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D2.4 Sub-Model APECOSM functional coupling with phytoplankton models

**User Guide for
ROMS-PISCES-APECOSM coupling**

Eric Machu, January 2010

Contents:

This work is done in synergy with the development of NEMO-PISCES-APECOSM carried out by Olivier Aumont (IRD/LPO), Olivier Maury (IRD/EME) and Thomas Gorgues (Post-doc LPO).

Note: The Fortran code for the models in the coupling can be requested from the developers/user groups: ROMS (http://www.myroms.org/), NEMO (http://www.nemo-ocean.eu/), PISCES (http://www.lodyc.jussieu.fr/~aumont/OPA_model.html or Olivier Aumont, Olivier.Aumont@ird.fr), APECOSM (Olivier Maury; maury@ird.fr)

1. Description of the models

1.1. Hydrodynamic model ROMS (Regional Oceanic Modeling System)

The Regional Oceanic Modeling System (ROMS; Shchepetkin and McWilliams, 2005) is an evolutionary descendent from the S-Coordinate Rutgers University Model (SCRUM: Song and Haidvogel, 1994). It solves the incompressible, hydrostatic, primitive-equation model with a free sea surface, horizontal curvilinear coordinates, and a generalized terrain-following vertical coordinate that can be configured to enhance resolution at the sea surface or at the sea floor. ROMS was developed to simulate both coastal and oceanic regions and their interactions. Its computational methods allow for realistic, long-term integrations in a fine-mesh regional domain.

The finite-difference discretization algorithms are oriented toward non-oscillatory, high-order schemes, thus improving the effective resolution of the model (weighing accuracy against computational cost; see, e.g., Sanderson, 1998). Once a grid resolution passes a certain threshold with viscosity decreased accordingly, the simulated flow becomes turbulent. Experience in computational fluid dynamics for turbulent flows has shown that conventional, second-order, discretized advection schemes are not satisfactory in comparison with higher order schemes. In ROMS the advection operator is third order and upstream biased, designed to reduce dispersive errors and the excessive dissipation rates needed to maintain smoothness, thereby effectively enhancing the resolution on a given grid (Shchepetkin and McWilliams, 1998). The pressure gradient formulation usually used in simulations of upwelling coastal areas is a variation of the density Jacobian formulation of Song (1998), with an optimized correction for vertical grid stretching. The vertical mixing in the interior and planetary boundary layers is calculated with the nonlocal, K-Profile Parameterization scheme (KPP: Large et al., 1994) that performs well in both measurement comparisons and large domain model solutions (Large and Gent, 1999; Li et al., 2001), and was adapted to the C-grid structure of ROMS. A mode-splitting technique allows the separation of the barotropic and baroclinic components in the model with internal and external time steps. The mode splitting is done using a time filter, which ensures that the continuity equation is satisfied on the discrete level, thus removing previous restrictions of small free-surface changes. The time stepping is a leapfrog/Adams–Moulton, predictor–corrector scheme, which is third-order accurate in time and has good dispersive properties for the advection equation. An expanded regime of stability allows larger time steps. The vertical diffusion terms are treated with a semi-implicit, Crank–Nicholson scheme to avoid time step restrictions due to large vertical mixing rates in the boundary layers and in the interior when static stability needs to be restored. The reader is referred to SMA and SMB for a more complete report.

Recently, a specific advection scheme has been designed to correct the spurious diapycnal mixing that can take place in terrain-following coordinate models for certain resolutions (Marchesiello et al., 2008).

The primitive equations of motion in Cartesian coordinates can be written:

$$\frac{\partial u}{\partial t} + \vec{v}.\nabla u - fv = -\frac{\partial \Phi}{\partial x} + F_u + D_u$$

$$\frac{\partial v}{\partial t} + v.\nabla v + fu = -\frac{\partial \Phi}{\partial y} + F_v + D_v$$

$$\frac{\partial T}{\partial t} + \vec{v}.\nabla T = F_T + D_T$$

$$\frac{\partial S}{\partial t} + \vec{v}.\nabla S = F_s + D_s$$

$$\rho = \rho(T, S, P)$$

$$\frac{\partial \Phi}{\partial z} = -\frac{\rho g}{\rho_0}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0.$$

The first two equations express the momentum balance in the *x*- and *y*-directions, respectively. The time evolution of the potential temperature and salinity fields, $T(x,y,z,t)$ and $S(x,y,z,t)$, are governed by the two next advective-diffusive equations. The equation of state is given by equation #5. In the Boussinesq approximation, density variations are neglected in the momentum equations except in their contribution to the buoyancy force in the vertical momentum equation (#6). Under the hydrostatic approximation, it is further assumed that the vertical pressure gradient balances the buoyancy force. Last equation expresses the continuity equation for an incompressible fluid. The effects of forcing and dissipation are here represented by the schematic terms *F* an *D*, respectively.

ROMSTOOLS (Penven et al., 2006), a collection of global data sets and a series of Matlab programs collected in an integrated toolbox, developed for generating the grid, the surface forcing, initial conditions, open boundary conditions, and tides for climatological and inter-annual ROMS ocean simulation will be adapted to account for APECOSM set-up in the future.

1.2. Biogeochemical model: PISCES

PISCES is a biogeochemical model which simulates the marine biological productivity that describes the biogeochemical cycles of carbon and of the main nutrients (P, N, Si, Fe). This model can be categorized as one of the many Monod models (Monod, 1942) since it assumes a constant Redfield ratio and phytoplankton growth depends on external concentration of nutrients.
However, when modeling silicate, iron and/or chlorophyll, assuming constant ratios is not justified anymore as these ratios can vary a lot (for instance, one order of magnitude for the Fe/C ratio). Thus, the elemental ratios of Fe, Si and Chl are prognostically predicted based on external concentrations of the limiting nutrients like in the quota approach (McCarthy, 1980; Droop, 1983). PISCES has currently twenty-four compartments. These are five modeled limiting nutrients for phytoplankton growth: Nitrate and Ammonium, Phosphate, Silicate and Iron. Phosphate and Nitrate+Ammonium are not really independent nutrients in PISCES since they are linked by constant Redfield ratios but the nitrogen pool undergoes nitrogen fixation and denitrification.
Four living compartments are represented: two phytoplankton size-classes/groups corresponding to nanophytplankton and diatoms, and two zooplankton size classes which are microzooplankton and mesozooplankton. For phytoplankton, prognostic variables are total biomass, the iron, chlorophyll and silicon contents. This means that the Fe/C, Chl/C and Si/C ratios of both phytoplankton groups are fully predicted by the model. For zooplankton, only the total biomass is modeled. For all species, the O/C/N/P ratios are supposed constant (172/122/16/1) and are not allowed to vary.
In addition, the Fe/C ratio for both zooplankton groups is kept constant. No silicified zooplankton is assumed and the bacterial pool is not explicitly modeled.

The evolution of any biological tracer concentration C_i is determined by an advective-diffusive equation:

$$\frac{\partial C_i}{\partial t} = -\nabla.(uC_i) - A_\rho \nabla^2 C_i + \frac{\partial}{\partial z}\left(K_\rho \frac{\partial C_i}{\partial z}\right) + SMS(C_i)$$

where the first term on the right-hand side accounts for advection (by currents *u*), the second accounts for horizontal diffusion (with A_ρ representing the horizontal eddy diffusion coefficient), and the third term represents vertical mixing with turbulent diffusion coefficient K_ρ. The last term is the source-minus-sink (SMS) term due to biological processes. A full description of the SMS terms and the parameters used can be found in Aumont and Bopp (2006) and in "description des equations".

PISCES has been first coupled to the OPA model (Madec et al., 1998). In 2004, a stable release of the model is made available to the community on the OPA website (www.lodyc.jussieu.fr/opa). It can be freely used and changed by anybody after subscription to the OPA system. More recently, a beta version of PISCES coupled to ROMS has been made. The code can be obtained by sending an email to this address (olivier.aumont@ird.fr). It will soon be freely available for use and development after subscription to the European ROMS development core team (ROMS/AGRIF v2.0: http://gforge.inria.fr/projects/romsagrif/).

1.3. Open Ocean Pelagic Communities: APECOSM

APECOSM (Apex Predators ECOSystem Model) is a recent spatially explicit size-based model of open-ocean ecosystems (Maury et al., 2007a; Maury et al., 2007b) developed in the framework of the GLOBEC-CLIOTOP modelling Working Group. APECOSM's philosophy is to specify a very generic and robust structure of marine ecosystems from which particular regional ecosystem organization are emerging due to interactions with the environment. It relies on very few general rules from which the structure of the model and the parameterizations are derived mechanistically. APECOSM represents the flow of energy through the ecosystem with a size-resolved structure in four dimensions (space x, y, time t, and size l). The uptake and use of energy for growth, maintenance and reproduction by the organisms are modelled according to the DEB (dynamic energy budget) theory (Kooijmann, 2000) and the size-structured nature of predation is explicit. Distinction between the epipelagic community, the mesopelagic community and the migratory community which experiences nyctemeral vertical movements and hence transfers energy between the two other communities is expressed. Their habitat depends mainly on the light profile. Thus, size and spatio-temporal co-occurrence of organisms structure trophic interactions.

The different features taken explicitly into account by the model and supposed to be determinant in the dynamics of the open ocean pelagic ecosystem, its spatial distribution and its accessibility to top predators can be summarized as follow:
- Size-structured opportunistic trophic interactions where producers are potential preys for consumers and where all consumer species are considered to be potentially prey and predator at the same time (Shin and Cury, 2004);
- Predators competition for preys;
- Allocation of energy between growth and reproduction;
- Somatic as well as maturity maintenance based on the Dynamic Energy Budget (DEB) theory (Kooijman, 2000, 2001; Nisbet, Muller, Lika & Kooijman, 2000);
- Size-dependent non predatory mortality;
- Starvation mortality;
- Temperature-dependence of organism's physiological rates;
- Passive movements driven by marine currents;
- Size- and food-dependent active movements;

In APECOSM, passive (driven by the ocean circulation) and active (with a behavioral origin) movements of organisms play an essential role in energy transfer between regions, dispersion and concentration of organisms. It is also expected that taking explicitly into account the size structured predation and growth processes helps to better understand the various mode of energy transfer through trophic levels and the regional differences in the pelagic ecosystem size structure.

The resulting balance equation (eqs 1) is used to describe the spatialized energy fluxes through the weight range of consumers. It combines 3D spatial diffusion and advection terms with an advection term for representing the growth process and three sink terms for predatory, non predatory and starvation mortality processes:

$$
\begin{aligned}
\partial_t \xi^i = div_{x,y}\left(d^i \nabla_{x,y}\xi^i - v^i \xi^i\right) + \partial_z\left(d_z^i \partial_z \xi^i - v_z^i \xi^i\right) \\
- \partial_w\left(\gamma^i \xi^i\right) \\
- \left(\lambda^i + m^i + s^i\right)\xi^i \qquad in \quad \Omega \times \left]w_{egg}, w_{\max}\right] \times \left(0, t_{\max}\right)
\end{aligned} \tag{3}
$$

Where ∇ and *div* are the usual differential operators on the spatial domain Ω.
This equation is completed with initial conditions,

$$
\xi^i_{0,x,y,z,w} = \xi^{i,0}_{x,y,z,w}, \qquad \forall (x,y,z,w) \in \Omega \times \left]w_{egg}, w_{\max}\right], \tag{1.}
$$

boundary conditions in size

$$
\gamma_{t,x,y,z,w_{egg}} \xi^c_{t,x,y,z,w_{egg}} = r_{t,x,y,z}, \quad \forall (x,y,z,t) \in \Omega \times \left[0, t_{\max}\right] \tag{2.}
$$

and Neuman boundary conditions in space

$$\nabla \xi^i_{t,x,v,z,w} \bullet n(x, y, z) = 0, \quad in \quad \partial\Omega, \quad \forall (w, t) \in \left]w_{egg}, w_{max}\right] \times \left[0, t_{max}\right], \tag{3.}$$

where $n(x, y, z)$ is the unit normal vector pointing outside Ω, d and d_z (m^2.s^{-1}) are the horizontal and vertical diffusivity coefficients, u, v and v_z (m.s^{-1}) are the zonal, meridional and vertical components of the spatial advection, γ (kg.s^{-1}) is the growth rate, s (s^{-1}) is the mortality rate due to predation, m (s^{-1}) is the loss of energy from the system due to non predatory mortality and s (s^{-1}) is the starvation mortality rate. The input of eggs r_t (J.s^{-1}) into the system due to reproduction is taken into account through the boundary condition in $w=w_{egg}$.

Focus species can then be "extracted" from the global size-spectrum without loosing mass balance and represented with more physiological or behavioural details (Maury, 2009). For these focus species, physiology acts as a transfer function between environment and behaviour.

More informations about APECOSM parameterization of source and sink terms can be obtained in Maury et al. (2007a). Parameterization of vertical habitat, biological diffusion and behavioural advection can be read in Maury et al. (submitted).

1.4. ROMS-PISCES-APECOSM coupling

Physical forcings (vertical turbulence, temperature, salinity and current fields) and biogeochemical forcings (light and oxygen fields in addition to primary production) will have an effect on the metabolic rates, the habitat definitions or the advection and diffusion (physical and biological) of the different Open Ocean Pelagic Communities (OOPC). These fields are provided by the physical-biogeochemical model ROMS-PISCES which simulates the ocean dynamics as well as the cycling of the main nutrients (C, N, P, Si, Fe) and the dynamics of the lowest trophic levels (nanophytoplankton, diatoms and microzooplankton). Hence, energy is provided at the basis of the model through primary production and transferred through the spatially explicit size-spectrum.

The feedback of the APECOSM model is insured through the predation of pelagic communities on autotrophs and microzooplankton. Mortality, Egestion and excretion of pelagic communities will also inject energy into the cycle of particulate organic matter. The coupling between PISCES and APECOSM can be schematized in Figure1.
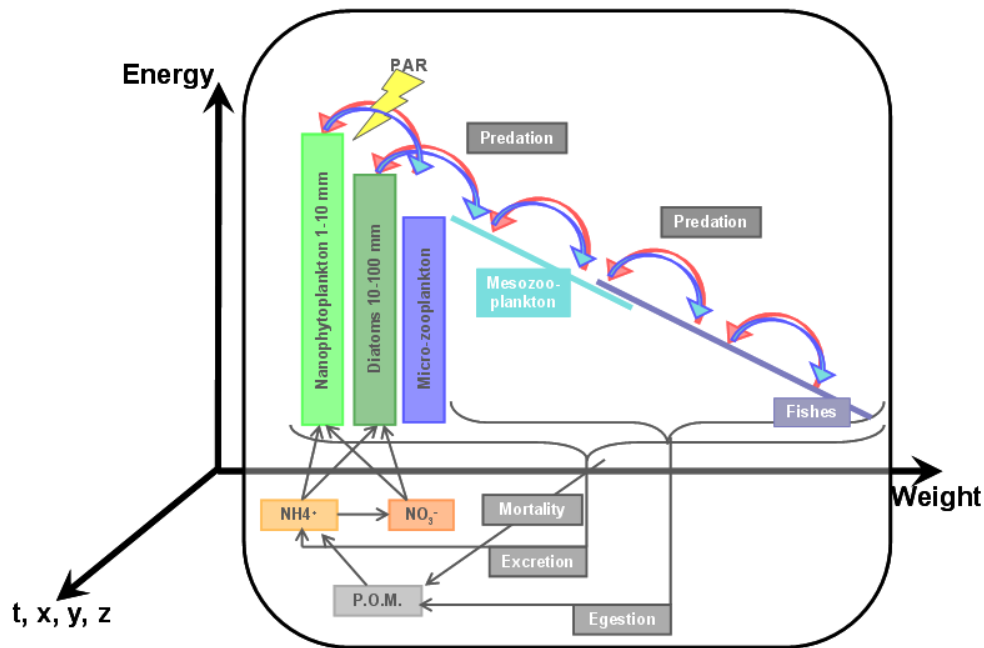

Figure 1: Scheme of the coupling of the PISCES-APECOSM models. Blue arrows represent the energy gained by predators and red arrows represent the energy lost by preys. Each blue arrow is compensated by a red arrow for the model to be mass balanced.

> **A fundamental characteristic of the resulting model is that mass is rigorously conserved**

To summarize, the online coupling of the three state of the art oceanic models that consider explicitly physical, biogeochemical and ecosystem levels provides a coherent formalism and makes possible to study the bottom-up and top-down controls that interact and propagate and finally determine the dynamics of marine ecosystems.

2. Technical coupling of ROMS-PISCES-APECOSM

The coupling of biogeochemical modules to ROMS has already been documented (http://roms.mpl.ird.fr/documentation.html) and published (e.g. Koné et al., 2005; Gruber et al., 2006; Echevin et al., 2008) and therefore will not be presented in this report. However it could be of interest to keep in mind that the solver for biogeochemical SMS terms is iterative to achieve implicit discretization of the biological interactions. During the iterative procedure a series of fractional time steps is performed in a chained mode (splitting by different biological conversion processes) in sequence nutrients, phytoplankton, zooplankton, detritus, that is the main food chain. In all stages the concentration of the component being consumed is treated in fully implicit manner, so that the algorithm guarantees non-negative values, no matter how strong is the concentration of active consuming component (phyto- or zooplankton component).

2.1. Time-stepping for Open Ocean Pelagic Communities

In the offline version of APECOSM, the time step is of one day. The mesopelagic migratory community experiences vertical nyctemeral movements and hence experiences different environmental conditions between day and night. Furthermore, because of the vertical migrations and because of light-dependent foraging behaviors, trophic interactions between the three communities are different between day and night. In order to determine the terms related to growth and mortality by starvation, an energy budget is computed at the end of the day. Depending on the result of this budget, growth and reproduction terms are either affected to the growth/reproduction process, or added to the starvation mortality (Maury et al., submitted). In the present coupled version, the time step used for OOPC variables is the same as physical and biogeochemical variables (order of one hour, depending on the resolution). Carrying the budget of energy after one day (i.e. *x* time steps) would be impossible to do since mass would not be conserved at each time step. Consequently, we divided each time step into 2 contributions (*dn*=0,1) to represent a day and a night fraction of the time step. The day/night loop is embedded into the time stepping and the energy budget is computed at the end of the night fraction of each time step (*dn=1*). The fraction of day and night for each time step depends on latitude and day of the year and is computed as follow:

$$day/night\_fraction_{i,j} = (1 - dn) \cdot zstrn_{i,j} / 24 + dn \cdot (1 - zstrn_{i,j} / 24)$$

dn = 0 for the day fraction and 1 for the night fraction. *i* and *j* represent the ROMS ζ and η direction indexes and *zstrn* the number of hours of light per day. This day/night fraction is then multiplied by the time step *dt* for computing the temporal evolution of pelagic communities.

2.2. 3D-implicit advection and diffusion calculation

Before computing SMS terms for pelagic communities, two-dimensional energy content of epipelagic, migratory and mesopelagic communities are projected vertically according to the definition of their habitat (see section 2.4.1.). The habitats of the different communities are defined with a Gaussian distributions centred on optimal light or temperature. Light-dependent and temperature-dependent profiles are respectively parameterized for epipelagic community and mesopelagic/migratory communities. According to Maury et al. (submitted), parameterizations taking better into account behavioural responses could be implemented to represent the sensitivity of epipelagic communities to oxygen concentration and temperature for instance.

Once OOPC variables are projected vertically according to their habitat, biological interactions (SMS terms) are computed in 3D. After taking into account the interactions between pelagic communities, the vertical distribution of energy is normalized and the profile likely defined provides the vertical weights for computing the 2D horizontal field of current and diffusion (to be explicitly introduced) that will be respectively used to advect and diffuse OOPC variables.

2.3. Computing temporal evolution of OOPC variables

APECOSM dynamic, originally computed in APECOSM by the routines dynamique() and calc_adv() is now carried on by ROMS thanks to its architecture and the numerical schemes associated to it.

Step.F is called by the main program to time step the 3-D momentum and tracers (potential temperature, salinity and biogeochemical state variables). Within this routine, the APECOSM state variables are implemented according to the other state variables of the model and specially the biogeochemical state variables where SMS terms (biological interactions) are to be considered. The timing of the operations is presented below.

Description of the sequence of operation in the ROMS architecture

main.F → init_oopc (initialize variables needed by APECOSM)
       → step (time step evolution of state variables)

step.F → step3d_t (advection followed by biogeochemical SMS terms)
       → **step2d_oopc** (APECOSM SMS terms followed by advection)
       → t3dmix (tracer horizontal and vertical mixing)
       → oopc2d_mix (OOPC variable horizontal mixing)

step2d_oopc.F:
       → bridge_oopc
            do dn=0,1 (day/night)
            → calc_habitat   (vertical habitat definition for epi-, meso- and migratory pelagic communities)
            → ff_updt (flux feeding)
            → calc_pred (predation mortality, source & sink terms related to growth: excretion, egestion, maintenance, reproduction)
            → <u>if dn=1</u> : growth (growth advection term, starvation, non-predatory mortality)
            → calc_adv (compute behavioural advection and biological diffusion)
            → calc_meso (mesozooplankton computed from oopc size spectra)
            → updt_bgc (update biogeochemical variables)
            enddo

       do dn=0,1
       → calc_vmoy (Vertical average to advect and diffuse 2D OOPC variables)
       enddo
       Compute horizontal advection (U+U_active)
       Compute horizontal diffusion (physical+biological)
       → oopc2dbc (treatment of the boundary conditions)

2.4. Initialization and boundary conditions

2.4.1. Initialization of OOPC variables

The energy associated to pelagic community *c* of weight *w* and length *l* is initialized as:

$$\xi_{i,j,w,0}^{c} = 100 \cdot l_{w}^{c\,(-3.17)}$$

Day/night (*dn* = 0,1) vertical profiles are considered homogeneous and are initially defined by:

$$profile_{i,j,k,w,dn,0}^{c} = 1/h_{i,j}$$

where *w* represents the weight index of the energy content of pelagic community *c* and *h* is the maximum water depth at point *i,j. profile* is used to project 2D OOPC variables on the vertical dimension:

$$\xi_{i,j,k,w}^{c} = profile_{i,j,k,w,dn}^{c} \cdot \xi_{i,j,w}^{c}$$

Initial state is obtained after running the model during a fifty year "spin-up" using climatological forcing fields when starting from the spatial distribution of phytoplankton field and the following allometric relationship corresponding to the stationary size-spectrum of 0-D simulations (Maury et al., submitted):

$$\xi_{t,x,y,w}^{i} = \frac{1}{i}\xi_{t,x,y,0}^{i}w^{-1.06} \quad \forall(t,x,y,w) \in (0,T_{spinup}) \times \Omega \times (0,w_{max})$$

2.4.2 Open Boundary Conditions (OBCs) for OOPC variables

OBCs for the regional domain are provided by the global NEMO-PISCES-APECOSM model and treated following the same scheme as other physical or biogeochemical tracers (Marchesiello et al., 2001).
For the moment, outside values used to compute boundary conditions are taken from a constant profile which is (shape and function of size)
In a second step, OOPC fields will be provided by the coupled physical-biogeochemical-ecosystem model NEMO-PISCES-APECOSM (Aumont and Bopp, 2006 for PISCES; Madec et al., 2007 for NEMO) which is developed in a global configuration.

2.5. New routines

2.5.1. Cpp-keys
OOPC = New cpp-key introduced to allow the computation of Open Ocean Pelagic Communities (OOPC) evolution

Compatibility:
- BIOLOGY, PISCES and DIURNAL_FLUX must be defined before defining OOPC key
- AGRIF option to allow embedded grid is under development

2.5.2. New routines for the ROMS code
Three common blocks are introduced:
- oopc.h → Declaration of APECOSM common variables
- oopc_cst.h → Setting of biological constants
- set_oopc.h → Set values for parameters related to OOPC variables

And six subroutines:
- init_oopc.F → Initialisation of APECOSM variables (weight/size scale, vertical profile, selectivity, parameters as a function of group and size, …)
- step2d_oopc.F → Compute the evolution for OOPC variables (equivalent to step3d_t.F for T, S and biogeochemical tracers)
- bridge.F → Compute APECOSM source-minus-sink terms (vertical habitat calculation, flux feeding, predation mortality, growth advection term, excretion, egestion, maintenance, reproduction, biological advection and diffusion terms, starvation, non-predatory mortality)
- oopc2dbc.F → Set lateral boundary conditions for OOPC variables for the parent grid
- oopc2dmix.F → Compute horizontal mixing for OOPC variables

The Makefile and the jobcomp files have been modified accordingly.

2.5.3. Modified routines

Here is the list of the ROMS routines that have been modified to implement the computation of the evolution of OOPC state variables:

ana_initial.F,
ana_initracer.F,
analytical.F,
averages.h,
climat.h,
cppdefs.h,
def_his.F,
get_srflux.F,
init_arrays.F,
init_scalars.h,
main.F,
output.F,
param.h,
read_inp.h,
scalars.h,
set_avg.F,
step.F,
wrt_avg.F

2.7. Outputs

The writing of output files is achieved by ROMS. Output data consist of temporally averaged (frequency defined in roms.in) bi-dimensional size-spectra for each pelagic community. APECOSM state variables are saved in separated netcdf files to reduce the usual size of output files.
The possibility of starting the run from a restart file has not yet been implemented.

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