

Delft3D-FM Simulation Configuration and Input File Generation

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CONTENTS

EXECUTIVE SUMMARY	E-1
1. INTRODUCTION	1
1.1 Background	1
2. MODEL DIRECTORY SET-UP	1
2.1 Directory Configuration and Contents	2
3. MODEL INPUT FILES	3
3.1 Model Run Script and DIMR Configuration File	3
3.2 Grid and Bathymetry Generation	3
3.3 Observation Points File	4
3.4 Hydrodynamic Boundary Conditions	4
3.5 Meteorological Forcing	6
3.6 File Transfer to HPC	7
3.7 External Forcing Files	8
3.8 Master Definition File for Hydrodynamics	10
3.9 Coupling with Waves	10
4. STARTING FROM AN EXISTING SIMULATION	10
4.1 Approach	11
4.2 HPC Directory Structure Creation	11
4.3 Model Run Script and DIMR Input File	11
4.4 Unstructured Grid File and Observation Points File	12
4.5 Boundary Condition Creation	12
4.6 Meteorological Forcing Creation	13
4.7 File Transfer to HPC	13
4.8 External Forcing Files	13
4.9 Master Definition File for FLOW Model	15
4.10 Water Depth and Curvilinear Grid Files	16
4.11 Master Definition File for WAVE Model	16
4.12 Model Execution	16
5. CREATING A PARAMETER ENSEMBLE	17
5.1 Introduction	17
5.2 Ensemble Directory Structure	17
5.3 Required Instantiate Files	18
5.4 Modification to Model Files	19
5.5 Running Instantiate	19
5.6 Preparing to Launch the Ensemble Simulation	20
5.7 Launching the Ensemble Simulation	21

REFERENCES	21
APPENDIX A—Python Code for Boundary Condition and Meteorological Forcing Creation	23
A.1 generate_BC_NCOM.py	23
A.2 coamps2meteo.py	34

EXECUTIVE SUMMARY

The purpose of this document is to give an overview of the setup of Delft3D-Flexible Mesh (DFM) (coupled FLOW and WAVE) on the Navy DoD Supercomputing Resource Center (Navy DSRC) High Performance Computing (HPC) system and to serve as a step-by-step guide for model setup starting from existing model input files of a specific domain.

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DELFT3D-FM SIMULATION CONFIGURATION AND INPUT FILE GENERATION

1. INTRODUCTION

This report outlines the set up of Delft3D-Flexible Mesh (DFM) coupled FLOW and WAVE modeling system on the DoD High Performance Computers (HPC). The primary focus is to serve as a step-by-step guide for model setup from an existing model input files of a given domain. Section 2 provides a description of model input file creation. This section is included to familiarize the user with the set-up process and input files, but is not intended to serve as a step-by-step guide to a new model setup. Section 5 outlines the required steps for parameter ensemble creation.

1.1 Background

The US Navy has employed the Delft3D4 (D3D4) modeling system [1] to provide forecasts of water levels, currents, and surface waves in coastal and nearshore environments for over a decade. Delft3D4 allows for coupled circulation and wave simulations on structured grids with quadrilateral elements.

The capacity for high model resolution is crucial because the quality of simulated water levels, currents, and wave parameters in nearshore and coastal environments depends significantly on bathymetric features with short horizontal length scales (tens of meters or less). Though the D3D4 system is capable of producing dependable forecasts at the desired resolution, it requires a cumbersome, nested approach of grids with increasing resolutions in areas of interest [2].

A flexible mesh capability was recently developed for the D3D4 modeling suite: Delft3D-Flexible Mesh (DFM) [3]. The advantage of DFM is that the computational grid for the circulation model is not restricted to quadrilateral elements. The elements can range from triangles to hexagons. Therefore, a flexible mesh of varying resolutions can be generated by combining multiple structured grids using triangular, pentagonal, and hexagonal elements. This allows for simulation of large areas combining lower resolution grids with higher resolution grids in areas of interest.

Replacing the structured grid with the new flexible mesh is expected to allow operators to highly resolve processes and improve predictions close to the coastline without compromising computational time or requiring a cumbersome nested approach. A current limitation of the DFM system is that it can perform only barotropic simulations. At the time of this report, the baroclinic version of DFM remains in Beta testing [2].

2. MODEL DIRECTORY SET-UP

This section outlines the recommended configurations for a model directory setup on a DoD HPC including the necessary files for running the model and the required directory structure.

2.1 Directory Configuration and Contents

2.1.1 Top-level Directory

The top-level directory should be named using the model `<run-id>` [3]. Here we use the example of “regionA” to denote a model domain setup in a given domain.

The required subdirectories in the top-level directory `regionA` for the example are:

```
regionA/dflowfm
regionA/wave
regionA/winds
```

The `dflowfm` directory contains all the input files for the FLOW circulation module, including the hydrodynamic lateral boundary conditions forcing the simulation. The `wave` directory contains all the input files for the WAVE module, including wave lateral boundary conditions forcing the simulation. The `winds` directory contains the wind forcing files used by both the FLOW and WAVE modules.

Additionally, the top-level directory should contain the Portable Bash Script (PBS) run script that will be submitted to the PBS batch queue on the HPC machine and the model configuration file:

```
run_dimr.pbs    model simulation PBS batch script
dimr_config.xml DIMR model configuration file
```

The location of the compiled DFM model executable is indicated in the model PBS run script, `<.pbs>`. The executable can exist in the user’s home directory, or in the home directory of another user in the group with the correct permissions.

2.1.2 dflowfm Subdirectory

The `dflowfm` subdirectory contains all the input files required to run the FLOW module of DFM:

```
<_net.nc>  unstructured grid file
  <.pli>    boundary condition location file(s) (polyline file format)
  <.bc>     lateral boundary forcing file(s)
<_bnd.ext> file containing lateral boundary conditions files’ specifications
  <.ext>    file containing meteorological forcing files’ specifications
  <.xyn>    list of point locations (lat,lon) of observation stations with columns x, y, station name
  <.mdu>    master definition file for parameters in the FLOW model
```

2.1.3 wave Subdirectory

The `wave` subdirectory contains all the input files required to run the WAVE module of DFM:

```
<.dep>    bathymetry or water depth file
<.grd>    curvilinear grid file
<.mdw>    master definition file for parameters in the WAVE model
```

2.1.4 winds Subdirectory

The winds subdirectory contains the meteorological files that are forced at the air-sea boundary of FLOW and WAVE:

- <.amp> meteorological forcing file (pressure)
- <.amu> meteorological forcing file (wind, u-component)
- <.amv> meteorological forcing file (wind, v-component)

3. MODEL INPUT FILES

Generating the model input files for DFM is similar to D3D4. Locally accessible tools are first used to configure model settings and inputs. The input files are then transferred to the DoD HPC machines where the simulation is executed. The required inputs include a grid file, bathymetry (depth) file, circulation (FLOW) model boundary conditions, meteorological boundary conditions, and wave (WAVE) model boundary conditions [2].

3.1 Model Run Script and DIMR Configuration File

Two files need to be placed in the top-level directory. They are the model run script, `run_dimr.pbs`, and the DIMR input file, `dimr_config.xml` file.

3.1.1 Model Run Script

The model run script, `run_dimr.pbs`, is used to launch the simulation on HPC. The run script we use was written especially for our HPC configuration and can be copied from the directory of another user in the group.

3.1.2 DIMR Input File

Both FLOW and WAVE are used as dynamic libraries. DIMR is the executable that steers both dynamic libraries. It prescribes when the FLOW computation should be paused to perform a WAVE calculation. The input file is usually named `dimr_config.xml` [3].

If a copy of `dimr_config.xml` is not created during initial model setup, one can be copied from the directory of another user in the group.

3.2 Grid and Bathymetry Generation

The model grid consists of mostly rectangular grid cells. The grid cell size is refined (i.e., reduced) in areas of the highest interest or where higher resolution is necessary. Triangular grid cells are used to transition from areas of low resolution to areas of high resolution. Grid and bathymetry generation utilizes Delft DashBoard (DDB), the RGFGrid Graphical User Interface (GUI), the DeltaShell GUI, and shell scripts (`refine_netfile_gebco.sh` and `refine_netfile_gcbco.sh`). Shell scripts are run on the Navy DoD Supercomputing Resource Center (Navy DSRC). DDB is used to generate a beginning (base) grid and to access bathymetry for the base grid (The General Bathymetric Chart of the Oceans (GEBCO 2019)) [4] and for areas of refinement (Coastal Relief Model (CRM)) [5] [6] [7] [8]. The base grid and bathymetry information are inputs to the shell scripts. Given the inputs and several tunable parameters, the shell scripts determine the refined mesh areas. The GUIs are used to save the refined grids in usable formats. Step-by-step instructions for grid generation and refinement can be found in Appendix A of *An Evaluation of Delft3D Flexible Mesh Applied to Southern California and the Gulf of Mexico* [2]. The `<_net.nc>` file results from this procedure.

3.3 Observation Points File

The points file with observation stations, `<.xyn>`, indicates the location of point output, which will be written to the `<_his.nc>` file. The `<_his.nc>` file contains time series with DFM model results for a number of stations. The `<.xyn>` file is generated using DDB at the time the base grid is created. If you choose not to create it in this manner, it can be created in a text editor, such as Vim. Each entry belongs on its own line. Its format is longitude (-180 to 180 convention), latitude, and station ID contained in quotes.

Example of `<.xyn>` file contents:

```
-84.516000 28.501000 "42036"
-86.008000 28.788000 "42039"
-88.226000 29.208000 "42040"
```

3.4 Hydrodynamic Boundary Conditions

3.4.1 Delft DashBoard Method

The DDB Model Maker Toolbox is used to define open boundaries and generate astronomic water level and normal velocity boundary conditions. Polyline files, `<.pli>`, are made during this process.

3.4.2 Python Method Using Naval Operational Model Sources

An alternative approach to generate boundary conditions is to pull boundary condition information from a regional model, like the Navy Coastal Ocean Model (NCOM) [9]; this approach to generate boundary conditions utilizes external software written in Python (`generate_BCs_NCOM.py`), not DDB [2]. In order to use this alternative method, one needs polyline files made for the domain, which is done using DDB.

The inputs to `generate_BCs_NCOM.py` include `<.pli>` file(s), a network Common Data Form (NetCDF) file containing the regional model (e.g., NCOM) output (`ncFile`), and the quantity from the model to be used for boundary condition creation (`quantity`). The command syntax is as follows:

```
>> python generate_BCs_NCOM.py [-h] --pli-list [PLI_LIST [PLI_LIST ...]]
[--bc-filename BC_FILENAME] [--nlevels N] [--depth-avg] [--plot] ncFile quantity
```

positional arguments

<code>ncFile</code>	NCOM NetCDF output containing boundary support points and duration of Delft3D simulation
<code>quantity</code>	NCOM variable; must be either <code>salinity</code> , <code>water_temp</code> , <code>velocity</code> , or <code>surf_el</code>

optional arguments

<code>-h, -help</code>	show this help message and exit
<code>-pli-list [PLI_LIST [PLI_LIST ...]]</code>	list of boundary support point polyline filenames
<code>-bc-filename BC_FILENAME</code>	optional filename for Delft3D boundary condition filename
<code>-nlevels N</code>	optional number of vertical levels for 3D boundary conditions
<code>-depth-avg</code>	flag to enable depth averaged output
<code>-plot</code>	flag to enable plotting

See Appendix A.1 for the `generate_BCs_NCOM.py` Python code.

Creation of NetCDF Files Used as Input to Python Method

The starting point for boundary condition creation from NCOM is the creation of the `ncFile` used as input to `generate_BCs_NCOM.py`. A Python script, `pull_NCEI_data.py`, along with its accompanying input file, `NCEI_input.yml`, are used to obtain the NetCDF files [10]. The routine retrieves NCOM model output from the National Centers for Environmental Information (NCEI) Environmental Research Division's Data Access Program (ERDDAP) server and saves it in a NetCDF file. The data pulled is determined by variables supplied in the `NCEI_input.yml` yaml file that is named on the command line.

Syntax for running `pull_NCEI_data.py` is as follows:

```
>>python pull_NCEI_data.py -y NCEI_input.yml -o . -i .
```

Values needed for `NCEI_input.yml`:

<code>dataset:</code>	The dataset (model and 2D or 3D variables) requested from the NCEI database
<code>variable:</code>	METOC variable requested
<code>start_time:</code>	The beginning of the time range (yyyy-mm-dd HH:MM:SS)
<code>end_time:</code>	The end of the time range (yyyy-mm-dd HH:MM:SS)
<code>latitude_min:</code>	The minimum of the latitude range
<code>latitude_max:</code>	The maximum of the latitude range
<code>longitude_min:</code>	The minimum of the longitude range
<code>longitude_max:</code>	The maximum of the longitude range

The `pull_NCEI_data.py` code can be used for obtaining results from both 2D and 3D models. A 2D dataset containing surface elevation (`surf_e1`) is needed for the creation of water level boundary conditions. When using `pull_NCEI_data.py` to obtain 2D NCOM output, only one netCDF file is made. 3D NCOM output (`water_u` and `water_v`) is needed for creating velocity boundary conditions. For obtaining 3D NCOM, the script automatically pulls two files per day (AM and PM) for all days in the range. Then it concatenates the 3D NCOM netCDF files to arrive at a single `ncFile` for input to `generate_BCs_NCOM.py`.

Date range and spatial coverage for NCOM can be found at:

<https://www.ncei.noaa.gov/products/weather-climate-models/fnmoc-regional-navy-coastal-ocean>

The `pull_NCEI_data.py` Python code and `NCEI_input.yml`, its accompanying yaml input file, are available in the US Naval Research Laboratory (NRL) Memorandum Report, *Automated Method to Extract Oceanographic and Atmospheric Data from Online Sources* [10].

Once the 2D `ncFile` and the 3D `ncFile` are obtained/constructed, they can be used with `generate_BCs_NCOM.py` to create the needed BCs, in this example, `WaterLevel.bc` and `Velocity.bc`.

Execution of `generate_BC_NCOM.py`

A Python environment, `dfm`, must be created before using `generate_BC_NCOM.py` [11]. After it is created, it must be activated:

```
>> conda activate dfm
```

After activation, execute the routine from the command line.

In the below example, the `polyline` files and the `ncFiles` are in the directory where the boundary condition creation scripts are executed. The `<.bc>` file will be written to the directory where `generate_BC_NCOM.py` is executed.

Example usage for water level boundary condition creation:

```
>> python3 /path/to/generate_BC_NCOM.py --pli-list bnd001.pli bnd002.pli  
--bc-filename WaterLevel.bc amseas2d_subset_20130420_20130511.nc surf_el
```

Example usage for velocity boundary condition creation (depth-averaged):

```
>> python3 /path/to/generate_BC_NCOM.py --pli-list bnd001.pli bnd002.pli --bc-  
filename Velocity.bc --depth-avg amseas3d_subset_20130420_20130511.nc velocity
```

3.5 Meteorological Forcing

External code written in Python is used to generate atmospheric forcing files. Meteorological forcing is obtained from the Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS) model using `coamps2meteo.py`. If COAMPS forcing is unavailable or unsuitable, meteorological forcing can be obtained from the ERA5 model using `ERA5_to_meteo.py`. The user must first check to see that coverage is available for the time period and region. For COAMPS, connect to the host server and check the available dates, by year, for the area of interest.

Execution of `coamps2meteo.py`

The `coamps2meteo.py` code requires input of the name of a COAMPS region, a start date, an end date, and the path to the directory containing the COAMPS output. It accesses and reads the COAMPS output and writes the spatially varying meteorological input files `<.amu>`, `<.amv>`, and `<.amp>` for use in DFM [2].

The `dfm` Python environment, used when creating boundary conditions from NCOM output, must also be used when running `coamps2meteo.py`. It must be activated before using the routines. After activation, execute the routine from the command line.

The command syntax for running `coamps2meteo.py` is as follows:

```
>> python coamps2meteo.py [-h] -r REGION -s STR_DATE -e END_DATE -d DATADIR
```

where

REGION is one of:

arctic	cencoos_n3	e_pac_comp	europa2	hawaii_n3	mbay_n4
n_ind2	southwest_asia	useast	cen_amer	centam	eqam
europa3	indo	mideast	nwatl	southwest_asia2	was3
cen_america	centio	eqam_comp	fukushima	mbay_n1	MREA04
nwpac	southwest_asia2_n3	w_atl	cencoos_n1	eafr	euro
hawaii	mbay_n2	nepac	socal	southwest_asia3	w_pac
cencoos_n2	e_pac	europa	hawaii_comp	mbay_n3	n_ind
somalia	test2	w_pac2			

STR_DATE start date in YYYYMMDD format
 END_DATE end date in YYYYMMDD format
 DATADIR location of the COAMPS output files

DATADIR currently requires file tree to be analogous to NOGAPS/COAMPS tree (e.g., DATADIR/region/YYYY).

The following files are produced:

```
coamps\_start\_date\_end\_date\_region.amp \\
coamps\_start\_date\_end\_date\_region.amu \\
coamps\_start\_date\_end\_date\_region.amv \\
coamps\_region\_start\_date\_end\_date\_today.log \\
```

Example usage for coamps2meteo.py:

```
>> python3 /path/to/coamps2meteo.py -r w_atl -s 20130425 -e 20130511 -d /path/to/NOGAPS/COAMPSg/
```

See Appendix A.2 for the coamps2meteo.py Python code.

3.6 File Transfer to HPC

If boundary conditions files and meteorological forcing files were created on your local system, you can scp them to the directories on the HPC. If any changes were made to the polyline files, transfer the updated polyline files that correspond to the boundary condition files as well. To do this, one has to have an active ticket on the HPC. The following command is performed in the local directory containing the files.

The form of the scp command follows:

```
>> scp <file> user@system.hpc_center.hpc.mil:/p/work1/user/regionA/dflowfm
```

An example of the scp command is:

```
>> scp *.bc user@gaffney.navydsrc.hpc.mil:/p/work1/user/regionA/dflowfm
```

The files that need to be copied to HPC are:

```
<*.bc>    to dflowfm  
<*.pli>   to dflowfm  
<*.am*>  to winds
```

Then login to the HPC system to confirm successful transfer of the new files:

```
>> ls /p/work1/user/regionA/dflowfm/
```

```
bnd001.pli  
bnd002.pli  
Velocity.bc  
WaterLevel.bc
```

```
>> ls /p/work1/user/regionA/winds/
```

```
coamps_20130425_20130511_w_atl.amp  
coamps_20130425_20130511_w_atl.amu  
coamps_20130425_20130511_w_atl.amv
```

3.7 External Forcing Files

The files containing lateral boundary conditions files' specifications, `<_bnd.ext>`, and the meteorological forcing files' specifications, `<.ext>`, are known as external forcing files. They are not the boundary condition files or the spatially-varying meteorological forcing files themselves; they contain the meta data for the actual forcing data files. They are made in DeltaShell. The names of the boundary conditions files and meteorological forcing files are needed for making `<_bnd.ext>` and `<.ext>`, respectively.

Two definition files for the external forcing are supported, each with their own format. The `<.ext >` is the old style, and details about meteorological forcing must be contained in this kind of external forcing file. Boundary conditions may use this kind of file [3]. The `<_bnd.ext>` file is the new style and can be used for boundary conditions but not meteorological forcing files [3]. The final step in specifying boundary conditions is pointing to the `<_bnd.ext>` and `<.ext>` files in the `<.mdu>` file [3]. For further explanation see Section 4.9.

If you do not create these files in DeltaShell, they can be created using a text editor such as Vim.

3.7.1 New Style External Forcing File: <_bnd.ext>

In the <_bnd.ext> file, there is one [boundary] entry per polyline file per boundary condition. The following code taken from a <_bnd.ext> file is for a simulation using two polyline files (bnd001.pli and bnd002.pli) and two boundary conditions (contained in WaterLevel.bc and Velocity.bc).

Example of <_bnd.ext> file contents:

```
[boundary]
quantity=waterlevelbnd
locationFile=bnd001.pli
forcingFile=WaterLevel.bc
returnTime=0.00000000e+000
```

```
[boundary]
quantity=waterlevelbnd
locationFile=bnd002.pli
forcingFile=WaterLevel.bc
returnTime=0.00000000e+000
```

```
[boundary]
quantity=uxuyadvectionvelocitybnd
locationFile=bnd001.pli
forcingFile=Velocity.bc
returnTime=0.00000000e+000
```

```
[boundary]
quantity=uxuyadvectionvelocitybnd
locationFile=bnd002.pli
forcingFile=Velocity.bc
returnTime=0.00000000e+000
```

quantity needs to match the information in the respective <.bc> file. Keywords and information about the file format can be found in DFM manual [3].

3.7.2 Old Style External Forcing File: <.ext>

Example of <.ext> file contents:

```
QUANTITY=windx
FILENAME=../winds/coamps_20130425_20130511_w_atl.amu
FILETYPE=4
METHOD=2
OPERAND=+
```

```
QUANTITY=windy
FILENAME=../winds/coamps_20130425_20130511_w_atl.amv
FILETYPE=4
METHOD=2
OPERAND=+
```

```
QUANTITY=atmosphericpressure
FILENAME=../winds/coamps_20130425_20130511_w_atl.amv
FILETYPE=4
METHOD=2
OPERAND=+
```

The location of the meteorological forcing files is given with respect to the location of the `<.ext>` file.

3.8 Master Definition File for Hydrodynamics

The master definition file is created by the DeltaShell GUI. The bathymetric sample files are imported and interpolated to the grid to form the bathymetric surface. The boundary definitions and conditions are imported; the atmospheric forcing files are imported, and the observation points for point output are imported. The user checks default model parameter settings and makes adjustments, if needed. The model configuration is saved and ported to a HPC machine where it can be run in parallel or serial using PBS scripting [2].

3.9 Coupling with Waves

After successful configuration of a FLOW circulation model, it can be coupled with the WAVE model if desired. Configuring the WAVE model begins with development of the grid, `<.grd>`, and bathymetry, `<.dep>`, using the Model Maker Toolbox in DDB. The WAVE model can be forced by only the meteorological boundary conditions or a combination of the meteorological boundary conditions and wave boundary conditions at the grid boundaries. Because the atmospheric forcing is shared with the FLOW model, the user must ensure that the atmospheric input files cover the WAVE grid, which is typically larger than the FLOW grid. If wave boundary conditions are desired at the grid boundaries, they are generated from a regional model like Simulating WAVes Nearshore (SWAN) or WaveWatch 3. In this case, the DeltaShell GUI is used to define the WAVE boundaries along the grid boundaries with spectral points evenly distributed on the boundaries. These points are added to the regional wave model as output locations, and the regional model is set to produce 2D spectra (in the SWAN format) at the output point locations for input to the DFM model. The 2D spectra filenames are added to the WAVE master definition file, `<.mdw>` [2].

The WAVE grid, bathymetry, and lateral boundary conditions (if applicable) are imported to DeltaShell, and switches to couple the FLOW and WAVE models are engaged. The coupled model configuration is ported to an HPC machine, where it can be run in parallel using PBS scripting.

4. STARTING FROM AN EXISTING SIMULATION

It is common to run multiple models using the same domain. The purpose of this section is to detail what information can be duplicated from an existing model of a specific domain and the required information

updates. Some files will need to be created for each unique study period. In those cases, the user will be directed to the descriptions of file creation in Section 3.

4.1 Approach

By starting from a previous model of your domain, many of the required files already exist and are ready for use in a new model. If the study period is changed, new boundary conditions and meteorological forcing will require recreation. The following files can be copied from a previous simulation that uses the same domain. Whether a file can be used without changes or whether it may require updating, is listed below:

model run script <.pbs>	may require update
DIMR input file <.xml>	may require update
unstructured grid file <_net.nc>	no changes
observation points file <.xyn>	may require update
polyline file(s) <.pli>	may require update (usually not)
new style external forcing file <_.bnd.ext>	may require update (usually not)
old style external forcing file <.ext>	may require update
mater definition file for FLOW <.mdu>	may require update
water depth file <.dep>	no changes
curvilinear grid file <.dep>	no changes (unless new bathymetry is acquired)
mater definition file for WAVE <.mdw>	may require update

4.2 HPC Directory Structure Creation

Set up the directory structure on HPC according to guidance in Section 2.1.

4.3 Model Run Script and DIMR Input File

Two files are required in the top-level directory. They are the model run script, `run_dimr.pbs`, and the DIMR input file, `dimr_config.xml`.

The `run_dimr.pbs` and `dimr_config.xml` can be copied from a previous simulation's directory.

Example of the PBS commands in the header of `run_dimr.pbs`:

```
#!/bin/bash
#PBS -A NRLSS06632HCF
#PBS -q high
#PBS -N regionA
#PBS -o log.dimr
#PBS -M sunni.schoenauer@nrlssc.navy.mil
#PBS -m be
#PBS -j oe
#PBS -W umask=0022
#PBS -l walltime=18:00:00
#PBS -l select=1:ncpus=24
#PBS -l place=scatter:excl
```

PBS commands in `run_dimr.pbs` that may require updating:

```
-A HPC_project
-q queue_priority
-N job_name
-M e-mail_address
-l wall_time
```

Additionally, any commands pertaining to archiving the completed simulation (at bottom of script) may require updating.

In `dimr_config.xml`, check `workingDir` names and `inputFile` names in both the Waves and FlowFM sections. What is visible in the below code, taken from `dimr_config.xml`, corresponds to a FLOW subdirectory named `dflowfm` and a WAVE subdirectory named `wave`. The names of the `<.mdw>` and `<.mdu>` files should match the names of the files in your `wave` and `dflowfm` sub-directories.

Example of sections of `dimr_config.xml` that may require updating:

```
<component name="Waves">
<workingDir>wave</workingDir>
<inputFile>regionA.mdw</inputFile>

<component name="FlowFM">
<workingDir>dflowfm</workingDir>
<inputFile>regionA.mdu</inputFile>
```

4.4 Unstructured Grid File and Observation Points File

The unstructured grid file, `<_net.nc>`, and the points file with observation stations, `<.xyn>`, can be copied from an existing model of your domain to the `dflowfm` directory. The unstructured grid file `<_net.nc>` will not need to be changed. The points file with observation stations `<.xyn>` may need to be updated to include observation points corresponding to the instruments deployed during your study period.

The following was added to the `<.xyn>` file for the `regionA` study period:

```
-85.673510  30.080170  "QuadPod07m"
-85.688940  30.050390  "QuadPod20m"
```

For more information about `<.xyn>` file contents, see Section 3.3

4.5 Boundary Condition Creation

Boundary conditions need to be created for each new study period. Refer to Section 3.4 for instructions.

4.5.1 *ncFiles for Input to Boundary Condition Creation Routine*

Use `pull_NCEI_data.py` to obtain the needed `ncFiles` for input to `generate_BC_NCOM.py`. (Refer to instructions in Section 3.4.2.)

4.5.2 Polyline Files

It is important to note that if NCOM is used for creating boundary conditions and the previous model used astronomic tides for boundary forcing, not all support points in the polyline files may have NCOM results available. If this is the case, any points that missing (e.g., on land) in NCOM can be removed, and performance may be increased.

4.5.3 Executing the Boundary Condition Creation Routine

Execute `generate_BCs_NCOM.py` according to the instructions in Section 3.4.

4.6 Meteorological Forcing Creation

Meteorological forcing needs to be created for each new study period. Refer to Section 3.5 for instructions.

4.7 File Transfer to HPC

Transfer any files you have created (or changed) on your local system to your directories on HPC. The boundary conditions file(s), `<.bc>`, and the polyline file(s), `<.pli>`, will need to be copied into the `dflowfm` subdirectory. The meteorological forcing files, `<.am*>`, will need to be copied into the `winds` subdirectory. Refer to the instructions in Section 3.6.

4.8 External Forcing Files

4.8.1 New Style External Forcing File: `<_bnd.ext>`

The file containing the lateral boundary conditions files' specifications, `<_bnd.ext>`, can be copied from an existing model of your domain to the `dflowfm` directory. It may need to be updated to match the names of the polyline files and the boundary condition types if any changes have been made since the previous simulation. In the `<_bnd.ext>` file, there is one [boundary] entry per polyline file per boundary condition.

The contents from a `<_bnd.ext>` file (shown below) are for a simulation using two polyline files (`bnd001.pli` and `bnd002.pli`), and two boundary conditions (contained in `WaterLevel.bc` and `Velocity.bc`).

```
[boundary]
quantity=waterlevelbnd
locationFile=bnd001.pli
forcingFile=WaterLevel.bc
returnTime=0.00000000e+000
```

```
[boundary]
quantity=waterlevelbnd
locationFile=bnd002.pli
forcingFile=WaterLevel.bc
returnTime=0.00000000e+000
```

```
[boundary]
quantity=uxuyadvectionvelocitybnd
locationFile=bnd001.pli
forcingFile=Velocity.bc
returnTime=0.0000000e+000
```

```
[boundary]
quantity=uxuyadvectionvelocitybnd
locationFile=bnd002.pli
forcingFile=Velocity.bc
returnTime=0.0000000e+000
```

The quantity value needs to match the information in the respective boundary condition file. For example, WaterLevel.bc's Quantity line (pictured below) matches the quantity listed in the <_bnd.ext> file. Similarly, Velocity.bc file's Vector line (pictured below) matches the quantity listed in the <_bnd.ext> file.

Header lines of WaterLevel.bc:

```
[forcing]
      Name = bnd001_0001
      Function = timeseries
Time-interpolation = linear
      Quantity = time
      Unit = seconds since 2013-04-25 00:00:00
      Quantity = waterlevelbnd
      Unit = m
```

Header lines of Velocity.bc:

```
[forcing]
      Name = bnd001_0001
      Function = timeseries
Time-interpolation = linear
      Quantity = time
      Unit = seconds since 2013-04-25 00:00:00
      Vector = uxuyadvectionvelocitybnd:ux,uy
      Quantity = ux
      Unit = -
      Quantity = uy
      Unit = -
```

4.8.2 Old Style External Forcing File: <.ext>

The file containing the meteorological forcing files' specifications, <.ext>, can be copied from an existing model of your domain to the dflowfm directory. The meteorological forcing file names contained in the

<.ext> file, i.e., FILENAME, need to match the names of files contained in the winds subdirectory. The location must be supplied with respect to the location of the <.ext> file. Specifically, since the <.ext> file is located in the dflowfm directory, the path to the <*.am*> files from dflowfm needs to match the path listed after FILENAME.

```
QUANTITY=windx
FILENAME=../winds/coamps_20130425_20130511_w_atl.amu
FILETYPE=4
METHOD=2
OPERAND=+
```

```
QUANTITY=windy
FILENAME=../winds/coamps_20130425_20130511_w_atl.amv
FILETYPE=4
METHOD=2
OPERAND=+
```

```
QUANTITY=atmosphericpressure
FILENAME=../winds/coamps_20130425_20130511_w_atl.amp
FILETYPE=4
METHOD=2
OPERAND=+
```

4.9 Master Definition File for FLOW Model

A copy of the master definition file for the FLOW model, <.mdu>, can be copied from an existing model of your domain to the dflowfm directory. The name of the <.mdu> file will need to match the name specified in the dimr_config.xml file (Section 4.3). The recommended naming convention is <run-id>.mdu, where <run-id> consists of only letters and numbers, up to 252 characters [3].

The following <.mdu> file contents may require updating:

```
[geometry]
  NetFile must match the name of the <_net.nc> in dflowfm

[time]
  RefDate often the time the model starts
  TStart start time w.r.t. RefDate (in TUnit)
  TStop stop time w.r.t. RefDate (in TUnit)

[external forcing]
  ExtForceFile must match name of <.ext> file in dflowfm
  ExtForceFileNew must match name of <_bnd.ext> file in dflowfm

[output]
  ObsFile must match name of <.xyn> file in dflowfm
```

Boundary condition and forcing coverage must be available between (and including) TStart and TStop.

4.10 Water Depth and Curvilinear Grid Files

The `<.dep>` and `<.grd>` files can be copied from an existing model of your domain to the wave directory. No changes will need to be made to these files.

4.11 Master Definition File for WAVE Model

A copy of the master definition file for the WAVE model, `<.mdw>`, can be copied from an existing model of the domain to the wave directory. The name of the file will need to match the name specified in the `dimr_config.xml` file (Section 4.3). The recommended naming convention is `<run-id>.mdw`, where `<run-id>` consists of only letters and numbers, up to 252 characters [3].

The following `<.mdw>` file contents may require updating:

```
[General]
```

```
ReferenceDate must match RefDate from the <.mdu> file
```

```
[Output]
```

```
COMFile = ../dflowfm/output/<run-id>_com.nc
```

```
(Note: <run-id> must match in <.mdu> and <.mdw> files)
```

```
[Domain]
```

```
Grid must match name of <.grd> file in wave
```

```
BedLevel must match name of <.dep> file in wave
```

4.12 Model Execution

Now that the directory structure with the model inputs has been set-up, verify that its contents match the requirements described in Section 2.1. Then, submit the run from the top-level directory using the following command:

```
>> qsub run_dimr.pbs
```

The PBS run id will be output to the command line:

```
3675481.pbsserver
```

To check the status of the job, you can use the `qstat` or `qview` command. The `-u` flag followed by your username will allow you to see only your jobs.

For example:

```
>> qstat -u siqueira
```

pbsserver:

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	S	Elap Time
-----	---	---	----	--	-	-	--	--	-	--
3675481.pbs*	siqueira	high	regionA	22002	1	24	-	18:00	R	01:14

Once the simulation is complete, copy the results file, `<_his.nc>`, to your local directory for the model. To do this, logout of the HPC system, change to the local directory where you want to save the results file, and perform a scp:

```
>> exit
```

```
logout
```

```
Connection to gaffney.navydsrc.hpc.mil closed.
```

```
>> cd Documents/cases/regionA/
```

```
>> scp siqueira@gaffney.navydsrc.hpc.mil:/p/work1/siqueira/regionA/
dflowfm/output/regionA_0000_his.nc .
```

5. CREATING A PARAMETER ENSEMBLE

5.1 Introduction

Once all of the inputs for the model have been completed, a parameter ensemble can be created. A parameter ensemble is a group of simulations whose members are identical in all ways except for the model parameter(s) being tested. These ensembles allow for model parameter sensitivity studies (e.g., using the Generalized Likelihood Uncertainty Estimation (GLUE) method [12]). A set of Python and Bash scripts called `instantiate` creates the inputs (e.g., unique `<.mdu>` or `<.mdw>` files) for each ensemble member. The code and further information are available on the NRL HPC GitLab repository, `instantiate_dfm` [13].

We recommend a version of Python (e.g., Miniconda [14], or Anaconda) be installed in your local HPC home directory versus using the HPC version of Python to allow for greater control over the libraries and packages. The user must initialize conda (either within the user's `.bashrc` file or manually after login). It is also recommended that the user activate the Python `dfm` environment to ensure the required libraries and packages are installed.

5.2 Ensemble Directory Structure

A directory structure with a `template` directory should be created. The contents of the `template` directory will be used to create each ensemble member's directory, `case_00**`. For example:

```

regionA
regionA/template
regionA/template/dflowfm
regionA/template/wave
regionA/winds

```

To save disk space, the winds directory should only be in the top-level directory and not in each ensemble member's directory. Verify that the meteorological forcing files are in the correct directory, and the `<.ext>` file includes the correct path location:

```

>> cd case_0000/dflowfm/
>> vim ESTCP2021.ext

```

Copy the name of one of the meteorological forcing files from the `<.ext>` file, including path. Use it in the following `ls` command:

```

>> ls ../../winds/coamps_20210402_20210604_nwat1.amp

```

The output below shows it is visible from the location of the `<.ext>` file.

```

../../winds/coamps_20210402_20210604_nwat1.amp

```

5.3 Required Instantiate Files

The `01_generate_ensembles_and_submission_script.py` Python script uses the template directory and instantiates it for every possible combination of values of variables as described in an input file, `input_params.txt`. Each instance is placed within a numbered "case_NNNN" in a user-defined output path [13].

In addition to the files described in Section 2.1, a copy of the `instantiate` script (`01_generate_ensembles_and_submission_script.py`) and the input parameter file (`input_params.txt`) must be in the top-level directory.

Example contents of `input_params.txt`:

```

UnifFrictCoef      0.005  0.035  7
UnifFrictCoef1D   0                               # REQUIRED so UnifFrictCoef val is not replaced
UnifFrictCoefLin  0                               # REQUIRED so UnifFrictCoef val is not replaced
Vicouv            0.0    20.0  9

```

This example file specifies that 7 values of `UnifFrictCoef` should be used, ranging from 0.005 to 0.035 in evenly spaced increments. Note that the next two lines specify that `UnifFrictCoef1D` and `UnifFrictCoefLin` will be written as 0 so the code does not replace their values with the `UnifFrictCoef` values. This legacy code bug should be fixed in the future. The final line specifies that 9 values of `Vicouv` will be used, ranging from 0.0 to 20.0 in evenly spaced increments. In this example, the parameters intended for replacement with the specified values are all in the `<.mdu>` file.

5.4 Modification to Model Files

No changes need to be made to the model input files in the `template` directory EXCEPT for the `run_id` name. In order for a unique job name to be written to each ensemble member's `run_dimr.pbs` file, the characters `@(f'run_id')` must be inserted into the `run_dimr.pbs` file contained in the `template` directory:

```
#PBS -N regionA_@(f'run_id')
```

This modification will allow for unique job names in the batch queue of the HPC system, allowing for ease of model simulation tracking.

5.5 Running Instantiate

A typical command on HPC for instantiating an ensemble is:

```
>> python 01_generate_ensembles_and_submission_script.py -i './template/
input_params.txt' -t './template/' -o './'
```

Command line switches for `01_generate_ensembles_and_submission_script.py` include:

```
'-i' '-input-filename' help=input file describing ensembles
                        default='input_params.txt'
'-t' '-template-dir'   help=input template directory
                        default='./template'
'-o' '-output-dir'     help=output directory
                        default='./output'
'-q' '-quiet'          help=do not print anything except error msgs
                        action=store_true
'-y' '-yes'            help=confirm all
                        action=store_true
```

When executed, the program prints the values that will be written to each ensemble member's files. Make sure to verify they are correct. If so, answer `y` to the prompts:

```
Continue instantiating? (y/n)
Delete yamls when done parsing? (y/n)
```

The `case_00*` directories will be created after giving confirmation.

5.5.1 *Confirming Values in Ensemble Members' Files*

It is a good practice to use `grep` commands to confirm the values in the files.

Command syntax is as follows:

```
>> grep <parameter> case_00*/dflowfm/<run-id>.mdu
>> grep <run-id> case_00*/run_dimr.pbs
```

Example of the `grep` commands:

```
>> grep Vicouv case_00*/dflowfm/regionA.mdu
>> grep regionA case_00*/run_dimr.pbs
```

5.6 **Preparing to Launch the Ensemble Simulation**

The `01_generate_ensembles_and_submission_script.py` code generates a script, `02_submit_all_cases.sh`, that is used to submit the batch scripts to all of the ensemble simulation cases to the PBS queue. The file will be created in a write-protected mode.

You then must change the permissions of the `02_submit_all_cases.sh` script:

```
>> chmod 755 02_submit_all_cases.sh
```

Consider making copies of `02_submit_all_cases.sh` with partial lists of cases to submit so under 100 jobs are submitted at once. For example, make three submission scripts with the submission commands for only a portion of the simulations. For an ensemble with 63 members, consider three groups and duplicate the submission script, `02_submit_all_cases.sh`.

```
group1  0-20
group2  21-41
group3  42-62
```

```
>> cp 02_submit_all_cases.sh 02_submit_all_cases_group1.sh
>> cp 02_submit_all_cases.sh 02_submit_all_cases_group2.sh
>> cp 02_submit_all_cases.sh 02_submit_all_cases_group3.sh
```

To quickly eliminate the unwanted lines from each files, use Vim line editor command, `dd N`, to delete `N` lines from the cursor location.

5.7 Launching the Ensemble Simulation

The `02_submit_all_cases.sh` file(s) can be executed from the command line from the top-level directory.

```
>> ./02_submit_all_cases.sh
```

5.7.1 HPC Reservations

If you use a reservation for running the ensemble, remove the `-q` and `-A` lines from the `run_dimr.pbs` in the `template` directory, and include the queue and project info contained in the reservation as part of each line beginning with `qsub` in the `02_submit_all_cases.sh` file.

Example instructions from a HPC reservation e-mail:

Please note that you need to submit a job to your reservation in order to make use of it:

"`qsub -q R3755198 -A NRLSS06632054 jobfile`" will assign the job to your reservation.

Example lines from modified `02_submit_all_cases.sh`:

```
cd ./case_0000
qsub -q R3755198 -A NRLSS06632054 run_dimr.pbs
cd ../
sleep 2
```

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Appendix A

PYTHON CODE FOR BOUNDARY CONDITION AND METEOROLOGICAL FORCING CREATION

A.1 generate_BC_NCOM.py

The following section contains the generate_BC_NCOM.py Python code used to create lateral boundary condition files, <*.bc>.

```
1 #!/usr/bin/env python
2 # coding: utf-8
3
4 # version 0.1    2020/01/08    -- Cody Johnson
5
6 """
7 # Updates:
8 # 2021/09/05 - Jay Veeramony
9 #             Added ability to output water level boundary conditions
10
11 Issues identified:
12
13 1. If the boundary point in Delft3D-FM is a land point in the NCOM/HYCOM output
14 due to resolution issues, this routine throws an error. There needs to be a
15 check for this
16 """
17
18 #import sys
19 from pathlib import Path
20
21 import argparse
22 import cartopy.crs as ccrs
23 #import cartopy.feature as cfeature
24 import cmocean.cm as cmo
25 import matplotlib
26 import matplotlib.pyplot as plt
27 import numpy as np
28 import pandas as pd
29 import xarray as xr
30 import sys
31
32 ### functions ###
33 def write_wl_for_pli(bc_fn, gcm, pli, quantity):
34     """
35     append or write 2D boundary conditions for water level
36
37     bc_fn = path to write or append boundary condition data
38     gcm = general circulation model output which contains boundary points (xr.
39     DataArray)
40     pli = table of boundary support points (pd.DataFrame)
41     quantity = variable to output to the BC files (salinity or water_temp)
42     depth_avg = flag to enable depth averaging
```

```

42 """
43
44 with open(bc_fn, "a") as f:
45
46     gcm_refd, ref_date = assign_seconds_from_refdate(gcm)
47
48     for _, (x_pli, y_pli, pli_point_name) in pli.iterrows():
49
50         if x_pli < 0:
51             x_pli_east = x_pli + 360
52         else:
53             x_pli_east = x_pli
54
55         bc_data = waterlevel_to_pli_point(gcm_refd, x_pli_east, y_pli)
56
57         write_wl_record(f, bc_data, pli_point_name, ref_date)
58
59 def write_wl_record(f, bc_data, pli_point_name, ref_date):
60     """
61     append or write time series water level boundary conditions
62
63     f = file descriptor for writing boundary condition output
64     bc_data = data at with percent bed coords (xr.DataFrame)
65     pli_point_name = name for entry
66     ref_date = date used to calculate offset of the record in seconds
67     """
68
69     # write a record
70     f.write("[forcing]\n")
71     f.write(f"Name                = {pli_point_name}\n")
72     f.write(f"Function                 = timeseries\n")
73     f.write(f"Time-interpolation       = linear\n")
74     f.write(f"Quantity                  = time\n")
75     f.write(f"Unit                      = seconds since {ref_date}\n")
76     f.write(f"Quantity                  = waterlevelbnd\n")
77     f.write(f"Unit                      = m\n")
78
79     # write data after converting to dataframe and iterating over the rows
80     for td, value in bc_data.to_dataframe()['surf_el'].iteritems():
81         value = f"{value:.03f}"
82         f.write(f"{td} {value}\n")
83
84     f.write("\n")
85
86
87 def write_t3d_for_pli(bc_fn, gcm, pli, quantity, nlevels, depth_avg):
88     """
89     append or write 3D boundary conditions for quantities
90
91     bc_fn = path to write or append boundary condition data
92     gcm = general circulation model output which contains boundary points (xr.
93     DataArray)
94     pli = table of boundary support points (pd.DataFrame)
95     quantity = variable to output to the BC files (salinity or water_temp)
96     depth_avg = flag to enable depth averaging
97     """
98     with open(bc_fn, "a") as f:

```

```

98
99     gcm_refd, ref_date = assign_seconds_from_refdate(gcm)
100
101     for _, (x_pli, y_pli, pli_point_name) in pli.iterrows():
102
103         if x_pli < 0:
104             x_pli_east = x_pli + 360
105         else:
106             x_pli_east = x_pli
107
108         if (quantity == "salinity") or (quantity == "water_temp"):
109             bc_data = interpolate_to_pli_point(
110                 gcm_refd, quantity, x_pli_east, y_pli, nlevels
111             )
112
113             if depth_avg:
114                 write_ts2d_record(f, bc_data, pli_point_name, quantity, ref_date)
115             else:
116                 write_ts3d_record(f, bc_data, pli_point_name, quantity, ref_date)
117
118             # in the case of velocity both components are interpolated
119             elif quantity == "velocity":
120                 bc_data = interpolate_to_pli_point(
121                     gcm_refd, ["water_u", "water_v"], x_pli_east, y_pli, nlevels
122                 )
123                 if depth_avg:
124                     write_vector_2d_record(f, bc_data, pli_point_name, quantity,
ref_date)
125                 else:
126                     write_vector_3d_record(f, bc_data, pli_point_name, quantity,
ref_date)
127
128 def write_vector_2d_record(f, bc_data, pli_point_name, quantity, ref_date):
129     """
130     append or write time series boundary conditions for depth averaged velocity
131
132     f = file descriptor for writing boundary condition output
133     bc_data = data at with percent bed coords (xr.DataFrame)
134     pli_point_name = name for entry
135     quantity = variable to output to the BC files
136     ref_date = date used to calculate offset of the record in seconds
137     """
138
139     # get units for quantity
140     if quantity == "velocity":
141         vector = "uxuyadvectionvelocitybnd:ux,uy"
142         quantbndx = "ux"
143         quantbndy = "uy"
144         x_comp = "water_u"
145         y_comp = "water_v"
146         units = "-"
147     else:
148         print('quantity should be "velocity"\n')
149         raise ValueError
150
151     # write a record
152     f.write("[forcing]\n")

```

```

153     f.write(f"Name                = {pli_point_name}\n")
154     f.write("Function              = timeseries\n")
155     f.write("Time-interpolation      = linear\n")
156     f.write("Quantity                    = time\n")
157     f.write(f"Unit                  = seconds since {ref_date}\n")
158     f.write(f"Vector                  = {vector}\n")
159     f.write(f"Quantity                    = {quantbndx}\n")
160     f.write(f"Unit                  = {units}\n")
161     f.write(f"Quantity                    = {quantbndy}\n")
162     f.write(f"Unit                  = {units}\n")
163
164     # write data after converting to dataframe and iterating over the rows
165     for td, values in (
166         bc_data.to_dataframe()[[x_comp, y_comp]].unstack().iterrows()
167     ):
168         x_comp_val = values.water_u.mean()
169         y_comp_val = values.water_v.mean()
170
171         #values_str = [ f'{x_comp_val:0.2f}' ' ' f'{y_comp_val:.02f}' ]
172         f.write(f"{td} {x_comp_val:0.2f} {y_comp_val:.02f}\n")
173
174     f.write("\n")
175
176 def write_ts2d_record(f, bc_data, pli_point_name, quantity, ref_date):
177     """
178     append or write time series boundary conditions for depth averaged quantities
179
180     f = file descriptor for writing boundary condition output
181     bc_data = data at with percent bed coords (xr.DataFrame)
182     pli_point_name = name for entry
183     quantity = variable to output to the BC files
184     ref_date = date used to calculate offset of the record in seconds
185     """
186
187     # get units for quantity
188     if quantity == "salinity":
189         quantbnd = "salinitybnd"
190         units = "ppt"
191     elif quantity == "water_temp":
192         quantbnd = "temperaturebnd"
193         units = "deg_C"
194     else:
195         print('quantity needs to be either "salinity" or "water_temp"\n')
196         raise ValueError
197
198     # write a record
199     f.write("[forcing]\n")
200     f.write(f"Name                = {pli_point_name}\n")
201     f.write("Function              = t3d\n")
202     f.write("Quantity                    = time\n")
203     f.write(f"Unit                  = seconds since {ref_date}\n")
204     f.write(f"Quantity                    = {quantbnd}\n")
205     f.write(f"Unit                  = {units}\n")
206
207     # write data after converting to dataframe and iterating over the rows
208     for td, values in bc_data.to_dataframe()[quantity].unstack().iterrows():
209

```

```

210     # take mean of values to get depth averaged
211     value = values.mean()
212
213     # see results of interpolation
214     if value > 100.0:
215         print(
216             f"Problem with {quantity} exceeding maximum allowed value: {values.max
217             ().__format__('.03f')} ppt."
218         )
219     elif value < 0.0:
220         print(
221             f"Problem with {quantity} becoming negative: {values.max().__format__('.03f')} ppt."
222         )
223         print(f"Negative value for {quantity} has been set to 0.01 {units}.")
224         value = 0.01
225
226     value = f"{value:.02f}"
227     f.write(f"{td} {value}\n")
228
229 f.write("\n")
230
231 def write_vector_3d_record(f, bc_data, pli_point_name, quantity, ref_date):
232     """
233     append or write 3D boundary conditions for quantities
234
235     f = file descriptor for writing boundary condition output
236     bc_data = data at with percent bed coords (xr.DataFrame)
237     pli_point_name = name for entry
238     quantity = variable to output to the BC files
239     ref_date = date used to calculate offset of the record in seconds
240     """
241
242     if quantity == "velocity":
243         vector = "uxuyadvectionvelocitybnd:ux,uy"
244         quantbndx = "ux"
245         quantbndy = "uy"
246         x_comp = "water_u"
247         y_comp = "water_v"
248         units = "-"
249     else:
250         print('quantity should be "velocity"\n')
251         raise ValueError
252
253     # convert percent from bed into formatted string
254     pos_spec = [f"{perc:.02f}" for perc in bc_data.perc_from_bed.data]
255     pos_spec_str = " ".join(pos_spec[::-1]) # reverse order for D3D
256
257     # write a record
258     f.write("[forcing]\n")
259     f.write(f"Name = {pli_point_name}\n")
260     f.write(f"Function = t3d\n")
261     f.write(f"Time-interpolation = linear\n")
262     f.write(f"Vertical position type = percentage from bed\n")
263     f.write(f"Vertical position specification = {pos_spec_str}\n")
264     f.write(f"Vertical interpolation = linear\n")
265     f.write(f"Quantity = time\n")

```

```

266 f.write(f"Unit                = seconds since {ref_date}\n")
267 f.write(f"Vector              = {vector}\n")
268
269 # loop over number of vertical positions
270 for vert_pos in range(1, len(pos_spec) + 1):
271     f.write(f"Quantity          = {quantbndx}\n")
272     f.write(f"Unit              = {units}\n")
273     f.write(f"Vertical position  = {vert_pos}\n")
274
275     f.write(f"Quantity          = {quantbndy}\n")
276     f.write(f"Unit              = {units}\n")
277     f.write(f"Vertical position  = {vert_pos}\n")
278
279 # write data after converting to dataframe and iterating over the rows
280 for td, values in (
281     bc_data.to_dataframe()[[x_comp, y_comp]].unstack().iterrows()
282 ):
283
284     # get componets as array in order to format for d3d input
285     x_comp_vals = values[x_comp].values[::-1] # reverse order for D3D
286     y_comp_vals = values[y_comp].values[::-1] # reverse order for D3D
287     values = [
288         f"{x_comp_val:.02f} {y_comp_val:.03f}"
289         for x_comp_val, y_comp_val in zip(x_comp_vals, y_comp_vals)
290     ]
291     values_str = " ".join(values)
292     f.write(f"{td} {values_str}\n")
293
294 f.write("\n")
295
296
297 def write_ts3d_record(f, bc_data, pli_point_name, quantity, ref_date):
298     """
299     append or write 3D boundary conditions for quantities
300
301     f = file descriptor for writing boundary condition output
302     bc_data = data at with percent bed coords (xr.DataFrame)
303     pli_point_name = name for entry
304     quantity = variable to output to the BC files
305     ref_date = date used to calculate offset of the record in seconds
306     """
307
308     # get units for quantity
309     if quantity == "salinity":
310         quantbnd = "salinitybnd"
311         units = "ppt"
312     elif quantity == "water_temp":
313         quantbnd = "temperaturebnd"
314         units = "deg_C"
315     else:
316         print('quantity needs to be either "salinity" or "water_temp"\n')
317         raise ValueError
318
319     # convert percent from bed into formated string
320     pos_spec = [f"{perc:.02f}" for perc in bc_data.perc_from_bed.data]
321     pos_spec_str = " ".join(pos_spec[::-1]) # reverse order for D3D
322

```

```

323 # write a record
324 f.write("[forcing]\n")
325 f.write(f"Name                = {pli_point_name}\n")
326 f.write("Function                = t3d\n")
327 f.write("Time-interpolation          = linear\n")
328 f.write("Vertical position type       = percentage from bed\n")
329 f.write(f"Vertical position specification = {pos_spec_str}\n")
330 f.write("Vertical interpolation        = linear\n")
331 f.write("Quantity                      = time\n")
332 f.write(f"Unit                          = seconds since {ref_date}\n")
333
334 # loop over number of vertical positions
335 for vert_pos in range(1, len(pos_spec) + 1):
336     f.write(f"Quantity                = {quantbnd}\n")
337     f.write(f"Unit                    = {units}\n")
338     f.write(f"Vertical position        = {vert_pos}\n")
339
340 # write data after converting to dataframe and iterating over the rows
341 for td, values in bc_data.to_dataframe()[quantity].unstack().iterrows():
342
343     # see results of interpolation
344     if values.max() > 100.0:
345         print(
346             f"problem with {quantity} exceeding maximum allowed value: {values.max():.03f} ppt"
347         )
348     elif values.min() < 0.0:
349         print(f"problem with {quantity} becoming negative: {values.max():.03f} ppt")
350
351         print(f"Negative values for {quantity} has been set to 0.01 {units}.")
352         values.where(values > 0.01, 0.01, inplace=True)
353
354     values = [f"{value:.02f}" for value in values]
355     values_str = " ".join(values[::-1]) # reverse order for D3D
356     f.write(f"{td} {values_str}\n")
357
358 f.write("\n")
359
360 def assign_seconds_from_refdate(gcm):
361     """
362     This func assigns seconds from a user specified ref date as coords.
363     This is how D3D interpolates the boundary conditions in time.
364
365     gcm = model output to add coords to
366     """
367     ref_date = gcm.time.data[0]
368     ref_dt = pd.to_datetime(ref_date)
369     ref_date_str = ref_dt.strftime("%Y-%m-%d %H:%M:%S")
370     timedeltas = pd.to_datetime(gcm.time.data) - ref_dt
371     seconds = timedeltas.days * 24 * 60 * 60 + timedeltas.seconds
372     gcm = gcm.assign_coords(coords={"seconds_from_ref": ("time", seconds)})
373     return gcm.swap_dims({"time": "seconds_from_ref"}), ref_date_str
374
375
376 def interpolate_to_pli_point(gcm_refd, quantity, x_pli_east, y_pli, nlevels):
377     """interpolates the quantities to the sigma depths and pli coords

```

```

378
379 gcm_refd = gcm with new time coordinates
380 quantity = variable to output to the BC files (salinity or water_temp)
381 x_pli_east = longitude of pli point in degrees east from meridian (NCOM convention
)
382 y_pli = latitude
383 """
384
385 # interpolate to pli point and drop data below bed level at nearest gcm_refd point
386 bc_data = (
387     gcm_refd[quantity]
388     .interp(lon=x_pli_east, lat=y_pli)
389     .dropna(dim="depth")
390     .squeeze()
391 )
392
393 # add coordinate for percent from bed. D3D uses this in its bc file format
394 gcm_refd_zb = bc_data.depth[-1] # get bed level of gcm_refd point
395 if nlevels > 1:
396     sigma_lvls = np.arange(nlevels)/(nlevels-1)*100
397     zlvls = sigma_lvls[:] * gcm_refd_zb.data / 100
398     bc_data = bc_data.interp(depth=zlvls)
399
400 perc_from_bed = 100 * (-1 * bc_data.depth + gcm_refd_zb) / gcm_refd_zb
401 bc_data = bc_data.assign_coords(coords={"perc_from_bed": ("depth", perc_from_bed.
data)})
402
403 return bc_data
404
405 def waterlevel_to_pli_point(gcm_refd, x_pli_east, y_pli):
406     """interpolates the quantities to the sigma depths and pli coords
407
408     gcm_refd = gcm with new time coordinates
409     x_pli_east = longitude of pli point in degrees east from meridian (NCOM convention
)
410     y_pli = latitude
411     """
412
413     # interpolate to pli point and drop data below bed level at nearest gcm_refd point
414     bc_data = (
415         gcm_refd['surf_el']
416         .interp(lon=x_pli_east, lat=y_pli)
417         .squeeze()
418     )
419
420     return bc_data
421
422
423 ### main loop ###
424 if __name__ == "__main__":
425
426     ### arguments ###
427     parser = argparse.ArgumentParser()
428     parser.add_argument(
429         "nc",
430         help="NCOM NetCDF output containing boundary support points and duration of
Delft3D simulation",

```

```
431 )
432 parser.add_argument(
433     "quantity",
434     help='NCOM variable. Must be either "salintiy", "water_temp", or "velocity"',
435 )
436 parser.add_argument(
437     "--pli-list",
438     nargs="*",
439     type=str,
440     help="list of boundary support point polyline filenames",
441     required=True,
442     dest="pli_list",
443 )
444 parser.add_argument(
445     "--nlevels",
446     default=11,
447     type=int,
448     help="Number of vertical levels",
449     dest="nlevels",
450 )
451 parser.add_argument(
452     "--bc-filename",
453     help="Optional filename for Delft3D boundary condition filename",
454     type=str,
455     dest="bc_filename",
456 )
457 parser.add_argument(
458     "--depth-avg",
459     help="flag to enable depth averaged output",
460     default=False,
461     action="store_true",
462     dest="depth_avg",
463 )
464 parser.add_argument(
465     "--plot",
466     help="flag to enable plotting",
467     default=False,
468     action="store_true",
469     dest="plot",
470 )
471
472 args = parser.parse_args()
473
474 gcm = args.nc
475 quantity = args.quantity
476 pli_list = args.pli_list
477 depth_avg = args.depth_avg
478 plot = args.plot
479 nlevels = args.nlevels
480
481 # validate arguments
482 if (
483     (quantity != "salinity")
484     and (quantity != "water_temp")
485     and (quantity != "velocity")
486     and (quantity != "surf_el")
487 ):
```

```

488     print(
489         f'<quantity> was specified as {quantity}, but should be either "salinity",
"water_temp", "velocity" or "surf_el".'
490     )
491     raise ValueError
492
493 # open gcm NetCDF output as Xarray dataset
494 try:
495     gcm = xr.open_dataset(Path(gcm), drop_variables="tau")
496 except FileNotFoundError as e:
497     print("f<NCOM output> should be path to NCOM NetCDF output")
498     raise e
499
500 # Some netcdf files have "latitude" and "longititude" instead of "lat" and "lon"
501 # In such cases, rename the indices
502 try:
503     gcm = gcm.rename({'latitude':'lat', 'longititude':'lon'})
504 except ValueError:
505     pass
506
507 # set default boundary condition filename depending on quantity
508 bc_fn = args.bc_filename
509 if bc_fn == None:
510     if quantity == "salinity":
511         bc_fn = Path("Salinity.bc")
512     elif quantity == "water_temp":
513         bc_fn = Path("Temperature.bc")
514     elif quantity == "velocity":
515         bc_fn = Path("Velocity.bc")
516     elif quantity == "surf_el":
517         bc_fn = Path("Waterlevel.bc")
518
519 # Overwrite the file on the first instance (i.e., clean up whatever is in the file
520 )
521 # There is probably a more elegant way to do this?
522 with open(bc_fn, 'w') as f:
523     f.write("")
524
525 # pli files opened as Pandas DataFrames
526 pli_points = []
527 for pli_fn in pli_list:
528     print(f"Reading in file: {pli_fn}")
529     pli = pd.read_csv(
530         pli_fn, sep="\s+", skiprows=2, header=None, names=["x", "y", "point_id"]
531     )
532
533 # Check if there are points in the pli file outside the lat/lon extent in the
534 # input file. If the points are outside the domain in the provided netcdf file
535 # this will either throw Nan's (for water level BCs) or cause interpolation
536 # errors (for the other boundary conditions)
537 pli_lat, pli_lon = pli["y"].values, pli["x"].values+360
538 latmin, latmax = min(gcm.coords["lat"].values), max(gcm.coords["lat"].values)
539 lonmin, lonmax = min(gcm.coords["lon"].values), max(gcm.coords["lon"].values)
540 if (any(pli_lon < lonmin) or any(pli_lon > lonmax) or
541     any(pli_lat < latmin) or any(pli_lat > latmax)):
542     if (all(pli_lon < lonmin) or all(pli_lon > lonmax) or
543         all(pli_lat < latmin) or all(pli_lat > latmax)):

```

```

543         print("All points in the pli file are outside the domain in the netcdf
file")
544         print("Please fix before continuing.")
545         print("Exiting routine...")
546     else:
547         print("Some points in the pli file are outside the domain in the
netcdf file")
548         print("Please remove these from the pli before continuing.")
549         print("Exiting routine...")
550         for i in range(pli_lon.size):
551             if (pli_lon[i] < lonmin or pli_lon[i] > lonmax or
552                 pli_lat[i] < latmin or pli_lat[i] > latmax):
553                 print(f"{pli_lon[i]-360:0.05f}, {pli_lat[i]:.05f} ")
554         sys.exit()
555
556     # Move forward if all points in the pli file are inside the domain
557     if quantity == "surf_el":
558         write_wl_for_pli(bc_fn, gcm, pli, quantity)
559     else:
560         write_t3d_for_pli(bc_fn, gcm, pli, quantity, nlevels, depth_avg=depth_avg)
561
562     # add points to list for visualization
563     pli_points.append(pli)
564
565     # concat pli points
566     pli_points = pd.concat(pli_points)
567
568
569
570     ### visualization ###
571     # color map depending on quantity
572     if plot:
573         matplotlib.use('Agg')
574         if quantity == "salinity":
575             cmap = cmo.haline
576         elif quantity == "water_temp":
577             cmap = cmo.thermal
578         elif quantity == "velocity":
579             cmap = "jet"
580         elif quantity == "surf_el":
581             cmap = "jet"
582
583     # setup orthographic projection for geographic data
584     fig, ax = plt.subplots(
585         1, 1, subplot_kw={"projection": ccrs.PlateCarree()}, figsize=(16, 9)
586     )
587     ax.gridlines(draw_labels=True)
588     ax.coastlines(resolution='50m')
589
590     # plot initial quantity at surface
591     if (quantity == "salinity") or (quantity == "water_temp"):
592         gcm[quantity].isel(time=0, depth=0).plot(
593             ax=ax, transform=ccrs.PlateCarree(), cmap=cmap
594         )
595     elif quantity == "velocity":
596         tmp = gcm.isel(time=0, depth=0)
597         tmp["magnitude"] = np.sqrt(tmp["water_u"] ** 2 + tmp["water_v"] ** 2)

```

```

598     tmp["magnitude"].plot(
599         ax=ax,
600         transform=ccrs.PlateCarree(),
601         cmap=cmap,
602         cbar_kwargs={"label": "velocity magnitude [m/s]"},
603     )
604     elif quantity == "surf_el":
605         gcm[quantity].isel(time=0).plot(
606             ax=ax, transform=ccrs.PlateCarree(), cmap=cmap
607         )
608
609     # add coastline for reference
610     # ax.add_feature(cfeature.COASTLINE, edgecolor="0.3")
611
612     # boundary condition support points
613     pli_points.plot.scatter(
614         "x", "y", marker="x", color="k", ax=ax, transform=ccrs.PlateCarree()
615     )
616
617     fig.savefig("point_output_locations.png", bbox_inches="tight")
618

```

A.2 coamps2meteo.py

The following section contains the coamps2meteo.py Python code used to create meteorological forcing files, `<.amp>`, `<.amu>`, and `<.amv>`.

```

1 # -*- coding: utf-8 -*-
2 """
3     Given a region, start date and end date creates meteorological forcing
4     files from COAMPS
5
6     Usage:
7     $ python coamps2meteo.py --region COAMPSREGION --start-date start_date
8     --end-date end_date --datadir COAMPS_DATADIR
9     date format: YYYYMMDD
10
11     Examples:
12
13     $ python coamps2meteo.py --region eqam --start-date 20190101 --end-date
14     20190107 --datadir /u/NOGAPS/COAMPSg
15
16     $ python coamps2meteo.py -r eqam -s 20190101 -e 20190107 -d
17     /u/NOGAPS/COAMPSg
18 """
19 # Created By: Jay Veeramony
20 # Version: 1.1
21 # Created on: Unknown
22 # Last modified: 2022-07-22
23 #     Various modifications to bring code in line with python best practice
24 #     Combined routines
25
26
27 import argparse
28 import logging
29 import os

```

```
30 import time
31 import sys
32 import shutil
33
34 from datetime import date, datetime, timedelta
35 from pathlib import Path
36 from subprocess import call
37
38 import numpy as np
39 from scipy.io import loadmat
40
41
42 def list_inputfiles(coamps_region, sdtg, edtg, ddir, component):
43     """
44     Creates list of input files that are read from the COAMPS database
45
46     Args:
47         coamps_region (str): Model region from which data is needed
48         sdtg (str): Start date for data retrieval (YYYYMMDD format)
49         edtg (str): End date for data retrieval (YYYYMMDD format)
50         ddir (str): Data directory
51         component: Meteorological component to retrieve, valid values are
52             "pres", "wnd_ucmp", "wnd_vcmp"
53
54     Returns:
55         List of files that contain the data. These files could be gzipped.
56
57     """
58     sdtg = datetime.strptime(sdtg, '%Y%m%d')
59     edtg = datetime.strptime(edtg, '%Y%m%d')
60
61     ddir = Path(ddir).resolve()/coamps_region
62
63     dirs = list(ddir.glob('20*'))
64     print("Type of dirs:", type(dirs))
65     print("Size of dirs:", len(dirs))
66
67     # check if directory is empty (likely a typhoon mounting error)
68     if not dirs:
69         print('dirs is empty')
70         sys.exit('directory empty or nonexistant. Check mount of typhoon')
71
72     # initial file
73     fileslist = list(dirs[0].glob(coamps_region+'_'+component+'.*'))
74
75     # rest of files
76     for idir in range(1, len(dirs)):
77         fileslist.extend(dirs[idir].glob(coamps_region+'_'+component+'.*'))
78
79     file_dates = list()
80     for filename in fileslist:
81         file_dates.append(str(filename).split('.')[1])
82
83     #
84     # sort files and dates, necessary bc zipped files
85     #
86     file_dates = np.asarray(file_dates, dtype='int')
```

```

87     idx = np.argsort(file_dates)
88     file_dates = file_dates[idx]
89
90     fileslist = np.array(fileslist)
91     fileslist = fileslist[idx]
92
93     tstart = int(sdtg.strftime('%Y%m%d%H'))
94     tend = int(edtg.strftime('%Y%m%d%H'))
95
96     idx = (file_dates >= tstart)*(file_dates <= tend)
97     return fileslist[idx]
98
99
100 def append_met_data(met_file, ref_time, datafile, nlon, nlat):
101     """
102     Appends the data to the meteorological file
103
104     Args:
105         met_file: file being written
106         ref_time: Reference time
107         datafile: file from list of files between start/end date
108         nlon, nlat: size of data array (obtained from model info)
109
110     """
111     print('reading file: ', datafile)
112     if str(datafile).endswith('gz'):
113         print('zipped file to be copied locally/unzipped')
114         zipfile = os.path.basename(files[0])
115         shutil.copyfile(files[0], './'+zipfile)
116         call(['gunzip', zipfile])
117
118         # reassign datafile to just unzipped file
119         cols = zipfile.split('.')
120         datafile = './'+cols[0]+'.'+cols[1]
121
122         file_time = cols[1]
123         time_array = datetime.strptime(file_time, '%Y%m%d%H') + \
124             np.arange(12) * timedelta(hours=1)
125         data = read_coamps(datafile, nlon, nlat, 12)
126
127         with open(metfile, 'a') as fid:
128             for i in range(len(time_array)):
129                 tc = time.mktime(time_array[i].timetuple()) - \
130                     time.mktime(ref_time.timetuple())
131                 logging.info('TIME = %.3f hours since %s # %s', tc/3600,
132                             ref_time.strftime('%Y%m%d%H'),
133                             time_array[i].strftime('%Y%m%d%H'))
134                 fid.write('TIME = {0} hours since {1} # {2}'.
135                           format(tc/3600, ref_time, time_array[i]))
136                 fid.write('\n')
137                 for m in reversed(range(data.shape[1])):
138                     for j in data[i, m, :]:
139                         fid.write('%0.2f ' % j)
140                     fid.write('\n')
141
142         os.remove(datafile)
143     else:

```

```

144     file_time = str(datafile).split('.')[1]
145     time_array = datetime.strptime(file_time, '%Y%m%d%H') + \
146         np.arange(12) * timedelta(hours=1)
147     data = read_coamps(datafile, nlon, nlat, 12)
148     with open(met_file, 'a') as fid:
149         for i in range(len(time_array)):
150             tc = time.mktime(time_array[i].timetuple()) - \
151                 time.mktime(ref_time.timetuple())
152             logging.info('TIME = %.3f hours since %s # %s',
153                         tc/3600, ref_time.strftime('%Y%m%d%H'),
154                         time_array[i].strftime('%Y%m%d%H'))
155             fid.write('TIME = {0} hours since {1} # {2}'.
156                     format(tc/3600, ref_time, time_array[i]))
157             fid.write('\n')
158             for m in reversed(range(data.shape[1])):
159                 for j in data[i, m, :]:
160                     fid.write('%2f ' % j)
161                 fid.write('\n')
162
163
164 def get_modelinfo(area_name):
165     '''
166     Given the name of an area with met data, extract information about the grid
167     such as its location, grid size and grid resolution
168
169     Args:
170         area_name(str): COAMPS model region
171
172     Returns:
173         sdir (str): Sub-directory name to check for data.
174         ssubdir (str) : Sub-sub directory name
175         nx (int) : Number of longitude points on the grid.
176         ny (int) : Number of latitude points on the grid.
177         minlat (float) : Origin - latitude.
178         minlon (float) : Origin - longitude.
179         maxlat (float) : max extent of latitude.
180         maxlon (float) : max extent of longitude.
181
182     '''
183     path = os.path.dirname(os.path.abspath(__file__))
184     area = loadmat(path+'/modelinfo.mat') # load mat-file
185     mdata = area['modelinfo'] # variable in mat file
186     mdtype = mdata.dtype # dtypes of structures are "unsized objects"
187
188     # * SciPy reads in structures as structured NumPy arrays of dtype object *
189     # * The size of the array is the size of the structure array, not the number
190     # * elements in any particular field. The shape defaults to 2-dimensional. *
191     # * For convenience make a dictionary of the data using the names from dtype
192
193     ndata = {n: mdata[0][n] for n in mdtype.names}
194
195     # When reading in the Matlab mat file, the different integers and floats
196     # have varying dtypes, presumably because Matlab uses the lowest size
197     # needed to store the data to save space. Make them all uniform size here
198     # for convenience
199
200     ndata['nx'] = ndata['nx'].astype('int')

```

```

201 ndata['ny'] = ndata['ny'].astype('int')
202 ndata['minlat'] = ndata['minlat'].astype('float64')
203 ndata['minlon'] = ndata['minlon'].astype('float64')
204 ndata['maxlat'] = ndata['maxlat'].astype('float64')
205 ndata['maxlon'] = ndata['maxlon'].astype('float64')
206
207 # Get line number where data is to be retrieved from
208 iloc = np.squeeze(np.where(ndata['modell'] == area_name))
209
210 sdir = str(np.squeeze(ndata['modell1'][iloc]))
211 ssdir = str(np.squeeze(ndata['modell2'][iloc]))
212 # nx = ndata['nx'][iloc]
213 # ny = ndata['ny'][iloc]
214 # minlat = ndata['minlat'][iloc]
215 # minlon = ndata['minlon'][iloc]
216 # maxlat = ndata['maxlat'][iloc]
217 # maxlon = ndata['maxlon'][iloc]
218 # return sdir, ssdir, nx, ny, minlat, minlon, maxlat, maxlon
219 area_info = {'sdir': sdir,
220             'ssdir': ssdir,
221             'nx': ndata['nx'][iloc],
222             'ny': ndata['ny'][iloc],
223             'minlat': ndata['minlat'][iloc],
224             'minlon': ndata['minlon'][iloc],
225             'maxlat': ndata['maxlat'][iloc],
226             'maxlon': ndata['maxlon'][iloc]}
227 return area_info
228
229
230 def read_coamps(data_file, nlon, nlat, ntime):
231     """
232     Given a binary file with meteorology data in /u/NOGAPS,
233     reads it into a data array Parameters
234
235     Args:
236         data_file (str): File containing binary data.
237         nlon (int) : Number of longitude locations.
238         nlat (int) : Number of latitude locations.
239         ntime (int) : Number of taus.
240
241     Returns:
242         data (float) : Matrix of size (nlon, nlat, ntime) containing the data.
243     """
244     header = np.zeros(ntime)
245     footer = np.zeros(ntime)
246     data = np.zeros((nlon, nlat, ntime))
247
248     with open(data_file, 'rb') as fid:
249         for j in range(ntime):
250             header[j] = np.fromfile(fid, dtype='>u4', count=1)
251             local_data = np.fromfile(fid, dtype='>f4', count=nlon*nlat)
252             footer[j] = np.fromfile(fid, dtype='>u4', count=1)
253
254             # Reshape the matrix in fortran order
255             local_data = np.reshape(local_data, (nlon, nlat), order='F')
256             data[:, :, j] = local_data
257

```

```

258     if header[0] != footer[0]:
259         print('Header ' + str(header[0]))
260         print('Footer ' + str(footer[0]))
261         print('File seems to be corrupt or read order is wrong')
262
263     # To keep it same as the openearth tools structure, permute
264     # the array to have time loop on the first dimension and
265     # longitude on the third dimension
266     data = data.transpose(2, 1, 0)
267
268     return data
269
270
271 def write_met_header(met_var, met_file, nlon, nlat, minlon, maxlon,
272                    minlat, maxlat):
273     """
274     Writes header for meteorological file
275
276     """
277     dlon = (maxlon - minlon)/(nlon - 1)
278     dlat = (maxlat - minlat)/(nlat - 1)
279
280     with open(met_file, 'w') as fid:
281         fid.write('### START OF HEADER\n')
282         fid.write('FileVersion      = 1.03\n')
283         fid.write('filetype         = meteo_on_equidistant_grid\n')
284         fid.write('n_cols           = %5d \n' % nlon)
285         fid.write('n_rows          = %5d \n' % nlat)
286         fid.write('grid_unit       = ' + 'deg' + '\n')
287         fid.write('x_llcorner      = %5.2f \n' % minlon)
288         fid.write('y_llcorner      = %5.2f \n' % minlat)
289         fid.write('dx              = %5.2f \n' % (dlon))
290         fid.write('dy              = %5.2f \n' % (dlat))
291         fid.write('n_quantity      = 1 \n')
292
293         if met_var == 'pres':
294             fid.write('quantity1       = ' + 'air_pressure' + '\n')
295             fid.write('unit            = ' + 'Pa' + '\n')
296             nodata_value = 101300.0
297         elif met_var == 'wnd_ucmp':
298             fid.write('quantity1       = ' + 'x_wind' + '\n')
299             fid.write('unit            = ' + 'm/s' + '\n')
300             nodata_value = 0.0
301         elif met_var == 'wnd_vcmp':
302             fid.write('quantity1       = ' + 'y_wind' + '\n')
303             fid.write('unit            = ' + 'm/s' + '\n')
304             nodata_value = 0.0
305         else:
306             sys.exit('Incorrect variable names')
307
308         fid.write('NODATA_value    = %.2f \n' % (nodata_value))
309         fid.write('### END OF HEADER\n')
310
311     """
312     Start of the main routing
313     """
314

```

```

315 if __name__ == "__main__":
316     valid_choices = ['arctic', 'cencoos_n3', 'e_pac_comp', 'europe2',
317                    'hawaii_n3', 'mbay_n4', 'n_ind2', 'southwest_asia',
318                    'useast', 'cen_amer', 'centam', 'eqam', 'europe3',
319                    'indo', 'mideast', 'nwat1', 'southwest_asia2', 'was3',
320                    'cen_america', 'centio', 'eqam_comp', 'fukushima',
321                    'mbay_n1', 'MREA04', 'nwpac', 'southwest_asia2_n3',
322                    'w_atl', 'cencoos_n1', 'eafr', 'euro', 'hawaii',
323                    'mbay_n2', 'nepac', 'social', 'southwest_asia3', 'w_pac',
324                    'cencoos_n2', 'e_pac', 'europe', 'hawaii_comp',
325                    'mbay_n3', 'n_ind', 'somalia', 'test2', 'w_pac2']
326
327     parser = argparse.ArgumentParser()
328     parser.add_argument("-r", "--region",
329                        type=str,
330                        help="COAMPS region of interest",
331                        choices=valid_choices,
332                        required=True)
333     parser.add_argument("-s", "--start-date",
334                        type=str,
335                        help="data start date YYYYMMDD",
336                        required=True,
337                        dest="str_date")
338     parser.add_argument("-e", "--end-date",
339                        type=str,
340                        help="data end date YYYYMMDD",
341                        required=True,
342                        dest="end_date")
343     parser.add_argument("-d", "--datadir",
344                        type=str,
345                        help="DATADIR = data directory",
346                        default='/u/NOGAPS/COAMPSg',
347                        required=True,
348                        dest="datadir")
349
350     args = parser.parse_args()
351     region = args.region
352     str_date = args.str_date
353     end_date = args.end_date
354     if str_date > end_date:
355         sys.exit('input error: {} occurs before {}'.format(end_date, str_date))
356
357     datadir = args.datadir
358
359     logfilename = ('coamps_'+region+'_'+str_date+'_'+end_date+'_'
360                  + date.today().strftime('%Y%h%d')+'.log')
361
362     logging.basicConfig(filename=logfilename, level=logging.INFO,
363                        format='%(levelname)s:%(message)s')
364     logging.info('Command line arguments: %s %s %s', sys.argv[1],
365                sys.argv[2], sys.argv[3])
366     coampsdata = get_modelinfo(region)
367     nx = coampsdata['nx']
368     ny = coampsdata['ny']
369     minlon = coampsdata['minlon']
370     maxlon = coampsdata['maxlon']

```

```
372 minlat = coampsdata['minlat']
373 maxlat = coampsdata['maxlat']
374
375 # note that 'pres' is only used for getting dates
376 files = list_inputfiles(region, str_date, end_date, datadir, 'pres')
377 if len(files) > 0:
378     print('Available range of files:')
379     print(str(files[0]).split('.')[1])
380     print(str(files[-1]).split('.')[1])
381 else:
382     sys.exit('No files found, check dates and region')
383
384 pars = ['pres', 'wnd_ucmp', 'wnd_vcmp']
385
386 for var in pars:
387     if var == 'pres':
388         metfile = Path('./coamps_'+str_date+'_'+end_date+'_'+region+'.amp')
389         write_met_header(var, metfile, nx, ny, minlon, maxlon,
390                         minlat, maxlat)
391         files = list_inputfiles(region, str_date, end_date, datadir, var)
392         # fileTime = files[0].split('.')[1]
393         fileTime = str(files[0]).split('.')[1]
394         refTime = datetime.strptime(fileTime, '%Y%m%d%H')
395         for f in files:
396             logging.info('****Reading coamps file %s****', f)
397             append_met_data(metfile, refTime, f, nx, ny)
398     elif var == 'wnd_ucmp':
399         metfile = Path('./coamps_'+str_date+'_'+end_date+'_'+region+'.amu')
400         write_met_header(var, metfile, nx, ny, minlon, maxlon,
401                         minlat, maxlat)
402         files = list_inputfiles(region, str_date, end_date, datadir, var)
403         fileTime = str(files[0]).split('.')[1]
404         refTime = datetime.strptime(fileTime, '%Y%m%d%H')
405         for f in files:
406             logging.info('****Reading coamps file %s****', f)
407             append_met_data(metfile, refTime, f, nx, ny)
408     elif var == 'wnd_vcmp':
409         metfile = Path('./coamps_'+str_date+'_'+end_date+'_'+region+'.amv')
410         write_met_header(var, metfile, nx, ny, minlon, maxlon,
411                         minlat, maxlat)
412         files = list_inputfiles(region, str_date, end_date, datadir, var)
413         fileTime = str(files[0]).split('.')[1]
414         refTime = datetime.strptime(fileTime, '%Y%m%d%H')
415         for f in files:
416             logging.info('****Reading coamps file %s****', f)
417             append_met_data(metfile, refTime, f, nx, ny)
418     else:
419         sys.exit('Incorrect variable names')
```