)
              ! offline ocean input files
ln dynrnf
                   .true.
                           ! runoffs option enabled (T) or not (F)
In dynrnf depth = .false. ! runoffs is spread in vertical (T) or not (F)
cn dir
                     ! root directory for the ocean data location
           file name
                                ! frequency (hours)!
                                                       variable ! time interp.! clim ! 'yearly'/!
                               (if <0 months) !
                                                                  (logical)! (T/F)! 'monthly'
                                                      name
                                                        , 'thetao'
'so'
            = 'dvna grid
sn tem
                                             120.
                                                                        .true.
                                                                               , .true. , 'yearly'
                                             120.
           = 'dyna\_grid\_T'
sn sal
                                                                      .true. , .true. , 'yearly
sn\_div
                                                       , 'hdivtr'
            = 'dyna_grid_
                                             120
                                                                       .true.
                                                                               , .true. , 'yearly
sn mld
            = 'dyna_grid_T'
                                             120
                                                          'mldr10 1
                                                                          .true. , .true. , 'yearly
sn_emp
             = \ 'dyna\_grid\_
                                              120
                                                          'wfo'
                                                                        .true. , .true. , 'yearly
                                                                                           'vearly
sn\_empb
             = 'dyna\_grid_
                                              120
                                                           'wfob'
                                                                                , .true. ,
                                                                         .true.
            = 'dyna_grid_T
                                                                                  .true.,
                                             120.
                                                         'fmmflx
sn fmf
                                                                         .true.
                                                                                          'vearly
                                             120.
            = 'dyna_grid_T
                                                         'runoffs'
sn rnf
                                                                       .true.
                                                                               , .true. ,
                                                                                         'vearly
           = 'dyna_grid_
                                             120.
sn ice
                                                         'siconc
                                                                       .true.
                                                                               , .true. ,
                                                                                        'yearly
                                                                               , .true. , 'yearly
            = 'dyna_grid_
                                                       , 'rsntds'
                                                                       .true.
sn_qsr
             = 'dyna\_grid_
                            T'
                                              120.
                                                          'windsp'
                                                                         . true.
                                                                                , .true. , 'yearly
sn\_uwd
             = 'dyna\_grid\_U'
                                              120.
                                                          'uocetr_eff',
                                                                          .true.
                                                                                 , .true. , 'yearly
sn\_vwd
                                                                                 , .true. , 'yearly
             = 'dyna_grid_V
                                              120.
                                                          'vocetr_eff'
                                                                          .true.
             = 'dyna_grid_
                                               120
                                                            'wocetr eff'.
sn wwd
                                                                           .true.
                                                                                   . .true. . 'vearly
            = 'dyna_grid_W
                                              120.
                                                          'difvsolog' ,
sn_avt
                                                                        .true. , .true. , 'yearly
sn\_ubl
            = 'dyna_grid_U'
                                             120.
                                                         'ahu_bbl'
                                                                         .true.
                                                                                 , .true. , 'yearly
sn\_vbl
            = 'dyna_grid_
                                             120.
                                                       , 'ahv bbl'
                                                                         .true.
                                                                                 , .true. , 'yearly
```

Additionally, temperature, salinity, and mixed layer depth are needed to compute slopes for isopycnal diffusion. Some ecosystem models like PISCES need sea ice concentration, short-wave radiation at the ocean surface, and wind speed (or at least, wind stress).

The so-called offline mode is useful since it has lower computational costs for example to perform very longer simulations – about 3000 years - to reach equilibrium of $\rm CO_2$ sinks for climate-carbon studies.

The offline interface is located in the code repository: <repository>/src/OFF/. It is activated by adding the key_offline CPP key to the CPP keys list. There are two specifics routines for the offline code:

- dtadyn.F90: this module reads and computes the dynamical fields at each model time-step
- nemogcm.F90 : a degraded version of the main nemogcm.F90 code of NEMO to manage the time-stepping

2.3. Forcing and Boundary conditions (BC)

2.3.1. Tracer boundary conditions

In TOP, different types of boundary conditions can be specified 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 (see also Sec. 6.2 of NEMO manual). Through the same facility one can apply coastal inputs/loads (coastal boundary conditions) and to specify the treatment of lateral open boundary conditions. For the latter, the spatial interpolation functionality should not be activated.

The entire set of boundary conditions is activated with the paramter ln_trcbc = .true. in namtrc_cfg (more details in Model Setup section).

Surface and lateral boundaries

The namelist &namtrc_bc is in file namelist_top_cfg and allows to specify the name of the files, the frequency of the input and the time and space interpolation as done for any other field using the fld_read interface.

```
! data for boundary conditions
&namtrc bc
  cn\_dir\_sbc
                            root directory for the location of SURFACE data files
                            root directory for the location of COASTAL data files
  cn\_dir\_cbc
  cn\_dir\_obc
                            root directory for the location of OPEN data files
                        ! Remove runoff dilution on tracers with absent river load
  ln rnf ctl
               = .false.
                = 86400.
                              Time scaling factor for SBC data (seconds in a day)
  rn sbc time
                            ! Time scaling factor for CBC data (seconds in a day)
                 = 86400.
  rn cbc time
```

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Lateral open boundaries

The BDY for passive tracer are set together with the physical oceanic variables (ln?bdy =.true.). Boundary conditions are set in the structure used to define the passive tracer properties in the « obc » column. These boundary conditions are applied on the segments defined for the physical system, as described in the BDY section of NEMO manual.

- cn_trc_dflt : the type of OBC applied to all the tracers
- $\bullet\,$ cn_trc : the boundary condition used for tracers with data file

2.3.2. Sea-ice interface

Sea-ice growth and melt effect

NEMO provides three options for the specification of tracer concentrations in sea ice: (-1) identical tracer concentrations in sea ice and ocean, which corresponds to no concentration/dilution effect upon ice growth and melt; (0) zero concentrations in sea ice, which gives the largest concentration-dilution effect upon ice growth and melt; (1) specified concentrations in sea ice, which gives a possibly more realistic effect of sea ice on tracers. Option (-1) and (0) work for all tracers, but (1) is currently only available for PISCES.

Antarctic Ice Sheet tracer supply

The external input of biogeochemical tracers from the Antarctic Ice Sheet (AIS) is represented by associating a tracer content with the freshwater flux from icebergs and ice shelves (Person et al., 2019). This supply is currently implemented only for dissolved Fe (figure 2.1) and is effective in model configurations with south-extended grids (e.g., eORCA1 and eORCA025). As the ORCA2 grid does not extend south into Antarctica, the external source of tracers from the AIS cannot be enabled in this configuration.

For icebergs, a homogeneous distribution of biogeochemical tracers is applied from the surface to a depth that can be defined in &namtrc_ais, with a default values of 120 m. It should be noted that the freshwater flux from icebergs affects only the ocean properties at the surface. For ice shelves, biogeochemical tracers follow the explicit or parameterized representation of freshwater flux distribution modeled by the NEMO physical core. The AIS tracer supply is activated by setting ln_tracis to true in the &namtra section.

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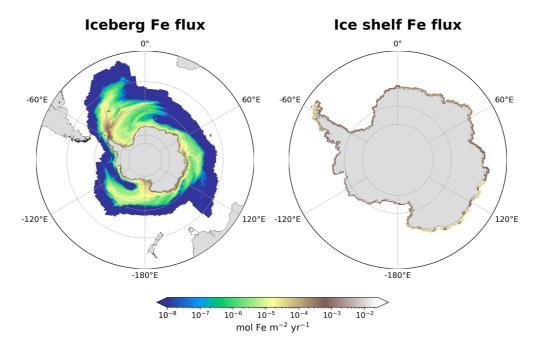


Figure 2.1.: Annual Fe fluxes from icebergs and ice shelves in the Southern Ocean.

2.3.3. Light vertical attenuation

A dedicated module (troopt) allows to compute form the sea surface solar radiation the amount of light that penetrate into the ocean interior depending on the chlorophyll field. The visible part of solar radiation is used to derive the photosynthetic available radiation (PAR) using a simplified version of the model by Morel (1988), as described in Lengaigne et al. (2007).

In a nutshell, visible light is split into three wavebands (blue: 400–500 nm, green: 500–600 nm, red: 600–700 nm) and for each one the chlorophyll-dependent attenuation coefficients are fitted to the coefficients computed from the full spectral model of Morel (1988) (as modified in Morel and Maritorena (2001)) assuming the same power-law expression.

The available light is then converted to PAR using a time-space constant value (parlux) or by prescribing a spatially variable distribution of the fraction of the downwelling shortwave radiation (sn_par), as specified with the logical parameter ln_varpar.

The light_loc parameter allows to select the way that light is computed within the gridcell volume, namely as the mean value at the cell center ('center') or integrated within the cell ('integral').

```
! light availability in the water column
&namtrc opt
              file name
                             ! frequency (hours) ! variable ! time interp. ! clim ! 'yearly' / ! weights ! rotation ! land/sea mask !
                            (if <0 months) ! name ! (logical) ! (T/F)! monthly ! filename! pairing! filename
                                    24
                                                  'fr_par'
                                                             .true.
                                                                       , .true. , 'yearly' , '
  cn_dir
                          ! root directory for the location of the dynamical files
  ln varpar
               =
                   .true.
                            ! Read PAR from file
  parlux
              = 0.43
                           ! Fraction of shortwave as PAR
  light_loc
                           ! Light location in the water cell ('center', 'integral')
              = 'center
```

2.4. "Source minus Sinks" modules (SMS)

2.4.1. Ideal Age

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An 'ideal age' tracer is integrated online in TOP when ln_age = .true. in namelist namtrc. This tracer marks the duration in units of years that fluid has spent in the interior of the ocean, insulated from exposure to the atmosphere (figure 2.2 and figure 2.3).

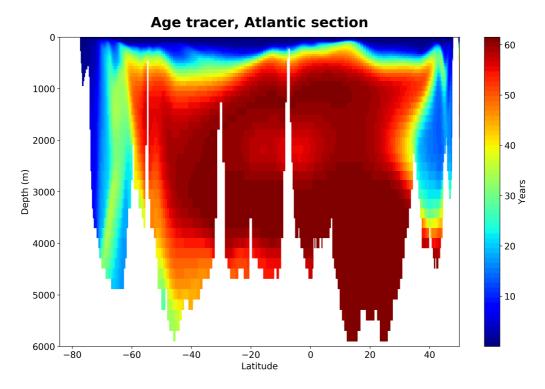


Figure 2.2.: Vertical distribution of the Age tracer in the Atlantic Ocean at 35°W from a 62-year simulation.

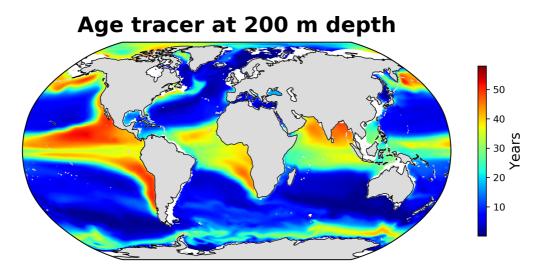


Figure 2.3.: Age tracer at 200 m depth from a 62-year simulation.

Thus, away from the surface for $z < -H_{Age}$ where H_{Age} is specified by the namage namelist variable rn_age_depth, whose default value is 10 m, there is a source SMS_{Age} of the age tracer A:

$$SMS_{Age} = 1yr^{-1} = 1/T_{year},$$
 (2.3)

where the length of the current year $T_{\rm year} = 86400 * N_{\rm days\ in\ current\ year}$ s, where $N_{\rm days\ in\ current\ year}$ may be 366 or 365 depending on whether the current year is a leap year or not. Near the surface, for $z > -H_{\rm Age}$, ideal age is relaxed back to zero:

$$SMS_{Age} = -\lambda_{Age}A, \qquad (2.4)$$

where the relaxation rate λ_{Age} (units s⁻¹) is specified by the namage namelist variable rn_age_kill_rate and has a default value of 1/7200 s. Since this relaxation is applied explicitly, the relaxation rate should in principle

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not exceed $1/\Delta t$, where Δt is the time step used to step forward passive tracers (2 * nn_dttrc * rn_rdt when the default leapfrog time-stepping scheme is employed).

Currently the 1-dimensional reference depth of the grid boxes is used rather than the dynamically evolving depth to determine whether the age tracer is incremented or relaxed to zero. This means that the age tracer module only works correctly in z-coordinates. To ensure that the forcing is independent from the level thicknesses, where the tracer cell at level k has its upper face z = -depw(k) above the depth $-H_{Age}$, but its lower face z = -depw(k+1) below that depth, then the age source is computed as:

$$SMS_{Age} = -f_{kill}\lambda_{Age}A + f_{add}/T_{vear}, \qquad (2.5)$$

where

$$f_{\text{kill}} = e3t_k^{-1}(H_{\text{Age}} - depw(k)),$$
 (2.6)

$$f_{\text{add}} = 1 - f_{\text{kill}}. (2.7)$$

This implementation was first used in the CORE-II intercomparison runs described in Danabasoglu et al. (2014).

2.4.2. Inert carbons tracer

Chlorofluorocarbons 11 and 12 (CFC-11 and CFC-12) and sulfur hexafluoride (SF6) are synthetic chemicals manufactured for industrial and domestic applications from the early 20th century onwards. CFC-11 (CCl₃F) is a volatile liquid at room temperature, and was widely used in refrigeration. CFC-12 (CCl₂F₂) is a gas at room temperature, and, like CFC-11, was widely used as a refrigerant, and additionally as an aerosol propellant. SF6 (SF_6) is also a gas at room temperature, with a range of applications based around its property as an excellent electrical insulator (often replacing more toxic alternatives). All three gases are relatively inert chemicals that are both non-toxic and non-flammable, and their wide use has led to their accumulation in the atmosphere. Large-scale production of CFC-11 and CFC-12 began in the 1930s, while production of SF6 began in the 1950s, and the time-histories of their atmospheric concentrations are shown in Figure 1.4. As can be seen in the figure, while the concentration of SF6 continues to rise to the present day, concentrations of both CFC-11 and CFC-12 have levelled off and declined since around the 1990s. These declines have been driven by the Montreal Protocol (effective since August 1989), which has banned the production of CFC-11 and CFC-12 (as well as other CFCs) because of their role in the depletion of stratospheric ozone (O_3) , critical in decreasing the flux of ultraviolet radiation to the Earth's surface. All three chemicals are also significantly more potent greenhouse gases than CO₂ (especially SF6), although their relatively low atmospheric concentrations limit their role in climate change.

The ocean is a notable sink for all three gases, and their relatively recent occurrence in the atmosphere, coupled to the ease of making high precision measurements of their dissolved concentrations, has made them valuable in oceanography. Because they only enter the ocean via surface air-sea exchange, and are almost completely chemically and biologically inert, their distribution within the ocean interior reveals ventilation of the latter via transport and mixing. Measuring the dissolved concentrations of these gases – as well as the mixing ratios between them – shows circulation pathways within the ocean as well as water mass ages (i.e. the time since has been last in contact with the atmosphere). This feature has made them valuable across a wide range of oceanographic problems. In ocean modelling, they can be used to evaluate the realism of the simulated circulation and ventilation patterns, which is key for understanding the behaviour of modelled marine biogeochemistry (e.g. (Dutay et al., 2002; Palmiéri et al., 2015)).

Modelling these gases (henceforth CFCs) in NEMO is done within the passive tracer transport module, TOP, using the conservation state equation equation 2.1

Advection and diffusion of the CFCs in NEMO are calculated by the physical module, TRP, whereas sources and sinks are done by the CFC module within TOP. The only source of CFCs to the ocean is via air-sea gas

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exchange at its surface, and since CFCs are generally stable within the ocean, we assume that there are no sinks (i.e. no loss processes) within the ocean interior. Consequently, the sinks-minus-sources term for CFCs consists only of their air-sea fluxes, F_{cfc} , as described in the Ocean Model Inter-comparison Project (OMIP) protocol (Orr et al., 2017):

$$F_{cfc} = K_w \cdot (C_{sat} - C_{surf}) \cdot (1 - f_i) \tag{2.8}$$

Where K_w is the piston velocity (in m s⁻¹), as defined in Equation equation 2.10; C_{sat} is the saturation concentration of the CFC tracer, as defined in Equation equation 2.9; C_{surf} is the local surface concentration of the CFC tracer within the model (in mol m⁻³); and f_i is the fractional sea-ice cover of the local ocean (ranging between 0.0 for ice-free ocean, to 1.0 for completely ice-covered ocean with no air-sea exchange).

The saturation concentration of the CFC, C_{sat} , is calculated as follows:

$$C_{sat} = Sol \cdot P_{cfc} \tag{2.9}$$

Where Sol is the gas solubility in mol m⁻³ pptv⁻¹, as defined in Equation equation 2.12; and P_{cfc} is the atmosphere concentration of the CFC (in parts per trillion by volume, pptv). This latter concentration is provided to the model by the historical time-series of Bullister (2017). This includes bulk atmospheric concentrations of the CFCs for both hemispheres – this is necessary because of the geographical asymmetry in the production and release of CFCs to the atmosphere. Within the model, hemispheric concentrations are uniform, with the exception of the region between 10°N and 10° in which they are linearly interpolated.

The piston velocity K_w is a function of 10 m wind speed (in m s⁻¹) and sea surface temperature, T (in °C), and is calculated here following Wanninkhof (1992):

$$K_w = X_{conv} \cdot a \cdot u^2 \cdot \sqrt{\frac{Sc(T)}{660}}$$
(2.10)

Where $X_{conv} = \frac{0.01}{3600}$, a conversion factor that changes the piston velocity from cm h⁻¹ to m s⁻¹; a is a constant re-estimated by Wanninkhof (2014) to 0.251 (in $\frac{cm\ h^{-1}}{(m\ s^{-1})^2}$); and u is the 10 m wind speed in m s⁻¹ from either an atmosphere model or reanalysis atmospheric forcing. Sc is the Schmidt number, and is calculated as follow, using coefficients from Wanninkhof (2014) (see Table table 2.2).

$$Sc = a0 + (a1 \cdot T) + (a2 \cdot T^2) + (a3 \cdot T^3) + (a4 \cdot T^4)$$
(2.11)

The solubility, Sol, used in Equation equation 2.9 is calculated in mol l^{-1} atm⁻¹, and is specific for each gas. It has been experimentally estimated by Warner and Weiss (1985) as a function of temperature and salinity:

$$\ln(Sol) = a_1 + \frac{a_2}{T_X} + a_3 \cdot \ln T_X + a_4 \cdot T_X^2 + S \cdot (b_1 + b_2 \cdot T_X + b_3 \cdot T_X^2)$$
(2.12)

Where T_X is $\frac{T+273.16}{100}$, a function of temperature; and the a_x and b_x coefficients are specific for each gas (see Table table 2.1). This is then converted to mol m⁻³ pptv⁻¹ assuming a constant atmospheric surface pressure of 1 atm. The solubility of CFCs thus decreases with rising T while being relatively insensitive to salinity changes. Consequently, this translates to a pattern of solubility where it is greatest in cold, polar regions (see Figure figure 2.5).

The standard outputs of the CFC module are seawater CFC concentrations (in mol m⁻³), the net air-sea flux (in mol m⁻² d⁻¹) and the cumulative net air-sea flux (in mol m⁻²). Using XIOS, it is possible to obtain outputs such as the vertical integral of CFC concentrations (in mol m⁻²; see Figure figure 2.6). This property, when divided by the surface CFC concentration, estimates the local penetration depth (in m) of the CFC.

Notes

In comparison to the OMIP protocol, the CFC module in NEMO has several differences:

For instance, C_{sat} is calculated for a fixed surface pressure of 1atm. This may be corrected in a future version of the module.

2.4.3. Radiocarbon

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Table 2.1.: Coefficients for fit of the CFCs solubility (Eq. equation 2.12).

Gas	a1	a2	a3	a4	b1	b2	b3
CFC-11	-218.0971	298.9702	113.8049	-1.39165	-0.143566	0.091015	-0.0153924
CFC-12	-229.9261	319.6552	119.4471	-1.39165	-0.142382	0.091459	-0.0157274
SF6	-80.0343	117.232	29.5817	0.0	0.0335183	-0.0373942	0.00774862

Table 2.2.: Coefficients for fit of the CFCs Schmidt number (Eq. equation 2.11).

Gas	a0	a1	a2	a3	a4
CFC-11	3579.2	-222.63	7.5749	-0.14595	0.0011874
CFC-12	3828.1	-249.86	8.7603	-0.1716	0.001408
SF6	3177.5	-200.57	6.8865	-0.13335	0.0010877

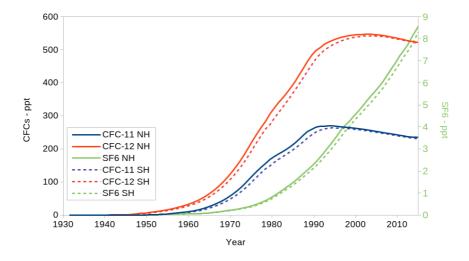


Figure 2.4.: Atmospheric CFC11, CFC12 and SF6 partial pressure evolution in both hemispheres.

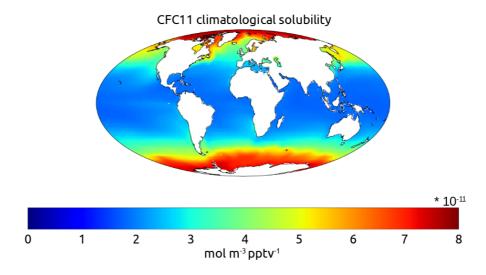


Figure 2.5.: CFC11 solubility in mol m^{-3} ppt v^{-1} , calculated from the World Ocean Atlas 2013 temperature and salinity annual climatology.

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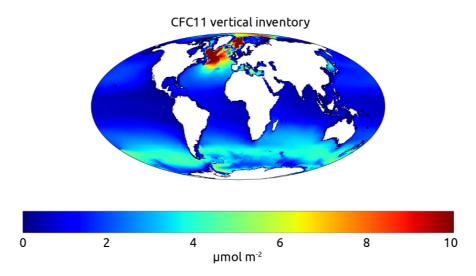


Figure 2.6.: CFC11 vertical inventory in μ mol m⁻², from one of the UK Earth System Model 1 model (UKESM1 - which uses NEMO as ocean component, with TOP for the passive tracers) historical run at year 2000.

The C14 package has been implemented in NEMO by Anne Mouchet Δ^{14} C. It offers several possibilities: Δ^{14} C as a physical tracer of the ocean ventilation (natural 14 C), assessment of bomb radiocarbon uptake, as well as transient studies of paleo-historical ocean radiocarbon distributions.

Method

Let 14 R represent the ratio of 14 C atoms to the total number of carbon atoms in the sample, i.e. 14 C/C. Then, radiocarbon anomalies are reported as:

$$\Delta^{14}C = \left(\frac{^{14}R}{^{14}R_{ref}} - 1\right)10^3, \tag{2.13}$$

where $^{14}R_{ref}$ is a reference ratio. For the purpose of ocean ventilation studies, $^{14}R_{ref}$ is set to one.

Here we adopt the approach of Fiadeiro (1982) and Toggweiler et al. (1989a,b) in which the ratio 14 R is transported rather than the individual concentrations C and 14 C. This approach calls for a strong assumption, i.e., that of a homogeneous and constant dissolved inorganic carbon (DIC) field (Toggweiler et al., 1989a; Mouchet, 2013). While in terms of oceanic Δ^{14} C, it yields similar results to approaches involving carbonate chemistry, it underestimates the bomb radiocarbon inventory because it assumes a constant air-sea CO₂ disequilibrium (Mouchet, 2013). Yet, field reconstructions of the ocean bomb 14 C inventory are also biased low (Naegler, 2009) since they assume that the anthropogenic perturbation did not affect ocean DIC since the pre-bomb

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epoch. For these reasons, bomb 14 C inventories obtained with the present method are directly comparable to reconstructions based on field measurements.

This simplified approach also neglects the effects of fractionation (e.g., air-sea exchange) and of biological processes. Previous studies by Bacastow and Maier-Reimer (1990) and Joos et al. (1997) resulted in nearly identical Δ^{14} C distributions among experiments considering biology or not. Since observed ¹⁴R ratios are corrected for the isotopic fractionation when converted to the standard Δ^{14} C notation (Stuiver and Polach, 1977) the model results are directly comparable to observations.

Therefore the simplified approach is justified for the purpose of assessing the circulation and ventilation of OGCMs.

The equation governing the transport of $^{14}\mathrm{R}$ in the ocean is

$$\frac{\partial}{\partial t}^{14} \mathbf{R} = - \nabla \cdot (\mathbf{u}^{14} \mathbf{R} - \mathbf{K} \cdot \nabla^{14} \mathbf{R}) - \lambda^{14} \mathbf{R}, \tag{2.14}$$

where λ is the radiocarbon decay rate, u the 3-D velocity field, and K the diffusivity tensor.

At the air-sea interface a Robin boundary condition (Haine, 2006) is applied to equation 2.14, i.e., the flux through the interface is proportional to the difference in the ratios between the ocean and the atmosphere

$$\mathcal{F} = \kappa_R(^{14}R - ^{14}R_a), \tag{2.15}$$

where \mathcal{F} is the flux out of the ocean, and 14 R_a is the atmospheric 14 C/C ratio. The transfer velocity κ_R for the radiocarbon ratio in equation 2.15 is computed as

$$\kappa_R = \frac{\kappa_{\text{CO}_2} K_0}{\overline{\text{C}_{\text{T}}}} \, \text{p}_{\text{CO}_2}^{\text{a}} \tag{2.16}$$

with κ_{CO_2} the carbon dioxide transfer or piston velocity, K_0 the CO₂ solubility in seawater, $p_{\text{CO}_2}^{\text{a}}$ the atmospheric CO₂ pressure at sea level, and $\overline{\text{C}_{\text{T}}}$ the average sea-surface dissolved inorganic carbon concentration.

The CO₂ transfer velocity is based on the empirical formulation of Wanninkhof (1992) with chemical enhancement (Wanninkhof and Knox, 1996; Wanninkhof, 2014). The original formulation is modified to account for the reduction of the air-sea exchange rate in the presence of sea ice. Hence

$$\kappa_{\text{CO}_2} = (K_W \,\text{w}^2 + b) \,(1 - f_{\text{ice}}) \,\sqrt{660/Sc},$$
(2.17)

with w the wind magnitude, f_{ice} the fractional ice cover, and Sc the Schmidt number. K_W in equation 2.17 is an empirical coefficient with dimension of an inverse velocity. The chemical enhancement term b is represented as a function of temperature T (Wanninkhof, 1992)

$$b = 2.5(0.5246 + 0.016256T + 0.00049946 * T^{2}). (2.18)$$

Model setup

To activate the C14 package, set the parameter ln_c14 = .true. in namelist namtrc.

Parameters and formulations The radiocarbon decay rate (rlam14; in trcnam_c14 module) is set to $\lambda = (1/8267) \text{ yr}^{-1}$ (Stuiver and Polach, 1977), which corresponds to a half-life of 5730 yr.

The Schmidt number Sc, Eq. equation 2.17, is calculated using the formulation of Wanninkhof (2014). The CO_2 solubility K_0 in equation 2.16 is taken from Weiss (1974). K_0 and Sc are computed with the OGCM temperature and salinity fields (trcsms_c14 module).

The following parameters intervening in the air-sea exchange rate are set in namelist c14:

- The reference DIC concentration $\overline{C_T}$ (xdicsur) intervening in equation 2.16 is classically set to 2 mol m⁻³ (Toggweiler et al., 1989a; Orr et al., 2001; BUTZIN et al., 2005).
- The value of the empirical coefficient K_W (xkwind) in equation 2.17 depends on the wind field and on the model upper ocean mixing rate (Toggweiler et al., 1989a; Wanninkhof, 1992; Naegler, 2009; Wanninkhof, 2014). It should be adjusted so that the globally averaged CO₂ piston velocity is $\kappa_{\text{CO}_2} = 16.5 \pm 3.2$ cm/h (Naegler, 2009).
- Chemical enhancement (term b in Eq. equation 2.18) may be set on/off by means of the logical variable ln_chemh.

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Experiment type The type of experiment is determined by the value given to kc14typ in namelist_c14. There are three possibilities:

1. natural Δ^{14} C: kc14typ=0

2. bomb Δ^{14} C: kc14typ=1

3. transient paleo-historical Δ^{14} C: kc14typ=2

Natural or Equilibrium radiocarbon kc14typ=0

Unless otherwise specified in namelist_c14, the atmospheric $^{14}R_a$ (rc14at) is set to one, the atmospheric CO_2 (pco2at) to 280 ppm, and the ocean ^{14}R is initialized with rc14init=0.85, i.e., $\Delta^{14}C$ =-150%(typical for deep-ocean, Fig 6 in Key et al., 2004).

Equilibrium experiment should last until 98% of the ocean volume exhibit a drift of less than 0.001‰/year (Orr et al., 2000); this is usually achieved after few kyr (Fig. figure 2.7).

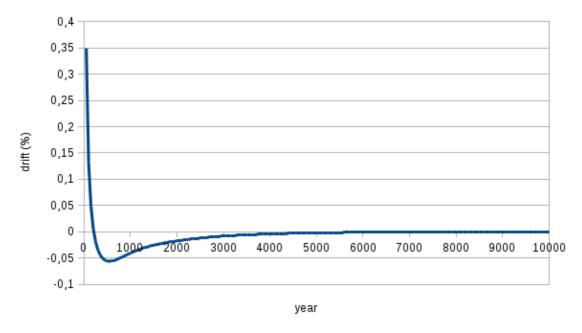


Figure 2.7.: Time evolution of 14 R inventory anomaly for equilibrium run with homogeneous ocean initial state. The anomaly (or drift) is given in % change in total ocean inventory per 50 years. Time on x-axis is in simulation year.

Transient: Bomb kc14typ=1

Performing this type of experiment requires that a pre-industrial equilibrium run has been performed beforehand (ln_rsttr should be set to .TRUE.).

An exception to this rule is when performing a perturbation bomb experiment as was possible with the package C14b. It is still possible to easily set-up that type of transient experiment for which no previous run is needed. In addition to the instructions given in this section, it is however necessary to adapt the atmc14.dat file so that it does no longer contain any negative Δ^{14} C values (Suess effect in the pre-bomb period).

The model is integrated from a given initial date following the observed records provided from 1765 AD on (Fig. figure 2.8). The file atmc14.dat (G Enting et al., 1994, & I. Levin, personal comm.) provides atmospheric Δ^{14} C for three latitudinal bands: 90S-20S, 20S-20N & 20N-90N. Atmospheric CO₂ in the file splco2.dat is obtained from a spline fit through ice core data and direct atmospheric measurements (Orr et al., 2000, & J. Orr, personal comm.). Dates in these forcing files are expressed as yr AD.

To ensure that the atmospheric forcing is applied properly as well as that output files contain consistent dates and inventories, the experiment should be set up carefully:

- Specify the starting date of the experiment: nn_date0 in namelist. nn_date0 is written as Year0101 where Year may take any positive value (AD).
- Then the parameters nn_rstctl in namelist (on-line) and nn_rsttr in namelist_top (off-line) must be set to 0 at the start of the experiment (force the date to nn_date0 for the first experiment year).
- These two parameters (nn_rstctl and nn_rsttr) have then to be set to 2 for the following years (the date must be read in the restart file).

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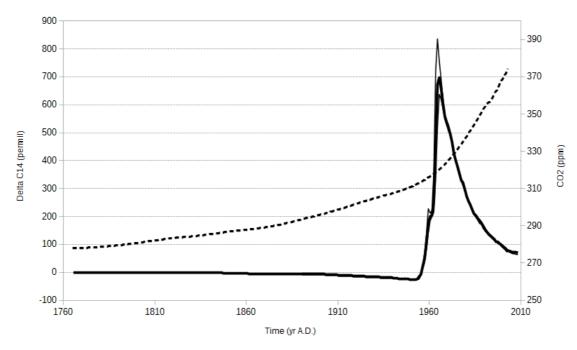


Figure 2.8.: Atmospheric $\Delta^{14}C$ (solid; left axis) and CO₂ (dashed; right axis) forcing for the ^{14}C -bomb experiments. The $\Delta^{14}C$ is illustrated for the three zonal bands (upper, middle, and lower curves correspond to latitudes > 20N, \in [20S, 20N], and < 20S, respectively.

If the experiment date is outside the data time span, the first or last atmospheric concentrations are then prescribed depending on whether the date is earlier or later. Note that tyrc14_beg (namelist_c14) is not used in this context.

Transient: Past kc14typ=2

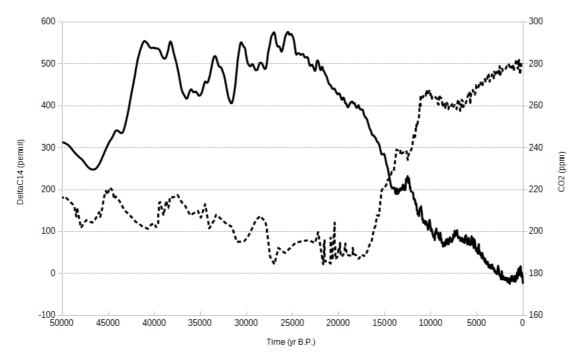


Figure 2.9.: Atmospheric Δ^{14} C (solid) and CO₂ (dashed) forcing for the Paleo experiments. The CO₂ scale is given on the right axis.

This experiment type does not need a previous equilibrium run. It should start 5–6 kyr earlier than the period to be analyzed. Atmospheric $^{14}R_a$ and CO_2 are prescribed from forcing files. The ocean ^{14}R is initialized with the value attributed to rc14init in namelist_c14.

The file intcal13.14c (Reimer et al., 2013) contains atmospheric Δ^{14} C from 0 to 50 kyr cal BP*. The CO₂

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^{*}cal BP: number of years before 1950 AD

forcing is provided in file ByrdEdcCO2.txt. The content of this file is based on the high resolution record from EPICA Dome C (Monnin et al., 2004) for the Holocene and the Transition, and on Byrd Ice Core CO2 Data for 20–90 kyr BP (Ahn and Brook, 2008). These atmospheric values are reproduced in Fig. figure 2.9. Dates in these files are expressed as yr BP.

To ensure that the atmospheric forcing is applied properly as well as that output files contain consistent dates and inventories the experiment should be set up carefully. The true experiment starting date is given by tyrc14_beg (in yr BP) in namelist_c14. In consequence, nn_date0 in namelist MUST be set to 00010101.

Then the parameters nn_rstctl in namelist (on-line) and nn_rsttr in namelist_top (off-line) must be set to 0 at the start of the experiment (force the date to nn_date0 for the first experiment year). These two parameters have then to be set to 2 for the following years (read the date in the restart file).

If the experiment date is outside the data time span then the first or last atmospheric concentrations are prescribed depending on whether the date is earlier or later.

Model output All output fields in Table table 2.3 are routinely computed. It depends on the actual settings in iodef.xml whether they are saved or not.

Field	Type	Dim	Units	Description		
RC14	ptrc	3-D	-	Radiocarbon ratio		
DeltaC14	diad	3-D	‰	$\Delta^{14}\mathrm{C}$		
C14Age	diad	3-D	yr	Radiocarbon age		
RAge	diad	2-D	yr	Reservoir age		
qtr_c14	diad	2-D	$\mathrm{m}^{-2}~\mathrm{yr}^{-1}$	Air-to-sea net ¹⁴ R flux		
qint_c14	diad	2-D	m^{-2}	Cumulative air-to-sea ¹⁴ R flux		
AtmCO2	scalar	0-D	ppm	Global atmospheric CO ₂		
AtmC14	scalar	0-D	‰	Global atmospheric $\Delta^{14}C$		
K_CO2	scalar	0-D	${\rm cm}~{\rm h}^{-1}$	Global CO_2 piston velocity $(\overline{\kappa_{CO_2}})$		
K_C14	scalar	0-D	${ m m~yr^{-1}}$	Global ¹⁴ R transfer velocity $(\overline{\kappa_R})$		
C14Inv	scalar	0-D	10^{26} atoms	Ocean radiocarbon inventory		

Table 2.3.: Standard output fields for the C14 package .

The radiocarbon age is computed as $(-1/\lambda) \ln (^{14}R)$, with zero age corresponding to $^{14}R = 1$.

The reservoir age is the age difference between the ocean uppermost layer and the atmosphere. It is usually reported as conventional radiocarbon age; i.e., computed by means of the Libby radiocarbon mean life (8033 yr; Stuiver and Polach, 1977)

$$^{14}\tau_{\rm c} = -8033 \ln\left(1 + \frac{\Delta^{14}C}{10^3}\right),$$
 (2.19)

where $^{14}\tau_{\rm c}$ is expressed in years B.P. Here we do not use that convention and compute reservoir ages with the mean lifetime $1/\lambda$. Conversion from one scale to the other is readily performed. The conventional radiocarbon age is lower than the radiocarbon age by $\simeq 3\%$.

The ocean radiocarbon inventory is computed as

$$N_A^{14} R_{\text{oxa}} \overline{C_T} \left(\int_{\Omega} {}^{14} R d\Omega \right) / 10^{26},$$
 (2.20)

where N_A is the Avogadro's number ($N_A = 6.022 \times 10^{23} \text{ at/mol}$), $^{14}\text{R}_{\text{oxa}}$ is the oxalic acid radiocarbon standard ($^{14}\text{R}_{\text{oxa}} = 1.176 \times 10^{-12}$; Stuiver and Polach, 1977), and Ω is the ocean volume. Bomb ^{14}C inventories are traditionally reported in units of 10^{26} atoms, hence the denominator in equation 2.20.

All transformations from second to year, and inversely, are performed with the help of the physical constant rsiyea the sideral year length expressed in seconds[†].

The global transfer velocities represent time-averaged[‡] global integrals of the transfer rates:

$$\overline{\kappa_{\text{CO}_2}} = \int_{\mathcal{S}} \kappa_{\text{CO}_2} d\mathcal{S} \text{ and } \overline{\kappa_R} = \int_{\mathcal{S}} \kappa_R d\mathcal{S}$$
(2.21)

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[†]The variable (nyear_len) which reports the length in days of the previous/current/future year (see oce_trc.F90) is not a constant. ‡ the actual duration is set in iodef.xml

2.4.4. PISCES biogeochemical model

PISCES is a biogeochemical model that simulates the lower trophic levels of marine ecosystem (phytoplankton, microzooplankton, and mesozooplankton) and the biogeochemical cycles of carbon and of the main nutrients (P, N, Si, and Fe) (figure 2.10 and figure 2.11).

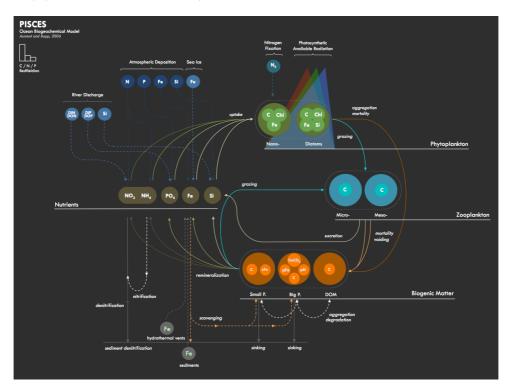


Figure 2.10.: Schematic view of the PISCES-v2 model (figure by Jorge Martinez-Rey).

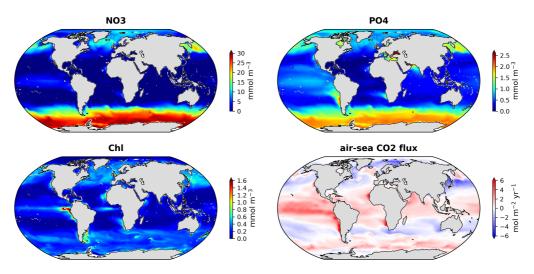


Figure 2.11.: Surface concentrations of NO₃, PO₄, total chlorophyll, and air-sea CO₂ flux from the last year of a 62-year simulation.

The model is intended to be used for both regional and global configurations at high or low spatial resolutions as well as for short-term (seasonal, interannual) and long-term (climate change, paleoceanography) analyses. Two versions of PISCES are available in NEMO v4.0:

• PISCES-v2, by setting ln_p4z = .true. in namelist_pisces_ref. This version can be seen as one of the many Monod models (Monod, 1958). It assumes a constant Redfield ratio and phytoplankton growth depends on the external concentration in nutrients. There are twenty-four prognostic variables (tracers) including two phytoplankton compartments (diatoms and nanophytoplankton), two zooplankton size-classes (microzooplankton and mesozooplankton) and a description of the carbonate chemistry. Formulations in PISCES-v2 are based on a mixed Monod/Quota formalism: On one hand, stoichiometry of C/N/P is

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fixed and growth rate of phytoplankton is limited by the external availability in N, P, and Si. On the other hand, the iron and silicium quotas are variable and growth rate of phytoplankton is limited by the internal availability in Fe. Various parameterizations can be activated in PISCES-v2, setting for instance the complexity of iron chemistry or the description of particulate organic materials.

• PISCES-QUOTA, by setting ln_p5z = .true. in namelist_pisces_ref. This version has been built on the PISCES-v2 model described in Aumont et al. (2015). PISCES-QUOTA has thirty-nine prognostic compartments. Phytoplankton growth is controlled by five modeled limiting nutrients: Nitrate and Ammonium, Phosphate, Silicate, and Iron. Five living compartments are represented: Three phytoplankton size classes/groups corresponding to picophytoplankton, nanophytoplankton, and diatoms, and two zooplankton size classes, which are microzooplankton and mesozooplankton. For phytoplankton, the prognostic variables are the carbon, nitrogen, phosphorus, iron, chlorophyll and silicon biomasses (the latter only for diatoms). This means that the N/C, P/C, Fe/C, and Chl/C ratios of the three phytoplankton groups as well as the Si/C ratio of diatoms are prognostically predicted by the model. Zooplankton are assumed to be strictly homeostatic (e.g., Sterner and Elser, 2003; Woods and Wilson, 2013; Meunier et al., 2014). As a consequence, the C/N/P/Fe ratios of these groups are maintained constant and are not allowed to vary. In PISCES, the Redfield ratios C/N/P are set to 122/16/1 (Takahashi et al., 1985) and the -O/C ratio is set to 1.34 (Körtzinger et al., 2001). No silicified zooplankton is assumed. The bacterial pool is not yet explicitly modeled.

There are three non-living compartments: Semi-labile dissolved organic matter, small sinking particles, and large sinking particles. As a consequence of the variable stoichiometric ratios of phytoplankton and of the stoichiometric regulation of zooplankton, elemental ratios in organic matter cannot be supposed constant anymore as that was the case in PISCES-v2. Indeed, the nitrogen, phosphorus, iron, silicon, and calcite pools of the particles are now all explicitly modeled. The sinking speed of the particles is not altered by their content in calcite and biogenic silicate ("The ballast effect", (Honjo, 1996; Armstrong et al., 2001)). The latter particles are assumed to sink at the same speed as the large organic matter particles. All the non-living compartments experience aggregation due to turbulence and differential settling as well as Brownian coagulation for DOM.

2.4.5. MY_TRC interface for coupling external BGC models

NEMO-TOP has one built-in biogeochemical model - PISCES - but there are several BGC models - MEDUSA, ERSEM, BFM or ECO3M - which are meant to be used within the NEMO plateform. Therefore it was necessary to provide to the users a framework to easily add their own BGCM model. The generalized interface is pivoted on MY_TRC module that contains template files to build the coupling between NEMO and any external BGC model. Call to MY_TRC is activated by setting ln_my_trc = .true. in namelist namtrc.

The following 6 fortran files are available in MY_TRC with the specific purposes here described.

- \bullet par_my_trc.F90 : This module allows to define additional arrays and public variables to be used within the MY_TRC interface
- trcini_my_trc.F90: Here are initialized user defined namelists and the call to the external BGC model initialization procedures to populate general tracer array (trn and trb). Here are also likely to be defined suport arrays related to system metrics that could be needed by the BGC model.
- trcnam_my_trc.F90: This routine is called at the beginning of trcini_my_trc and should contain the initialization of additional namelists for the BGC model or user-defined code.
- trcsms_my_trc.F90: The routine performs the call to Boundary Conditions and its main purpose is to contain the Source-Minus-Sinks terms due to the biogeochemical processes of the external model. Be aware that lateral boundary conditions are applied in trcnxt routine. IMPORTANT: the routines to compute light penetration along the water column and the tracer vertical sinking should be defined/called in here, as generalized modules are still missing in the code.
- trcice_my_trc.F90: Here it is possible to prescribe the tracers concentrations in sea ice that will be used as boundary conditions when ice formation and melting occurs (nn_ice_tr =1 in namtrc_ice). See e.g. the correspondent PISCES subroutine.
- trcwri_my_trc.F90: This routine performs the output of the model tracers using IOM module (see NEMO manual Chapter on Output and Diagnostics). It is possible to place here the output of additional variables produced by the model, if not done elsewhere in the code, using the call to iom put.

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The usage of TOP is activated i) by including in the configuration definition the component TOP and ii) by adding the macro key_top in the configuration CPP file (see for more details "Learn more about the model"). As an example, the user can refer to already available configurations in the code, ORCA2_ICE_PISCES being the NEMO biogeochemical demonstrator and GYRE_BFM to see the required configuration elements to couple with an external biogeochemical model (see also Section 4).

Note that, since version 4.0, TOP interface core functionalities are activated by means of logical keys and all submodules preprocessing macros from previous versions were removed.

Below is the list of preprocessing keys that apply to the TOP interface (beside key_top):

- key_xios use XIOS I/O
- key_agrif enables AGRIF coupling
- key_trdtrc and key_trdmxl_trc trend computation for tracers

There are only two entry points in the NEMOGCM model for passive tracers:

- initialization (trcini): general initialization of global variables and parameters of BGCM
- time-stepping (trcstp): time-evolution of SMS first, then time evolution of tracers by transport

3.1. Setting up a passive tracer configuration

```
&namtrc
                ! tracers definition
  jp_bgc
               = 0
                             ! Number of passive tracers of the BGC model
                             ! Run PISCES BGC model
  ln\_pisces
               = .false.
                = .false.
                              ! Run MY_TRC BGC model
  ln\_my\_trc
                            ! Run the sea water age tracer
               = .false.
                               Run the CFC11 passive tracer
  ln_cfc11
               = .false.
                             ! Run the CFC12 passive tracer
  ln cfc12
               = .false.
                            ! Run the SF6 passive tracer
  ln sf6
               = .false.
                            ! Run the Radiocarbon passive tracer
  ln_c14
               = .false.
                = .false. ! Initialisation from data input file (T) or not (F)
  ln trcdta
  ln trcdmp
                = .false. ! add a damping termn (T) or not (F)
  In_trcdmp_clo = .false. ! damping term (T) or not (F) on closed seas In_trcbc = .false. ! Surface, Lateral or Open Boundaries conditions
  ln\_trcais
               = .false. ! Antarctic Ice Sheet nutrient supply
  jp_dia3d
                           ! Number of 3D diagnostic variables
  jp\_dia2d
                = 0
                           ! Number of 2D diagnostic variables
                name!
                                  title of the field
                                                           ! units
                                                                      ! init from file !
 sn_tracer(1) = 'tracer ', 'Tracer Concentration
                                                                           , .false.
```

As a reminder, the revisited structure of TOP interface now counts for five different modules handled in namelist_top :

- PISCES, default BGC model
- MY_TRC, template for creation of new modules couplings (see section 3.2) or user defined passive tracer dynamics
- CFC, inert tracers dynamics (CFC₁₁,CFC₁₂,SF₆) updated based on OMIP-BGC guidelines (Orr et al, 2016)
- C14, radiocarbon passive tracer
- AGE, water age tracking

For inert, C14, and Age tracers, all variables settings (sn_tracer definitions) are hard-coded in trc_nam_* routines. For instance, for Age tracer:

```
! Variable setting
ctrcnm (jp_age) = 'Age'
ctrcln (jp_age) = 'Sea water age since surface contact'
ctrcun (jp_age) = 'year'
ln_trc_ini(jp_age) = .false.
ln_trc_cbc(jp_age) = .false.
ln_trc_obc(jp_age) = .false.
ln_trc_obc(jp_age) = .false.
```

The modular approach was also implemented in the definition of the total number of passive tracers (jptra) which is specified by the user in namtrc.

3.2. TOP Tracer Initialization

Two main types of data structure are used within TOP interface to initialize tracer properties and to provide related initial and boundary conditions. In addition to providing name and metadata for tracers, the use of initial and boundary conditions is also defined here (sn_tracer). The data structure is internally initialized by the code with dummy names and all initialization/forcing logical fields are set to false. Below are listed some features/options of the TOP interface accessible through the namelist_top_ref and modifiable by means of namelist_top_efg (as for NEMO physical ones).

There are three options to initialize TOP tracers in the namelist_top_file: (1) initialization to hard-coded constant values when ln_trcdta at false, (2) initialization from files when ln_trcdta at true, and (3) initialisation from restart files by setting ln_rsttr to true in namelist.

In the following, an example of the full structure definition is given for four tracers (DIC, Fe, NO₃, PHY) with initial conditions and different surface boundary and coastal forcings for DIC, Fe, and NO₃:

```
! tracers definition
&namtrc
  jp_bgc
                = 24
  ln\_pisces
                = .true.
                     .false.
  ln_my_trc
                = .false.
  ln_age
  ln\_cfc11
                = .false.
  ln_cfc12
                   .false.
  \ln_c14
                   .false.
  ln trcdta
                = .true. ! Initialisation from data input file (T) or not (F)
  ln trcdmp
                 = .false. ! add a damping termn (T) or not (F)
  ln_trcdmp_clo = .false. ! damping term (T) or not (F) on closed seas
                = .true. ! Surface, Lateral or Open Boundaries conditions
  ln trcbc
  \ln\_{\rm trcais}
                  .true.
                          ! Antarctic Ice Sheet nutrient supply
                                                                                                  ! obc
                                   title of the field
                                                              ! units
                                                                          ! init
                                                                                  ! sbc ! cbc
                 name
  sn\_tracer(1)
                 = 'DIC
                                'Dissolved inorganic Concentration
                                                                            'mol-C/L', .true., .false., .true., .false., .false.
                                                                          'mol-C/L', .true. , .true. , .true. , .false. , .true. 'mol-C/L', .true. , .true. , .true. , .false. , .false.
                 = \, {}^{\scriptscriptstyle |}\mathrm{Fer}
                            , 'Dissolved Iron Concentration
  sn tracer(2)
                 = 'NO3
                               , 'Nitrates Concentration
                                                                            sn_tracer(3)
  sn_tracer(4)
                 = 'PHY
                                 'Nanophytoplankton Concentration
```

You have to activate which tracers (sn_tracer) you want to initialize by setting them to true in the column.

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```
&namtrc dta
                   ! Initialisation from data input file
                                  ! frequency (hours) ! variable ! time interp. ! clim ! 'yearly',
               file name
                                                                   (logical) ! (T/F) ! 'monthly' !
                                ! (if <0 months)! name!
                                                                 'PiDIC' , .false. , .true. , 'yearly' 
'Fer' , .true. , .true. , 'yearly'
  sn trcdta(1) = 'data DIC nomask.nc',
                                                    -12
  sn_trcdta(2) = 'data_FER_nomask.nc',
  sn_trcdta(3) = 'data_NO3_nomask.nc',
                                                                 'NO3'
  rn\_trfac(1) =
                    1.028e-06! multiplicative factor
                =
                    1.0e-06
  rn trfac(2)
                     7.6e-06
  \operatorname{rn} \operatorname{trfac}(3) =
```

In namtrc_dta, you prescribe from which files the tracer are initialized (sn_trcdta). A multiplicative factor can also be set for each tracer (rn_trfac).

3.3. TOP Boundaries Conditions

3.3.1. Surface and lateral boundaries

Lateral and surface boundary conditions for passive tracers are prescribed in namtrc_bc as well as whether temporal interpolation of these files is enabled. Here we show the cases of Fe and NO_3 from dust and rivers with different output frequencies.

```
&namtrc bc
                   ! data for boundary conditions
                                 ! frequency (hours) ! variable
                                                                     ! time interp. ! clim ! 'yearly' / !
               file name
                                                      name
                                                                      (logical) ! (T/F) ! 'monthly' !
                              ! (if <0 months) !
  sn_trcsbc(2) = 'dust.orca.new' , -1
sn_trcsbc(3) = 'ndeposition.orca', -12
                                                       , 'dustfer'
                                                                       , .true.
                                                                                     , .true. , 'yearly
                                                         , 'ndep'
                                                                        , .false.
                                                                                     , .true. , 'yearly
  rn_{trsfac(2)} = 6.266e-04
                                 ! Multiplicative factor
  rn\_trsfac(3) = 5.4464e\text{-}01 !
                                     , -12
                                                       , 'riverdic'
  sn trccbc(1) = 'river.orca'
                                                                     , .true.
                                                                                   , .true. , 'yearly'
                                    , -12
, -12
                                                       , 'riverdfe'
                                                                     , .true.
  sn trccbc(2) = 'river.orca'
                                                                                   , .true. , 'yearly
  sn trccbc(3) = 'river.orca'
                                                                                   , .true. , 'yearly
                                                       , 'riverdin'
                                                                        .true.
  rn\_trcfac(1) = 1.0! Multiplicative factor
  \operatorname{rn\_trcfac}(2) = 1.0
  rn\_trcfac(3) = 1.0 !
  rn_cbc_time = 3.1536e+7 ! Time scaling factor for CBC data (seconds in a year)
```

3.3.2. Antarctic Ice Sheet tracer supply

As a reminder, the supply of passive tracers from the AIS is currently implemented only for dissolved Fe. The activation of this Fe source is done by setting ln_trcais to true and by adding the Fe tracer (sn_tracer(2) = .true.) in the 'ais' column in &namtrc (see section 2.2).

As the external source of Fe from the AIS is represented by associating a sedimentary Fe content (with a solubility fraction) to the freshwater fluxes of icebergs and ice shelves, these fluxes have to be activated in namelist_cfg. The reading of the freshwater flux file from ice shelves is activated in namisf with the namelist parameter ln_isf set to true.

You have to choose between two options depending whether the cavities under ice shelves are open or not in your grid configuration:

- ln isfcav mlt = .false. (resolved cavities)
- ln_isfpar_mlt = .true. (parameterized distribution for unopened cavities)

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```
spe = fwfisf is read from a forcing field
                                  ! Spe = Iwins is read from a lording field | 12eq = ISOMIP | like: 2 equations formulation (Hunter et al., 2006 for a short description) | 3eq = ISOMIP | like: 3 equations formulation (Asay-Davis et al., 2016 for a short description | ! thickness of the top boundary layer (Losh et al. 2008) | 0 => thickness of the tbl = thickness of the first wet cell
                       = 30.
    rn_htbl
     !* 'spe' and 'oasis' case
                   ! file name ! frequency (hours) ! variable ! time interp.! clim \,! 'yearly'/ !
                                     ! (if <0 months) ! name ! (logical) ! (T/F) ! 'monthly'
    sn_isfcav_fwf = 'isfmlt_cav', -12. , 'fwflisf' , .false. , .true. , 'yearly
                ---- cavities parametrised ---
\label{eq:ln_isfpar_mlt} \begin{split} &\ln\_{isfpar\_mlt} = .true. & ! \ ice \ shelf \ melting \ parametrised \\ &cn\_{isfpar\_mlt} = {}^{!}spe^{!} \ ! \ ice \ shelf \ melting \ parametrisation \ (spe/bg03/oasis) \\ &! \ spe = fwfisf \ is \ read \ from \ a \ forcing \ field \end{split}
  ! ! file name ! frequency (hours) ! variable ! time interp.! clim ! 'yearly' / ! ! (if <0 months) ! name ! (logical) ! (T/F) ! 'monthly' ! sn_isfpar_zmax = 'runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc' , -12
                                                                                                                                                      , 'sodepmax_isf' , .false. , .true. , 'yearly
   sn_isfpar_zmin = 'runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc', -12
!* 'spe' and 'oasis' case
                                                                                                                                                      ,'sodepmin_isf' , .false. , .true. , 'yearly'
         'spe' and 'oasis' case
    \label{eq:sn_isfpar_fwf} sn\_isfpar\_fwf = 'runoff-icb\_DaiTrenberth\_Depoorter\_eORCA1\_JD.nc' \;, \; -12 \qquad , 'sornfisf' \;, \quad .false.
                                                                                                                                                                                         , .true. , 'yearly'
```

Runoff from icebergs is activated by setting ln_rnf_icb to true in the &namsbc_rnf section of namelist_cfg.

```
&namsbc_rnf ! runoffs
                                                                                                                                                                                                                                                                                                          (\ln_{rnf} = T)
           ln\_rnf\_mouth = .false.
                                                                                                                                   ! specific treatment at rivers mouths
                    rn_hrnf = 15.e0 ! depth over which enhanced vertical mixing is used (ln_rnf_mouth=T rn_avt_rnf = 1.e-3 ! value of the additional vertical mixing coef. [m2/s] (ln_rnf_mouth=T) a_rfact = 1.e0 ! multiplicative factor for runoff
                                                                                                                                                                                                                                                                                                                                                                                                             (ln\_rnf\_mouth=T)
           rn rfact
           ln_rnf_icb = .true. ! read iceberg flux
           cn\_dir = './'! root directory for the location of the runoff files
         ! ! (if <0 months) ! name ! (logical) ! (T/F)! 'monthly' ! sn_rnf = 'runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc', -1 sn_cnf = 'runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc', -1 sn_sn_s_rnf = 'runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc', 0 , sn_s_rnf = 'runoffs' , 24. , 'rosaline', true true 'rosaline' , tru
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        , .true. , 'yearly'
                                                                                                                                                                                                                                                                                                                                                                                                                              , 'sorunoff', .true. , .true. , 'yearly' , 'Icb_flux', .true. , .true. , 'yearly' , 'socoefr' , .false. , .true. , 'yearly'
                                                                                                                                      , 24. , 'rosaline', .true. , .true. , 'yearly'
, 24. , 'rotemper', .true. , .true. , 'yearly'
, 0. , 'rodepth' , .false. , .true. , 'yearly'
                                                                    = 'runoffs'
           sn t rnf
           sn_dep_rnf = runoffs
```

The freshwater flux from ice shelves and icebergs is based on observations and modeled climatologies and is available for eORCA1 and eORCA025 grids:

- runoff-icb_DaiTrenberth_Depoorter_eORCA1_JD.nc
- $\bullet \ \ runoff\text{-}icb_DaiTrenberth_Depoorter_eORCA025_JD.nc$

Two options for tracer concentrations in iceberg and ice shelf can be set with the namelist parameter nn_ais_tr:

- 0 : null concentrations corresponding to dilution of BGC tracers due to freshwater fluxes from icebergs and ice shelves
- 1 : prescribed concentrations set with the rn_trafac factor

The depth until which Fe from melting iceberg is delivered can be set with the namelist parameter rn_icbdep. The value of 120 m is the average underwater depth of the different iceberg size classes modeled by the NEMO iceberg module, which was used to produce the freshwater flux climatology of icebergs.

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3.4. Coupling an external BGC model using NEMO framework

The coupling with an external BGC model through the NEMO compilation framework can be achieved in different ways according to the degree of coding complexity of the Biogeochemical model, like e.g., the whole code is made only by one file or it has multiple modules and interfaces spread across several subfolders.

Beside the 6 core files of MY_TRC module, see (see , let's assume an external BGC model named "MYBGC" and constituted by a rather essential coding structure, likely few Fortran files. The new coupled configuration name is NEMO_MYBGC.

The best solution is to have all files (the modified MY_TRC routines and the BGC model ones) placed in a unique folder with root <MYBGCPATH> and to use the makenemo external readdressing of MY_SRC folder.

Before compiling the code it is necessary to create the new configuration folder

```
*[nemo-code-root]> mkdir cfgs/NEMO_MYBGC
```

and add in it the configuration file cpp_MYBGC.fcm whose content will be

```
bld::tool::fppkeys key_xios key_top
```

The compilation with makenemo will be executed through the following syntax, by including OCE and TOP components

```
[nemo-code-root]>./makenemo -r GYRE_PISCES -n NEMO_MYBGC -d "OCE TOP" -m <arch_my_machine> -j <math display="inline">8 -e \hookrightarrow < MYBGCPATH>
```

The makenemo feature -e was introduced to readdress at compilation time the standard MY_SRC folder (usually found in NEMO configurations) with a user defined external one. After the compilation, the coupled configuration will be listed in work cfg.txt and it will look like

```
NEMO_MYBGC OCE TOP
```

The compilation of more articulated BGC model code & infrastructure, like in the case of BFM (Lovato et al., 2020), requires some additional features.

As before, let's assume a coupled configuration name NEMO_MYBGC, but in this case MYBGC model root becomes <MYBGCPATH> that contains 4 different subfolders for biogeochemistry, named initialization, pelagic, and benthic, and a separate one named nemo_coupling including the modified MY_SRC routines. The latter folder containing the modified NEMO coupling interface will be still linked using the makenemo -e option.

In order to include the BGC model subfolders in the compilation of NEMO code, it will be necessary to extend the configuration cpp_NEMO_MYBGC.fcm file to include the specific paths of MYBGC folders, as in the following example

where MYBGC_MACROS is the space delimited list of macros used in MYBGC model for selecting/excluding specific parts of the code. The BGC model code will be preprocessed in the configuration BLD folder as for NEMO, but with an independent path, like NEMO_MYBGC/BLD/MYBGC/<subfolders>.

The compilation of more articulated BGC model code & infrastructure, like in the case of BFM (Lovato et al., 2020), requires some additional features.

As before, let's assume a coupled configuration name NEMO_MYBGC, but in this case MYBGC model root becomes <MYBGCPATH> that contains 4 different subfolders for biogeochemistry, named initialization, pelagic, and benthic, and a separate one named nemo_coupling including the modified MY_SRC routines. The

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latter folder containing the modified NEMO coupling interface will be still linked using the makenemo -e option.

In order to include the BGC model subfolders in the compilation of NEMO code, it will be necessary to extend the configuration cpp_NEMO_MYBGC.fcm file to include the specific paths of MYBGC folders, as in the following example

where MYBGC_MACROS is the space delimited list of macros used in MYBGC model for selecting/excluding specific parts of the code. The BGC model code will be preprocessed in the configuration BLD folder as for NEMO, but with an independent path, like NEMO_MYBGC/BLD/MYBGC/<subfolders>.

The compilation will be performed similarly to in the previous case with the following

```
makenemo -r NEMO_MYBGC -m <arch_my_machine> -j 8 -e <MYBGCPATH>/nemo_coupling
```

Note that, the additional lines specific for the BGC model source and build paths, can be written into a separate file, e.g. named MYBGC.fcm, and then simply included in the cpp_NEMO_MYBGC.fcm as follow:

```
bld::tool::fppkeys key_zdftke key_dynspg_ts key_xios key_top inc <MYBGCPATH>/MYBGC.fcm
```

This will enable a more portable compilation structure for all MYBGC related configurations.

Important: the coupling interface contained in nemo_coupling cannot be added using the FCM syntax, as the same files already exists in NEMO and they are overridden only with the readdressing of MY_SRC contents to avoid compilation conflicts due to duplicate routines.

All modifications illustrated above, can be easily implemented using shell or python scripting to edit the NEMO configuration cpp.fcm file and to create the BGC model specific FCM compilation file with code paths.

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Coding Rules

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A "model life" is more than ten years. Its software, composed of a few hundred modules, is used by many people who are scientists or students and do not necessarily know every aspect of computing very well. Moreover, a well thought-out program is easier to read and understand, less difficult to modify, produces fewer bugs and is easier to maintain. Therefore, it is essential that the model development follows some rules:

- well planned and designed
- well written
- well documented (both on- and off-line)
- maintainable
- · easily portable
- flexible.

To satisfy part of these aims, NEMO is written with a coding standard which is close to the ECMWF rules, named DOCTOR (Gibson, 1986). These rules present some advantages like:

- to provide a well presented program
- to use rules for variable names which allow recognition of their type (integer, real, parameter, local or shared variables, etc.).

This facilitates both the understanding and the debugging of an algorithm.

A.1. Introduction

This document describes conventions used in NEMO coding and suggested for its development. The objectives are to offer a guide to all readers of the NEMO code, and to facilitate the work of all the developers, including the validation of their developments, and eventually the implementation of these developments within the NEMO platform.

A first approach of these rules can be found in the code in ./src/OCE/module_example where all the basics coding conventions are illustrated. More details can be found below.

This work is based on the coding conventions in use for the Community Climate System Model *, the previous version of this document ("FORTRAN coding standard in the OPA System") and the expertise of the NEMO System Team. After a general overview below, this document will describe:

- \bullet The style rules, *i.e.* the syntax, appearance and naming conventions chosen to improve readability of the code;
- The content rules, i.e. the conventions to improve the reliability of the different parts of the code;
- The package rules to go a step further by improving the reliability of the whole and interfaces between routines and modules.

A.2. Overview and general conventions

NEMO has 3 major components: ocean dynamics (./src/OCE), sea-ice (./src/ICE) and marine biogeochemistry (./src/MBG). In each directory, one will find some FORTRAN files and/or subdirectories, one per functionality of the code: ./src/OCE/BDY (boundaries), ./src/OCE/DIA (diagnostics), ./src/OCE/DOM (domain), ./src/OCE/DYN (dynamics), ./src/OCE/LDF (lateral diffusion), etc...

All name are chosen to be as self-explanatory as possible, in English, all prefixes are 3 digits.

English is used for all variables names, comments, and documentation.

Physical units are MKS. The only exception to this is the temperature, which is expressed in degrees Celsius, except in bulk formulae and part of SI³ sea-ice model where it is in Kelvin. See .src/OCE/DOM/phycst.F90 files for conversions.

*UCAR conventions

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A.3. Architecture

Within each directory, organisation of files is driven by orthogonality, *i.e.* one functionality of the code is intended to be in one and only one directory, and one module and all its related routines are in one file. The functional modules are:

- SBC surface module
- IOM management of the I/O
- NST interface to AGRIF (nesting model) for dynamics and biogeochemistry
- OBC, BDY management of structured and unstructured open boundaries
- C1D 1D (vertical) configuration for dynamics, sea-ice and biogeochemistry
- OFF off-line module: passive tracer or biogeochemistry alone
- ...

For example, the file domain.F90 contains the module domain and all the subroutines related to this module (dom_init, dom_nam, dom_ctl).

A.4. Style rules

A.4.1. Argument list format

Routine argument lists will contain a maximum 5 variables per line, whilst continuation lines can be used. This applies both to the calling routine and the dummy argument list in the routine being called. The purpose is to simplify matching up the arguments between caller and callee.

```
SUBROUTINE tra_adv_eiv( kt, pun, pvn, pwn )

CALL tra_adv_eiv( kt, zun, zvn, zwn )
```

A.4.2. Array syntax

Except for long loops (see below), array notation should be used if possible. To improve readability the array shape must be shown in brackets, e.g.:

```
onedarraya(:) = onedarrayb(:) + onedarrayc(:)
twodarray (:,:) = scalar * anothertwodarray(:,:)
```

When accessing sections of arrays, for example in finite difference equations, do so by using the triplet notation on the full array, e.g.:

```
 \begin{array}{lll} twodarray(:,2:len2) = & scalar & \& \\ \& & * (twodarray2(:,1:len2-1) & \& \\ \& & - twodarray2(:,2:len2)) \end{array}
```

For long, complicated loops, explicitly indexed loops should be preferred. In general when using this syntax, the order of the loops indices should reflect the following scheme (for best usage of data locality):

```
DO jk = 1, jpk
DO jj = 1, jpj
DO ji = 1, jpi
DO ji = 1, jpi
threedarray(ji,jj,jk) = ...
END DO
END DO
```

A.4.3. Case

All FORTRAN keywords are in capital: DIMENSION, WRITE, DO, END DO, NAMELIST, ... All other parts of the NEMO code will be written in lower case.

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A.4.4. Comments

Comments in the code are useful when reading the code and changing or developing it.

The full documentation and detailed explanations are to be added in the reference manual (TeX files, aside from the code itself).

In the code, the comments should explain variable content and describe each computational step.

Comments in the header start with "!!". For more details on the content of the headers, see Content rules/Headers in this document.

Comments in the code start with "!".

All comments are indented (3, 6, or 9 blank spaces).

Short comments may be included on the same line as executable code, and an additional line can be used with proper alignment. For example:

```
zx = zx *zzy ! Describe what is going on and if it is
! ! too long use another! for proper
! ! alignment with automatic indentation
```

More in-depth comments should be written in the form:

```
! Check of some namelist values
```

or

```
!
! !<<<<<<<<<<<<<<<<>
! Bottom boundary condition on the
! !<<<<<<<<<<<<<>><<<<>>! !<<<<<>>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! ! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! ! ! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! ! ! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>! !</>
```

Key features of this style are

- 1. it starts with a "!" in the column required for proper indentation,
- 2. the text is offset above and below by a blank line or a content line built for underlying.

A.4.5. Continuation lines

Continuation lines can be used with precise alignment for readability. For example:

Code lines, which are continuation lines of assignment statements, must begin to the right of the column of the assignment operator. Due to the possibility of automatic indentation in some editor (emacs for example), use a "&" as first character of the continuing lines to maintain the alignment.

A.4.6. Declaration of arguments and local variables

In a routine, input arguments and local variables are declared 1 per line, with a comment field on the same line as the declaration. Multiple comment lines describing a single variable are acceptable if needed. For example:

```
INTEGER :: kstp ! ocean time-step index
```

A.4.7. F90 Standard

NEMO software adheres to the Fortran 90language standard (specifically, the Fortran 2003 standard) and does not rely on any specific language or vendor extensions.

A.4.8. Free-Form Source

Free-form source will be used. The F90/95 standard allows lines of up to 132 characters, but a self-imposed limit of 80 should enhance readability, or print source files with two columns per page. Multi-line comments that extend to column 100 are unacceptable.

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A.4.9. Indentation

Code as well as comment lines within loops, if-blocks, continuation lines, MODULE or SUBROUTINE statements will be indented 3 characters for readability (except for CONTAINS that remains at first column).

```
MODULE mod1
REAL(wp) xx
CONTAINS
SUBROUTINE sub76( px, py, pz, pw, pa, & & & pb, pc, pd, pe )
<instruction>
END SUBROUTINE sub76
END MODULE mod1
```

A.4.10. Loops

Loops, if explicit, should be structured with the do-end do construct as opposed to numbered loops. Nevertheless non-numeric labels can be used for a big iterative loop of a recursive algorithm. In the case of a long loop, a self-descriptive label can be used (*i.e.* not just a number).

A.4.11. Naming Conventions: files

A file containing a module will have the same name as the module it contains (because dependency rules used by "make" programs are based on file names). †

A.4.12. Naming Conventions: modules

Use a meaningful English name and the "3 letters" naming convention: first 3 letters for the code section, and last 3 to describe the module. For example, zdftke, where "zdf" stands for vertical diffusion, and "tke" for turbulent kinetic energy.

Note that by implication multiple modules are not allowed in a single file. The use of common blocks is deprecated in Fortran90 and their use in NEMO is strongly discouraged. Modules are a better way to declare static data. Among the advantages of modules is the ability to freely mix data of various types, and to limit access to contained variables through the use of the ONLY and PRIVATE attributes.

A.4.13. Naming Conventions: variables

All variable should be named as explicitly as possible in English. The naming convention concerns prefix letters of these name, in order to identify the variable type and status.

Never use a Fortrankeyword as a routine or variable name.

The table below lists the starting letter(s) to be used for variable naming, depending on their type and status:

A.4.14. Operators

Use of the operators <, >, <=, >=, =, /= is strongly recommended instead of their deprecated counterparts (.lt., .gt., .le., .ge., .eq., .ne.). The motivation is readability. In general use the notation: < Blank > < Operator > < Blank >

A.4.15. Pre processor

Where the use of a language pre-processor is required, it will be the C pre-processor (cpp).

The cpp key is the main feature used, allowing to ignore some useless parts of the code at compilation step. The advantage is to reduce the memory use; the drawback is that compilation of this part of the code isn't checked.

The cpp key feature should only be used for a few limited options, if it reduces the memory usage. In all cases, a logical variable and a FORTRAN IF should be preferred. When using a cpp key key_optionname, a corresponding logical variable lk_optionname should be declared to allow FORTRAN IF tests in the code and a FORTRAN module with the same name (*i.e.* optionname.F90) should be defined. This module is the only place where a "#if defined" command appears, selecting either the whole FORTRAN code or a dummy module.

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[†]For example, if routine A "USE"s module B, then "make" must be told of the dependency relation which requires B to be compiled before A. If one can assume that module B resides in file B.o, building a tool to generate this dependency rule (e.g. A.o: B.o) is quite simple. Put another way, it is difficult (to say nothing of CPU-intensive) to search an entire source tree to find the file in which module B resides for each routine or module which "USE"s B.

Type	integer	real	logical	character	double	complex
/ Status					precision	
public	m n	abefgho	1	С	d	У
or	but not	q to x	but not	but not	but not	but not
module	nn_	but not	lp ld ll ln_	cp cd cl	dp dd dl	yp yd yl
variable		fs rn_		cn_	dn	
dummy	k	р	ld	cd	dd	yd
argument	but not	but not				
	kf	pp pf				
local	i	Z	11	cl	cd	yl
variable						
loop	j					
control	but not					
	jp					
parameter	jp	pp	lp	ср	dp	yp
namelist	nn_	rn_	ln_	cn_	dn_	
CPP	kf	sf				
macro						

For example, the assimilation increments module name is asminc.F90, the CPP key is key_asminc and the associated logical is lk_asminc.

The following syntax:

```
#if defined key_optionname
!! Part of code conditionally compiled if cpp key key_optionname is active
#endif
```

Is to be used rather than the #ifdef abbreviate form since it may have conflicts with some Unix scripts. Tests on cpp keys included in NEMO at compilation step:

- The CPP keys used are compared to the previous list of cpp keys (the compilation will stop if trying to specify a non-existing key)
- If a change occurs in the CPP keys used for a given experiment, the whole compilation phase is done again.

A.5. DO LOOP macros

Another aspect of the preprocessor is the use of macros to substitute code elements. In some cases these are used to reduce unnecessary array dimensions. A good example are the substitutions introduced by the key_qco key:

```
#if defined key_qco # define e3t(i,j,k,t) (e3t_0(i,j,k)*(1._wp+r3t(i,j,t)*tmask(i,j,k))) ... #elif defined key_linssh # define e3t(i,j,k,t) e3t_0(i,j,k) ... #endif
```

which are used to reduce 4-d arrays to a 3-d functional form or an invariant, 3-d array depending on other options. Such macros should be located in files with _substitute.h90 endings to their names (e.g. domzgr_substitute.h90).

From 4.2, a more pervasive use of macros has been introduced in the form of DO LOOP macros. These macros have replaced standard nested, loops over the spatial dimensions. In particular:

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and white-space variants thereof.

The macro naming convention takes the form: DO_2D(L, R, B, T) where:

- L is the Left offset from the PE's inner domain
- R is the Right offset from the PE's inner domain
- B is the Bottom offset from the PE's inner domain
- T is the Top offset from the PE's inner domain

So, given an inner domain of 2, jpim1 and 2, jpjm1, a typical example would replace:

```
DO jj = 2, jpj
DO ji = 1, jpim1

END DO
END DO
```

with:

```
DO_2D( 1, 0, 0, 1 )
.:
END_2D
```

similar conventions apply to the 3D loops macros. jk loop limits are retained through macro arguments and are not restricted. This includes the possibility of strides for which an extra set of DO_3DS macros are defined.

The purpose of these macros is to enable support for extra-width halos. The width of the halo is determined by the value of the namelist parameter:nn_hls. Version 4.2 will work with either nn_hls=1 or nn_hls=2 but there is currently a performance penalty to using nn_hls=2 since more development is needed before any benefits are realised. Code developers should consider whether or not loops need to be over:

- The inner domain only (e.g. DO_2D(0, 0, 0, 0))
- The entire domain (e.g. DO_2D(nn_hls, nn_hls, nn_hls, nn_hls))
- All but the outer halo (e.g. DO_2D(nn_hls-1, nn_hls-1, nn_hls-1, nn_hls-1))
- A mixture on different boundaries (e.g. DO_2D(nn_hls, nn_hls-1, nn_hls, nn_hls-1))

The correct use of these macros will eventually lead to performance gains through the removal of unnecessary computation and a reduction in communications.

A.6. Content rules

A.6.1. Configurations

The configuration defines the domain and the grid on which NEMO is running. From 4.2 onwards, all configuration-specific settings should be read from variables in, or attributes of, the domain configuration file (or set in usrdef supplied subroutines). See ?? for more details.

A.6.2. Constants

Physical constants (e.g. π , gas constants) must never be hard-wired into the executable portion of a code. Instead, a mnemonically named variable or parameter should be set to the appropriate value, in the setup routine for the package. We realize than many parameterizations rely on empirically derived constants or fudge factors, which are not easy to name. In these cases it is not forbidden to leave such factors coded as "magic numbers" buried in executable code, but comments should be included referring to the source of the empirical formula. Hard-coded numbers should never be passed through argument lists.

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A.6.3. Declaration for variables and constants

Rules

Variables used as constants should be declared with attribute PARAMETER and used always without copying to local variables, in order to prevent from using different values for the same constant or changing it accidentally.

- Usage of the DIMENSION statement or attribute is required in declaration statements
- The "::" notation is quite useful to show that this program unit declaration part is written in standard FORTRAN syntax, even if there are no attributes to clarify the declaration section. Always use the notation

 three blanks> to improve readability.
- Declare the length of a character variable using the CHARACTER (len=xxx) syntax ‡
- For all global data (in contrast to module data, that is all data that can be access by other module) must be accompanied with a comment field on the same line §. For example:

```
REAL(wp), DIMENSION(jpi,jpj,jpk) :: ua ! i-horizontal velocity (m/s)
```

Implicit None

All subroutines and functions will include an IMPLICIT NONE statement. Thus all variables must be explicitly typed. It also allows the compiler to detect typographical errors in variable names. For modules, one IMPLICIT NONE statement in the modules definition section is needed. This also removes the need to have IMPLICIT NONE statements in any routines that are CONTAINS'ed in the module. Improper data initialisation is another common source of errors ¶. To avoid problems, initialise variables as close as possible to where they are first used.

Attributes

PRIVATE / PUBLIC: All resources of a module are PUBLIC by default. A reason to store multiple routines and their data in a single module is that the scope of the data defined in the module can be limited to the routines which are in the same module. This is accomplished with the PRIVATE attribute.

INTENT: All dummy arguments of a routine must include the INTENT clause in their declaration in order to improve control of variables in routine calls.

A.6.4. Headers

Prologues are not used in NEMO for now, although it may become an interesting tool in combination with ProTeX auto documentation script in the future. Rules to code the headers and layout of a module or a routine are illustrated in the example module available with the code: $./src/OCE/module_example$

A.6.5. Interface blocks

Explicit interface blocks are required between routines if optional or keyword arguments are to be used. They also allow the compiler to check that the type, shape and number of arguments specified in the CALL are the same as those specified in the subprogram itself. FORTRAN 95 compilers can automatically provide explicit interface blocks for routines contained in a module.

A.6.6. I/O Error Conditions

I/O statements which need to check an error condition will use the iostat=<integer variable> construct instead of the outmoded end= and err=.

Note that a 0 value means success, a positive value means an error has occurred, and a negative value means the end of record or end of file was encountered.

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[†]The len specifier is important because it is possible to have several kinds for characters (e.g. Unicode using two bytes per character, or there might be a different kind for Japanese e.g. NEC).

[§]This allows a easy research of where and how a variable is declared using the unix command: "grep var *90 | grep !:".

[¶]A variable could contain an initial value you did not expect. This can happen for several reasons, e.g. the variable has never been assigned a value, its value is outdated, memory has been allocated for a pointer but you have forgotten to initialise the variable pointed to.

A.6.7. PRINT - ASCII output files

Output listing and errors are directed to numout logical unit =6 and produces a file called ocean.output. Usually, this is produced by only the first ranked process in an MPP environment. This process will have the lwp logical variable set and this can be used to restrict output. For example: to output an error from a routine, one can use the following template:

```
IF( nstop /= 0 .AND. lwp ) THEN ! error print
    WRITE(numout,cform_err)
    WRITE(numout,*) nstop, ' error have been found'
ENDIF
```

At run-time, the user can use sn_cfctl options to have output from more processes in MPP.

A.6.8. Precision

Parameterizations should not rely on vendor-supplied flags to supply a default floating point precision or integer size. The F95 KIND feature should be used instead. In order to improve portability between 32 and 64 bit platforms, it is necessary to make use of kinds by using a specific module ./src/OCE/par_kind.F90 declaring the "kind definitions" to obtain the required numerical precision and range as well as the size of INTEGER. It should be noted that numerical constants need to have a suffix of _kindvalue to have the corresponding size. Thus wp being the "working precision" as declared in ./src/OCE/par_kind.F90, declaring real array zpc will take the form:

```
REAL(wp), DIMENSION(jpi,jpj,jpk) :: zpc ! power consumption
```

A.6.9. Structures

The TYPE structure allowing to declare some variables is more often used in NEMO, especially in the modules dealing with reading fields, or interfaces. For example:

```
! Definition of a tracer as a structure
TYPE PTRACER
CHARACTER(len = 20) :: sname ! short name
CHARACTER(len = 80) :: lname ! long name
CHARACTER(len = 20) :: unit ! unit
LOGICAL :: lini ! read in a file or not
LOGICAL :: lsav ! ouput the tracer or not
END TYPE PTRACER

TYPE(PTRACER) , DIMENSION(jptra) :: tracer
```

Missing rule on structure name??

A.7. Packages coding rules

A.7.1. Bounds checking

NEMO is able to run when an array bounds checking option is enabled.

Thus, constructs of the following form are disallowed:

```
REAL(wp) :: arr(1)
```

where "arr" is an input argument into which the user wishes to index beyond 1. Use of the (*) construct in array dimensioning is forbidden also because it effectively disables array bounds checking.

A.7.2. Communication

A package should refer only to its own modules and subprograms and to those intrinsic functions included in the Fortran standard.

All communication with the package will be through the argument list or namelist input.

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The point behind this rule is that packages should not have to know details of the surrounding model data structures, or the names of variables outside of the package. A notable exception to this rule is model resolution parameters. The reason for the exception is to allow compile-time array sizing inside the package. This is often important for efficiency.

A.7.3. Error conditions

When an error condition occurs inside a package, a message describing what went wrong will be printed (see PRINT - ASCII output files). The name of the routine in which the error occurred must be included. It is acceptable to terminate execution within a package, but the developer may instead wish to return an error flag through the argument list, see stpctl.F90.

A.7.4. Memory management

The main action is to identify and declare which arrays are PUBLIC and which are PRIVATE.

As of version 3.3.1 of NEMO, the use of static arrays (size fixed at compile time) has been deprecated. All module arrays are now declared ALLOCATABLE and allocated in either the <module_name>_alloc() or <module_name>_init() routines. The success or otherwise of each ALLOCATE must be checked using the stat=<integer variable> optional argument.

In addition to arrays contained within modules, many routines in NEMO require local, "workspace" arrays to hold the intermediate results of calculations. These arrays are mostly declared in such a way as to be automatically allocated on the stack when the routine is called. Examples of an automatic arrays are:

```
SUBROUTINE sub(n)
REAL(wp) :: za(n)
REAL(wp), DIMENSION(jpi,jpj) :: zhdiv ! 2D workspace
...
END SUBROUTINE sub
```

Sometimes these local arrays are only required for specific options selected at run-time. Allocatable arrays should be used to avoid unnecessary use of stack storage in these cases. For example:

```
SUBROUTINE wzv(...)
...
REAL(wp), ALLOCATABLE, DIMENSION(:,:,:) :: zhdiv ! 3D workspace
...
If (ln_vvl_ztilde .OR. ln_vvl_layer ) THEN
ALLOCATE( zhdiv(jpi,jpj,jpk) )
...
DEALLOCATE( zhdiv )
ELSEIF
...
END SUBROUTINE sub
```

A.7.5. Optimisation

Considering the new computer architecture, optimisation cannot be considered independently from the computer type. In NEMO, portability is a priority, before any too specific optimisation.

A.7.6. Package attribute: PRIVATE, PUBLIC, USE, ONLY

Module variables and routines should be encapsulated by using the PRIVATE attribute. What shall be used outside the module can be declared PUBLIC instead. Use USE with the ONLY attribute to specify which of the variables, type definitions etc... defined in a module are to be made available to the using routine.

A.7.7. Parallelism using MPI

NEMO is written in order to be able to run on one processor, or on one or more using MPI. From 4.2, this is the default assumption but a non-MPI, single processor executable can be compiled by activating the cpp key: key_mpi_off .

The domain decomposition divides the global domain in cubes (see NEMO reference manual). Whilst coding a new development, the MPI compatibility has to be taken in account (see ./src/LBC/lib_mpp.F90) and should be tested. By default, the x-z part of the decomposition is chosen to be as square as possible. However, this may be overriden by specifying the number of sub-domains in latitude and longitude in the nammpp section of the namelist file.

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A.8. Features to be avoided

The code must follow the current standards of FORTRAN and ANSI C. In particular, the code should not produce any WARNING at compiling phase, so that users can be easily alerted of potential bugs when some appear in their new developments. Below is a list of features to avoid:

- COMMON block (use the declaration part of MODULE instead)
- EQUIVALENCE (use POINTER or derived data type instead to form data structure)
- Assigned and computed GOTO (use the CASE construct instead)
- Arithmetic IF statement (use the block IF, ELSE, ELSEIF, ENDIF or SELECT CASE construct instead)
- Labelled DO construct (use unlabelled END DO instead)
- FORMAT statement (use character parameters or explicit format- specifiers inside the READ or WRITE statement instead)
- GOTO and CONTINUE statements (use IF, CASE, DO WHILE, EXIT or CYCLE statements or a contained?)
- PAUSE
- ENTRY statement: a sub-program must only have one entry point.
- RETURN is obsolete and so not necessary at the end of program units
- FUNCTION statement
- Avoid functions with side effects. **
- DATA and BLOCK DATA (use initialisers)

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^{**}First, the code is easier to understand, if you can rely on the rule that functions don't change their arguments. Second, some compilers generate more efficient code for PURE functions (in FORTRAN 95 there are the attributes PURE and ELEMENTAL), because they can store the arguments in different places. This is especially important on massive parallel and as well on vector machines.

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CPP keys

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