A Quick Introduction to TMM

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Abstract

This document goes through how to use the Transport Matrix Model (TMM) using computational resources at the University of Minnesota's Minnesota Supercomputing Institution (MSI). All the source codes and documents (including this tutorial) that Tanioka made to TMM is available at my github website (https://github.com/tanio003/tmm/tree/TT_Release).

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1 Setting up

1.1 Flow Chart

Before you do anything, read "README.txt" by Samar Khatiwala at the following website: https://github.com/samarkhatiwala/tmm. I will go over each of these steps specifically aimed at audiences using the computational cluster *Mesabi*.

- 1. Installing and configuring PETSc
- 2. Downloading all the scripts and transport matrices into your own local directory
- 3. Compiling the model (we use the BGC model MOPS2 for this example)
- 4. Running the model
- 5. Processing the model outputs
- 6. Displaying the model outputs

1.2 Steps

1.2.1 Step 0: Logging into MSI and Mesabi

Open the terminal (assuming that you have a MAC or Linux environment) on your computer and log in to MSI with your x500 account:

```
$ ssh -Yt youremail@umn.edu
```

Log in to Mesabi:

```
$ ssh -X mesabi
```

Make a new directory called TMM2 in your home directory and enter into this directory. Everything related to TMM will go into this directory.

```
$ mkdir TMM2
$ cd TMM2
```

1.2.2 Step 1: Installing and configuring PETSc

Download the latest version of PETSc and save it in your TMM2 directory and unzip this package. If opened properly, you should see the new directory petsc-3.13.5.

```
$ wget http://ftp.mcs.anl.gov/pub/petsc/release-snapshots/petsc-lite-3.13.5.tar.gz
$ tar -xvf petsc-lite-3.13.5.tar.gz
$ ls
petsc-3.13.5
```

Import the required modules: (1) impi, (2) impi/intel, and (3) cmake. Also make sure that you are using python 3, not python 2 (= default for MSI).

```
$ module purge
$ module load intel
$ module load impi/intel
$ module load cmake
$ module load python3
$ module list
Currently Loaded Modulefiles:
1) intel/2018.release(default) 4) cmake/3.10.2(default)
2) intel/2018/release 5) python3/3.7.1_anaconda
3) impi/intel(default)
```

Set up \$PETSC_DIR to your petsc-3.13.5 directory. For your future uses, I would advise you to set \$PETSC_DIR in your .bashrc as well.

```
$ export PETSC_DIR=$HOME/TMM2/petsc-3.13.5
$ echo $PETSC_DIR
/.../TMM2/petsc-3.13.5
```

Configure PETSc. Although this part is quite tricky you can copy and use my config file

"reconfigure-arch-linux-c-opt.py". If the config file does not work properly, let me know and I can show you a way to compile without using this .py file.

```
$ cd petsc-3.13.5
$ cp ~/../tanio003/TMM2/petsc-3.13.5/config/reconfigure-arch-linux-c-opt.py config/
$ config/reconfigure-arch-linux-c-opt.py
```

Don't worry about some warning signs. It takes few minutes to compile. If it's compiled properly you should see the notice "Conifgure stage complete." Then build PETSc library:

```
$ make all
```

Building process takes about 15-30 minutes. If you're very lucky it will go through in a single shot. But in most cases, it fails during the middle of the process. Don't worry if it fails the first time. Simply type "\$ make all" again and hopefully it will finish building from where it left off. If built properly, you should see the message "Now to check if the libraries are working do:...". Then type,

```
$ make check
...
Completed test examples
```

If you get this far, you've managed to build the PETSc successfully and you're ready to go to the next step. If it failed, read the error messages, debug, and try again. **Building PETSc is harder than it looks** so you need to be patient.

As more of a technical note, the procedure above uses the Intel compilers and Intel MPI library. By loading the cmake, the PETSc build system can learn more about the host machine. In addition to taking advantage of compiler

optimizations and vectorization, the procedure above builds PETSc against the Intel Math Kernel Library (MKL) for BLAS, LAPACK and ScaLAPACK which gives a performance gain over the reference implementations. For the FORTRAN compiler, we specifically need to use mpiifort, and not mpif90 (the default compiler), because TMM codes are written in both F77 and F90. Also, since we don't require C++ for TMM we put the flag in the config file, --with-cxx=0. The reason we need to use MPI compilers, not regular gcc compilers, is because we want to run PETSc in a parallel mode (i.e., by using the command mpiexec in the runscript). For more details about building PETSc please check out https://www.mcs.anl.gov/petsc/documentation/installation.html.

1.2.3 Step 2: Downloading all the scripts and transport matrices

 First download Matlab scripts from http://kelvin.earth.ox.ac.uk/spk/Research/TMM/tmm_matlab_code.tar.gz and put into the first level of your TMM2 folder Path. You could also get my copy.

```
$ cp -r ~/../tanio003/TMM2/tmm_matlab_code $HOME/TMM2/
```

2. Download transport matrices and related data for the model of your choice:

http://kelvin.earth.ox.ac.uk/spk/Research/TMM/TransportMatrixConfigs/ and put into he first level of your TMM2 folder Path. You can download all 6 configurations but I warn you that MITgcm_ECCO_v4 and UVicKielIncrIsopycDiffTransient take a very long time. For the ones that I have you could also grab my copy (e.g., to copy MITgcm_ECCO):

```
$ cp -r ~/../tanio003/TMM2/MITgcm_ECCO $HOME/TMM2/
```

Alternatively, you can get download these TMM files from the web directly (e.g., to download MITgcm_ECCO):

```
$ wget kelvin.earth.ox.ac.uk/spk/Research/TMM/TransportMatrixConfigs/MITgcm_ECCO.tar
$ tar -xvf MITgcm_ECCO.tar
```

 Download miscellaneous data called OceanCarbon from http://kelvin.earth.ox.ac.uk/spk/Research/TMM/MiscData/. You can get my copy by:

```
$ cp -r ~/../tanio003/TMM2/OceanCarbon $HOME/TMM2/
```

4. Download source codes for TMM and models:

```
$ git clone https://github.com/tanio003/tmm
```

This directory (/TMM2/tmm) contains the source codes from Khatiwala's master branch ("master") and my public release branch ("TT_Release"). For our exercise, we will be using some of my new codes so you need to switch from the master branch to my branch in the newly created tmm directory:

```
$ cd tmm
(master) $ ls
driver HOWTO.txt LICENSE.txt models README.txt
(master) $ git checkout TT_Release
(TT_Release) $ ls
driver HOWTO.txt LICENSE.txt models README.txt Tutorial_MSI
```

Notice that in the branch TT_Release, there is a new directory Tutorial_MSI, which was not present in the master branch.

(Optional) If you want to make start making your own changes to the source codes, I would suggest making a new branch in your local computer (e.g., yournewrepo), and leave master and TT_Release untouched.

```
(TT_Release) $ git checkout -b yournewrepo
(yournewrepo) $ git branch --show-current
yournewrepo
```

5. Set the environment variable TMMROOT to point to the top level of the TMM directory.

```
(TT_Release) $ export TMMROOT=$HOME/TMM2/tmm
(TT_Release) $ echo $TMMROOT
/home/.../TMM2/tmm
```

For your future convenience, I would advise you to set TMMROOT in your .bashrc as well so you don't need to set the variable every time you log in to MSI.

6. To synchronize your tmm folder with the remote repository (e.g., syncing TT_Release with my updates), use the git pull command your terminal. I suggest you do this regularly to keep your files up to date.

```
$ cd $TMMROOT
$ git checkout TT_Release
$ git pull origin TT_Release
```

1.2.4 Step 3: Compiling the model

Here, let's try compiling the biogeochemical MOPS. If you want to learn about the basic architecture of MOPS, read the model description paper by Kriest and Oschlies (2015) at https://gmd.copernicus.org/articles/8/2929/2015/.

1. For each model there are model-specific source codes in the directory (\$TMMROOT/models/current/mops2/) and we need to import some of them to the run directory. First, we create a new run directory. I make a new base directory called "Runs" and in that directory, I make subdirectories for specific experiments. I call it Runs/MOPS/Test_spinup and copy here all the files needed.

```
$ cd ~/TMM2
$ mkdir -p Runs/MOPS/Test_spinup
$ cd Runs/MOPS/Test_spinup
$ cp -p $TMMROOT/models/current/mops2.0/src/Makefile .
$ cp -p -R $TMMROOT/models/current/mops2.0/matlab/* .
$ cp -p $TMMROOT/models/current/mops2.0/runscripts/* .
$ cp -p $TMMROOT/models/current/mops2.0/parameters/* .
```

2. Compile mops. Make sure that all the modules are loaded and \$PETSC_DIR is set correctly before you compile mops.

```
$ module load intel
$ module load impi/intel
$ module load cmake
$ make cleanall
$ make mops
```

If compiled properly, you'd find a new executable "mops" created along with a bunch of objective .o files.

```
BGC_INI.o
BGC_MODEL.o
CAR_CHEM.o
CAR_INI.o
                                          n7fluxes28.m
                                          n7physics.m
                                          n7tracers28.m
                                          n7tracersavg28.m
perry1996-runoff-noarctic_noname.txt
external_forcing_mops_biogeochem.o
                                          perry1996-runoff_noname.txt
insolation.o
load_output.m
                                          petsc_matvec_utils.o
load_output_time_avg.m
                                          petsc_signal_utils.o
load_pco2.m
                                          process_output.m
                                          runscript
make_input_files_for_mops_model.m
                                          runscr
make_rivers.m
misfit_mops_biogeochem.o
                                          tmm_external_bc.o
                                          tmm_forcing_utils.o
                                          tmm_forward_step.o
                                          tmm_main.o
mops_biogeochem_copy_data.o
mops_biogeochem_diagnostics.o
mops_biogeochem_ini.o
                                          tmm_monitor.o
                                          tmm_profile_utils.o
mops_biogeochem_misfit.o
                                          tmm_timer.o
mops_biogeochem_model.o
                                          tmm_write.o
mops_biogeochem_set_params.o
                                          biogem_params.txt
```

3. Edit the file make_input_files_for_mops_model.m. First thing to do is to make sure that variable base_path point to the right directory for the TMM configuration.

```
% make_input_files_for_mops_model.m
% Set toplevel path to GCMs configuration
% base_path='/data2/spk/TransportMatrixConfigs/MITgcm_2.8 deg';
% base_path='/data2/spk/TransportMatrixConfigs/MITgcm_ECCO';
% base_path='/data2/spk/TransportMatrixConfigs/MITgcm_ECCO_v4';
base_path='~/TMM2/MITgcm_2.8 deg';
%base_path='~/TMM2/MITgcm_ECCO';
addpath(genpath('~/TMM2/MITgcm_ECCO';
addpath(genpath('~/TMM2/tmm_matlab_code'));% add tmm_matlab_code to the search path oceanCarbonBasePath='~/TMM2/OceanCarbon'; % add OceanCarbon to the search path atmosDataPath=fullfile(oceanCarbonBasePath,'AtmosphericCarbonData');
```

In the same matlab file, there are different switches (0 = no and 1 = yes). For this spin-up exercise, we **couple MOPS to a simple OCMIP-like carbon model** and **fix atmospheric** pCO₂ **at 280 ppm**. So set the switches as following:

```
% make_input_files_for_mops_model.m
...
periodicForcing=1
periodicMatrix=1

dt=43200; % time step to use (43200s for ECCO and MIT2.8; 28800s for any other TMMs)
rearrangeProfiles=1
```

```
bigMat=0
writeFiles=1
writeTMs=1
useCoarseGrainedMatrix=0
writePCFiles=0
READ SWRAD=0
                                    % Read short-wave radiation?
useCarbon=1
                                    % Use simple inorganic carbon model?
useOrgCarbon=0
                                    % Use organic carbon module?
useAtmModel=0
                                    % Use prognostic 1-box atmosphere?
pCO2atm_ini=280.0
                                    % Initial pco2?
                                   % Use prescribed pco2 pathway?
% Use DIC and Alk to calculate E-P?
% Scaling factor for E-P (default = 1)
useTimeVaryingPrescribedCO2=0
useVirtualFlux=1
empScaleFactor = 1.0
% Modified by Tatsuro Tanioka 200907 to allow for Atmospheric CO2 option
% For a prescribed pCO2 run, useTimeVaryingPrescribedCO2=1 and choose a scenario
% Available options: 'historical', 'RCP3PD', 'RCP45', 'RCP6' and 'RCP85'
co2Scenario='RCP85';
```

Then open MATLAB and run make_input_files_for_mops_model.m

This creates a bunch of periodic forcing files (xxx_01, xxx_02,...), initial tracer concentrations (po4ini.petsc, no3ini.petsc,...), and binary files (.bin and .petsc) related to model geometry and forcing.

4. Edit the parameter file. biogem_params.txt. We only need to set the first 7 parameters because we are not using organic carbon module for this exercise. We will use the calibrated values for MOPS/MIT2.8 follwiing Kriest et al. (2020).

```
1.39
          #01. detmartin = Martin Curve exponent of Detritus [1.39 for MIT2.8, 1.46 for ECCO]
          \#02. ro2ut = Refield -O2:P
                                                                     [173.7 for MIT2.8, 151.1 for ECCO]
173.7
0.00119
          #03. nfix = Max growth rate (1/d) of N-fixers
                                                                     [0.00119 for MIT2.8, 0.00229 for ECCO]
          #04. subdin = No denitrification below this level of DIN (mmol/m3) #05. ACkbaco2 = Half sat-constant for oxic degradation (mmol/m3)
15.8
                                                                                                   [15.8, 16.0]
1.01
                                                                                                    [1.01, 1.07]
          #06. ACkbacdin = Half sat-constant for suboxic degradation
                                                                                                    [32.0, 23.1]
32.0
               alimit = Min. value for the degradation of PHY and DOP [0.001 for mops, 0.01 for mops_ep]
0.001
```

1.2.5 Step 4: Running the model

MSI systems use job queues to efficiently and fairly manage when computations are executed. The queuing system at MSI is called Slurm and to submit a job to a queue users create Slurm job scripts. The script contains information on the resources requested for calculation, as well as the commands for executing the calculation.

Below is the custom Slurm script for submitting a new job to run MOPS2 using Mesabi. It's called runscript_msi and should be in the current directory already.

```
#!/bin/bash -l
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=24
#SBATCH --time=06:00:00
#SBATCH --time=06:00:00
#SBATCH --mail-type=ALL
#SBATCH --mail-user=tatsurobkkuk@gmail.com
#SBATCH -p small
#SBATCH -- output=%j.out

cd $SLURM_SUBMIT_DIR

module load intel
module load impi/intel
module load cmake
```

The first line defines which type of shell the script will be read. Here we will use the bash. Commands for the Slurm queuing system begin with #SBATCH. Lines 2 to 4 in the above sample script contain the Slurm resource

request. The current job will require about 6 hours, 1 node each with 24 processor cores, and 2GB of memory per core . The two lines containing #SBATCH --mail are both commands having to do with sending message emails to the user. The first of these lines instructs the Slurm system to send a message email when the job aborts, begins, or ends. The second command specifies the email address to be used. Using the message emails is recommended because the reason for a job failure can often be determined using information in the emails. A Slurm script should contain the appropriate change directory commands to get to the job execution location. A Slurm script also needs to contain module load commands for any software modules that the calculation might need.

The follwing lines $(17\sim)$ in runscript_msi contain the commands to execute and start a specific program. Different flags need to be change accordingly depending on the nature of experiments. For more information on different options available, read "HOWTO.txt" by S. Khatiwala located in \$TMMROOT. Do not put these # comments in the actual file.

```
# 360 days per year with a time step of 2 steps per day: mpirun -np 24 ./mops \ # number of cores, models
             -numtracers 9 \ # number of tracers (i.e. state variables)
            -i po4ini.petsc, dopini.petsc, oxyini.petsc, phyini.petsc, zooini.petsc, detini.petsc, no3ini.petsc, dicini.petsc, alkini.petsc \ # files for initialization of BGC state variables
-me Ae \ # the name of the explicit transport matrix
-mi Ai \ # the name of the implicit transport matrix
            -t0 0.0 -iter0 0 \
            -deltat_clock 0.001388888888888 \ # starting time[years] starting time[timesteps]: for initial run
            -max_steps 2160000 \ # total number of timesteps to be evaluated (here 3000 yr -write_time_steps 72000 \ # output frequency(in timesteps, here every 100 yrs)
            -o po4out.petsc,dopout.petsc,oxyout.petsc,phyout.petsc,zooout.petsc,detout.petsc,no3out.petsc,dicout.petsc,alkout.petsc \ # files for output of 9 BGC state variables
-external_forcing \ # calculate BGC explicitly
            -use_profiles \
                                 # number of layers in euphotic zone (2 for MIT2.8, 6 for ECCO)
            -biogeochem_deltat 43200.0 -days_per_year 360.0 \ # ocean timestep[seconds]
            -burial_sum_steps 720 \ # sum burial over a period of 720 timesteps = 1 yr -pco2atm 280.0 \ # use fixed pCO2 of 280 ppm
    -use_virtual_flux \ # use the global surface mean DIC and Alk to calculate E-P
-periodic_matrix \ # use of periodic transport matrix # the unit of time is year and circulation has a periodicity of 1 year; monthly mean tranport matrix (12 TMs/year)
            -matrix_cycle_period 1.0 -matrix_num_per_period 12 \
            -periodic_biogeochem_forcing \
            -periodic_biogeochem_cycle_period 1.0 -periodic_biogeochem_num_per_period 12 \
-num_biogeochem_steps_per_ocean_step 8 \ # the number of BGC timestep per ocean step
-separate_biogeochem_time_stepping \ # timestep BGC model separately from ocean step
            -time_avg -avg_start_time_step 2159281 -avg_time_steps 60 \
            # initial timestep for diagnostic fluxes (for final year); avg over 60 timesteps = 1 month
            -avg_files po4avg.petsc,dopavg.petsc,oxyavg.petsc,phyavg.petsc,zooavg.petsc,detavg.petsc,no3avg.petsc,
            dicavg.petsc, alkavg.petsc \ # avg file names
            -bgc_params_file biogem_params.txt \ # parameter files to be read
-num_bgc_params 7 \ # number of parameters read
-calc_diagnostics -diag_start_time_step 2159281 -diag_time_steps 60 \
            # initial timestep for diagnostic fluxes (for final year); avg over 60 timesteps = 1 month
             -diag_files fbgc1.petsc,fbgc2.petsc,fbgc3.petsc,fbgc4.petsc,fbgc5.petsc,fbgc6.petsc,fbgc7.petsc,
            fbgc8.petsc \ # diagnsotic flux files names > log # outputting to logfile
```

Currently BGC model writes the following 8 diagnostics into the different files:

- 1. fbgc1.petsc: primary production in each box [mmolP/m³/oceantimestep]
- 2. fbgc2.petsc: zooplankton grazing in each box [mmolP/m³/oceantimestep]
- 3. fbgc3.petsc: detritus sedimentation through upper boundary of each box [mmolP/m²/oceantimestep]
- 4. fbgc4.petsc: remineralization of detrius and DOP in each box [mmolP/m³/oceantimestep]
- 5. fbgc5.petsc: river runoff [mmolP/m³/oceantimestep]
- 6. fbgc6.petsc: nitrogen fixation [mmolN/m³/oceantimestep]
- 7. fbgc7.petsc: denitrification [mmolN/m³/oceantimestep]
- 8. fbgc8.petsc: Irradiance at the top of every layer in euphotic zone $[W/m^2]$, added by T.Tanioka (2020/11)

To submit the job to the queue, type on the command line:

```
$ chmod u+x runscript_msi
$ sbatch runscript_msi
```

To check your job status at MSI, type:

```
$ squeue -u yourusername
```

1.2.6 Step 5: Processing the model outputs

When the run is completed, you should receive an email from MSI (if you set it so in the runscript). You should also check you log file and the bottom of the log file should say "Wall clock time xxx seconds". As the output files are binary and cannot be opened on its own, we have to convert from the binary format into either netcdf (.nc) or Matlab (.mat) files using Matlab scripts.

(Option 1, recommended): To convert to .nc files you are going to use the following 5 scripts:

1. n7tracers28.m: This file converts each tracer snapshot .petsc file (e.g., po4put.petsc) into a single .nc file. The MATLAB syntax is:

>> n7tracers28('filename1.nc')

Make sure to set the basepath correctly and set useCarbon=1 (when carbon model is used) and useOrgCarbon=0. Also make sure that there is no .nc file with the same name already in the directory.

2. n7tracersavg28.m: This file converts each tracer time-averaged .petsc file (e.g., po4avg.petsc) into a single .nc file. The MATLAB syntax is:

>> n7tracersavg28('filename2.nc')

Make sure to set the basepath correctly and set useCarbon=1 and useOrgCarbon=0.

3. n7fluxes28.m: This file converts each diagnostic flux .petsc file (e.g., fbgc1.petsc) into a single .nc file. The MATLAB syntax is:

>> n7fluxes28('filename3.nc')

Make sure to set the basepath correctly and and set useOrgCarbon=0.

4. n7physics.m: This file makes single .c files with monthly mean temperature and salinity. The MATLAB syntax is:

>> n7physics('filename4.nc')

Make sure to set the basepath correctly and make sure that there is no .nc file with the same name already in the directory.

5. load_pco2.m: This file makes a global mean atmospheric pCO₂ file ("pco2.nc") and surface CO₂ air-sea flux file ("co2airseaflux.nc"). CO₂ is in ppm and CO₂ air-sea flux is in [mmolC/m²/timestep] (positive flux means CO₂ is going into the sea from air). The MATLAB syntax is

>> load_pco2

Make sure to set the basepath and the CO₂ run options correctly.

6. process_output.m (optinal): To run all 5 scripts at once, edit and use this file. The MATLAB syntax is

>> process_output

(Option 2): To convert to .mat files you are going to run 2 scripts:

- 1. load_output.m: This file converts each tracer snapshot .petsc file (e.g., po4put.petsc) to .mat file. Make sure to edit the base_path and add tmm_matlab_code to search path in lines 2 and 3.
- 2. load_output_time_avg.m: This file converts each tracer average concentration .petsc file (e.g., po4avg.petsc) to .mat file. Make sure to edit the base_path and search path correctly.
- 3. Unfortunately I don't have scripts for creating .mat diagnostic flux files, physics files, and CO_2 files. But this should not be too hard to do and all you have to do is to modify other .m files.

1.2.7 Step 6: Displaying the model outputs

(Option 1): To view .nc files, I recommend the software *Ferret* developed by NOAA. It is already installed in MSI, and to launch Ferret, type on the command line:

```
filename1.nc filename2.nc filename3.nc filename4.nc co2airseaflux.nc pco2.nc
  module load ferret/7.6.0
        NOAA/PMEL TMAP
        PyFerret v7.6 (optimized)
Linux 4.15.0-1089-azure - 06/25/20
11-Nov-20 16:51
    load filename1.nc
ves? sho d
    currently SET data sets:
   1> ./filename1.nc (default)
           title
P04
OXYGEN
PHYT0
                                                              1:64
Z00
                                                              1:64
DET
                                                              1:64
                                                                          1:15
NO3
                                                              1:64
```

I won't go into too much detail here but to learn more about Ferret, visit NOAA's website and take a tutorial at https://ferret.pmel.noaa.gov/Ferret/documentation/ferret-tutorials. You can make all kinds of graphs and figures with Ferret.

(Option 2): If you want to visualize .mat files, I recommend the MATLAB package m_map. Again, I would not go into much detail here but if you want to learn about it, download the package and take the tutorial from the developer's website: https://www.eoas.ubc.ca/~rich/map.html. Compared to Ferret, you have more freedom for customizing graphs. The downside is that you are going to have to write much longer codes.

2 Case Studies

2.1 Study 1: Postindustrial CO₂ uptake with MOPS+MIT2.8

In the first case study, we will simulate postindustrial CO_2 uptake using MOPS and MITgcm2.8 under IPCC's RCP8.5 scenario from 1765 to 2265. We are going to do the continuous run from the spinup run (Section 1) so make sure that you have completed that run before you proceed.

1. Update source codes in your tmm directly by doing git pull from the remote repository.

```
$ cd $TMMROOT
$ git checkout TT_Release
$ git pull origin TT_Release
```

2. Make a new run directory. Let's call it Test_co2historyRCP85 and copy all the files needed into this directory.

```
$ cd ~/TMM2
$ mkdir -p Runs/MOPS/Test_co2historyRCP85
$ cd Runs/MOPS/Test_co2historyRCP85
$ cp -p $TMMROOT/models/current/mops2.0/src/Makefile .
$ cp -p $TMMROOT/models/current/mops2.0/matlab/* .
$ cp -p $TMMROOT/models/current/mops2.0/runscripts/* .
$ cp -p $TMMROOT/models/current/mops2.0/parameters/* .
```

3. Compile mops as we have done in the spinup run. Don't forget to load modules and make sure that environmental variables \$TMMROOT and \$PETSC_DIR are set up properly.

```
$ make cleanall
$ make mops
```

4. Copy the file pickup.petsc from the spinup run directory into the current working directory and give it a new name (restart.petsc). This petsc files contains the tracer concentrations from the final year of the run and is required for the continuous run.

\$ cp ../Test_spinup/pickup.petsc restart.petsc

Also, copy the file pickup_runoff.bin from the spinup run directory. This binary file contains the global sedimentation from the final year of the previous run.

```
$ cp ../Test_spinup/pickup_runoff.bin restart_runoff.bin
```

(Optional) Instead of copying files, you can also create symbolink links so that you would know exactly where these restart files actually come when you do \$1s -1.

```
$ ln -s ../Test_spinup/pickup.petsc restart.petsc
$ ln -s ../Test_spinup/pickup_runoff.bin restart_runoff.bin
$ ls -l restart.petsc
lrwxrwxrwx. 1 tanio003 matsumot 26 Sep 28 12:33 restart.petsc -> ../Test_spinup/pickup.petsc
```

5. Edit the input generation file (make_input_files_for_mops_model.m). The key here is to set useTimeVaryingPrescribedC02=1 and choosing the appropriate co2Scenario, in this case RCP85.

```
% make_input_files_for_mops_model.m
% Set toplevel path to GCMs configuration
% base_path = '/data2/spk/TransportMatrixConfigs/MITgcm_2.8 deg';
% base_path = '/data2/spk/TransportMatrixConfigs/MITgcm_ECCO';
% base_path = '/data2/spk/TransportMatrixConfigs/MITgcm_ECCO_v4';
base_path='~/TMM2/MITgcm_2.8 deg';
%base_path = '~/TMM2/MITgcm_ECCO';
addpath(genpath(`\sim/TMM2/tmm_matlab\_code')); \% \ add \ tmm_matlab\_code \ to \ the \ search \ path \ oceanCarbonBasePath=`\sim/TMM2/OceanCarbon'; \ \% \ add \ OceanCarbon \ to \ the \ search \ path \ atmosDataPath=fullfile(oceanCarbonBasePath , `AtmosphericCarbonData');
READ_SWRAD=0
                                            % Read short-wave radiation?
useCarbon=1
                                            % Use simple inorganic carbon model?
useOrgCarbon\!=\!0
                                            % Use organic carbon module?
                                            % Use prognostic 1-box atmosphere?
% Initial pco2? (will be ignored as useAtmModel=0)
useAtmModel=0
pCO2atm_ini=280.0
                                            % Use prescribed pco2 pathway?
% Use DIC and Alk to calculate E-P?
useTimeVaryingPrescribedCO2=1
useVirtualFlux=1
                                            % Scaling factor for E-P (default = 1)
empScaleFactor = 1.0
% Modified by Tatsuro Tanioka 200907 to allow for Atmospheric CO2 option
% For a prescribed pCO2 run, useTimeVaryingPrescribedCO2=1 and choose a scenario
% Available options: co2Scenario='RCP85';
                             'historical', 'RCP3PD', 'RCP45', 'RCP6' and 'RCP85'
```

6. Open Matlab and make input files:

```
$ matlab -nodesktop
...
>> make_input_files_for_mops_model
```

- 7. Edit runscript_msi. Important changes are commented with blue (do not actually put these comments after line 13 on the script). You can manually edit the script or copy my script from
 - ${\tt \sim/.../tanio003/TMM2/Runs/MOPS/Testruns/Slurm/Test_co2historyRCP85_slurm.}$

```
#!/bin/bash -1
   #SBATCH -- nodes=1
 3 #SBATCH —ntasks—per—node=24
 4 #SBATCH --mem-per-cpu=2gb
5 #SBATCH --time=00:60:00
   #SBATCH -- mail-type=ALL
   #SBATCH --mail-user=tatsurobkkuk@gmail.com
   #SBATCH -p small
#SBATCH --output=%j.out
10
11 cd $SLURM_SUBMIT_DIR
13 module load intel
14 module load impi/intel
15 module load cmake
16
17 # 360 days per year with a time step of 2 steps per day:
18 mpirun -np 24 ./mops \
19 -numtracers 9 \
     -pickup restart.petsc \ # read initial values from file
20
2.1
      -me Ae \
2.2
     -mi Ai \
```

```
-t0 1765.0 -iter0 0 \
                                   # start from year 1765
      -deltat_clock 0.0013888888888888 \
     -max_steps 360000 \ # run for 720*500 timesteps = 500 years

-write_time_steps 7200 \ # output every 720*10 timestep = 10 years
25
26
2.7
     -o po4out.petsc, dopout.petsc, oxyout.petsc, phyout.petsc, zooout.petsc,
detout.petsc, no3out.petsc, dicout.petsc, alkout.petsc \
     -external_forcing \
     -use_profiles \
29
30
     -nzeuph 2 \
     -biogeochem_deltat 43200.0 -days_per_year 360.0 \
32
     -burial_sum_steps 720 \
33
     -runoff_ini_file restart_runoff.bin \ # read global sedimentation of previous run
     -periodic_matrix \
-pco2atm_history TpCO2.bin,pCO2atm.bin \ # read prescribed pCO2 and time
34
35
     -use_virtual_flux \
      -matrix_cycle_period 1.0 -matrix_num_per_period 12 \
38
      -periodic_biogeochem_forcing
      -periodic\_biogeochem\_cycle\_period \ 1.0 \ -periodic\_biogeochem\_num\_per\_period \ 12 \ \backslash
39
40
     -num_biogeochem_steps_per_ocean_step 8 \
41 -separate_biogeochem_time_stepping \
42 -time_avg -avg_start_time_step 169201 -avg_time_steps 720 \
# output annual avg. from year 2000 (235 years after 1765)
43
      -avg_files po4avg.petsc,dopavg.petsc,oxyavg.petsc,phyavg.petsc,zooavg.petsc,
detavg.petsc,no3avg.petsc,dicavg.petsc,alkavg.petsc \ 44     -bgc_params_file biogem_params.txt \ 45     -num_bgc_params 7 \
45
     -calc_diagnostics -diag_start_time_step 169201 -diag_time_steps 720 \
# output annual mean fluxes from 2000 (235 years after 1765)
       -diag_files fbgc1.petsc,fbgc2.petsc,fbgc3.petsc,fbgc4.petsc,fbgc5.petsc,
fbgc6.petsc,fbgc7.petsc,fbgc8.petsc \
48
     > log
```

8. Make sure that paramter file (biogem_params.txt) is same as the one used in the spinup run. You can simply copy that file into the current directory.

```
$ cp ../Test_spinup/biogem_params.txt
```

9. Submit the job to MSI queue.

```
$ sbatch runscript_msi
```

10. Processing and outputting results. Use 5 Matlab scripts (n7tracers28.m,n7tracersavg28.m,n7fluxes28.m,n7physics.m,load_pco2.m) to create .nc files. Here, I will show you how to plot CO_2 timeseries and global annual mean air-sea flux of CO_2 using Ferret. The script is also at

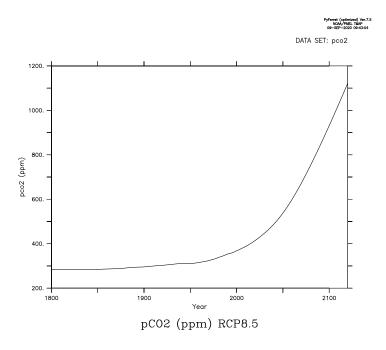


Figure 1: CO₂ concentration pathway under RCP8.5 scenario (Meinshausen et al., 2011).

Figure 1 ($Ferret:w\ I$) shows the change in CO_2 under RCP8.5 scenario. There is a rapid increase in CO_2 concentration from the late 1990s.

Figure 2 compares annual mean CO_2 flux in 2010 (Ferret:w 2) and 2100 (Ferret:w 3). Notice that in 2010, large parts of the equatorial regions are net source of CO_2 but in 2100, larger parts are becoming sink. Also, greater part of the Southern Ocean is also expected to absorb more CO_2 in 2100 compared to 2010.

Figure 3 is a CO_2 flux in 2010 from a study by Woolf et al. (2019) who used Surface CO_2 atlas and wind data. If you compare with the left panel of Figure 2, you can see that our MOPS model does a quite good job in reproducing the large scale pattern.

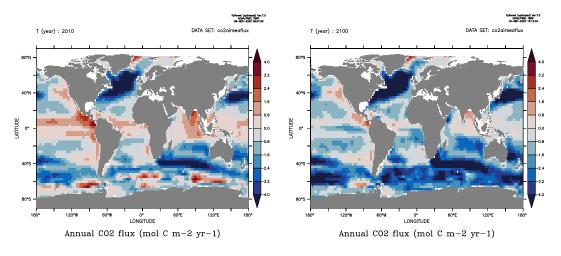


Figure 2: Modeled map of annual CO₂ flux for 2010 (Left) and for 2100 (Right). Upward fluxes are defined as positive.

Figure 4 (*Ferret:w* 4) is a globally integrated sea-air CO_2 flux projections under RCP8.5 scenario. The negative value means net uptake of CO_2 by ocean. For a comparison, we show the similar projection using the CESM and CMIP5 (Figure 5a-b.) from Lovenduski et al. (2016). Again, notice that MOPS's result is largely consistent in terms of the magnitude.

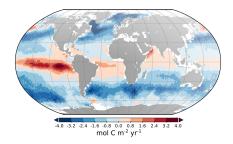


Figure 3: Map of annual CO₂ flux in 2010 from CO₂ and wind data (from Woolf et al., 2019). Compare this with Figure 2.

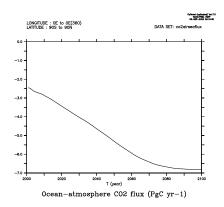


Figure 4: Modeled annual-mean globally integrated sea-air CO₂ flux projections under RCP8.5 scenario.

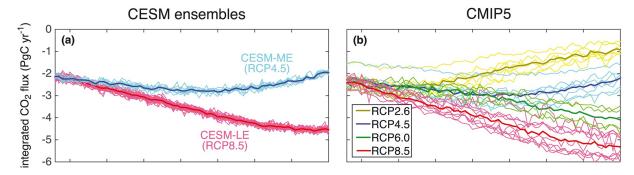


Figure 5: Modeled annual-mean globally integrated sea-air CO₂ flux projections (from Lovenduski et al., 2016) with CESM (a) and CMIP5 models (b). Compare this with Figure 4.

2.2 Study 2: Using MOPS+ECCO to simulate flexible C:P

In the second case study, we will use the modified MOPS code to study the spatiotemporal variability in organic matter C:P ratio under steady-state scenario. We are going to do a 3000-yr spinup run where C:P of phytoplankton is flexible but C:P of zooplankton is homeostatic (i.e. less flexible). We will use the TMM model 12 monthly mean TMs derived from the Estimating the Circulation and Climate of the Ocean (ECCO) project, which provides circulation fields that yield a best fit to hydrographic and remote sensing observations over a 10-year period, on a spatial grid of 1-by-1 degree horizontal resolution with 23 vertical levels

We model P:C uptake ratio of phytoplankton using the power-law as a function of nutrients, temperature, and light following Tanioka and Matsumoto (2020):

$$(P:C)_{uptake,phyto} = (P:C)_{ref} \left(\frac{[PO_4]}{[PO_4]_0}\right)^{s_{PO_4}^{P:C}} \left(\frac{[NO_3]}{[NO_3]_0}\right)^{s_{NO_3}^{P:C}} \left(\frac{[T]}{[T]_0}\right)^{s_T^{P:C}} \left(\frac{[I]}{[I]_0}\right)^{s_I^{P:C}} \tag{1}$$

Exponent $s_{\text{driver}}^{P:C}$ is constant and describe the strength of a given driver on P:C.

Zooplankton P:C uptake ratio is also computed using the power-law as a function of phytoplankton P:C of biomass:

$$(P:C)_{\text{uptake},zoo} = (P:C)_{\text{ref},zoo}^{1-H} \cdot (P:C)_{\text{biomass},\text{phyto}}^{H}$$
(2)

Parameter H is a zooplankton homeostatic parameter that describes how variable zooplankton P:C is affected

by phytoplankton P:C. When H = 0, P:C uptale equals a fixed reference P:C and is independent of phytoplankton P:C. When H = 1, uptake P:C equals cellular P:C of phytoplankton. Here we will use the value of H = 0.08 following Persson et al. (2010), who conducted meta-analysis on zooplankton C:P.

In order to cope with the mismatch between required P:C and P:C of prey, zooplankton can excrete excess P or C as dissolved and particulate organic matter. At steady state, uptake P:C ratio should equal the biomass P:C ratio for both phytoplankton and zooplankton.

In implementing flexible C:P, I added 4 new tracers: (1) Phytoplankton C biomass, (2) Zooplankton C biomass. (3) DOC, and (4) POC. The total number of tracers is now 13.

1. Update source codes in your tmm directly by doing git pull from the remote repository.

```
$ cd $TMMR00T
$ git checkout TT_Release
$ git pull origin TT_Release
```

2. Make a new run directory. Here, we call it Test_ECCO_CP and copy all the files needed into this directory. I also created a new directory called paramters which contains an ASCII text file (biogem_params.txt) with biogeochemical parameters.

```
$ cd ~/TMM2
$ mkdir -p Runs/MOPS/Test_ECCO_CP
$ cd Runs/MOPS/Test_ECCO_CP
$ cp -p $TMMROOT/models/current/mops2.0/src/Makefile .
$ cp -p $TMMROOT/models/current/mops2.0/matlab/* .
$ cp -p $TMMROOT/models/current/mops2.0/runscripts/* .
$ cp -p $TMMROOT/models/current/mops2.0/parameters/* .
```

3. Compile mops. The new model with flexible C:P is called mops_cp.

```
$ make cleanall
$ make mops_cp
```

- 4. Edit the file make_input_files_for_mops_model.m and run it on Matlab. First thing to do is to make sure that variable base_path point to the right directory for the TMM ECCO configuration. Also make sure that option useORGCARBON is set to 1. The options useORGCARBON creates new initial concentrations arrays for DOC, POC, ZooC, and PhytoC. This initizalization process takes much longer than that of the first case study.
- 5. Edit the parameter input file biogem_params.txt. In the first run, rows 1-6 should be the default values for MOPS + ECCO following Kriest et al. (2020). Parameters 12-21 correspond to the P:C power-law formulations of phytoplankton and zooplankton from Equations (1)-(2). Reference P:C for both phytoplankton and zooplankton is 1/117 = 8.547 permil (line 12).

```
1.46
                 #01. detmartin = Martin Curve exponent of Detritus
                                                                                          [1.39 for MIT2.8, 1.46 for ECCO]
                 #02. ro2ut = Refield -O2:P
                                                                                           [173.7 for MIT2.8, 151.1 for ECCO]
   151.1
 3 0.00229
                 #03. nfix = Max growth rate (1/d) of N-fixers
                                                                                           [0.00119 for MIT2.8, 0.00229 for ECCO]
 4 16.0
                 #04. subdin = No denitrification below this level of DIN (mmol/m3)
                                                                                                                                [15.8, 16.0]
                #05. ACkbaco2 = Half sat-constant for oxic degradation (mmol/m3) #06. ACkbacdin = Half sat-constant for suboxic degradation
                                                                                                                                [1.01,
 5 1.07
   23.1
                                                                                                                                [32.0, 23.1]
 6
                #07. alimit = Min. value for the degradation of PHY and DOP [0.001 for mops, 0.01 for mop #08. detmartin_c = Martin Curve Exponent of POC. For pref. remin, change from #01 [1.39,
   0.01
 8 1.46
                 #09. cp_option (1 = Power-law, 2: Galbraith and Martiny, 0: Redfield)
                #10. maxcp = upper bound C:P
#11. mincp = lower bound C:P
10 250.0
11 50 0
                                                                                                                                [50.01]
                #12. par_bio_pc0 = Reference P:C (permil) for power-law
#13. par_bio_po4_ref = Reference PO4 (mmolP/m3) for power-law
#14. par_bio_no3_ref = Reference NO3 (mmolN/m3) for power-law
12 8.547
                                                                                                                                [8.547]
13 0.57
                                                                                                                                [0.57]
14 5.7
                                                                                                                                [5.7]
15 18.0
                 #15. par_bio_temp_ref = Reference Temp (deg C) for power-law
                                                                                                                                 [18.0]
                 #16. par_bio_light_ref = Reference Irradiance (W/m2) for power-law
#17. par_bio_spc_p = s_P:C^PO4 for power-law
#18. par_bio_spc_n = s_P:C^NO3 for power-law
16 70.0
                                                                                                                                 [70.0]
                                                                                                                                 [0.21]
17 0.21
18 0.0
                                                                                                                                [0.01]
                #19. par_bio_spc_i = s_P:C^I for power-law
#20. par_bio_spc_t = s_P:C^T for power-law
19 0.0
                                                                                                                                10.01
20 -3.6
                                                                                                                                  -3.6]
21 0.08
                 \#21. par_zoo_cp_hom = Homeostatic parameter for Zooplankton (0-1)
```

6. Edit runscript_msi. Here we are going to run the model for 15 hours with 10 nodes, 24 processors per core. Each processor is allocated with 2GB of memory. As we are using more than 9 nodes, we submit to the queue *large*. If you want the job to proceed quicker, you can increase the number of nodes from 10. (Note: Asking for more nodes will mean longer time in the queue. So this will require some trial and error to find the optimal node request.)

Here is the first 12 lines of the runscript. The script is also at

~/../tanio003/TMM2/Runs/MOPS/Testruns_ECCO/201108b/runscript_msi.

```
1 #!/bin/bash -l
2 #SBATCH --nodes=10
3 #SBATCH --ntasks-per-node=24
4 #SBATCH --mem-per-cpu=2gb
5 #SBATCH --time=15:00:00
6 #SBATCH --mail-type=ALL
7 #SBATCH --mail-user=tatsurobkkuk@gmail.com
8 #SBATCH -p large
9 #SBATCH --output=%j.out
10
11 cd $SLURM_SUBMIT_DIR
```

The following lines $(13\sim)$ contain the commands to execute and start the program mops_cp.

```
13 module load intel
    module load impi/intel
15
   module load cmake
16
17 # 360 days per year with a time step of 2 steps per day:
18 mpirun -np 240 ./mops_cp \ # use 240=24*10 cores, program = mops_cp
19 -numtracers 13 \ # use 13 tracers (9 tracers in mops + 4 new tracers)
20
               -i po4ini.petsc, dopini.petsc, oxyini.petsc, phyini.petsc, zooini.petsc, detini.petsc,
               no3ini.petsc, dicini.petsc, alkini.petsc, docini.petsc, pocini.petsc, phycini.petsc, zoocini.petsc \ # 13 initial tracer concentrations
               zoocini.petsc \
21
               -me Ae \
22
               −mi Ai \
               -t0 0.0 -iter0 0 \
23
24
               -deltat_clock 0.001388888888888 \
               -max_steps 2160000 \ # Run for 720 steps/year * 3000 years
2.5
               -write_time_steps 72000 \ # Output snapshot every 100 yeras
26
27
               -o po4out.petsc,dopout.petsc,oxyout.petsc,phyout.petsc,zooout.petsc,detout.petsc,
               ro3out.petsc, dicout.petsc, alkout.petsc, docout.petsc, pocout.petsc, phycout.petsc, zoocout.petsc , alkout.petsc, docout.petsc, pocout.petsc, phycout.petsc, zoocout.petsc \ # 13 output tracers
               -external_forcing \
29
               -use_profiles \
30
                                          # the default number of euphotic zones = 6 layers in ECCO
               -nzeuph 6 \
               -biogeochem_deltat 43200.0 -days_per_year 360.0 \
31
32
               -burial_sum_steps 720 \
33
               -pco2atm 280.0 \
                                         # Constant pCO2 at 280 ppm
34
               -use_virtual_flux \
35
               -periodic_matrix \
36
               -matrix\_cycle\_period \ 1.0 \ -matrix\_num\_per\_period \ 12 \ \backslash
37
               -periodic_biogeochem_forcing \
               -periodic_biogeochem_cycle_period 1.0 -periodic_biogeochem_num_per_period 12 \
38
               -num_biogeochem_steps_per_ocean_step 8 \
-separate_biogeochem_time_stepping \
-time_avg -avg_start_time_step 2159281 -avg_time_steps 60 \ # monthly avg in final year
39
40
41
42
               -avg_files po4avg.petsc,dopavg.petsc,oxyavg.petsc,phyavg.petsc,zooavg.petsc,detavg.petsc,
               no3avg.petsc,dicavg.petsc,alkavg.petsc,docavg.petsc,pocavg.petsc,phycavg.petsc,zoocavg.petsc\ # 4 new time-average tracers added
-bgc_params_file biogem_params.txt \ # telling to read the parameter file
43
                                                                     # the number of parameters to be read = 21
44
               -num_bgc_params 21 \
45
               -calc_diagnostics -diag_start_time_step 2159281 -diag_time_steps 60 \ # monthly diagnostic
               -diag_files fbgc1.petsc,fbgc2.petsc,fbgc3.petsc,fbgc4.petsc,fbgc5.petsc,fbgc6.petsc
fbgc7.petsc,fbgc8.petsc,fbgc9.petsc,fbgc10.petsc,fbgc11.petsc \ # 11 diagnostics
46
47
```

The important notes are commented with blue. The three new diagnostics related to organic carbon and flexible C:P module I added are:

- (a) fbgc9.petsc: POC sedimentation through upper boundary of each box [mmolC/m²/oceantimestep]
- (b) fbgc10.petsc: Phytoplankton C:P uptake ratio in molar units.
- (c) fbgc11.petsc: Zooplankton C:P uptake ratio in molar units.

Monthly-averaged disgnostics as well as mothly-averaged tracers will be computed in the final year (Year 2999) of the run.

7. To submit the job to the queue, type on the command line:

```
$ chmod u+x runscript_msi
$ sbatch runscript_msi
```

To check your job status at MSI, type:

```
$ squeue -u yourusername
```

- 8. Process the outputs using the Matlab Scripts as outlined previously. For each .m files (n7tracers28.m,n7tracersavg28.m,n7fluxes28.m,n7physics.m,load_pco2.m), make sure that variable base_path point to the right directory for the TMM ECCO configuration. Also make sure that option useORGCARBON is set to 1.
- 9. Analyze outputs. Here we will look at seasonal cycles of productivity at 4 different locations. These 4 locations are: (1) the high latitude bloomforming North Atlantic Ocean (NAT: 25W-35W, 45N-50N, black line), (2) the North Atlantic subtropical gyre (NASG: 25W-70W, 25N-35N, red line), (3) the South Pacific subtropical gyre (SPSG:90W-150W, 15S-40S, green line), and (4) the Equatorial upwelling region (EQU: 5S-5N, blue line). The code for making figrues is in my directory
 - ~/../tanio003/TMM2/Runs/MOPS/Testruns_ECCO/201108b/analyze_201108b.jnl.

Figure 6 shows the seasonal cycle of productivity (left) and the tracers/forcings (right). Notice that phytoplankton biomass exceeds zooplankton biomass throughout the year in all regions. The only exception is NAT where zooplankton biomass catches up with the phytoplankton biomass following the spring bloom. NPP peaks in early spring and export production lags NPP about a month or two.

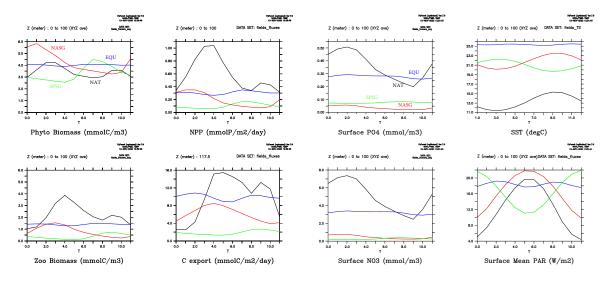


Figure 6: Modeled seasonal cycle of productivity (Left) and tracers (Right) at four geographical regions. North Atlantic Ocean (NAT: 25W-35W, 45N-50N, black line), (2) the North Atlantic subtropical gyre (NASG: 25W-70W, 25N-35N, red line), (3) the South Pacific subtropical gyre (SPSG:90W-150W, 15S-40S, green line)

Figure 7 shows the seasonal cycle of C:P. Phytoplankton C:P at NAT and NASG peaks in fall (~September) and is lowest during spring. This pattern generally follows that of SST and PO4, where low PO4/high SST leads to higher C:P. Seasonal variability of phytoplankton C:P at SPSG and EQU are smaller as the change in SST and nutrients are small. C:P of zooplankton remains around 117 even in gyres. As phytoplankton biomass is greater than that of zooplankton, C:P of bulk POM is similar in magnitude to that of phytoplankton. What's interesting is that C:P export is greater than C:P of phytoplankton and bulk POM at NASG, SPSG, and EQU. This is because excess carbon that is excreted by zooplankton is added to detrital POC pool leading to higher C:P of exported organic mater. At NAT, the different is relatively smaller because the stoichioemtric mismatch between phytoplankton C:P and zooplankton C:P is small.

10. (Optional) We can also calculate export of DOC and DOP. The code for making figrues is in my directory ~/../tanio003/TMM2/Runs/MOPS/Testruns_ECCO/201108b/analyze_dom_export.jnl.

Figure 8 shows that the total DOC export is around 3.0~PgC/yr which is factor of 2 greater than the previous modeling studies. This is mainly due to the fact that the DOC surface concentration at the moment is too high. This is something that need to be worked on. Majority of export occurs in the subtropical gyres by advection. Export due to diapycnal diffusion occurs in equatorial upwelling regions but the maginude is utmost 10%

The seasonal pattern of DOC:DOP export in Figure 9 is similar to that of POC:POP export. Compared to POC:POP export (Fig. 7(d)), temporal shift in DOC:DOP export is smaller. Another interesting thing is that DOC concentration (Fig. 9(d)) and DOC export (Fig. 9(c)) are not correlated in a predictable way. This shows the DOC export is much more nuanced as a result of interaction between physics (flow field) and biogeochemistry. DOC dynamics is something that has to be explored in more detail.

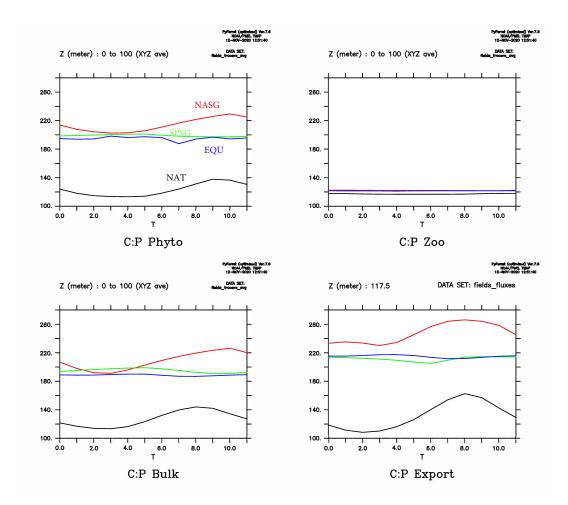


Figure 7: Modeled seasonal C:P of (a) Phytoplankton, (b) Zooplankton, (c) Bulk POM (= Detritus + Phytoplankton + Zooplankton), and (d) Export ratio at 100 m

2.3 Study 3: Using MOBI+UVic to simulate isotope dynamics, WORK IN PROGRESS

For this study, we will explore ocean biogeochemical dynamics using the second version of MOBI (Model of Ocean Biogeochemistry and Isotopes). MOBI includes:

- NO₃, PO₄, and DFe as interactive nutrients.
- 3 Phytoplankton classes (diazotrophs, coccolithophores, and other phytoplankton).
- Zooplankton.
- Detritus (dead POM).
- CaCO₃ is a prognostic variable and its production is calculated as a fraction of the detrirus produced by coccolithophores and zooplankton and it is sinking into the deep ocean where it dissolves.
- Nitrogen (¹⁵N) and carbon (¹³C) isotopes are included in all compartments.
- Radiocarbon (¹⁴C) is included only in the DIC compartment.
- Dissolved O₂ controls the water column denitrification. Benthic denitrification is calculated considerting subgridscale bathymetry.
- DOM is calculated separately for C, N, and P (DOC, DON, DOP).
- The most complex configuration has a total of 30 prognostic tracers.

To learn different configurations of MOBI, refer to the primer by A. Schmittner (https://github.com/tanio003/tmm/blob/TT_Release/Tutorial_MSI/MOBI2.0_Schmittner.pdf).

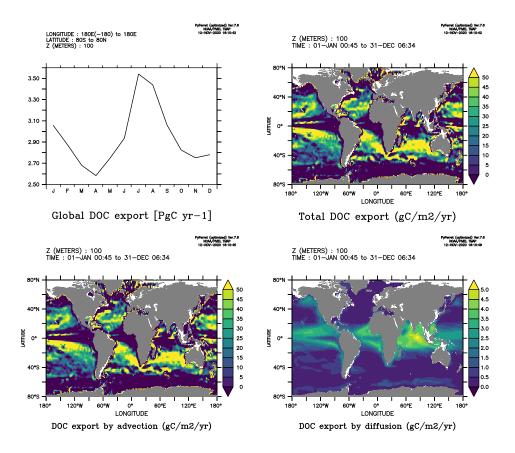


Figure 8: Modeled DOC export. (a) Monthly global DOC export at 100 m (b) Annual mean global DOC export (c) Annual mean global DOC export by advection, and (d) Annual mean global DOC export by diffusion.

In our exercise, we will try conducting a spin-up run for 3000 yrs using 30 prognostic tracers. Instructions will mostly follow that of S. Khatiwala.

1. Download the compatible versions of UVic ESCM 2.9 in the first level of your TMM directory

```
$ cd ~/TMM2
$ git clone https://github.com/your_github_username/UVic2.9
```

2. Download the TMM called UVicOSUpicdefault. Although you can download the original TMM from the Samar's repository, I found out when I did the preliminary test that the original TMM does not have the flow field for river discharge. Therefore, I had to import the "foreign" river discharge field from another TMM called UVicKielIncrIsopycDiff (Maybe we could contact Samar to ask for the full configuration for UVicOSUpicdefault with river discharge?). To copy my TMM,

```
$ cp -r ~/../tanio003/TMM2/UVicOSUpicdefault_with_discharge $HOME/TMM2/
```

Currently, MOBI can only be coupled to this TMM configuration (UVicOSUpicdefault_with_discharge) because other TMMs like MITgcm models do not have bathymetry profile and hydrothermal Fe input masks.

3. Make a Run directory for TMM-MOBI. For this run, I call it Runs/MOBI/Test_spinup. Copy mobi2.0/src/Makefile and mobi2.0/src/MOBI_TMM_OPTIONS.h to this directory.

```
$ cd ~/TMM2
$ mkdir -p Runs/MOBI/TMM_spinup
$ cd Runs/MOBI/TMM_spinup
$ cp -p $TMMROOT/models/current/mobi2.0/src/Makefile .
$ cp -p $TMMROOT/models/current/mobi2.0/src/MOBI_TMM_OPTIONS.h .
```

Also, following the instructions at the top of Makefile, set the environmenta variable \$UVICESCMROOT to point to the top level of the UVic ESCM 2.9. Add this to your .bashrc for cd your future convenience.

```
$ export UVICESCMROOT=$HOME/TMM2/UVic2.9
echo $UVICESCMROOT
/home/.../TMM2/UVic2.9
```

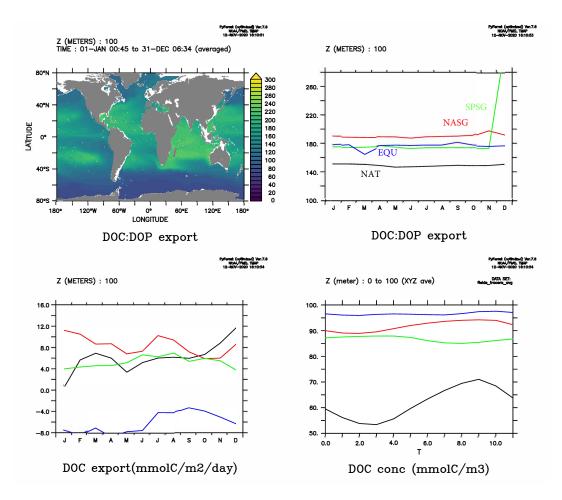


Figure 9: Modeled DOC:DOP and regional DOC export. (a) Annual mean DOC:DOP export ratio at 100 m, (b) Annual mean DOC:DOP at 4 different regions, (c) Annual mean DOC export, and (d) Annual mean surface DOC concentration.

4. Copy the contents (including the subdirectories) of mobi2.0/matlab and mobi2.0/runscripts to the test directory.

- 5. Edit the C preprocessor options in MOBI_TMM_OPTION.h as necessary. In particular, you have to define the directive O_co2_user (i.e., by # define O_co2_ccn_user). See Appendix ??? for what each of the options mean.
- 6. Build the model with:

```
$ make cleanall
$ make tmmmobi
```

If compiled properly, you would see an executable file tmmmobi created along with a bunch of objective .o files. Don't worry about various warnings as long as they are not fatal.

7. Generate the names tracers being simulated (as per the options set in MOBI_TMM_OPTIONS.h and their initial consitions. To do this, first set at the top of make_input_files_for_mobi_model_write_ic.m.

```
% make_input_files_for_mobi_model_write_ic.m
```

Execute in MATLAB.

>> make_input_files_for_mobi_model_write_ic

8. Compile and execute tmmmobiwrite.

\$ make tmmmobiwrite \$./tmmmobiwrite

This will write out MOBI_tracer_names.txt containing the tracer names, and a corresponding set of *.dat text files (e.g., dic.dat) containing the vertical profile of tracer concentration. These names and (horizontally uniform) profiles are used by make_input_files_for_mobi_model.m to generate initial condition files (e.g., dicini.petsc).

9. Make a directory InitialConditionProfiles and copy the *.dat files into it. By default make_input_files_for_mobi_model.m will look in this directory for the *.dat files.

\$ cp -p *.dat InitialConditionProfiles/

(Note-1): There are already copies of MOBI_tracer_names.txt and InitialConditionProfiles/ in matlab/ but S.Khawtiwala recommends you still go through this step to generate tracer names consistent with your version of UVic/MOBI and MOBI_TMM_OPTIONS.h.

(Note-2): The order of tracers in MOBI_tracer_names.txt is the same as that in which you specify initial condition, output and time average files in the TMM-MOBI run script. You can reduce the tedium (and chances of making a mistake) of generating the correct sequence to specify in the run script by executing this on the command line:

\$ printf "%sini.petsc," 'tr '\n' ' < MOBI_tracer_names.txt' | sed 's/,*\$//g'</pre>

(The tr replaces newlines with spaces to put all tracer names on a single line, the printf appends "ini.petsc," to each tracer name, and the sed strips out the final comma.)

(Note-3): tmmmobiwrite uses UVic routines where initial condition profiles are set. The code for this is hardwired for the standard UVic grid with 19 levels. If you're using TMs from a different ocean model you will need to modify make_input_files_for_mobi_model.maccordingly to specify initial conditions corresponding to your grid. You will also need to change the number of levels (km) in size.h.

10. Set the path at the top of make_input_files_for_mobi_model.m and execute in MATLAB. (See NOTE-3 in #9.)

% make_input_files_for_mobi_model.m

>> make_input_files_for_mobi_model

- 11. Edit the namelists in control.in as necessary. The important variables you must set are:
 - dtts in the &tsteps namelist: this MUST match the time step argument to the run time option -biogeochem_deltat in the runscript. This is the tracer advection-diffusion timestep.
 - co2ccn and dc14ccn in the &carbon namelist.
 - dtnpzd in the &npzd namelist. Set this so that dtts is a multiple of dtnpzd. For stability, dtnpzd (in seconds) should not exceed 1/3rd of a day (in seconds).

See Appendix 3.3 for what each of these other options mean in control.in.

12. Edit runscript as necessary. Also see (NOTE-2 in #9).

```
# runscript_msi
```

(NOTE-1): If turning on sediments and running on a smaller number of CPUs you should unlimit stacksize. Otherwise you may get a segmentation fault. Don't worry about this for MSI but you can check just in case by:

\$ ulimit -H -a
...
stack size (kbytes, -s) unlimited

- 13. Set the path at the top of the load*.m scripts to read in the output in Matlab.
- 14. Display output files in .nc. Currently, all the .nc files are spewed out one by one. If I get a time, I can make a scirpt to put all the variables into a single .nc file.

3 Appendix

3.1 Downloading PyFerret on MSI

1. Install miniconda on your home directory. This is a free cross-platform for Python distribution from Continuum Analytics.

```
$ cd ~
$ module purge
$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
$ bash Miniconda3-latest-Linux-x86_64.sh
```

Follow the prompts on the installer screens. If you are unsure about any setting, accept the defaults. To make the changes take effect, close and then re-open your terminal window. Once installed you should find new directory called miniconda3 on your home directory.

2. Execute the following command to install pyferret as well as ferret_datasets (the default Ferret datasets) into conda.

```
$ conda create -n PyFERRET -c conda-forge pyferret ferret_datasets --yes
```

PyFERRET is the environment name where pyferret is installed. You can change that to any name you like.

3. To start using PyFerret, execute the following commands (replace PyFERRET with whatever environment name you used):

```
(base) $ conda activate PyFerret
(PyFERRET) $ pyferret
NOAA/PMEL TMAP
PyFerret v7.6 (optimized)
Linux 4.15.0-1089-azure - 06/25/20
18-Sep-20 15:07
yes?
```

4. (Optional) You may with to add directories to FER_DATA and FER_GO:

```
(PyFERRET) $ export FER_DATA="$FER_DATA_/my/path/to/big/data/dir"
(PyFERRET) $ export FER_GO="$FER_GO_/my/path/to/custom/ferret/scripts"
```

5. Once you are done working with PyFerret you can leave this environment, if you wish, with the command:

```
(PyFERRET) $ conda deactivate
(base) $
```

3.2 General reference for MOPS and MOBI

Key references for MOPS:

- Kriest, I. and Oschlies, A. (2015). Mops-1.0: modelling the regulation of the global oceanic nitrogen budget by marine biogeochemical processes. *Geoscientific Model Development*, 8:2929–2957
- Kriest, I., Kähler, P., Koeve, W., Kvale, K. F., Sauerland, V., and Oschlies, A. (2020). One size fits all? Calibrating an ocean biogeochemistry model for different circulations. *Biogeosciences*, 17(12):3057–3082
- Niemeyer, D., Kriest, I., and Oschlies, A. (2019). The effect of marine aggregate parameterisations on nutrients and oxygen minimum zones in a global biogeochemical model. *Biogeosciences*, 16(15):3095–3111

Key references for MOBI:

- Khatiwala, S., Schmittner, A., and Muglia, J. (2019). Air-sea disequilibrium enhances ocean carbon storage during glacial periods. *Science advances*, 5(6):eaaw4981
- Muglia, J., Somes, C. J., Nickelsen, L., and Schmittner, A. (2017). Combined effects of atmospheric and seafloor iron fluxes to the glacial ocean. *Paleoceanography*, 32(11):1204–1218
- Somes, C. J., Schmittner, A., Muglia, J., and Oschlies, A. (2017). A three-dimensional model of the marine nitrogen cycle during the last glacial maximum constrained by sedimentary isotopes. *Frontiers in Marine Science*, 4:108

- Kvale, K. F., Meissner, K., Keller, D., Eby, M., and Schmittner, A. (2015). Explicit planktic calcifiers in the university of victoria earth system climate model, version 2.9. *Atmosphere-Ocean*, 53(3):332–350
- Yamamoto, A., Abe-Ouchi, A., Shigemitsu, M., Oka, A., Takahashi, K., Ohgaito, R., and Yamanaka, Y. (2015). Global deep ocean oxygenation by enhanced ventilation in the southern ocean under long-term global warming. *Global Biogeochemical Cycles*, 29(10):1801–1815

3.3 Paramters for MOBI (listed at control.in)

• contrl: Variables related to general control. Declared in \$UVICESCMROOT/source/common/switch.h.

Num	Parameters	Description	Unit	Default
1	init	This is a initial run (true) or from a restart	[true,false]	.false.
2	runlen	Integration period in "rununits"	[rununits]	36500.
3	rununits	Units of "runlen". Can be days, months, or years	[Days/Month/Years]	'days'
4	restrt	Write a restart at the end of the run	[true,false]	.true.
5	runstep	Integration period in timesteps	[timesteps]	2550000

• tsteps: Variables related to timestepping.

Num	Parameters	Description	Unit	Default
1	dtts	Timestep for density and tracers	[sec]	28800.
2	dtuv	Timestep of baroclininc velocity (internal mode)	[sec]	1125.
3	dtsf	Timestep of barotropic velocity	[sec]	1125.
4	dtatm	Timestep of atmospher	[sec]	54000.
5	namix	Timesteps between mixing	[timesteps]	10
6	segtim	Integration time is broken into number of segments each of length "segtim" days	[Days]	5.

• riglid: Variables related to numerical analysis thresholds.

Num	Parameters	Description	Unit	Default
1	mxscan	Max number of allowable scans for Poisson solvers	[-]	200
2	sor	Over-relaxation multiplier	[-]	1.60
3	tolrsf	Tolerance for stream function calculation	[-]	5.e8
4	tolrsp	Tolerance for surface pressure calcualtion	[-]	1.e-4
5	tolrfs	Tolerance for implicit free surface calculation	[-]	1.e-4

• mixing: Variables related to mixing. Most of these declared in \$UVICESCMROOT/source/mom/UVic_ESCM.F but no descriptions given for some.

Num	Parameters	Description	Unit	Default
1	am	?	?	1.5e9
2	ah	?	?	8.e6
3	ahbkg	?	?	0.
4	ambi	Constant lateral biharmine viscosity coefficient for momentum	[-]	1.e23
5	ahbi	Constant lateral biharmine diffusion coefficient for tracers	[-]	5.e22
6	kappa_m	Constant vertical viscosity coefficient	[cm ² /sec]	10.
7	kappa_h	Constant vertical dissusion coefficient	[cm ² /sec]	0.35
8	aidif	Coefficient for implicit time differencing for vertical diffusion	[-]	0.5
9	nmix	Number of timesteps between mixing timesteps	[timesteps]	16
10	eb	Conifgures for the use of a Euler Backward mixing timestep	[true,false]	.false.
11	ncon	Number of passes through convection routine	[-]	1
12	cdbot	Bottom drag coefficient	[-]	1.3e-3
13	acor	Implicit Coriolis Factor (0.0 => 1.0)	[-]	0.
14	dampts	Timescale for damping surface tracers to data	[Days]	30.,60.
15	dampdz	Ocean level thicknesss for converting Newtonian damping	[cm]	50.e2,50.e2

• **diagn**: Variables related to time integral. Descriptions are found in \$UVICESCMROOT/source/common/switch.h.

Num	Parameters	Description	Unit	Default
1	tsiint	Number of days between printing of time step integrals	[Days]	365.
2	tsiper	Averaging period for "time_step_monitor"	[Days]	365
3	timavgint	Interval for writing time mean data from the "averaging" grid	[Days]	36500.
4	timavgper	Averaging period for "time_averages"	[Days]	36500.
5	restint	Days between saving restarts	[Days]	36500.
6	tavgint	Days between regional tracer averages (under horizontal regions)	[Days]	-365000.

7	itavg	Write regional mask info the tracer average diagnostic	[true,false]	.true.
8	tmbint	Number of days over which tracer equation in averaged in depth and longitude	[Days]	-365000.
9	itmb	Write "msktmb" for tracer meridional balance diagnostic. True for the new runs.	[true,false]	.true.
10	trmbint	Days between momentum and tracer term balances	[Days]	-365000.
11	itrmb	Write regional mask info for the term balance diagnostic	[true,false]	.true.
12	tbtint	Averaging period for writing term balances	[Days]	-365000.
13	tbtper	Averaging period for tracer term balances	[Days]	-365.
14	glenint	Number of days between global energetics integrals	[Days]	-365000.
15	vmsfint	Number of days between calculation of vertical and meridional stream function	[Days]	-365000.
16	stabint	Number of days between sampling for various stability criteria	[Days]	-365000.
17	zmbcint	Number of days between calculation of zonal mean surface boundary conditions	[Days]	-365000.
18	gyreint	Number of days between calculation of traccer northward transport	[Days]	-365000.
19	extint	Number of days between printouts of external mode	[Days]	-365000.
20	prxzint	Number of days between printouts of x-z data	[Days]	-365000.
21	dspint	Number of days between surface pressure calculation	[Days]	-365000.
22	trajint	?	[Days]	-365000.
23	xbtint	Averaging period for xriting XBT data	[Days]	-365000.

• io: Variables related to ocean circulation module. Descriptions are found in \$UVICESCMROOT/source/common/iounit.h and \$UVICESCMROOT/source/common/diag.h.

Num	Parameters	Description	Unit	Default
1	expnam	60 character text string for experiment name	['Name']	, ,
2	iotavg	Control # for tracer averages	[-]	6
3	iotmb	Control # for writing meridional tracer budget	[-]	6
4	iotrmb	Control # for term balances for tracer and momentum	[-]	6
5	iozmbc	Control # for writing zonal mean surf boundary conditions	[-]	6
6	ioglen	Control # for writing global energetics integrals	[-]	6
7	iovmsf	Control # for writing meridional stream function	[-]	6
8	iogyre	Control # for writing gyre transport	[-]	6
9	ioprxz	Control # for writing x-z sections from latitudes	[-]	6
10	ioext	Control # for writing external mode (stream function)	[-]	6
11	iodsp	Control # for writing diagnostic surface pressure	[-]	6
12	iotsi	Control # for writing time step integrals	[-]	6
13	iotraj	?	[?]	6
14	ioxbt	Control # for writing time averaged xbt data	[-]	6
15	mrot	Regional mask region for max/min overturning	[-]	1
16	jsot	Starting j index for max/min overturning	[-]	65
17	jeot	Ending j index for max/min overturning	[-]	90
18	ksot	Starting k index for max/min overturning	[-]	3
19	keot	Ending k index for max/min overturning	[-]	17

• ictime: Variables related to time management. Descriptions are found in \$UVICESCMROOT/source/common/tmngr.h, \$UVICESCMROOT/source/common/tmngr.F, and \$UVICESCMROOT/source/common/switch.h.

Num	Parameters	Description	Unit	Default
1	eqyear	Use constant length year calendar?	[true,false]	.true.
2	eqmon	Use 12 equal months of monlen days each?	[true,false]	.false.
3	refinit	reference to initial condition time	[true,false]	.true.
4	refrun	referenced to the start of each run	[true,false]	.false.
5	init_time_in	sets input restart to initial time	[true,false]	.false.
6	init_time_out	sets output restart to initial time	[true,false]	.false.
7	year0	year of initial conditions	[year]	0
8	month0	month of initial conditions	[month]	1
9	day0	day of initial conditions	[day]	1
10	hour0	hour of initial conditions	[hour]	0
11	min0	minute of initial conditions	[minute]	0
12	sec0	second of initial conditions	[second]	0

Num	Parameters	Description	Unit	Default
1	AHV	Vertical diffusion coefficient	[-]	0.6

- **hlmix**: Variables related to horizontal mixing. Default = not given.
- **isopyc**: Variables related to the isopycnal mixing scheme. Descriptions are found in \$UVICESCMROOT/source/mom/isopycnal.F.

Num	Parameters	Description	Unit	Default
1	slmx	max slope of isopycnals	[-]	0.01
2	ahisop	isopycnal tracer diffusivity	[cm ² /sec]	1.2e7
3	athkdf	isopycnal thickness diffusivity	[cm ² /sec]	8.e6
4	del_dm	transition for scaling diffusion coefficient	[cm ² /sec]	0.4e-2
5	s_dm	half width scaling for diffusion coefficient	[cm ² /sec]	0.1e-2

- ppmix: Variables related to the Pacanowski/Philander vertical mixing scheme. Default = not given.
- smagnl: Variables related to the Smagorinsky nonlinear horizontal viscosity. Default = not given.
- embm: Variables related to the energy balance atmosphere model.

Num	Parameters	Description	Unit	Default
1	adiff	atmospheric diffusivity?	[?]	0.03

 $\bullet \ \ \, \textbf{carbon:} Variables \ related \ to \ carbon \ cycle \ in \ the \ energy \ balance \ atmosphere \ model. \ Descriptions \ are \ found \ in \ \$UVICESCMROOT/source/common/cembm.h. \\$

Num	Parameters	Description	Unit	Default
1	co2ccn	atmospheric CO2 concentration	[ppmv]	277.4412
2	dc14 ccn	atmospheric dC14 concentration	[permil]	0.0

• **paleo**: Variable related to paleoclimatology and paleoceanography. Descriptions are found in \$UVICESCMROOT/source/common/cembm.h.

Num	Parameters	Description	Unit	Default
1	pyear	default paleo calendar year (-/+ = BC/AD)	[year]	1765.

- ice: Variables related to ice module. Default = not given.
- **veg**: Variables related to land/vegetation module. Default = not given.
- mtlm: Variables related to land-surface and vegetation model. Descriptions are found in \$UVICESCMROOT/source/common/mtlm.h.

Num	Parameters	Description	Unit	Default
1	BF	Burn fraction	[-]	0.0

• **npzd**: Parameters related to biogeochemical NPZD model. Descriptions are from https://github.com/ OSU-CEOAS-Schmittner/UVicMOBI_fct_npzd_o2_n_fe_ca_caco3_c13_n15/blob/master/updates/npzd_src.

Num	Parameters	Description	Unit	Default
1	k1n	Half saturation constant for N uptake	$[mmol/m^3]$	0.7
2	capr	carbonate to carbon production ratio	[molar]	0.055
3	$abio_P$	a; Maximum growth rate parameter	[1/day]	0.6
4	alpha	Initial slope P-I curve	$[(W/m^2)^{-1}/day]$	0.16
5	nup	Specific mortality rate (Phytoplankton)	[1/day]	0.03
6	nupt0	Fast-recycling mortality rate (Phytoplankton)	[1/day]	0.001
7	redctn	C/N Redfield ratio	[molar]	7
8	geZ	Zooplankton growth efficiency	[-]	0.54
9	redotn	O2/N Redfield ratio	[molar]	11.0
10	kfemin	Minimum half saturation constant for Fe limitation	$[mmolFe/m^3]$	0.04e-3
11	kfemax	Maximum half saturation constant for Fe limitation	$[mmolFe/m^3]$	0.4e-3
12	kfemin_C	Minimum half saturation constant for Fe limitation (Cocco)	$[mmolFe/m^3]$	0.04e-3
13	kfemax_C	Maximum half saturation constant for Fe limitation (Cocco)	$[mmolFe/m^3]$	0.4e-3
14	kfe_D	Half saturation constant for Diaz Fe limitation	$[mmolFe/m^3]$	0.1e-3
15	zprefC	Zooplankton preference for C	[-]	0.21
16	zprefP	Zooplankton preference for P	[-]	0.24
17	dissk0	initial dissolution rate parameter	[-]	0.013
18	gbio	Maximum grazing rate	[1/day]	0.37
19	wd0	Sinking speed of detritus at surface	[m/day]	15
20	nuz	Quadratic mortality (zpk)	$[(mmol/m^3)^{-2}day^{-1}]$	0.06
21	jdiar	factor reducing the growth rate of diazotrophs	[-]	0.2
22	nud0	detritus remineralization rate	[1/day]	0.07

23	sgbdfac	sub-grid benthic denitrification rate factor	[-]	2.0
24	diazntp	diazotroph N:P ratio	[molar]	40.0
25	nup_D	Specific mortaility rate (Diazotrophs)	[1/day]	0.0001
26	$abio_C$	a; Maximum growth rate parameter (Cocco)	[1/day]	0.3
27	k1n_C	Half sat const for N uptake (Cocco)	$[mmol/m^3]$	0.35
28	alpha_C	Initial slope P-I curve (Cocco)	$[(W/m^2)^{-1}/day]$	0.1
29	nuct0	Fast-recycling mortality rate (Cocco)	[1/day]	0.013
30	$nupt0_D$	Fast-recyling mortality rate (Diazotrophs)	[1/day]	0.001
31	dfr	phyt mortality refractory/semi-labile DOM fraction	[-]	0.1
32	dfrt	phyt fast-recy refracotyr/semi-labile DOM fraction	[-]	0.08
33	dtnpzd	time step of biology	[s]	14400.0
34	hdop	DOP growth rate handicap	[-]	0.4
35	nudop0	DOP remineralization rate	[1/day]	2.0e-5
35	nudon0	DON remineralization rate	[1/day]	1.0e-5
36	eps_assim	Scaling factor for assimilation	[-]	6.0
37	eps_excr	Scaling factor for excretion	[-]	4.0
38	eps_recy	Scaling factor for recycling	[-]	1.3
39	eps_wcdeni	Scaling factor for water column denitrification	[-]	25.0
40	eps_bdeni0	Scaling factor for benthic denitrification	[-]	4.0
41	eps_nfix	Scaling factor for benthic N fixation	[-]	1.0
42	mwz	Depth where sinking below remains constant	[cm]	100000
43	mw	Sinking speed increase with depth	$[s^{-1}]$	0.055

To find out what these paramters actually do in the model, you may need to refer to several description papers:

- Original NPZD model (Oschlies and Garçon, 1999; Giraud et al., 2000; Schmittner et al., 2005, 2008).
- Zooplankton grazing formulation (Keller et al., 2012)
- Nitrogen isotope model (Somes et al., 2010a,b, 2013)
- Carbon isotope (¹³C) model (Schmittner et al., 2013)
- Prognostic CaCO₃, Coccolithophores, and balast (Kvale et al., 2015)
- Iron Model (Nickelsen et al., 2015)
- Benthic denitrification and sedimentary iron release (Somes and Oschlies, 2015; Muglia et al., 2017)
- sed: Variables related to sediment module. Default = not given.

References

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