Spectral light and bio-optical model in REcoM2

Last update: 22-March-2022

1. Introduction

The code presented couples a radiative transfer component with the biogeochemical ecosystem component REcoM2 in the dynamic three-dimensional physical framework of the MITgcm. The bio-optical component resolves the penetration of spectral irradiance as it is absorbed (and scattered) within the water column. It includes the effect of several optically water constituents (two phytoplankton types, detrital particles and coloured dissolved organic matter).

2. Configuration

radtrands package needs to be downloaded from MITgcm_contrib/darwin2 and copied to MITgcm/pkg. UPDATE: radtrans is in the standard distribution of MITgcm. Add radtrans to **packages.conf.**

3. Compile-time options

Parts of the WAVEBANDS/RADTRANDS code can be enabled or disabled at compile time via CPP preprocessor flags. These options are set in **RECOM_OPTIONS.h**. Next table summarizes these options.

CPP OPTION	**Description**
`RECOM_WAVEBANDS`	computes spectral downwelling radiation and waveband-dependent primary production
`RECOM_RADTRANS`	computes spectral down and upwelling radiation and waveband-dependent primary production
`OASIM`	enables the use of OASIM light as forcing field
`RECOM_CALC_ACDOM`	computes variable absorption by CDOM
`RECOM_CALC_APART`	uses mass-specific absorption, scattering and backscattering by detritus
`RECOM_CALC_APHYT`	computes variable absorption spectrum by phytoplankton, depending on PPC content
`RECOM_BMASS`	uses C-specific light scattering (m^2 $mmolC^{-1}$) instead of Chl-specific scattering (m^2 $mgChla^{-1}$) for phytoplankton
`RECOM_CALC_REFLEC`	exports waveband-specific diagnostics

RECOM_WAVEBANDS: It is comparable to Darwin-WAVEBANDS that is the code behind (Hickman et al., 2010). It considers the spectral absorption by constituents, resolves the downward light spectrum and computes spectral primary production. This is the model setup by default, all the other options modify the behaviour of RECOM_WAVEBANDS.

RECOM_RADTRANS: It is comparable to Darwin-DAR_RADTRANS that is the code behind (Dutkiewicz et al., 2015; 2018). In addition to spectral absorption, it computes the spectral scattering and backscattering by constituents and resolves the upwelling light spectrum and hence the water–leaving optical properties. RECOM_RADTRANS is not independent, it is additional to RECOM_WAVEBANDS and needs to be set together with it. Hence, all computations under RECOM_WAVEBANDS, regarding absorption of constituents, downwelling spectral light and primary production, are common to both options. RECOM_RADTRANS adds the computation of scattering and backscattering of constituents and resolves upwelling spectral irradiances.

OASIM: This option allows to use the output of the OASIM model (Gregg & Casey, 2009) as light input to the model (Section 6.2). Both RECOM_WAVEBANDS and RECOM_RADTRANS can be used alone or combined with OASIM forcing.

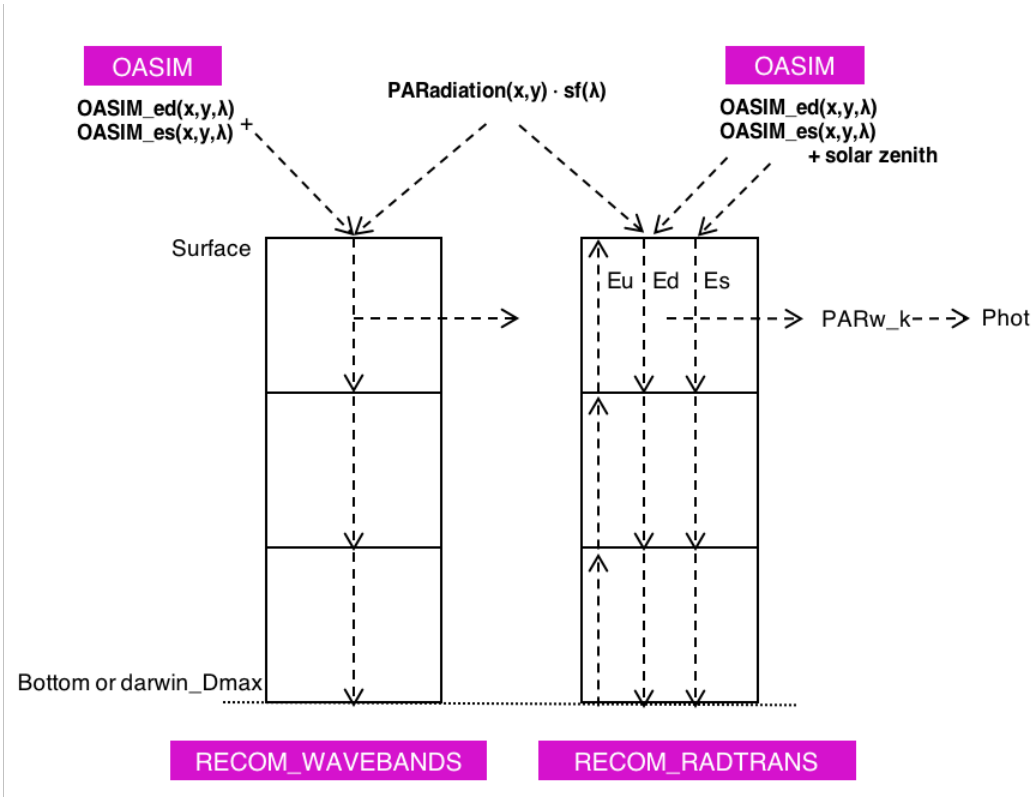

Figure 1. Differences between RECOM_WAVEBANDS and RECOM_RADTRANS regarding transmission of light in the water column. They both admit as input light the non-spectral value from standard REcoM provided a PAR-normalized spectrum is given in a file (sf, section 6.1). In this case only direct incoming irradiance is considered. OASIM option allows to consider both direct and diffuse incoming radiances.

The next options are related to the computation of spectral properties of the water constituents. coloured dissolved organic matter, detritus and phytoplankton. They all can be used with RECOM_WAVEBANDS and RECOM_RADTRANS independently.

RECOM_CALC_ACDOM: Computes absorption by CDOM considering either CDOM biomass if available or phytoplankton biomass. If this option is not used, assumed constant CDOM absorption needs to be provided in a file (Section 5.3).

RECOM_CALC_APART: Computes absorption by detritus considering mass-specific absorption at a reference wavelength. If this option is not used, spectral properties per particle of detritus need to be provided in a file and a conversion biomass per particle specified (Section 5.4).

RECOM_CALC_APHYT: Computes total absorption by each phytoplankton group considering the amount of non-photosynthetic pigments present. This option needs to be set together with RECOM_MARSHALL, that adds the fraction of active PSII as state variables (2 additional tracers) (Section 5.2).

RECOM_BMASS: instead of Chl-specific scattering (m^2 $mgChla^{-1}$) for phytoplankton, it uses C-specific scattering (m^2 $mmolC^{-1}$), the file *darwin_phytoabsorbFile* needs to be changed accordingly.

RECOM_CALC_REFLEC: Allows to export waveband-specific diagnostics in the 3D ocean, such as absorption/scattering/backscattering of constituents, Ed, Es, and Eu, and PAR (TO DO: figuring out how to export 4D diagnostics).

4. Default configuration: spectral parameters and files.

Under the option RECOM_WAVEBANDS alone, the model runs in its default configuration. **SPECTRAL_SIZE.h** sets the number of wavebands used (tlam) and **WAVEBANDS_PARAMS.h** the number of types of absorption spectra for phytoplankton (tnabp). **recom_readparams.F** (from darwin_readparams.F) creates two new namelists, `/DARWIN_SPECTRAL_PARM/` with parameters for the computation of spectral light, and `/SPECTRAL_FILES/` with the names of the files for absorption/scattering coefficients. The same routine gives default values for the parameter and file names, and both can be filled at runtime in **data.recom**.

In `/DARWIN_SPECTRAL_PARM/` darwin_waves or darwin_wavebands set the wavebands centers or the wavebands boundaries respectively. When tlam=13, wavecenters from 400 to 700 separated by 25 nm are considered by default. Note that the width of the first and the last waveband is 12.5 nm, whereas the rest have 25 nm.

/DARWIN_SPECTRAL_PARM/	
darwin_waves	Wavebands centers (defaults 400, 425, 450, 475, 500, 525, 550, 575, 600, 625, 650, 675, 700)
darwin_wavebands	Wavebands boundaries (tlam+1)

In /SPECTRAL_FILES/ the names of the files for absorption/scattering coefficients are set. Absorption/scattering files need to provide optical properties in the wavebands given by tlam and darwin_waves. The file for phytoplankton needs to provide the number of types of absorption/scattering spectra given by tnabp. All file names are also included in the commonblock /RECOM_FILENAMES/ in **RECOM.h**

/SPECTRAL_FILES/	
darwin_waterabsorbFile	
darwin_acdomFile	modified with RECOM_CALC_CDOM (Section 5.3)
darwin_particleabsorbFile	modified with RECOM_CALC_APART (Section 5.4)
darwin_phytoabsorbFile	modified with RECOM_CALC_APHYT (Section 5.2)
darwin_surfacespecFile	modified with OASIM (Section 6.2)

This default configuration can be modified enabling some of the other options.

5. Optical properties of constituents

wavebands_init_fixed.F reads the /SPECTRAL_FILES/ and extract input values for the optical properties of the difference constituents. This routine also computes the wavebands widths and total light width (wb_width and wb_totalWidth) used to compute wb-integrated and average values (e.g., PARlocal, alpha_mean, a_kave).

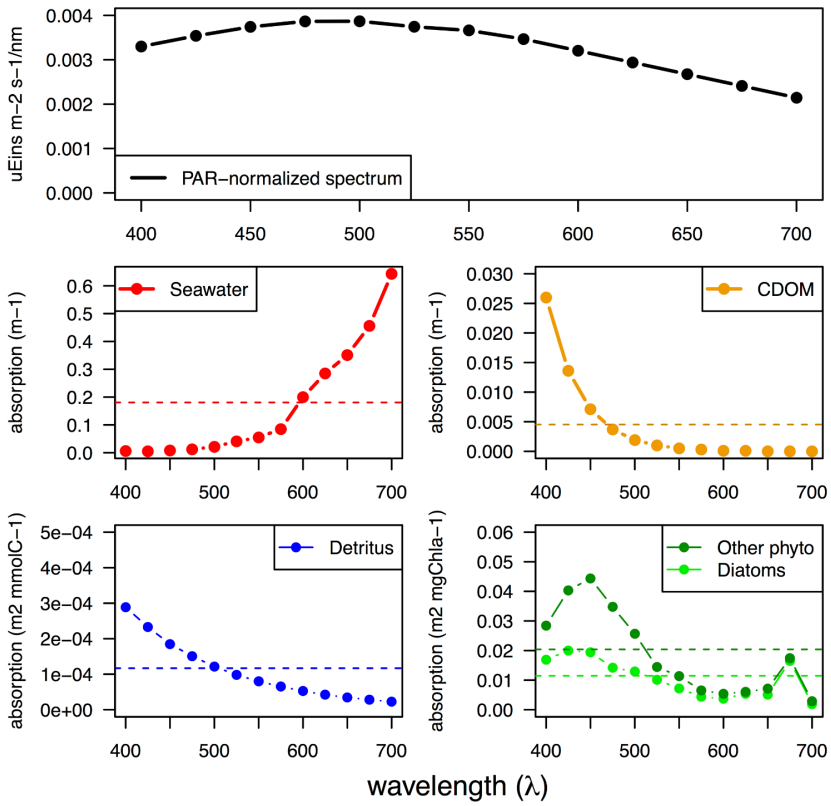

Figure 2. Spectral values in `/SPECTRAL_FILES/`. The surfacespecFile includes a PAR-normalized surface light spectrum (sf) to split single value PAR into spectral PAR at ocean surface (if OASIM input is not used). The files for water constituents indicate the values of absorption (and scattering and backscattering when relevant) for the center of the waveband (cdom and detritus) or for the waveband average (phyto).

5.1. Seawater

`darwin_waterabsorbFile`

Format: H6 (I5, F15.4, F10.4). Values: lambda (nm), absorption (m^{-1}), scatter (m^{-1}).

Example: /input/abw25par.dat

Source: Pope & Fry 1997, Smith & Baker 1981, Circio and Petty 1951, Maul 1985.

5.2. Phytoplankton

`darwin_phytoabsorbFile`

Format: H6 (I4, 3F10.4, F20.14). Values: lambda (nm), aph_chl (m^2 mg $Chla^{-1}$), aph_chl_psc (m^2 mg $Chla^{-1}$), scattering (m^2 mg $Chla^{-1}$), backscattering (m^2 mg $Chla^{-1}$)

Example: /input/phyto_optics_1bb_2groups_withbb.dat

Source: Hickman et al 2010, Gregg & Casey 2009, Moore et al 1993.

The phytoplankton file provides in the two first columns two values for absorption, both in m^2 $mgChla^{-1}$. ap (tnabp,λ) that sets absorption for all pigments and is used for light **attenuation**, and ap_ps(tnabp,λ) that sets the absorption only by photosynthetic pigments and is used for

phytoplankton **growth**. The third column is scattering and the fourth backscattering (computed from the backscattering ratio). Scattering can be provided in units of m^2 mg $Chla^{-1}$ (by default) or in units of m^2 $mmolC^{-1}$ (and defining at the same time RECOM_BMASS).

wavebands_init_vari.F assigns each type of absorption/scattering spectra to each phytoplankton group. In Darwin, npmax sets the number of phytoplankton groups and the absorption variables have one dimension npmax. Since REcoM have duplicated variables and parameters, one for diatoms and one for other phytoplankton, in this routine we split ap(tnabp,λ) into aphy_chl(λ) and aphy_chl_dia(λ), and ap_ps(tnabp,λ) into aphy_chl_ps(λ) and aphy_chl_ps_dia(λ).

recom_init_vari.F computes the actual slope of the production curve for each group, alpha_chl_nl(λ) and alpha_chl_nl_dia(λ), as absorption times efficiency of the photochemistry or quantum yield (QY). QY is set to different values to both phytoplankton groups, so the product of mean absorption by QY is equal to the value of alpha used in non-spectral REcoM2. The values for QYmax and QYmax_d are also set in `/DARWIN_SPECTRAL_PARM/`

`/DARWIN_SPECTRAL_PARM/`	
`QYmax=1.14D-4,`	Maximum photochemical efficiency non-diatoms
`Qymax_d=1.92D-4,`	Maximum photochemical efficiency diatoms
	(mmolC J-1)

Finally, an average value for alpha (alpha_mean) for each group is computed. These alpha_mean's should be comparable to the constant parameters alpha and alpha_d in non-spectral REcoM2.

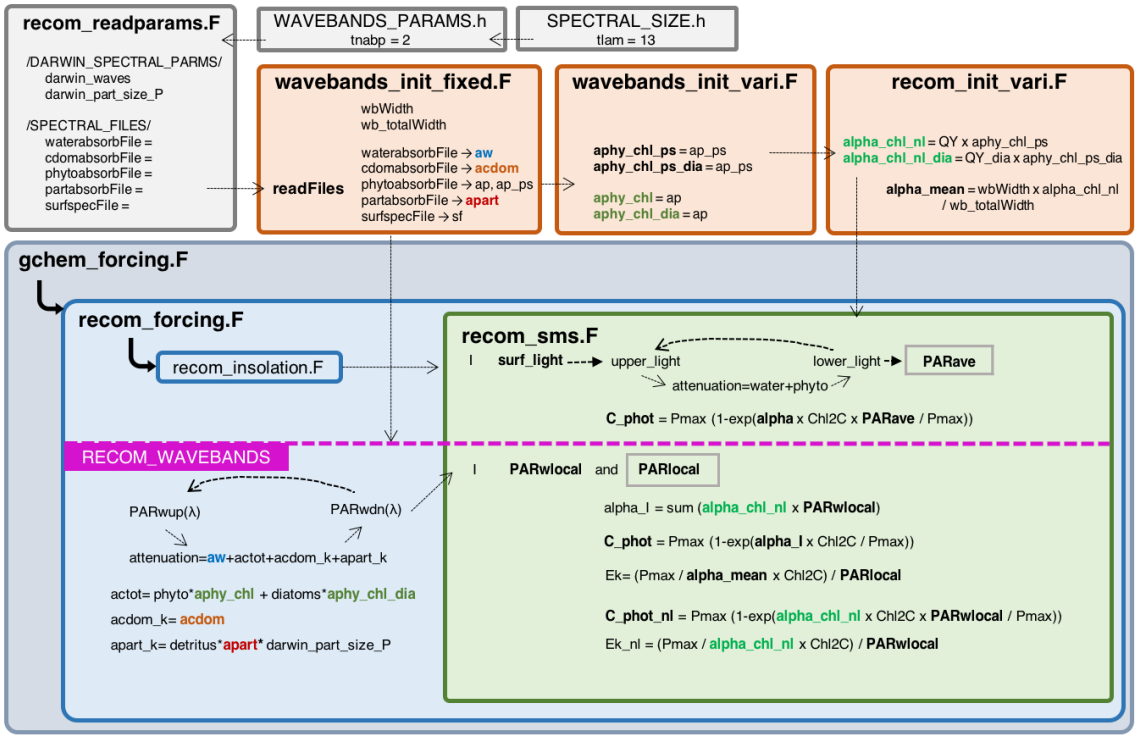

Figure 3. Default RECOM_WAVEBANDS taking optical properties of constituents from files in `/SPECTRAL_FILES/`.

For CDOM and detritus, in addition to read spectral properties from file, they can be calculated within the model using the options RECOM_CALC_ACDOM and RECOM_CALC_APART respectively. For phytoplankton, RECOM_CALC_APHYT can be set for calculating variable spectral properties for phytoplankton, but the file needs to be provided as well to prescribe the absorption of photosynthetic pigments, scattering and backscattering coefficients.

RECOM_CALC_APHYT

Under this option, the absorption by photosynthetic pigments, aphy_chl_ps(λ) and aphy_chl_ps_dia(λ), do not vary. As explained in section 5.2, these spectra are read from file (in **wavebands_init_fixed.F**) and assigned to each phytoplankton type (in **wavebands_init_vari.F**). On the other hand, total absorption, aphy_chl(λ) and aphy_chl_dia(λ), are modified based on the content of PPC:Chla of the respective phytoplankton type. To do that, the option RECOM_MARSHALL needs to be defined, as this option provides two additional state variables (id1 and id1d) that simulated the fraction of PSII active for photochemistry (active D1) for small phytoplankton and diatoms, respectively (Álvarez et al. 2019).

recom_forcing.F gets the values of these state variables (phyD1_k and diaD1_k) and pass them to **recom_aphyto_phy.F** and **recom_aphyto_dia.F**, respectively. From active D1, these routines compute the ratio PPC:Chla (PPC) and from PPC compute the spectral slope of the absorption spectrum between 488-532nm. The empirical relationships between the spectral slope of the absorption spectrum and the PPC:Chla ratio are obtained fitting a linear model to NOMAD v2 data (the slopes of the relationships are 0.00193 for small phyto and 0.00142 for diatoms). And finally, they reconstruct aphy_chl(λ) and aphy_chl_dia(λ) for wavebands equal or longer than 525nm. For wavebands longer than 525nm, aphy_chl(λ) is equal to aphy_chl_ps(λ) and aphy_chl_dia(λ) is equal to aphy_chl_ps_dia(λ).

Currently, the coefficients of the empirical relationship between the spectral slope of the absorption spectrum and the PPC:Chla ratio, as well as the wavelengths interval for the slope, are hardcoded. TO DO: put these values in a namelist and make the code find the closest wavebands to the interval of wavelengths for computing the spectral slope.

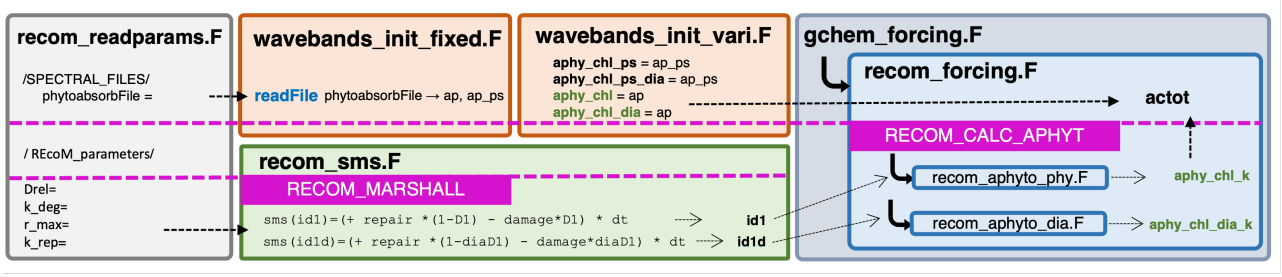

Figure 4. Option RECOM_CALC_APHYT.

5.3. CDOM

Optical properties of CDOM given in `darwin_acdomFile` assume constant contribution and hence are given in m^{-1}. The file only has one column because dissolved matter only absorbs, it does not scatter.

```
#ifndef RECOM_CALC_ACDOM
/SPECTRAL_FILES/
 darwin_acdomFile =
```

Format: H6 (F10.4). Values: absorption (m^{-1}).
Example: /input/aCDOM13amtVK2006.dat
Source: (Kitidis et al., 2006) (AMT13) (Hickman et al. 2010)

RECOM_CALC_ACDOM

With this option, absorption by CDOM is proportional to CDOM biomass. Absorption by CDOM (acdom) is calculated in **monod_acdom.F**. If RECOM_CDOM (ALLOW_CDOM in Darwin) is defined, acdom is computed from CDOM biomass, otherwise, acdom is computed from phytoplankton biomass and an additional parameter for converting phytoplankton to CDOM is required (default set to 20%). The computation is based on (Kitidis et al., 2006) that sets a biomass-specific value of absorption (`cdomcoeff`) at a reference wavelength (`darwin_lambda_aCDOM`) and a spectral slope (`darwin_Sdom`).

$$acdom = [\mathbf{C_{CDOM}}]*cdomcoeff *exp(-S*(\lambda-\lambda ref))$$

```
#ifdef RECOM_CALC_ACDOM
/DARWIN_SPECTRAL_PARM/
 darwin_Sdom = 0.021 nm-1
 darwin_lambda_aCDOM = 450
 cdomcoeff = 0.18 m2 mmolC

#ifndef RECOM_CDOM
 darwin_aCDOM_fac fac = 0.2
#endif
```

The exponential part of the function is computed in **wavebands_init_fixed.F.**

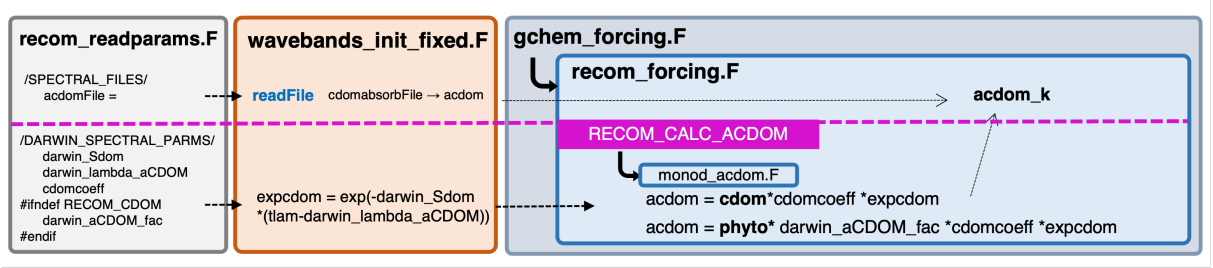

Figure 5. Option RECOM_CALC_ACDOM.

5.4. Detritus

In `darwin_particleabsorbFile`, the optical properties are given per particle (Stramski et al., 2001), hence an additional parameter to convert detritus biomass to particles needs to be provided. A value equivalent to the 1e-15 mmolP part^{-1} in (Dutkiewicz et al., 2015) is set as default.

#ifndef RECOM_CALC_APART	
/DARWIN_SPECTRAL_PARM/	
darwin_part_size_P=1.06e-13 mmolC part^{-1}	
/SPECTRAL_FILES/	
darwin_particleabsorbFile =	

Format: H6 (I4, 3E15.5). Values: lambda (nm), absorption (m^2 particle^{-1}), scattering (m^2 particle^{-1}), backscattering (m^2 particle^{-1}).

Example: /input/optics_detritus_3bb.dat

Source: (Stramski et al., 2001).

RECOM_CALC_APART

Under this option, optical properties of detritus are calculated from biomass-specific values taken from (Gallegos et al., 2011). This is the option used in (Gregg & Rousseaux, 2017). The computation of absorption needs a mass-specific value of absorption (`aparcoeff`) at a reference wavelength (`darwin_lambda_aPart`) and a spectral slope (`darwin_Sapar`).

apart = **[C_{DET}]** x aparcoeff x exp[-Sa x (λ-λref)]

The computation of scattering needs a mass-specific value of scattering (`bparcoeff`) at a reference wavelength (`darwin_lambda_bPart`) and a spectral exponent (`darwin_Sbpar`).

bpart = **[C_{DET}]** x bparcoeff x (λref/ λ)^Sb

#ifdef RECOM_CALC_APART	
/DARWIN_SPECTRAL_PARM/	
darwin_Sapar= 0.013 darwin_lambda_aPart= 440 aparcoeff =0.016 m^2 mmolC^{-1} darwin_Sbpar = 0.5 darwin_lambda_bPart = 550 bparcoeff = 0.345 m^2 mmolC^{-1} bb_to_b =0.05	

Similarly to CDOM, the exponential parts of the functions are computed in **wavebands_init_fixed.F**. Backscattering is computed in **recom_forcing.F** using the backacattering to total scattering ratio (bb_to_b).

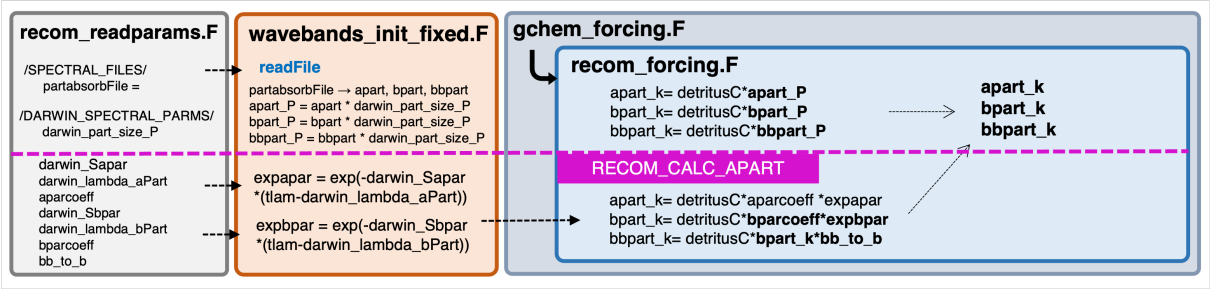

Figure 6. Option RECOM_CALC_APART.

6. Input light

There are two options for resolving spectrally the incoming light at surface. The default option is to use the same PAR as non-spectral REcoM2 and multiply it by a PAR-normalized spectrum. The other option, OASIM, provides spectral light as external forcing fields. In all cases light units are W m^{-2}, except for the light used to compute primary production where it is converted to µE m^{-2} s^{-1} with the function WtouEins(λ).

6.1. Light from short-wave downward solar radiation

Non-spectral REcoM2 computes PAR from the short-wave heat flux (Qsw) in **recom_insolation.F** in daily averages. To split incoming light into spectral light, it is necessary to provide a PAR-normalized surface light spectrum (µE m^{-2} s^{-1}/nm). It is specified in the `darwin_surfacespecFile`. It is read as *sf* and multiplies PARadiation in **recom_forcing.F**. Since *sf* is given in nm^{-1} it is necessary to convert it to per waveband multiplying by `wb_width(λ)`. Using this option as light input neglects the diffuse component at ocean surface.

`#ifndef OASIM`	
`/SPECTRAL_FILES/`	
`darwin_surfacespecFile =`	

Format: H3 (I5, F15.6)

Example: /input/surfspec_13amt6.dat

Source: (Hickman et al., 2010) (AMT13).

6.2. Light from OASIM

To get both direct and diffuse irradiance at surface we used the output of the OASIM model as forcing (Gregg & Casey, 2009).

6.2.1. Generate Ed and Es files

The option OASIM requires to provide one single file per waveband, so all they are 3D (x, y, time). TO DO: figuring out how to read directly 4D data into the model using EXF.

The original data are downloaded from the NASA-NOBM ftp (https://gmao.gsfc.nasa.gov/reanalysis/MERRA-NOBM/data/data_description.php). The spatial and temporal resolution are kept at 1°x1° and monthly means, the only pre-treatment to the data is to extract from each netCDF file the lambdas required and store the 12 monthly means of each lambda in a separate file. Additionally, a climatology averaging several years can be done. An R script that does that is available under `utils/R/generate_oasim_clim.R` It requires to specify the reading directory (where the original files are stored), the initial lambda, the final lambda, the initial year, the final year and the saving directory (where the final files will be stored).

6.2.2. Describing the files in data.recom

Comparably to other forcing fields specific to REcoM2, OASIM data files are defined in the namelist `/RECOM_PARMS01/` read by **RECOM.h**.

#ifdef OASIM	
/RECOM_PARMS01/	
darwin_oasim_edFile1 = darwin_oasim_edFile2 = … darwin_oasim_esFile1 = darwin_oasim_esFile2 = …	Ed_400_360x180x12_32b.bin Ed_425_360x180x12_32b.bin … Es_400_360x180x12_32b.bin Es_425_360x180x12_32b.bin …

If useEXF=.true., the start date and the period of the files need to be set under under the namelist `/RECOM_PARMS02/` read by **RECOM_EXF.h** The period can be given in seconds or as -12 for monthly means. If the option USE_EXF_INTERPOLATION is not used the input files must be user-interpolated to the model grid. Otherwise, the files can be given in any grid and they are interpolated on-the-fly to the model grid. This latter option requires to specify the dimensions of the input grid also under the namelist `/RECOM_PARMS02/`. These are the characteristics of the files provided in /input/:

useEXF = .true.	
/RECOM_PARMS02/	

OASIMstartdate1 = 00010115,
OASIMstartdate2 = 120000,
# OASIMperiod = 2592000., 	
OASIMperiod = -12,
# exf_inscal_OASIM = 1.0, 	
# exf_outscal_OASIM = 1.0, 	
	format: YYYYMMDD
	format: HHMMSS
	in seconds
	0 annual, -12 monthly
	optional re-scaling parameters

used in conjunction with EXF_USE_INTERPOLATION	

```
OASIM_lon0      = 0.5D0,
OASIM_lon_inc   = 1.0D0,
OASIM_nlon      = 360,
OASIM_lat0      = -89.5D0,
OASIM_lat_inc   = 179*1.,
OASIM_nlat      = 180,
```

recom_readparams.F reads both namelists from **RECOM.h** and **RECOM_EXF.h** respectively and gives default values. **recom_init_fixed.F** computes OASIMstartdate from OASIMstartdate1 (day) and OASIMstartdate2 (hour).

6.2.3. Loading external fields

The forcing fields where the input data will be stored (`oasim_ed` and `oasim_es`) are defined in **SPECTRAL.h** under the commonblock `/SPECTRAL_INPUT/`. Some auxiliary fields are defined under the commonblock `/SPECTRAL_INPUT_AUX/`.

/SPECTRAL_INPUT/	/SPECTRAL_INPUT_AUX/
oasim_ed (nx, ny, tlam) oasim_es (nx, ny, tlam)	oasim_ed0 (nx, ny, tlam) oasim_ed1 (nx, ny, tlam) oasim_es0 (nx, ny, tlam) oasim_es1 (nx, ny, tlam)

recom_init_vari.F initializes all the temporary fields (one per file) and finally, **recom_external_fields_load.F** (from darwin_fields_load.F) updates the fields for the current time step filling oasim_ed and oasim_es.

Oasim_ed and oasim_es are then used in **recom_forcing.F** as the source of light below ocean surface, assigning `oasim_ed` to Edwsf, `oasim_es` to Eswsf and total PAR at surface (PARwup) is the sum Edwsf +Eswsf.

Note: without using EXF, OASIM files are not read correctly. Maybe it is something to improve in the future, although not a priority now because ALLOW_EXF is always set to true.

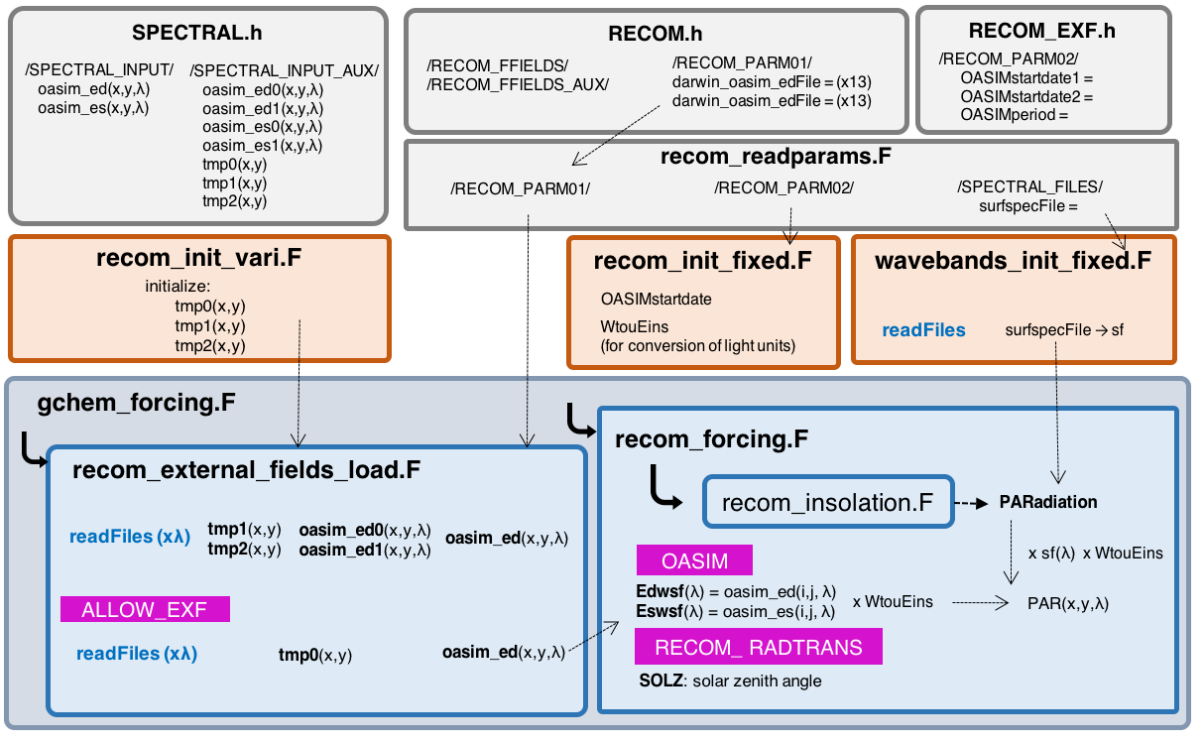

Figure 7. Light external forcing.

7. Light attenuation

Light attenuation is computed in **recom_forcing.F** (from monod_forcing.F).

7.1. Total absorption by constituent

First, it gathers the biomass of each component contributing to light attenuation using the names for tracers in REcoM2 (idetc, icdom, iphyc, ipchl, idiac and idchl). Then it gets the spectral absorption by each component, water (aw(λ)), cdom (acdom(λ)), particles (apart(λ)) and phytoplankton (aphy_chl(λ) and aphy_chl_dia(λ)).

7.2. Default light attenuation (RECOM_WAVEBANDS)

It computes total attenuation, and with it, it transforms PAR in the upper part of the layer into PAR in the lower part of the layer. With the two values, it computes the spectral PAR at the middle of the layer.

Attenuation by phytoplankton: actot(λ) = (aphy_chl(λ) x ipchl) + (aphy_chl_dia(λ) x idchl)

Total attenuation: a_k(λ) = aw(λ) + (acdom(λ) x icdom) + (apart(λ) x idetc) + actot(λ)

7.3. Full radiative transfer model (RECOM_RADTRANS)

The option RECOM_RADTRANS uses several new parameters set in `/DARWIN_SPECTRAL_PARM/` in **recom_readparams.F**

`#ifdef RECOM_RADTRANS`	
`/DARWIN_SPECTRAL_PARM/`	
`darwin_PAR_ilamLo = 1`	starting waveband index of PAR range
`darwin_PAR_ilamHi = tlam`	end waveband index of PAR range
`darwin_radmodThresh = 1e-4`	threshold for calling radmod
`darwin_Dmax = 500`	depth at which Ed is zero
`darwin_rmus = 1.0/0.83`	inverse average cosine of downward diffuse radiation
`darwin_rmuu = 1.0/0.4`	inverse average cosine of downward diffuse radiation
`darwin_bbmin = 0.0002`	minimum backscattering coefficient (not ratio)
`darwin_bbw = 0.5`	backscattering to forward scattering ratio for water
`darwin_bbphy(x2) = 0, 0`	backscattering to forward scattering ratio for Chlorophyll
`darwin_radtrans_kmax = Nr`	deepest layer to compute irradiances
`darwin_radtrans_niter = -2`	how to solve 3-stream equations: -2 means use direct solver (default) (see below for details).

Additionally to absorption, it needs the total scattering (bt_k) and total backscattering (bb_k) of constituents, that are passed together with total attenuation (a_k) to one of the routines to solve the 3-stream equations.

Scattering by phytoplankton: bctot(λ) = (bphy_chl(λ) x ipchl) + (bphy_chl_dia(λ) x idchl)

Total scattering: bt_k(λ) = bw(λ) + (bpart(λ) x idetc) + bctot(λ)

To resolve the 3-stream equations, RECOM_RADTRANS uses routines from the monod package (now in the code folder). The choice among the subroutines is set by the value of darwin_radtrans_niter. The default option is **monod_radtrans_direct.F** that is the method used in (Dutkiewicz et al., 2015).

monod_radtrans.F (`darwin_radtrans_niter = -1`)

Model of irradiance in the water column adapted from Watson Gregg's original (edeu.F). It accounts for three irradiance streams, all in Wm^{-2} per waveband: **Edz** (direct downwelling irradiance), **Esz** (diffuse downwelling irradiance) and **Euz** (diffuse upwelling irradiance). Propagation of these three streams is done in energy units and they are included in the output together with **Eutop** at the top of each layer. Also in the output are scalar radiance (**tirrq**) and PAR (**tirrwq**) at the grid cell center (both in $\mu Ein\ m^{-2}\ s^{-1}$) for phytoplankton growth. Conversion of unit is done with darwin_rmus.

monod_radtrans_iter.F (`darwin_radtrans_niter >= 0`)

It accounts for three irradiance streams, all in $W\ m^{-2}$ per waveband: **Edz** (=Edbot, direct downwelling irradiance), **Esz** (=Esbot, diffuse downwelling irradiance) and **Euz** (=Eubot, diffuse upwelling irradiance).
The Ed equation is integrated exactly. Es and Eu are first computed using a truncation to downward-decreasing modes as in (Aas, 1987) that makes Es continuous. Then, n iterations (prescribed by the value of `darwin_radtrans_niter`) alternating upward and downward integrations are performed, each time using Es at the top and Eu at the bottom of each layer as a boundary condition. The boundary condition in the deepest wet layer is always downward-decreasing modes only.
During upward integrations, Eu, and during downward integrations, Es, are made continuous respectively. At the end, Ed and Es are continuous, but Eu is so only approximately. Propagation is done in energy units. Ed, Es and Eu are included in the output together with **Eutop** at the top of each layer. Also in the output are scalar radiance (**tirrq**) and PAR (**tirrwq**) at the grid cell center (both in $\mu Ein\ m^{-2}\ s^{-1}$) for phytoplankton growth. Conversion of unit is done with WtouEins.

monod_radtrans_direct.F (`darwin_radtrans_niter <= -2`)

Model of irradiance in the water column that accounts for three irradiance streams (Ackleson et al., 1994), all defined at the bottom of each layer in $W\ m^{-2}$ per waveband: **Edz** (=Edbot, direct downwelling irradiance), **Esz** (=Esbot, diffuse downwelling irradiance) and **Euz** (=Eubot, diffuse upwelling irradiance).
Also computed are **Estop** and **Eutop** at the top of each layer which should be very close to Esbot and Eubot of the layer above. The Ed equation is integrated exactly, Es and Eu are computed by solving a set of linear equation for the amplitudes in the exact solution, see e.g. (Kylling et al., 1995). The boundary condition in the deepest wet layer is downward-decreasing modes only (i.e., zero irradiance at infinite depth, assuming the optical properties of the last layer). It needs the routine **solve_tridimensional_pivot.F** from monod, that needs to be in the

code folder.

Also in the output are scalar radiance (**tirrq**) and PAR (**tirrwq**) at the grid cell center (both in µEin m^{-2} s^{-1}) for phytoplankton growth. Conversion of unit is done with WtouEins.

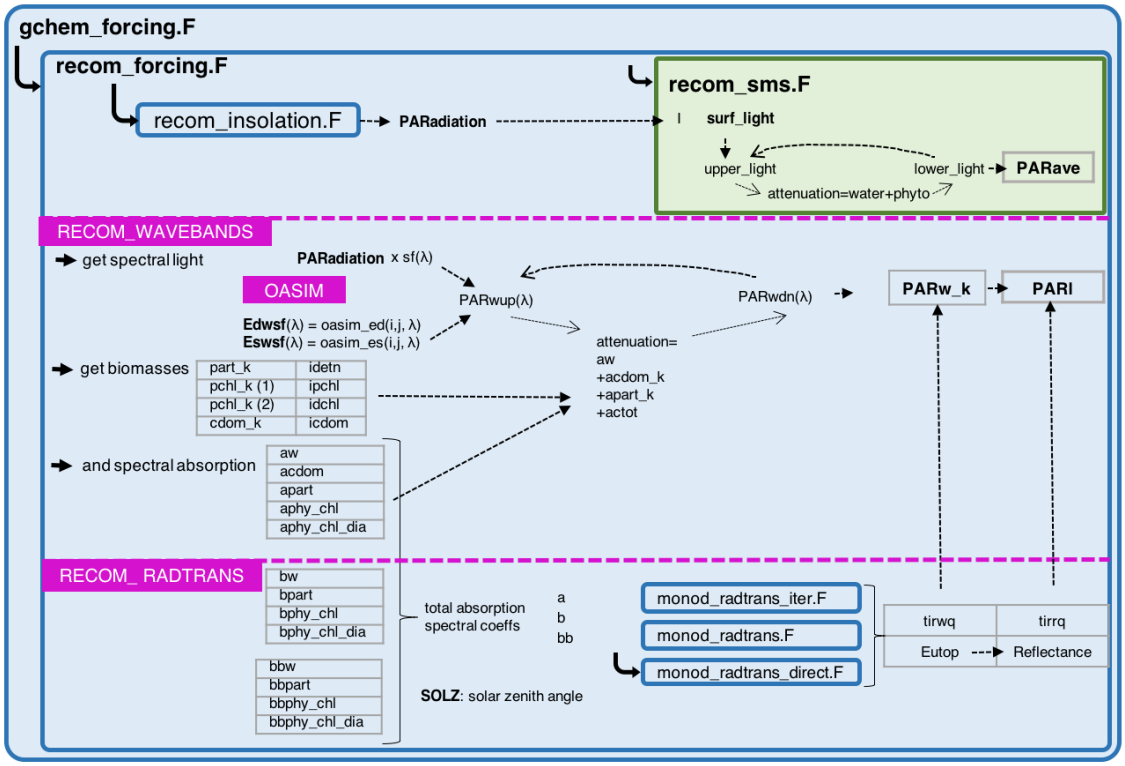

Figure 8. Details of light attenuation with and without RECOM_RADTRANS.

Any of the three routines resolves the upwelling stream of irradiance (Eutop), so, after resolving water column light penetration, surface reflectance is computed as the upwelling irradiance at the top of the most superficial layer relative to the incoming irradiance just below the surface and saved as a diagnostic (*reflecta*):

$$\text{Reflectance}(\lambda) = \text{Eutop}(\lambda)[k=1] / \text{Edwsf}(\lambda) + \text{Eswsf}(\lambda)$$

In order to compare to remotely sensed reflectance (Dutkiewicz et al., 2015) convert this model subsurface reflectance to slant upward radiance dividing by a bidirectional function Q. They assumed a constant value of Q=4 sr although in (Dutkiewicz et al., 2018) they considered Q=3 sr. This conversion is not done within the model.

8. Primary production

Once the spectral light at the middle of the cell is computed, the computation of primary production is common to all options. Darwin computes light at each layer in monod_forcing.F and then passes it to monod_plankton.F. We kept the same structure and therefore spectral light is computed in **recom_forcing.F** and passed to **recom_sms.F** as PARwlocal(λ) and the integral value as PARlocal (see Section 11 for timestep issues). The unit of light is μE m^{-2} s^{-1}.

The integration of light wavebands to production is made by integrating the product of alpha_chl_nl(λ) times PARwlocal(λ) to get alpha_I:

alpha_I = sum(alpha_chl_nl(λ) x PARwlocal(λ))

Cphot = Pmax x(1-exp(alpha_I x Chla:C/Pmax))

To keep coherence to non-spectral REcoM2 also the light limitation term is computed as:

llim = (1-exp(alpha_I x Chla:C/Pmax))

Also, PARave in non-spectral REcoM2 is used in other processes (damage of D1, photo-bleaching of CDOM, Fe ligands), so under RECOM_WAVEBANDS PARave is computed integrating PARwlocal(λ) over lambda and changing units to W m^{-2} with WtouEins(λ).

9. Available diagnostics

New diagnostic names exported under WAVEBANDS/RADTRANS are defined in **recom_diagnostics_init.F**. Diagnostics related to primary production that are computed in **recom_sms.F** are exported filling the array *recom_3Ddiags* (3) with the variable of interest in **recom_sms.F** and then filling the diagnostic name with the respective portion of the array in **recom_forcing.F**. Diagnostics related to light and absorption that are computed in **recom_forcing.F** are exported directly from this routine filling the diagnostic name with the variable of interest. Based on their dimensions, new diagnostics fall within three categories:

i) Diagnostic in the whole ocean: dimensions are longitude, latitude, depth (x,y,z) plus time. DiagCode is **MR** that indicates that the value is given for the middle of the cell in Nr levels. For spectral variables, that have an additional tlam dimension, diagnostic is exported as an average value (see Section 5 for details on how spectral average values are computed) or as the value in a specific waveband.
To export diagnostics in a specific waveband the option RECOM_CALC_REFLEC needs to be active and the desired waveband specified in the parameter `darwin_diag_acdom_ilam`. The default value is 450 nm.

`#ifdef RECOM_CALC_REFLEC`	
`/DARWIN_SPECTRAL_PARM/`	
`darwin_diag_acdom_ilam`	wavelength to export diagnostics

ii) Diagnostic in surface, spectrally resolved: dimensions are longitude, latitude and waveband (x,y,λ) plus time. DiagCode is **UX** that indicates that the value is given for the top of the cell in user-defined levels. Levels are set to tlam by calling to CALL DIAGNOSTICS_SETKLEV when defining the diagnostic name.

iii) Diagnostic for single value in surface: dimensions are longitude and latitude (x,y) plus time. DiagCode is **U1** that indicates that the value is given for the top of the cell only in the first level.

This is the complete list of diagnostics, the first 15 are common to all options.

```
-------------------------------------------------------------------------------
Num |<-Name->|Levs|mate|<- code ->|<-- Units -->|<- Tile (max=80c)
-------------------------------------------------------------------------------
621 |par3dw  | 30 |    |SM      MR|uE/m^2/s-1  |average spectral PAR
622 |Ek_phy  | 30 |    |SM      MR|            |phytoplankton spectral light saturation
623 |Ek_dia  | 30 |    |SM      MR|            |diatom spectral light saturation
624 |abtotave| 30 |    |SM      MR|m-1         |absorption total average
625 |acdomave| 30 |    |SM      MR|m-1         |absorption by cdom average
626 |abparave| 30 |    |SM      MR|m-1         |absorption by detritus average
627 |abphyave| 30 |    |SM      MR|m-1         |absorption by phytoplankton average
655 |abtotsur| 13 |    |SM      MX|m-1         |absorption total in surface
656 |acdomsur| 13 |    |SM      MX|m-1         |absorption by cdom in surface
657 |abparsur| 13 |    |SM      MX|m-1         |absorption by detritus in surface
658 |abphysur| 13 |    |SM      MX|m-1         |absorption by phytoplankton in surface
652 |par3doa | 13 |    |SM      UX|uE/m-2/s-1  |spectral PAR below surface
653 |edirect | 13 |    |SM      UX|W/m-2       |direct irradiance below surface
654 |ediffuse| 13 |    |SM      UX|W/m-2       |diffuse irradiance below surface
683 |par2doa |  1 |    |SM      U1|uE/m-2/s-1  |total PAR below surface
```

#ifdef RECOM_CALC_REFLEC

```
628 |par3d_wb| 30 |    |SM      MR|uE/m^2/s-1 |Light at selected wb
629 |abtot_wb| 30 |    |SM      MR|m-1       |absorption total at selected wb
630 |acdom_wb| 30 |    |SM      MR|m-1       |absorption by cdom at selected wb
631 |abpar_wb| 30 |    |SM      MR|m-1       |absorption by detritus at selected wb
632 |abphy_wb| 30 |    |SM      MR|m-1       |absorption by phytoplankton at selected wb
```

#ifdef RECOM_RADTRANS

```
633 |bttotave| 30 |    |SM      MR|m-1        |scattering total average
634 |btparave| 30 |    |SM      MR|m-1        |scattering by detritus average
635 |btphyave| 30 |    |SM      MR|m-1        |scattering by phytoplankton average
636 |bbtotave| 30 |    |SM      MR|m-1        |backscattering total average
637 |bbparave| 30 |    |SM      MR|m-1        |backscattering by detritus average
638 |bbphyave| 30 |    |SM      MR|m-1        |backscattering by phytoplankton average
661 |bttotsur| 13 |    |SM      MX|m-1        |scattering total in surface
662 |btparsur| 13 |    |SM      MX|m-1        |scattering by detritus in surface
663 |btphysur| 13 |    |SM      MX|m-1        |scattering by phytoplankton in surface
664 |bbtotsur| 13 |    |SM      MX|m-1        |backscattering total in surface
665 |bbparsur| 13 |    |SM      MX|m-1        |backscattering by detritus in surface
666 |bbphysur| 13 |    |SM      MX|m-1       |backscattering by phytoplankton in surface
659 |euptop  | 13 |    |SM      UX|W/m-2       |water-leaving irradiance
660 |reflecta| 13 |    |SM      UX|            |Reflectance
682 |rmudave |  1 |    |SM      U1|            |Inverse cosine zenith solar angle
```

#ifdef RECOM_CALC_REFLEC

```
639 |bttot_wb| 30 |    |SM      MR|m-1     |scattering total at selected wb
640 |btpar_wb| 30 |    |SM      MR|m-1     |scattering by detritus at selected wb
641 |btphy_wb| 30 |    |SM      MR|m-1     |scattering by phytoplankton at selected wb
642 |bbtot_wb| 30 |    |SM      MR|m-1     |backscattering total at selected wb
643 |bbpar_wb| 30 |    |SM      MR|m-1     |backscattering by detritus at selected wb
644 |bbphy_wb| 30 |    |SM      MR|m-1   |backscattering by phytoplankton at selected wb
645 |Edz_wb  | 30 |    |SM      LR|W m-2   |Ed at the bottom of the layer at selected wb
646 |Esz_wb  | 30 |    |SM      LR|W m-2   |Es at the bottom of the layer at selected wb
647 |Euz_wb  | 30 |    |SM      LR|W m-2   |Eu at the bottom of the layer at selected wb
648 |Estop_wb| 30 |    |SM      UR|W m-2   |Es at the top of the layer at selected wb
649 |Eutop_wb| 30 |    |SM      UR|W m-2   |Eu at the top of the layer at selected wb
650 |amp1_wb | 30 |    |SM      MR||amplitude of downward increasing mode at selected wb
651 |amp2_wb | 30 |    |SM      MR||amplitude of downward decreasing mode at selected wb
```

Other diagnostics to check:

```
646 |PARSURF |  1 |    |SM      U1|W/m-2 |Surface Photosynthetically Available Radiation
601 |par3d   | 30 |    |SM      MR|W/m^2        |photosynthetically available radiation
604 |llimdia | 30 |    |SM      MR|             |diatom light limitation
605 |llimphy | 30 |    |SM      MR|             |small phytoplankton light limitation
583 |gr_pps  | 30 |    |SM      MR|mmol/m^3/d   |small Phy gross primary production
584 |gr_ppd  | 30 |    |SM      MR|mmol/m^3/d   |diatom gross primary production
```

if used RECOM_PHOTODAMAGE:

```
613 |pphotdia | 30 |   |SM     MR|d-1       |photosynthesis rate diatoms
614 |pphotphy | 30 |   |SM     MR|d-1       |photosynthesis rate small phytoplankton
615 |ppmaxdia | 30 |   |SM     MR|d-1       |max photosynthesis rate diatoms
616 |ppmaxphy | 30 |   |SM     MR|d-1       |max photosynthesis rate small phytoplankton
617 |chlsydia | 30 |   |SM     MR|gChl/molC/d |chla synthesis rate diatom
618 |chlsyphy | 30 |   |SM     MR|gChl/molC/d |chla synthesis rate small phytoplankton
619 |kochldia | 30 |   |SM     MR|gChl/molC/d |degradation rate chla diatoms
620 |kochlphy | 30 |   |SM     MR|gChl/molC/d |degradation rate chal small phyto
```

if used RECOM_MARSHALL:

```
651 |alphaphy| 30 |    |SM     MR|m2 molC gChl-1 J  |initial slope PE Phyto Marshall
652 |alphadia| 30 |    |SM     MR|m2 molC gChl-1 J  |initial slope PE Diatoms Marshall
653 |ppcphy  | 30 |    |SM     MR|                  |ratio PPC:Chla small phyto
654 |ppcdia  | 30 |    |SM     MR|                  |ratio PPC:Chla diatoms
```

10. Run-time parameters

Run-time parameters are set in file **data.recom** which is read in **recom_readparms.F**. Run-time parameters are split into 4 categories:

`&DARWIN_SPECTRAL_PARM`: general flags and parameters

```
darwin_waves = 400,425,450,475,500,525,550,575,600,625,650,675,700
darwin_wavebands = 14*-1
darwin_part_size_P = 1.06e-13
darwin_Sdom = 0.021
darwin_lambda_aCDOM = 450
cdomcoeff = 0.18
darwin_aCDOM_fac fac = 0.2
darwin_Sapar= 0.013
darwin_lambda_aPart= 440
aparcoeff =0.016
darwin_Sbpar = 0.5
darwin_lambda_bPart = 550
bparcoeff = 0.345
bb_to_b =0.05
darwin_PAR_ilamLo = 1
darwin_PAR_ilamHi = tlam
darwin_radmodThresh = 1e-4
darwin_Dmax = 500
darwin_rmus = 1.0/0.83
darwin_rmuu = 1.0/0.4
darwin_bbmin = 0.0002
darwin_bbw = 0.5
darwin_bbphy(x2) = 0, 0
darwin_radtrans_kmax = Nr
darwin_radtrans_niter = -2
darwin_diag_acdom_ilam = 450
```

&SPECTRAL_FILES: names spectral files

```
darwin_waterabsorbFile='abw25par.dat',
darwin_phytoabsorbFile='optics_phyto_recom_carbon.dat'
darwin_particleabsorbFile='optics_detritus_3bb.dat'
darwin_acdomFile='aCDOM13amtVK2006.dat'
darwin_surfacespecFile='surfspec_13amt6.dat'
```

&RECOM_PARM01: names forcing and climatological fields

```
darwin_oasim_edFile01 = 'Ed_400_360x180x12_32b.bin'
darwin_oasim_edFile02 = 'Ed_425_360x180x12_32b.bin'
...
darwin_oasim_esFile01 = 'Es_400_360x180x12_32b.bin'
darwin_oasim_esFile02 = 'Es_425_360x180x12_32b.bin'
...
```

&RECOM_PARM02: attributes for each forcing and climatological field

```
OASIMstartdate1 = 00010115
OASIMstartdate2 = 120000
OASIMperiod     = -12
exf_inscal_OASIM = 1.0
exf_outscal_OASIM = 1.0
```

used in conjunction with EXF_USE_INTERPOLATION

```
OASIM_nlon      = 360
OASIM_nlat      = 180
OASIM_lon0      = 0.5D0
OASIM_lon_inc   = 1.0
OASIM_lat0      = -89.5D0
OASIM_lat_inc   = 179*1.0
```

11. Last remarks, improvements, code cleanup.

Code location

Original Darwin Monod code:

https://doi.org/10.7910/DVN/R12GTM

REcoM2 code modifications:

https://github.com/ealvarez-s/code_recom_radtrans.git

Runtime configuration files:

https://github.com/ealvarez-s/global_aphyt.git

Vector machines

At compiling time, there were some warnings about vectorization (in Stan). Simulations run but are very slow. Loops were reorganized following S. Losa instructions: loops over depth and lambda in the outer part and loops over the horizontal grid in the inner part. After the modifications, there was some time saving but not large. UPDATE: this issue has not been encountered in (Ollie, GALILEO and G100).

OASIM forcing files

Forcing fields for spectral light in surface need four dimensions, x, y, tlam and time. I couldn't figure out how to read 4D fields with EXF, so I used one forcing field per waveband (x,y,time), reading one by one 13+13 files, and stacking them in oasim_ed(x,y,tlam) and oasim_es(x,y,tlam).

Time lag between light and biology

Standard REcoM2 computes light attenuation and biology both in **recom_sms.F** and hence for the current timestep. Under WAVEBANDS/RADTRANDS light attenuation is computed in **recom_forcing.F** and passed to **recom_sms.F**, hence the concentrations used to compute attenuation and the resultant light are from the previous timestep. I guess this can be acceptable as long as the timestep is kept small.

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