

User Manual for PSOM

~ et. al

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1 Introduction

FROM README FILE :

* GENERAL DESCRIPTION

PSOM, pronounced "soam" (the nectar derived from the churning of the oceans in Indian mythology), stands for Process Study Ocean Model. It is a versatile, three-dimensional, non-hydrostatic, computational fluid dynamical model for oceanographic (as well as other) applications (Mahadevan et al., 1996a,b). The model uses the finite volume method on a structured grid with boundary fitted coordinates (topography conforming sigma grid in the vertical, and boundary conforming in the horizontal). The model has a free-surface. It can be used for large- and small-scale phenomena and can be run in hydrostatic or non-hydrostatic mode (Mahadevan, 2006). It uses a highly efficient solution procedure that exploits the skewness arising from the small geometrical aspect (depth to length scale) ratio of the ocean to speed up the solution of the non-hydrostatic pressure, which is solved by the multigrid method.

The model has been used for a number of process studies, including investigation of the vertical transport of nutrients for phytoplankton production (Mahadevan and Archer, 2000) and the dynamics of submesoscale processes (Mahadevan and Tandon, 2006; Mahadevan, Tandon and Ferrari, 2010). Since the non-hydrostatic model is well-posed with open boundaries, it can be used as a nested high-resolution model with time-varying boundary conditions applied from a coarser resolution general circulation model (Mahadevan and Archer, 1998). The model is thus ideally suited for high-resolution, limited-region modeling studies.

2 Headstart

FROM GET_STARTED_1

```
1 Here is the minimal set of actions required prior to starting using psom.
2
3 * step 1: Select the compiler you want to use. To do that, please edit the ./
  optfile to set the compiler you will use:      fcomp=... (ifort, pgf95
  etc.). If compiler is modified, the user is encouraged to scan through the
  ./optfile to make other necessary modifications (e.g., the directory of
  the gotm library if activated, the define\_parallel flag, etc.).
4
5 * step 2: By default, psom will produce both binary files and netcdf files. If
  you do not have netcdf library installed or simply do not want to use
  netcdf files,
```

```

6
7 — edit the file ./optfile          and set define\_netcdf to F.
8 — edit the file ./model/inc/cppdef and undefine output\_netcdf variable:
9 \#define file\_output\_cdf    by default
10 \#undef file\_output\_cdf    if you do not want to use netcdf.
11
12 These two actions will disable the netcdf output. The executable will only
    produce binary files.

```

3 Configure, compile, run sequence

FROM GET_STARTED_1

```

1
2 Once you have done that, you simply follow the "configure, compile, run"
    sequence:
3
4 * step 3: Configure.
5
6 sh tools/configure.sh
7
8 * step 4: Compile.
9
10 sh tools/compile.sh
11
12 * step 5: Run.
13
14 ./exe/nh $<$ ./namelist\_default
15
16
17 +  ADDITIONAL INFORMATION
18
19 Some explanations:
20
21 * About step 3.
22 — Step 3 will search for makedepend (which is necessary to create the makefile
    ). The script will stop if makedepend is not installed. The makefile file
    will only be created if makedepend can be called.

```

23 → Solution: download makedepend, which is free and widely accessible. For
 instance, on mac, you can simply `sudo port install makedepend` (if you have
 macport installed).

24 – Furthermore, if you chose to use netcdf, an attempt to use `nc-config` will be
 tried. Note that the code has only been tested with netcdf4 libraries.

25 → if `nc-config` is present, it will be used in order to set the links to
 netcdf libraries appropriately.

26 → if not, you can complete this step yourself by linking the executable to
 the netcdf libraries. To do so, edit `./optfile` before going through step
 3.

27

28 Step 3 has two effects:

29 – `./optfile` is modified ,

30 – `./namelist` is customized.

31

32 To sum up, if step 3 fails , the easiest way is to install makedepend and/or to
 install netcdf libraries (in case you want to use netcdf output). After
 having done that , repeat step 3.

33

34

35 * Step 4 will

36 – create the makefile in `./mkfile`

37 – compile

38

39 A failure during step 4 most likely indicates that there is an error in the
 fortran code.

40

41

42 * Step 5 will start and run the model.

43 By default , the namelist file contains the values of key parameters of the
 model, that you are likely willing to change. You can of course edit
 namelist to your convenience and repeat step 5.

44 By default , messages will appear on the screen and the output files will go to
`../output/`.

4 Particle tracking in PSOM

PSOM offers the option to release and track particles "online" (i.e., as part of the numerical simulation). To activate this option, the `allow_particle` options must be defined in `inc/cppdefs.h` by including (See Section 6.3):

```
#define allow_particle
```

The particle tracking code has been written for a rectangular grid only, and cannot be used "as is" for a non-rectangular model grid.

4.1 Non-sinking particles

While key particle parameters are set in `namelist` (e.g., particle number, frequency of outputs, etc.; see Section 6.8), the seeding and advection of particles is controlled by the code included in `particles.f90`. The file includes the following subroutines:

- open_parti_files*: This subroutine creates the output files where the particle characteristics will be saved. The number of output files is specified in `namelist` and must be a factor of the total number of particles (NPR). Increasing the number of output files reduced the size of the individual files, which proves to be useful when dealing with a very large number of particles. The output files are unformatted binary files.
- save_parti*: This subroutine loops through all the particles and writes the specified variables. The number of variables saved is important, as it must be known to read the unformatted binary output files.
- ini_particles*: This subroutine is called when the model timestep matches the particle initialization timestep specified in `namelist`. This is where the seeding of particle is defined. By default, all particles are released below the surface layer in the middle of the model domain. To personalize the release of particles, see Section 6.8.2.
- get_parti_vel*: This subroutine interpolates the physical model's velocity field onto the particles' positions (using *interp_trilinear*; see below). The *get_parti_vel* subroutine also interpolates variables of interest onto the particles position (e.g., salinity, temperature, density, vorticity, etc.).
- parti_forward*: This subroutine extrapolates the position of a particle at the next timestep $t+1$ using a 2nd order Adams-Bashforth scheme. As an example, the position of the particle in the zonal direction is computed using:

$$(i, j, k)_{t+1} = (i, j, k)_t + dtf \times \frac{1}{2}[3(u, v, w)_{t+1} - (u, v, w)_t]$$

Where (i, j, k) is the position of the particle in the model space, dtf is the non-dimensional model time step, (u, v, w) is the non-dimensional velocity field at the particle's location, and the subscripts represent the timestep. The corresponding code appears in `particles.f90` as (e.g., for the particle position in the zonal direction):

```
1 ! Assign i-position to particle.
2 parti(i)%i = parti(i)%i + 0.5d0 * dtf * (3d0 * parti(i)%u - parti(i)%u0)
```

At $t=0$, the velocities are assumed to be zero (set in `ini_particles`, and the 2^{nd} order Adams-Bashforth scheme simplifies to a one-step Euler scheme.

interp_trilinear This subroutine is used to interpolate 3D model variables onto a particle's position using a trilinear interpolation technique (e.g., velocities, density, etc.).

interp_bilinear This subroutine is used to interpolate 2D model variables onto a particle's position using a bilinear interpolation technique (e.g., depth of water column).

4.2 Sinking particles

The subroutine `get_parti_vel` includes the possibility to prescribe a vertical sinking velocity to the particles (set to 0 m/s by default). The prescribed velocity must be scaled appropriately to match the scaling used by PSOM. This requires information about the function used to compute the thickness of the model cells in the vertical, defined in `findzall.f90`. If this function is modified, the code in `particles.f90` **must be changed accordingly** (See Appendix 6.8.2 for important information). Although not implemented in the code, a horizontal velocity (e.g., to simulate swimming behavior) could also be easily prescribed to the particles following a similar method.

4.3 Reading unformatted binary output files

Particle-tracking output files are written as unformatted binary files. Information on how the output file is built is therefore required to be able to access the data. Two MATLAB routines to import or convert the particle-tracking output are provided with the model code:

- `particle_open_bin.m`: Imports the particle-tracking data into MATLAB as a 3D matrix (Nbr of particles, model time, # of recorded variables; see Appendix ??).

WARNING: This routine SHOULD NOT BE USED FOR LARGE FILES otherwise the 3D matrix will become too large and will crash MATLAB.

- `particle_bin2csv.m`: Converts the particle-tracking data into a CSV-file (see Appendix 6.8.2). This can be helpful when trying to import the particle-tracking data into another software (i.e., into an SQL database).

5 Test Cases

5.1 Wiggles

- 1 – `wiggle` : This is a testcase with a wiggling front over a flat topography.

5.2 NA

- 1 – `NA` : This is a much more complex simulation of three fronts that go unstable. This case has particles and tracers for biology.

5.3 Shelfbreak

- 1 – `shelfbreak` : Simulation of the Middle Atlantic Bight shelfbreak with a shelf front and a shelfbreak front. The topography includes a sharp slope at the break. It shows how to use the "user" namelist.

6 Setting up your PSOM simulation

Write a note about the superceding trick

6.1 Create your experiment directory

For every experiment you want to conduct, create a directory that will contain the source files specific to this experiment. As a example, you want to create an experiment named "my_experiment". First, create a directory `code/my_experiment`, in which you will create two subdirectories `/inc` and `/src`. You can either create this directory manually, or, in `code/`, you can run:


```
1 # Copies the template directory
2 cp -r expe_template my_experiment
```

Whether you are a user or a developer, **you are strongly invited to leave untouched the files contained in `code/model/`**. This directory is designed to contain the latest version of the model, which is common to every user at a given time. For every routine that will be specific to `my_experiment`, a new subroutine should be created in `code/my_experiment/src`. This can be achieved using the following command:

```
1 # Copies the initial conditions subroutine
2 cp model/src/ini_st.f90 my_experiment/src
```

The compiling step (**<FIX ME: see Section on compiling>**) includes a superseding procedure that will take into account the new version of `ini_st.f90` (in `code/my_experiment/src`) and disregard the standard version found in `code/model/src`. More precisely, it will create the makefile based on this new state of the model (in `./mkfile`), compile and create the executable `code/exe/nh_my_experiment`. More details on `compile.sh` may be found by running:

```
1 # Provides more information on compile.sh
2 sh tools/compile.sh --help
```

6.2 Defining your model grid

The grid size is defined in `size.h`. If you wish to modify the grid size, you must first copy `size.h` into your experiment's directory:

```
1 # Copies the grid file
2 cp model/inc/size.h my_experiment/inc
```

Grids used in previous experiments are listed in this file and commented out. If your grid appears in a commented line, Comment the uncommented line and uncomment the one you want. Be aware that if your grid set requires more than 2Go, you might experience compilation issues. If so, you may fix the issue by editing `tools/genmakefile1` to replace the default compiling options by:

```
fflags_o="-fpp -real-size 64 -mcmodel medium -shared-intel -stand 03 -u"
fflags_e="-fpp -real-size 64 -mcmodel medium -shared-intel -stand 03 -u"
```

If your grid set does not appear in `my_experiment/inc/size.h`, you can create the required line. Defining the model grid is not straight-forward, because of the multi-grid solver `mgrid` **<FIX ME: (See Section)>**. The multi-grid solver is used to allow the reuse of array space in `mgrid.f90` **<FIX ME: insert link to function?>**. Although this issue could now be circumvented by making use of `f90`'s dynamic allocation of memory, the code was originally in `fortran77`, explaining the need for space re-allocation. A step-by-step approach to defining your own grid is provided below:

1. Choose grid dimensions NI , NJ , and NK (i.e., the number of grid cells in x , y , and z directions) such that the grid can be subdivided a maximum number of times by a factor of 2 to form "*ngrid*" levels of grid. For example, choosing $NI = 48$, $NJ = 24$, and $NK = 32$ constrains the grid levels to 4 (i.e., $ngrid = 4$), because:

$NI : 48; 24; 12; 6; 3$	(5 grid levels)
$NJ : 24; 12; 6; 3$	(4 grid levels)
$NK : 32; 16; 8; 4; 2$	(5 grid levels)

The number of grid points possible for a specific *ngrid* can be computed by multiplying prime numbers (2, 3, 5, 7, etc.) by $2^{ngrid-1}$. Table 1 lists some of the most commonly used number of grid points, depending on the number of grid levels *ngrid*.

2. Compile `tools/preproc.f90`:

```
1 # Compiles preproc.f90 (e.g., using ifort)
2 ifort preproc.f90 -o preproc
```

3. Runs `preproc.f90` and fill the values that are asked:

```
1 # Runs preproc.f90
2 ./preproc.f90
```

4. Copy/Paste the last line the program provides in `my_experiment/inc/size.h`. Below is an example for $NI = 96$, $NJ = 160$, and $NK = 32$ (hence $ngrid = 5$, see Table 1):

```
1 ./preproc
```

Table 1: Number of grid points associated with a specific number of grid levels $ngrid$. These numbers can be computed by multiplying prime numbers (2, 3, 5, 7, etc.) by $2^{ngrid-1}$. Each experiment's number of grid levels is set by the minimum $ngrid$ associated with NI , NJ , and NK .

$ngrid$	Number of grid points (NI , NJ , or NK)							
4	16	24	40	56	88	104	136	152
5	32	48	80	112	176	208	272	304
6	64	96	160	224	352	416	544	608
7	128	192	320	448	704	832	1088	1216

```

2 number of grid levels in mgrid, ngrid =
3 5
4 input the grid info
5 NI =
6 96
7 NJ =
8 160
9 NK =
10 32
11 Number of grid points on fine grid: nx,ny,nz  96  160  32
12 m, ntint , ntout , nbc(m)  1      491520      539784      47104
13 m, ntint , ntout , nbc(m)  2      61440      73800      11776
14 m, ntint , ntout , nbc(m)  3      7680      10920      2944
15 m, ntint , ntout , nbc(m)  4      960      1848      736
16 m, ntint , ntout , nbc(m)  5      120      384      184
17 Copy the following line to size.h
18 INTEGER, PARAMETER :: NI=96, NJ=160, NK = 32, ngrid=5, maxout=626736,
    maxint=561720, int1=491520

```

6.3 cppdefs.h

This file defines the different options to be used in the experiment. Again, it is recommended to copy this file into the experiment folder (e.g., `my_experiment/inc/` before making any modifications. To include (exclude) an option, use `#define` (`#undef`) `option_name`. The file includes 13 options:

runtracmass : placeholder

periodic_ew : placeholder

periodic_ns : placeholder

allow_particle : If defined, allows the seeding of particles in the experiment. Please refer to section **<FIX ME: ref to particle section>** for a detailed explanation on particle seeding.

rhoonly : If defined, only the density field *rho* is used. The density field is stored in the salinity array (*s*; see `evalrho_rho.f90`). If not defined, *rho* is computed from the salinity (*s*) and temperature (*T*) fields (see `evalrho_sT.f90`).

relaxation : placeholder

red_bottom_thickness : placeholder

file_output : placeholder

file_output_cdf : placeholder

file_output_bin : placeholder

gotm_call : placeholder

implicit : placeholder

parallel : placeholder

6.4 namelist

This file defines key parameters relating to the experiment (e.g., grid resolution, time step, diffusion, output, ...). Again, it is recommended to copy this file into the experiment folder (e.g., `my_experiment/` before making any modifications. Each parameter in the file is either self-explanatory or include a short description as a comment.

6.5 Defining the initial conditions

Initial conditions can be specified either in the corresponding subroutines, or from an input file. The former approach is used in the Shelfbreak test-case (see Section 5.3), where the temperature and salinity distributions are determined from analytical expressions in DO-loops, and only requires a limited knowledge of the model grid. The latter approach can sometimes be more practical, especially when using available data products to initialize the model. However, this approach requires mapping the data used to initialize the experiment to the pre-defined model grid.

The horizontal grid is relatively straightforward to determine, given the grid size specified in `my_experiment/inc/size.h` (i.e., NI and NJ), and the grid resolution specified in `my_experiment/namelist` (i.e., dx and dy). The location of each grid point can be computed using the following equations:

$$x(i) = -dx/2 + idx; \quad i = (0, 1, 2 \dots NI, NI + 1) \quad (1)$$

$$y(j) = -dy/2 + jdy; \quad j = (0, 1, 2 \dots NJ, NJ + 1) \quad (2)$$

6.5.1 Temperature, salinity, and density

The initial conditions in the temperature and salinity

6.6 Wind stress

To specify a customized wind forcing, the code in `wind_stress.f90` can be modified. The wind stress at the surface is prescribed to the model through the variables `stress_top_x`, `stress_top_y`, and `stress_top`. The dimensions of these three variables are (NI, NJ) (see `header.f90`). The surface wind stress can be read from a file:

```
1 ! Import the wind stress time series for model forcing
2 if (step.eq.1) then
3   open(unit=17, file='youfilefullpath.in')
4   do i=1,nsteps
5     read(17,fmt="(F5.10,F5.10)") stressxTS(i),stressyTS(i)
6   end do
7   close (17)
8   PRINT*,"Read wind stress"
9 end if
10 stress_top_x = stressxTS(step)
11 stress_top_y = stressyTS(step)
```

or specified as a constant:

```
1 stress_top_x = 0.05d0
2 stress_top_y = 0.01d0
3 PRINT*, "Read Wind Stress"
```

If your domain includes solid boundary (i.e., no periodicity), it is recommended to damp the surface wind stress close to the boundaries, to avoid upwelling/downwelling. Below is an example of wind stress damping at the north/south boundaries using a tanh profile. A similar approach can be used in the east/west direction.

```
1 ! Apply a tanh profile in the meridional direction
2 ycenter = 0.5*(yc(NJ)+yc(1)) ! Find the middle of the domain
3 ywindmin = 10.0 ! Starts damping 10 km from southern boundary
4 ywindmax = yc(NJ)-10.d0 ! Starts damping 10 km from northern boundary
5 edge = 0.06 ! tightness of the padding in the wind stress
6
7 do j=1,NJ
8   if (yc(j).lt.ycenter) then
9     stressprofile(j) = 0.5*(tanh(edge*(yc(j)-ywindmin)*PI)+1.d0)
10  else
11    stressprofile(j) = -0.5*(tanh(edge*(yc(j)-ywindmax)*PI)-1.d0)
12  end if
13 end do
14
15 do j=1,NJ
16   do i=1,NI
17     stress_top_x(i,j) = stressxTS(step)*stressprofile(j)
18     stress_top_y(i,j) = stressyTS(step)*stressprofile(j)
19   end do
20 end do
```

6.7 Surface Heat Fluxes

6.8 Customizing Particle-tracking in PSOM

6.8.1 Parameters in `namelist`

To set up a particle-tracking experiment in PSOM, the `allow_particle` option must be defined in `inc/cppdefs.h` (See Section 6.3):

```
#define allow_particle
```

Four key variables related to particle-tracking are set in the `namelist` file:

1. The total number of Particles (NPR). NPR must be a multiple of the number of output files (see below).
2. The time step at which the particles are released (`ini_particle_time`). `ini_particle_time` **must be** greater than 0, or than `pickup_step` if pickup files are used to initialize the experiment (see Section ?? **<FIX ME: Refer to section about namelist and pick up files>**). If `ini_particle_time = pickup_step`, no particle output file will be written.
3. The number of output files to generate (`parti_file_num`). Increasing the number of files logically decreases the file size. This is especially useful when dealing with a very large number of particles, or when writing particles' position at high frequency. The number of file must be a factor of NPR (see above).
4. The frequency of particle outputs (`parti_outfreq`) in number of time steps.

6.8.2 particles.f90

a. Particle seeding

The seeding and tracking of the particles in PSOM are controlled by subroutines located in `particles.f90`. To personalize the seeding of particles in the model, the code in the subroutine `ini_particles` should be altered. By default, the particles are released below the surface layer, in the middle of the model domain:

```
1 ! User-defined particle positioning.
2 DO ip=1, NPR
3   parti(ip)%i=REAL(NI)/2d0 ! mid-domain in x
4   parti(ip)%j=REAL(NJ)/2d0 ! mid-domain in y
5   parti(ip)%k=REAL(NK)-5.  ! sub-surface cell
6
7   ! Converts model grid to distances (i,j,k) ==> (x,y,z)
8   parti(ip)%x = parti(ip)%i * dx
9   parti(ip)%y = parti(ip)%j * dy
10  ! Assign z-position to particle based on sigma level
11  ! Calculate the scaled z-depth
12  CALL sigma2z(parti(ip)%i, parti(ip)%j, parti(ip)%k, swap1)
```

```

13 parti(ip)%z = swap1 * DL
14 ENDDO

```

b. Sinking velocity

A sinking velocity can be prescribed to the particles (default = 0 m/s) by modifying the following line of code in *get_parti_vel*:

```

1 ! Then, specify the sinking velocity (in m/s), including the scaling factors
2 parti(ip)%wsink= -0d0/86400d0/WL*parti(ip)%wzf*EPS ! 0 m/day

```


Appendix A

Prescribing Sinking Velocity to Particles

M.Dever

July 18, 2017

How is sinking prescribed

The sinking velocity in the model (w_{sink}) is prescribed in the subroutine `get_parti_vel` in `particles.f90`. To match the physical model's velocity, w_{sink} must be scaled appropriately using:

```
1 parti(ip)%wsink= -ld0/86400d0/WL*parti(ip)%wzf*EPS ! lm/day
```

where WL non-dimensionalizes the vertical velocity, EPS is the Rossby number, and wzf is the coefficient scaling the vertical velocity with the size of the the k -cell in the k -space.

More on wzf

wzf can be thought of as $1/\Delta z$. It is the inverse of the (normalized) grid spacing in the vertical **at the cell faces**. The equivalent metric at the cell centers is wz .

Error on the vertical displacement

Motivation

The coefficient wzf needs to be determined for each particle position. The original way of determining wzf relied on (1) the linear interpolation of the cell-centered vertical grid spacing wz , and (2) the trilinear interpolation used in the particle code (see `particles.f90`).

```
1 ! Compute wz at face grids using linear interpolation
2 wzf = 0.5d0*(wz(:, :, 0:NK) + wz(:, :, 1:NK+1))
3
4 ! Compute wzf at the particle's location using trilinear interpolation
5 CALL interp_trilinear(dic,djc,dkc,wzf(ic:ic+1,jc:jc+1,kfc:kfc+1),parti(ip)%wzf)
```

Issues

The approach to determine the wzf coefficient onto the particle position in the vertical introduced some error in the vertical position of the particle. This error was identified by comparing the depth of a particle sinking at a constant rate as computed by the `particles.f90` routine, with the theoretical depth based on the sinking rate, the time elapsed, and the release depth:

```
1 model = w_sink * (t - t0) + z0
```

Figure 1 shows the error on the particle's vertical positioning with respect to the particle's depth. The error increases between the cell centers and faces (where the velocity is underestimated; see Figure 1), and decreases between cell faces and centers (where the velocity is overestimated). The error therefore oscillates and grows as k-cells become thicker. Future model variables (i.e., current velocities) will be interpolated onto the erroneous particle position, therefore introducing some cumulative effect in the errors associated with this method. Such errors are hard to quantify.

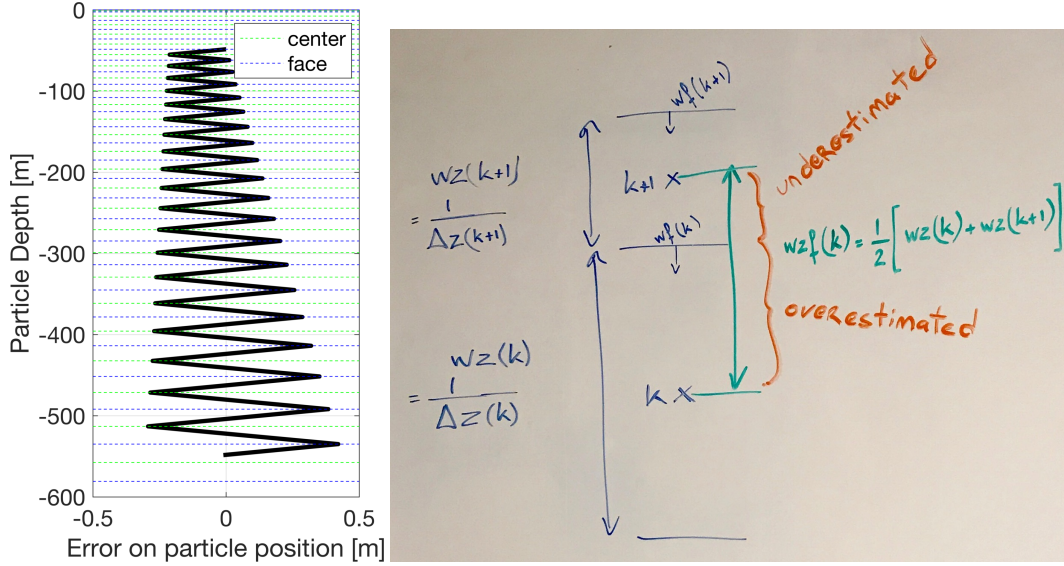


Figure 1: Error on particle vertical position due to the interpolation of wzf onto the particle position. Error is maximum at model grid cell centers and at grid cell faces. Error grows with depth, as grid cells become thicker, and is independent of the sinking velocity. Right panel shows the important variables and highlights the limitations of the original method.

New approach

Instead of relying on an interpolation of the discrete values of wzf , the continuous function that determines the depth of the k-levels (i.e., the vertical grid spacing), is used to exactly determine the value of wzf at the particle's location. The function is defined in the routine `findz_topmoves.f90`.

```
1  zc(i,j,k)= (exp(pfac*xfac)-1.d0)*epmlinv*(D(i,j)+dztop) -dztop
```

which can be re-written in terms of set parameters as:

$$zc(i,j,k) = \left(\frac{D(i,j) + dztop}{e^{pfac} - 1} \right) e^{pfac} e^{\frac{-pfac(k-0.5)}{NK-1}} + C \quad (1)$$

where zc is the depth of the cell-center, $D(i,j)$ is the dimensionless depth of the 0-th face z (at cell centers in x and y), $dztop$ is the dimensionless thickness of the uppermost cell, $pfac$ is the vertical stretching parameter used to define the sigma levels, NK is the number of vertical levels, and C is a constant.

What about the horizontal?

The error in the vertical described here arises from the fact that cell dimensions change with depth. A similar issue will therefore be present in the horizontal when using a non-rectangular grid. For a non-rectangular grid, uxf and vyf should be computed using a similar approach than the method outlined below. For a rectangular grid, the linear interpolation of ux and vy onto the faces is adequate.

What is the constant C?

The value of C is irrelevant in this context, as the difference between two z -levels is the quantity we are ultimately interested in.

The equation for the difference between two z-levels at k and $k+1$ (i.e., Δz) can thus be derived (Figure 2):

$$\begin{aligned}
 zc|_k &= \left(\frac{D + dz_{top}}{e^{pfac} - 1} \right) e^{pfac} e^{-\frac{pfac(k-0.5)}{Nk-1}} + C = \left(\dots \right) e^{pfac} e^{\frac{\frac{1}{2}pfac}{Nk-1}} e^{-\frac{pfac k}{Nk-1}} + C \\
 zc|_{k+1} &= \left(\dots \right) e^{pfac} e^{-\frac{pfac(k+0.5)}{Nk+1}} + C = \left(\dots \right) e^{pfac} e^{\frac{\frac{1}{2}pfac}{Nk+1}} e^{-\frac{pfac k}{Nk+1}} + C \\
 \Delta z &= zc|_{k+1} - zc|_k = \left(\dots \right) e^{pfac} e^{-\frac{pfac k}{Nk+1}} \left(e^{\frac{\frac{1}{2}pfac}{Nk+1}} - e^{\frac{\frac{1}{2}pfac}{Nk-1}} \right) + C - C
 \end{aligned}$$

Figure 2: Equations used to compute Δz at k -faces in particles.f90

The variable wzf can now be computed exactly at the particle's position by taking the inverse of Δz . Figure 3 shows the error (in meters, as well as in percentage of the particle's depth) on the particle vertical position after modifying the approach to compute wzf . The error grows linearly with depth, with a slope of 1.735×10^{-4} m per meter (i.e., 17.35 cm at 1000 m deep).

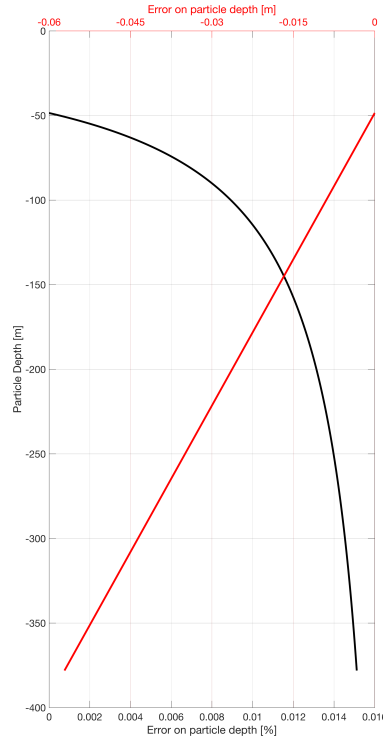


Figure 3: Error on particle vertical position after the approach used to compute wzf was modified.

What about the horizontal?

A slightly different equation than the one depicted in Figure 2 must be used if computing wz . While wzf must be computed using the depth of the z -cell centers zc , wz must be computed using the depths of the z -cell faces zf . this is achieved by using k instead of $(k - 0.5)$ in Equation 1.

Appendix B - particle_open_bin.m

```
1 clear
2
3 % ** This code imports the particle-tracking data directly from bin output
4 % files.
5 % ** The file path has to be specified.
6 % ** output is a 3D matrix where the 1st dimension is the particle number,
7 % the 2nd dimension is the model time, and the 3rd dimension is the
8 % recorded variables.
9
10 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
11 % WARNING
12 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
13 % This routine SHOULD NOT BE USED FOR LARGE FILES otherwise MATLAB matrices
14 % will become too large and will crash MATLAB.
15 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
16
17 %
18 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
19 % PARAMETERS
20 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
21
22 % number of files to import into matlab
23 number_of_files = 1;
24 % filepath
25 path = 'specify the path for the output files here';
26 % Number of variables recorded (see particles.f90)
27 number_of_variables = 20;
28
29 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
30 % CORE CODE
31 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
32
33 % Loops through the number of files to open
34 for filenum = 1:number_of_files
35
36 % Create fullpath
37 filename = ['op.parti-', num2str(filenum, '%03.f'), '.bin'];
38 fullpath = [path, '/', filename];
```

```

39
40 % Display the file being extracted
41 disp(filename);
42
43 % Open the file
44 fileID = fopen(fullpath);
45
46 % Extract the data (refer to particles.f90 to confirm that number)
47 A = fread(fileID,[number_of_variables Inf],'double');
48 A = A';
49
50 % Finds the number of particle per file using the ID numbers
51 if filenum == 1
52 partnum = max(A(:,1));
53 end
54
55 % write a matrix of dimensions:
56 % # of particles x timestep x recorded variables
57 for Np = (filenum-1)*partnum+1:(filenum-1)*partnum+partnum
58 ind = find(A(:,1) == Np);
59 data(Np, :, :) = A(ind, :);
60 end; clear Np ind
61
62 fclose(fileID);
63 clear A fileID filename path fullpath ans
64
65 end; clear filenum partnum

```

Appendix C - particle_bin2csv

```
1 clear
2
3 % This code converts the binary file output from the model into CSV files.
4 % This can be useful to open in other programs (e.g., import in a SQL
5 % database)
6
7 %%
8 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
9 % PARAMETERS
10 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
11
12 % number of files to import into matlab
13 number_of_files = 1;
14 % filepath of files to import
15 pathin = 'specify the path of the files to import here';
16 % Number of variables recorded (see particles.f90)
17 number_of_variables = 20;
18 % filepath of the csv-file to be written
19 pathout = 'specify the path where you would like to write the csv-files';
20
21 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
22 % CORE CODE
23 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
24
25 % Loops through the number of files to open
26 for filenum = 1:number_of_files
27
28     % Create fullpath
29     filename = ['op parti-', num2str(filenum, '%03.f'), '.bin'];
30     fullpath = [pathin, '/', filename];
31
32     % Display the file being extracted
33     disp(['Converting ', filename, ' into a CSV file ...']);
34
35     % Open the file
36     fileID = fopen(fullpath);
37
38     % Extract the data (refer to particles.f90 to confirm that number)
```

```

39  A = fread(fileID,[number_of_variables Inf],'double');
40  A = A';
41
42  % Remove all the zeros recorded
43  ind = find(A(:,1)==0);
44  if isempty(ind)~=1
45      warning(['Missing ',num2str(length(ind)),' records...!'])
46      A(ind,:) = [];
47  end; clear ind
48
49
50  % Re-write the file as CSV.
51  csvwrite([pathout,'/op.parti-',num2str(filenum,'%03.f'),'.csv'],A)
52
53  fclose(fileID);
54  clear A partnum fileID filename path fullpath
55
56 end; clear filenum

```


Glossary

D | E | N | P | S | U | V | W | Z

D

D Model depth

DL Characteristic depth scale

dtf non-dimensional time step

dx Grid-spacing in the x -direction (in m)

dy Grid-spacing in the y -direction (in m)

dztop Thickness of the uppermost cell (non-dimensional)

E

EPS Rossby number

N

NI Number of grid points in x-direction

NJ Number of grid points in y-direction

NK Number of grid points in z-direction

P

pfac Stretching coefficient used to determine vertical grid spacing

S

stress_top Surface wind stress magnitude

stress_top_x Surface wind stress in x-direction

stress_top_y Surface wind stress in y-direction

U

u Velocity in x -direction (non-dimensional)

UL Scaling coefficient for horizontal velocity

V

v Velocity in y -direction (non-dimensional)

W

w Velocity in z -direction (non-dimensional)

WL Scaling coefficient for vertical velocity

wsink Particle sinking velocity

wtotal Total particle vertical velocity (advection + sinking)

wz Inverse thickness of a given σ -layer $\Delta\sigma/\Delta z = 1/\Delta z$ at cell center

wzf Inverse thickness of a given σ -layer $\Delta\sigma/\Delta z = 1/\Delta z$ at cell faces

Z

zc Depth of the cell centers (non-dimensional)

zf Depth of the cell faces (non-dimensional)