NEMO-PISCES 1D demonstration guide

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This document is a demonstration guide of the PISCES marine biogeochemistry model using a 1D configuration of the NEMO-PISCES model. The document describes the various steps required to install and run the code of the 1D configuration of NEMO-PISCES at the BATS station. The instructions given here can be adapted to different ocean stations by changing the bathymetry, station coordinates, initial conditions and forcing files.

1. Brief description of PISCES

PISCES is constructed based on the assumption that phytoplankton growth is directly limited by the external availability of nutrients (Monod, 1942). This choice was mostly dictated by the computing cost as PISCES has been designed to suit a wide range of temporal and spatial scales, including quasi steady-state simulations on the global scale.

The model has 24 compartments (Figure 1). Phytoplankton growth can be limited by five different nutrients: nitrate, ammonium, phosphate, silicate and iron. Four living pools are represented: two phytoplankton size classes/groups (nanophytoplankton and diatoms) and two zooplankton size classes (microzooplankton and mesozooplankton). Diatoms differ from nanophytoplankton by their need for Si, by higher requirements in Fe (Sunda and Huntsman, 1995) and by higher half-saturation constants because of their larger mean size. For all living compartments, the ratios between C, N and P are kept constant to the values proposed by Takahashi et al. (1985). On the other hand, the internal contents in Fe of both phytoplankton groups and in Si of diatoms are prognostically simulated as a function of the external concentrations in nutrients and of the light level. The Chl/C ratio is modeled using a modified version of the photoadaptation model by Geider et al. (1998). All the elemental ratios of zooplankton are kept constant.

There are three non-living compartments: semi labile dissolved organic matter (with timescales of several weeks to several years), small and big sinking particles. The two particle size classes differ by their sinking speeds (2 m/d for the small size class and 50 to 200 m/d for the large size class). As for the living compartments, constant Redfield ratios are imposed for C/N/P. However, the iron, silicon and calcite pools of the particles are fully simulated. As a consequence, their ratios relative to organic carbon are allowed to vary. The impact of ballast minerals on particles' sinking speeds is not accounted for in the model (e.g., Armstrong et al., 2002).

Nutrients are supplied to the ocean from three different sources: atmospheric dust deposition, rivers and sediment mobilization. These sources are explicitly modeled and are extensively described in Aumont et al. (2015). Thus only the main aspects are presented here. The model considers the atmospheric supply of iron (Fe), silicon (Si), phosphorus (P), and nitrogen (N) elements. The aforementioned three sources have been estimated from climatological monthly maps of dust deposition simulated by the model of Tegen and Fung (1995) assuming constant values for the iron content and the solubility (e.g., Jickells and Spokes, 2001; Moore et al., 2004). River discharge of carbon is taken from the Global Erosion Model of Ludwig et al. (1996). Iron, N, P and Si supplies are derived from the same model output by considering globally constant Fe/P/N/Si/C ratios in the rivers. Reductive mobilization of iron from marine sediments has been recognized as a significant source to the ocean (e.g., Johnson et al., 1999; de Baar and de Jong, 2001). Unfortunately, almost no quantitative information is available to describe this potentially important source. In a way similar to Moore et al. (2004), we have very crudely parameterized this input of iron.





PISCES has been used, at the global scale, to study past climates (Bopp et al. 2003), to understand the mechanisms that explain interannual variability in marine productivity (Aumont et al. 2008) or ocean-atmosphere carbon fluxes (Rodgers et al. 2008), to assess the impact of climate change or ocean acidification on marine ecosystems and air-sea carbon fluxes (Bopp et al. 2001, Orr et al. 2005) and to evaluate geo-engineering strategies to mitigate climate change (Aumont and Bopp, 2006, Dutreuil et al. 2009).

2. The 1D vertical configuration NEMO-PISCES

In this demonstrator, we use a 1-D (vertical) configuration of NEMO-PISCES using the official NEMO release version 4.2.

The one-dimensional vertical model only considers the vertical -z, sigma or partial steps - coordinate and time as independent variables in the primitive equations, with no horizontal variations. All horizontal derivatives are set to zero. Thus, in this one-dimensional vertical configuration, there is no (both lateral and vertical) advection, no lateral mixing on tracers nor dynamics.

Temperature and salinity are thus only controlled by vertical diffusion equations and the density, needed for the turbulent mixing closure scheme, is computed using an equation of state of sea water:

•
$$\partial_t T = \partial_z (K_z \partial_z T) + 1/(\rho C_p) F(z)$$

with F(z) representing the penetrating solar flux. Bulk flux surface boundary conditions for T(z=0,t) are imposed (not detailed here). Vertical advection of temperature is not taken into account ($\partial_z(w,T) = 0$) as w=0 over the entire water column. The vertical mixing coefficient K_z is computed using a vertical mixing scheme (not detailed here) depending on the option selected in the dynamical namelist (Turbulent Kinetic Energy (TKE), K-profile-parameterization (KPP), Richardson or constant vertical mixing).

•
$$\partial_t S = \partial_z (K_z \partial_z S)$$

Surface boundary conditions for S(z=0,t) are applied (not detailed here).

For passive biogeochemical tracers C(z,t), only biogeochemical sources and sinks are taken into account together with vertical diffusion processes:

•
$$\partial_t C = \partial_z (K \partial_z C) + SMS_{bio}(z, t)$$

SMS_bio means "sources" minus "sinks". Surface boundary conditions are applied depending on the biogeochemical tracer (see Aumont et al., 2015 for details).

Information on the NEMO and PISCES namelists and parameters can be found at:

- NEMO-OCE : <u>https://doi.org/10.5281/zenodo.6334656</u>
- NEMO-MBG : <u>https://doi.org/10.5281/zenodo.1471700</u>

The 1D Station :

For this demonstrator, we will focus on one of the Joint Global Ocean Flux Study sites (<u>http://ijgofs.whoi.edu/</u>): the BATS station (Figure 2).

BATS : (64°W, 31.5°N)

http://bats.bios.edu/

However, the 1D model configuration can also be implemented at the following sites:

NABE : (20°W, 47°N) http://usjgofs.whoi.edu/research/nabe.html

HOT : (158°W, 22.45°N) http://hahana.soest.hawaii.edu/hot/

DYFAMED : (7.52°E, 43.27°N) http://www.obs-vlfr.fr/cd_rom_dmtt/sodyf_main.htm

KERFIX (68.25°E, 50.40°S) : http://www.obs-vlfr.fr/cd_rom_dmtt/OTHER/KERFIX/bacteries/kfx_bact_delille.htm.ht m



Figure 2: Mean SST from World Ocean Atlas and position of JGOFS sites

MODEL CONFIGURATION SET UP

1. System prerequisites

- Netcdf package installed on your computing machine
- XIOS package installed on your computing machine
- An arch file set to your computing machine (this just sets paths to XIOS, netcdf and the compiling option which depends on your compiler)

Information to install the necessary environment (libraries, dependencies) to run the NEMO ocean model on your computing machine can be found at : https://forge.ipsl.jussieu.fr/nemo/chrome/site/doc/NEMO/guide/html/install.html

2. Provided :

- Ocean and biogeochemical boundary and initial conditions and atmospheric forcing at the BATS station
- Namelists of the 1D NEMO-PISCES configuration adapted to the BATS station

You need to copy the tarball of the provided files to the working directory of your computing machine and extract the contents:

• tar xvzf PISCES Demonstrator.tgz

A PISCES_demonstrator folder should be installed in your working directory (i.e., \$WORK/PISCES_Demonstrator/).

3. Instructions

3.1 Compile XIOS

The outputs of NEMO are managed by the external library XIOS. This library allows a lot of flexibility in the choice of the output variables and output frequencies (amongst other things).

Information on the XIOS library can be found at : https://forge.ipsl.jussieu.fr/ioserver

Before running NEMO, we need to first compile the XIOS library.

 Connect to your computing system and go to your working directory and download the XIOS library :

```
cd $WORK
svn co http://forge.ipsl.jussieu.fr/ioserver/svn/XIOS/trunk@2331 xios
```

• Setup your arch files (one for the environment (.env), another for the compiler (.fcm) and a last one for the path (.path)):

```
cd $WORK/xios/arch
```

In the arch directory, examples of arch files can be found, e.g., arch-X64 JEANZAY.*

• Compile XIOS referring to the set of your arch files (example here for X64 JEANZAY):

```
cd $WORK/xios/
./make xios --arch X64 JEANZAY --full --prod --job 8
```

XIOS is now compiled.

3.2 Compile and create NEMO executable

Before running NEMO-PISCES, you need to compile the code on your computing machine.

• Get the NEMO code by cloning the gitlab repository :

```
cd $WORK
git clone https://forge.nemo-ocean.eu/nemo/nemo.git nemo-4.2.0
cd nemo-4.2.0
git switch --detach 4.2.0
```

In the nemo, directory, you can see the first level tree structure of NEMO :

- arch contains the compilation settings
- cfgs contains the reference configurations of NEMO
- doc contains the documentation
- ext contains external dependencies, e.g., the two-way nesting package of AGRIF
- mk contains the compilation scripts
- src contains the Fortran model routines, ie.e, the source code
- tests contains idealized test-cases
- tools contains the pre and post-processing tools

As for XIOS, you need to set the arch file relative to your computing machine environment to compile NEMO. See the NEMO user guide for instructions on setting up your archive file:

https://sites.nemo-ocean.io/user-guide/install.html#download-and-install-the-nemo-co de

here we used the arch/CNRS/arch-X64 JEANZAY.fcm

- In your arch file, you must ensure that the path to xios refers to your xios directory (i.e., \$WORK/xios). Indeed, as NEMO is compiled with the XIOS library, the makenemo compilation script refers to this arch file to create the executable.
- Create and compile the code for the 1D configuration :

The 1D configuration is made upon the reference NEMO configuration C1D_PAPA in which the horizontal and vertical grids are defined.

```
./makenemo -n ORCA_1D_PISCES -r GYRE_PISCES -m X64_JEANZAY -j 0
cp $WORK/PISCES_Demonstrator/MY_SRC/*
cfgs/ORCA_1D_PISCES/MY_SRC/.
cp cfgs/C1D_PAPA/MY_SRC/* cfgs/ORCA_1D_PISCES/MY_SRC/.
./makenemo -n ORCA 1D PISCES -r GYRE PISCES -m X64 JEANZAY -j 4
```

4. The NEMO-PISCES 1D configuration

In the 1-D configuration, the size of the domain is 1x1x75, 75 being the number of vertical levels. The user must set several parameters in the namelist of the configuration (namelist cfg):

- the ln_cld flag to .true.
- the longitude (rn_lon1d) and latitude (rn_lat1d) coordinates of the station
- the depth of the ocean at the given point rn bathy.

Input data (initial state and forcings) at the location under consideration are required, initial states being set to values of dimension 1x1x75.

Note that in the following, the settings of the 1D configuration namelists have already been made.

Go to the run directory for the BATS station :

```
cd $WORK/PISCES_Demonstrator/BATS/
```

Explore the run directory and observe the 1D station-specific configuration settings in the namelist files :

• namelist_cfg

This namelist file contains information about the configuration, initial conditions and the forcing of the physics (temperature, salinity and vertical mixing scheme):

- The ocean depth at the station:

```
!-----
&namusr_def ! GYRE user defined namelist
!-----
rn_bathy = 4556. ! depth in meters
/
```

- The geographical coordinates of the station:

- The initialisation files of seawater temperature and salinity at the station:

&namtsd	! Temperature & Sal	inity Data (init/dmp	(default: OFF)						
! ln_tsd_ir	! =T read nit = .true. ! o	T-S fields for: cean initialisation							
cn_dir	= './' ! root di	rectory for the T-S d	ata location						
!	! file name	! frequency (hours)	! variable	! time interp.!	clim ! 'year	'ly'/ !			

- The forcing atmospheric files at the station:

! &namsbc_blk	! namsbc_blk	generic Bulk form	ula	(ln_blk	=T)		
! ln_NCAR	! bulk = .true. ! "N	algorithm : ICAR" algorith	nm (Large and Yea	ager 2008)			
cn_dir =	'./' ! root direc	tory for the bulk	data location				
!	!	!		!		!	!!
!	! file nam	le !	frequency (hours)	! variable	! time interp.	! clim	! 'yearly'/ !
!	!	!	(if <0 months)	! name	(logical)	! (T/F)	! 'monthly' !
sn_wndi	= 'CORE2_NY_Forc	ings_6h_BATS.nc',	6.	, 'U_10_MOD'	, .false.	, .true.	, 'yearly',
sn_wndj	<pre>= 'CORE2_NY_Forc</pre>	ings_6h_BATS.nc',	6.	, 'V_10_MOD'	.false.	, .true.	, 'yearly' ,
sn_qsr	<pre>= 'CORE2_NY_Forc</pre>	ings_1d_BATS.nc',	24.	, 'SWDN_MOD'	.false.	, .true.	, 'yearly' ,
sn_qlw	<pre>= 'CORE2_NY_Forc</pre>	ings_1d_BATS.nc',	24.	, 'LWDN_MOD'	.false.	, .true.	, 'yearly' ,
sn_tair	= 'CORE2_NY_Forc	ings_6h_BATS.nc',	6.	, 'T_10_MOD'	, .false.	, .true.	, 'yearly' ,
sn_humi	= 'CORE2_NY_Forc	ings_6h_BATS.nc',	6.	, 'Q_10_MOD'	, .false.	, .true.	, 'yearly' ,
sn_prec	= 'CORE2_NY_Forc	ings_1m_BATS.nc',	-1.	, 'PRC_MOD1'	.false.	, .true.	, 'yearly' ,
sn_snow	= 'CORE2_NY_Forc	ings_1m_BATS.nc',	-1.	, 'SNOW'	.false.	, .true.	, 'yearly' ,
sn_slp	= 'CORE2_NY_Forc	ings_6h_BATS.nc',	6.	, 'SLP'	, .false.	, .true.	, 'yearly' ,

1

- The Chlorophyll for bio penetration:

&namtra_qsr	! penetrative	e solar radiation		(ln_traqsr =T)								
! ! ln_qsr_rgb	! = .true. !	type of penetration RGB light penetratio	on (Red-Green	(defaul -Blue)	t: NO selection)							
cn_dir !	= './' !	root directory for the	e chlorophyl (data location	!							
! ! sn_chl	! file name ! ='CHLA_BATS'	! frequency (hours) ! (if <0 months) , -1.	variable ! ! name ! , 'CHLA' ,	time interp.! (logical) ! .true. , .	clim ! 'yearly'/ (T/F) ! 'monthly' true. , 'yearly'							

• namelist_top_cfg

This namelist file contains information about the initial conditions and forcings of the biogeochemistry :

- PISCES initial data files

&n	amtrc_dta	ļ	Initialisation from data inp	put	t file									
!		!	file namei	!	frequency (hours)	!	- variable	!	time interp.	ļ	clim	ļ	'yearly'/	!
!		1		!	(if <0 months)	!	name	!	(logical)	!	(T/F)	!	'monthly'	!
	sn_trcdta(1)	=	'Glodapv2.1_annual_175_BATS.nc'	١,	-12.	,	'TDIC'	,	.false.	,	.true.	,	'yearly'	,
	sn_trcdta(2)	=	'Glodapv2.1_annual_175_BATS.nc'	١,	-12.	,	'Alkalini'	,	.false.	,	.true.	,	'yearly'	,
	sn_trcdta(3)	=	'WOA2009_monthly_175_BATS.nc'	,	-1.	,	'02'	,	.true.	,	.true.	,	'yearly'	,
	sn_trcdta(5)	=	'WOA2009_monthly_175_BATS.nc'	,	-1.	,	'P04'	,	.true.	,	.true.	,	'yearly'	,
	sn_trcdta(7)	=	'WOA2009_monthly_175_BATS.nc'	,	-1.	,	'Si'	,	.true.	,	.true.	,	'yearly'	,
	sn_trcdta(10)	=	'PISCES_monthly_175_BATS.nc'	,	-1.	,	'DOC'	,	.true.	,	.true.	,	'yearly'	,
	sn_trcdta(14)	=	'PISCES_monthly_175_BATS.nc'	,	-1.	,	'Fer'	,	.true.	,	.true.	,	'yearly'	,
	sn_trcdta(23)	=	'WOA2009_monthly_175_BATS.nc' ,	,	-1.	,	'NO3'	,	.true.	,	.true.	,	'yearly'	,

- Nutrients from external inputs (dust and nitrogen deposition at surface)

! &namtrc_bc !	!	data for bound	lary	conditions									
! ! sn_trcsbc(5)	! ! =	file name 'DustNew_BATS'	! ! ,	frequency (hours) (if <0 months) -1	! !	variable name 'dustpo4'	! ! ,	time interp. (logical) .true.	! !	clim (T/F) .true.	! !	'yearly'/ 'monthly' 'yearly'	! !
sn_trcsbc(7) sn_trcsbc(14) sn_trcsbc(23)	= = =	'DustNew_BATS' 'DustNew_BATS' 'Ndep_BATS'	, , ,	-1 -1 -12	, ,	'dustsi' 'dustfer' 'ndep2'	, , ,	.true. .true. .false.	, , ,	.true. .true. .true.	, , ,	'yearly' 'yearly' 'yearly'	, , ,

- Flag to disable advection & lateral diffusion

• The namelist_pisces_cfg

This namelist contains the input files for photosynthetically available radiation (PAR) and other nutrients, possible PISCES options and parameter values (not detailed)

- PAR from a file at the station

```
knampisopt ! parameters for optics
sn_par = 'par_fr_gewex_clim_BATS.nc' , 24. , 'fr_par' ,
cn_dir = './' ! root directory for the location of the dynamical files
ln_varpar = .true. ! boolean for PAR variable
parlux = 0.43 ! Fraction of shortwave as PAR
```

- Nutrients from external inputs (iron from sediments, sea ice, hydrothermal vents,...)

knampisbc	! parameters for inputs deposition														
sn_dust sn_ironsed ln_ironsed	! fil ! = 'Dus = 'pmc = .tr	e name :tNew_BATS' irge_etopo_BATS iue. ! boolec	! ! ;',	frequency (hours) (if <0 months) -1 -12. or Fe input from	! ! , se	variable name 'dust' 'bathy' diments	!	time interp. (logical) , .true. , .false.	!	clim (T/F) , .tr , .tr	! ! rue rue	'year] 'month · , ') · , ')	ly'/ ! hly' ! yearly yearly		

5. Run the model :

Copy the executable in your run directory and run the model :

```
cp $WORK/nemo-4.2.0/cfgs/ORCA_1D_PISCES/BLD/bin/nemo.exe .
./nemo.exe
```

The run takes a few minutes.

Note: you can do the same for the other stations by copying the executable in the proper station directory.

One file has been created containing the physical and biogeochemical variables :

```
ncdump -h BATSv420 1m 20100101 20121231 nemo.nc
```

6. Results

Here we briefly describe the results of some physical and biogeochemical variables simulated by the model at the BATS station.

Figure 3 shows the seasonal evolution of dynamic ocean variables that are important for marine biogeochemistry: sea surface temperature (sst), net downward flux of shortwave radiation at the sea surface (qsr), sea surface salinity (sss) and the mixed-layer depth (mld). The seasonal cycle is well developed and all tracers, except SSS, show a minimal drift between the second and third year.



Figure 3: Sea surface temperature, downward shortwave radiation, sea surface salinity and mixed-layer depth at the BATS station.

Seasonal cycles of surface nutrients (NO3, PO4, Si, Fe) and total chlorophyll concentrations highlight the non-equilibrium states of the biogeochemical fields simulated by the model over the three years of the run from the prescribed initial state (Figure 4).



Figure 4: Surface nitrate, phosphate, silicate, iron, oxygen and total chlorophyll (nchl+dchl) concentrations at the BATS station.

Monthly variations of temperature and NO3 concentration in the water column down to 200 m depth and the annual mean vertical profile of temperature and NO3 illustrate the behavior of the 1D model configuration, in particular the typical oligotrophic regime of the BATS station (Figure 5). Winter mixing induces a modest increase in NO3 in the upper ocean.



Figure 5: Hovmoller (time vs. depth) and vertical profiles averaged over the last year of the experiment (year 2012) of seawater temperature and NO3 concentration at the BATS station.

Figure 6 shows the correlation between the deep chlorophyll maximum and the depth of the nutricline as well as the entrainment of nutrients at the surface by the deepening of the mixed layer at the end of winter. This entrainement sustains an increase in surface chlorophyll, which is characteristic of the biogeochemical regime at BATS. Nevertheless, this increase remains modest. The strong limitation by NO3 during summer explains the very low chlorophyll concentrations at the surface.



Figure 6: Hovmoller (time vs. depth) of total chlorophyll and nitrate concentrations and seasonal cycles of surface total chlorophyll concentration and mixed layer depth at BATS.

Finally, the comparison with observations of seawater temperature and NO3 shows a reasonable skill of the model at representing the main observed patterns, despite a highly simplified physical 1-D framework.



Figure 7: Seasonal cycles of sea surface temperature and NO3 concentration and their respective vertical profiles in December at BATS in the observations (red) and the model (orange).

Conclusion

In this document we presented the different steps necessary to install, compile and run the NEMO-PISCES code in a low computational cost 1D configuration. This document does not aim to exhaustively detail all possible options for using the PISCES marine biogeochemistry model. To learn more about the architecture and the use of the PISCES model, training courses are proposed every year as part of the PISCO v2.0 project (LEFE-GMMC French funding). Announcements of these courses are published on the website dedicated to the PISCES community https://www.pisces-community.org/.

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