Sparse Hydrodynamic Ocean Code

V5199

User Manual

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The latest SHOC User Manual may be downloaded from:
http://www.emg.cmar.csiro.au/www/en/emg/software/EMS/hydrodynamics.html
Revision history is available at the same address.

1 Introduction

SHOC (Sparse Hydrodynamic Ocean Code) is a finite difference hydrodynamic model developed by the Environmental Modelling group at CSIRO (Commonwealth Scientific and Industrial Research Organization) Division of Marine Research (Herzfeld, 2006). This model is intended to be a general purpose model applicable to scales ranging from estuaries to regional ocean domains. Outputs from the model include three dimensional distributions of velocity, temperature, salinity, density, passive tracers, mixing coefficients and sea level. Inputs required by the model include forcing due to wind, atmospheric pressure gradients, surface heat and water fluxes and open boundary conditions (e.g. tides). **SHOC** is based on the three dimensional equations of momentum, continuity and conservation of heat and salt, employing the hydrostatic and Boussinesq assumptions. The equations of motion are discretized on a finite difference stencil corresponding to the Arakawa C grid.

The model uses a curvilinear orthogonal grid in the horizontal and fixed 'z' coordinates in the vertical. The 'z' vertical system allows for wetting and drying of surface cells, useful for modelling regions such as tidal flats where large areas are periodically dry. **SHOC** has a free surface and uses mode splitting to separate the two dimensional (2D) mode from the three dimensional (3D) mode. This allows fast moving gravity waves to be solved independently from the slower moving internal waves allowing the 2D and 3D modes to operate on different time-steps, resulting in a considerable contribution to computational efficiency. The model uses explicit time-stepping throughout except for the vertical diffusion scheme which is implicit. The implicit scheme guarantees unconditional stability in regions of high vertical resolution. A Laplacian diffusion scheme is employed in the horizontal on geopotential surfaces. **SHOC** can invoke several turbulence closure schemes, including k-ε, k-ω, Mellor-Yamada 2.5, Mellor-Yamada 2.0 and Csanady type parameterisations. Input and output is handled through netCDF data formatted files, with the option of submitting ascii text files for simple time-series forcing. The netCDF format allows input of spatially and temporally varying forcing and initialization data in a grid and time-step independent manner. **SHOC** is capable of performing particle tracking and may be coupled to ecological and sediment transport models.

SHOC uses a sparse coordinate system which maps all cells in the grid into a 1-dimensional vector. This process effectively eliminates all land from the domain representation in computer memory. Arbitrary domain composition can be efficiently performed, allowing **SHOC** to operate in a true distributed processing environment. The sparse representation leads to increases in speed and simplified housekeeping, allowing techniques such as distributed process, 2-way nesting and hybrid physics to be performed with no overhead.

SHOC is written in C and evolved during 2002 from the **MECO** model, with subsequent improvements post 2002.

This document is designed to assist the user in operating **SHOC**. For a description of the theory the model is based on refer to Herzfeld et al (2002).

2 Installation and operation

This section describes how to acquire, compile, and install **SHOC**. At present, **SHOC** is designed to run under the UNIX operating system. It has successfully been installed on SUN workstations, Silicon Graphics workstations, and Intel Linux which is the current development platform.

2.1 Getting the model source code

The source code to SHOC and associated libraries and utilities is available from CSIRO Marine Research, subject to approval and acceptance of a license agreement. If you wish obtain the source code, or require further information please contact John.Parslow@csiro.au.

2.2 Building and installing the model executable file

This section provides a brief description of how to compile and install **SHOC** and the supporting libraries**, ecology**, **sediments** and **tracerstats** as provided with the **SHOC** source distribution. Additional compilation and installation instructions are provided with each package (see the INSTALL file).

Note that all packages depend on the udunits and netCDF packages. Please ensure that udunits and netCDF have been installed before attempting to compile or install either **SHOC** or the libraries. netCDF and udunits are available from Unidata http://www.unidata.ucar.edu/.

SHOC resides in a directory structure called the Environmental Modelling Suite (ems), which also contains source code for various supporting libraries and the sediment transport and ecology models. Once ems is installed on the computer it must be configured. During this step a script checks for the presence of external and internal libraries, searches for compilers, linkers, and other utilities required to compile the source code. If `configure` was successful, it will generate a `makefile` which can be used to build the model and related utilities. The configure script is run as follows:

```
./conf/configure
```

By default the configure script searches for all architecture independent files (e.g. netCDF libraries) in the directory /usr/local. If an alternate path is required use:

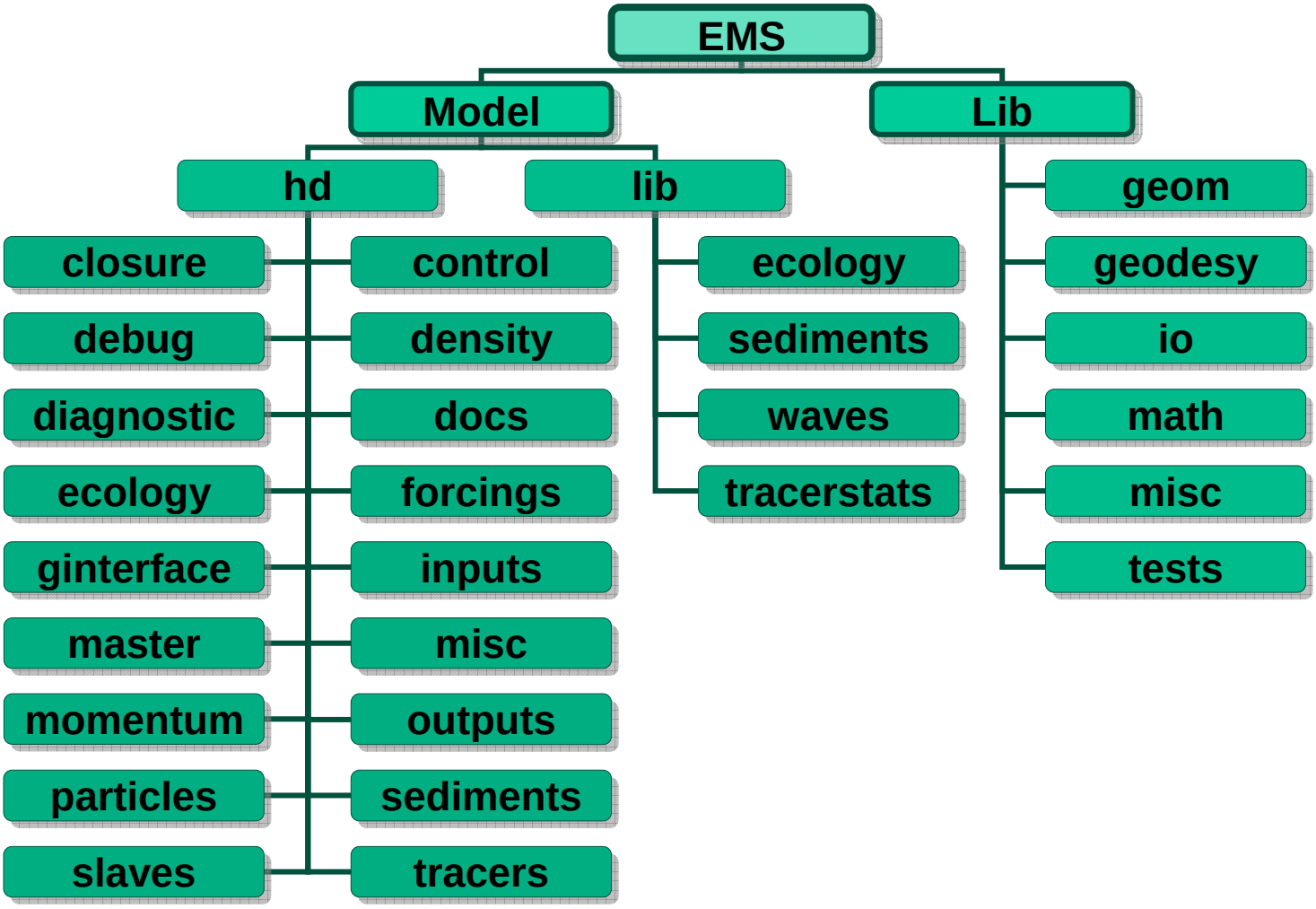
```
./conf/configure –prefix=PATH
```

For a full list of configure's command line options, enter `configure --help`. Once ems is configured, all source code is compiled using:

```
make
```

The libraries and executables are installed using the `make install` command. The directories are cleared of object files and executables by using `make clean` command. Additionally, `make distclean` removes any files created by configure, as well as all object files, etc. If `make distclean` is used, it will be necessary to re-run `./conf/configure` in order to re-build the model.
The ems packing is stand-alone in the sense that once it is installed the user is free to modify any of the libraries or core code without being dependent on external libraries or code. Individual components of ems can be compiled by using the `makefile` in the subdirectories of ems (the directory structure of ems is illustrated in Figure 2.1). For example to re-make **SHOC** if it has been modified, go to `/ems/model/hd` and type `make`.

Figure 2.1 : ems directory structure



2.3 Running the model

To set-up and run **SHOC**, it is necessary to provide a parameter file containing information about the model geometry, run parameters and forcing inputs. A specially formatted netCDF file is also required that contains the initial values for the model variables over the model grid. The netCDF file may be the result of a previous model run, or may be generated from the parameter file using the `-g` option (see section 8).

The parameter file contains essentially all the information needed to describe a particular model implementation, and its contents are described in detail in the Model setup section.

The model may be run in one of two modes. The auto-configuration mode is invoked via:

```
shoc -a prmname
```

where `prmname` is the name of the model auto-config file (see section 5). These files are vastly simplified versions of the full parameter file. In this mode **SHOC** will internally generate all parameters required for the run, write this information to a parameter file, generate a netCDF input file and commence the run. If the `-ag` option is used then **SHOC** will not commence the run but will terminate once all input files are created and written. In the auto

mode model parameters are set to fixed default values or are calculated from the bathymetry and grid geometry.

Alternatively, a run may be initiated using an existing complete parameter file and input netCDF file using:

```
shoc -p prmname
```

where `prmname` is the name of the model parameter file. Model parameters used for the run in this mode are those specified in the parameter file.

Various diagnostic information about the internal status of **SHOC** can be obtained using the `--debug` or `–l` command line option. This option is followed by a sequence of diagnostics types separated by commas `e.g. –debug time,dump`, where each type defines a desired diagnostic output. By default the output is written to the C standard error. Depending on the type requested, the diagnostic output may be quite voluminous. Some diagnostic types depend on the presence of others. **SHOC** will automatically enable any dependent diagnostics.

To display the command line arguments and a list of all diagnostic types **SHOC** should be run with the `-help` option. Following is an example output:

```
    % shoc –help

                SHOC: Sparse Hydrodynamic Ocean Code
Version:        v0.00 (beta) rev000
Run start:      Thu Jun 24 14:31:51 2004

Usage:
shoc -p prmfile <options>
  Run SHOC using standard parameter file.
  prmfile               Standard parameter file

shoc -g prmfile dumpfile <options>
  Generate initial dump using standard parameter file.
  prmfile               Standard parameter file
  dumpfile              Initialisation dump file

shoc -a prmfile <options>
  Run SHOC using autostart parameter file.
  prmfile               Autostart parameter file

shoc -ag prmfile <options>
  Generate initial dump using autostart parameter file.
  prmfile               Autostart parameter file

shoc –t tranfile <options>
  Run SHOC in transport mode.
  tranfile              Transport input file

shoc –ps prmfile
  Compute percentile statistics.
  prmfile               Parameter file.

shoc –v
  Print shoc version information.
```

```
options:
    -diag_log <file>|off  Enable/disable diagnostic log (default:
                          'diag.txt').

    -setup_log <file>|off Enable/disable setup log (default:
                          'setup.txt').

    -window_log on|off    Enable/disable window log (default: off). A
                          text file listing all master-slave mappings
                          is stored in 'window_map.txt' and the
                          spatial distribution of all windows in
                          'window_geom.txt'.

  -l tag,tag...           Set library log level. The more tags
                          listed, the more messages are printed. All
                          messages are printed to file 'runlog'. In
                          order of output detail, supported tags are:
       - main             # print information on major general events
       - info             # print information on minor general events
       - warn             # non-fatal warning information
       - debug            # print high level debug information
       - trace            # print low level debug information
       - metric           # information on time spent in routines,
                          # (for development only).

    -debug tag,tag,...    Set debug level. Supported debug tags are:
       - all                   # print all debug information
       - conversions           # list time unit conversions
       - time                  # list model time
       - dump        [ time ]  # list next dump
       - particles   [ time ]  # list particle resets
       - init_m                # master initialisation info
       - init_w                # slave initialisation info
       - ecology               # ecology info
       - sediments             # sediment info
```

Examples :

```
shoc –g input.prm in.nc –debug init_m,init_w

shoc –p input.prm –l main,info,warn –window_log on
```

It is often useful to run the model as a background process with the output captured into a file. How this is done, depends on the UNIX shell being used. For a csh the following command is sufficient:

```
shoc -p prmname >&! logfile &
```

3 Model setup

3.1 Setting up a model application

There are many steps required to successfully configure **SHOC**. Following are some of the major steps:

- Installation of the model software. This is described in section 2.
- Definition of the horizontal and vertical geometry of the model grid. This may require the use of an interactive grid generation program with the ability to plot coastlines, etc, or may be a simple specification of a test area such as a ‘swimming pool'.
- Construction of the model parameter file. This step incorporates the grid geometry obtained above along with information about bathymetry and the location and types of boundary points. As well, forcing data sets are specified, and the physical parameters (mixing, friction, etc) are chosen. With the auto-config mode this file is automatically generated.
- Creation of the model variable initialisation netCDF file, either from the parameter file by using the `-g` option, described in section 8, or by using output from a previous model run.
- Running the model. Commands needed to do this are described in section 4.
- Examination of the results. This is done either by using an interactive viewer (`jvismeco, olive`), or by producing plots with various scripts or tools such as `gnuplot`.

To set up the model for a particular area or application, it is necessary to gather together a diverse set of parameter specifications and input data. These are all defined in the model parameter file, an easily edited ASCII file which completely defines the model for a particular application and run. Amongst other things, the parameter file describes the model geometry, forcing data, run period and where and how to write results. This section describes the various datasets that are needed to create a model parameter file, and the elements of the parameter file itself.

4 The parameter file

The parameter file is an ASCII text file containing comments, keywords and values. Its contents completely describe a particular model implementation and run parameters (apart, possibly, from initial values for model variables). All lines starting with a # character are considered as comment lines. Comment lines are valuable for documenting certain choices of parameter values, or for reminders of the significance of certain infrequently used parameters. Comment lines and blank lines are generally ignored by the model itself, but may not appear in certain positions described below. Other lines typically contain a keyword (the parameter name) and a value. Parameter values may be strings, integers, floating point values, arrays of floating point values or more complex lists (such as boundary point lists, or time series point lists). The order in which parameters appear in the file is largely unimportant.

Examples of string parameters are:

```
PARAMETERHEADER  River model
file0.name       out
```

Examples of boolean parameters (and comment lines) are:

```
# All boolean parameters may be set with either {TRUE|FALSE},
# {YES|NO}, {1|0}, {INCLUDE|EXCLUDE}. Case is not important.
NONLINEAR  TRUE
CALCDENS   no
```

Examples of integer and floating point parameters are:

```
NCE1        20
G           9.81
```

Arrays are entered by giving the keyword and the number of values in the array on the same line, followed on the next lines by the array values separated by spaces, tabs or new lines. Comment lines may not appear in the middle of the list of array values. Following are two examples:

```
# Fills the bathymetry array with four values.
BATHY 4
0.002 0.0025
0.0026
0.0027

# If insufficient data is provided, then the last value
# is used to pad out the array
BATHY 4
0.002
```

Having described the general syntax of the parameters, the following sections describe the wide range of parameters needed to specify a particular model application.

4.1 Parameter header

Most parameter files begin with some comment lines which describe the model application, and mandatory parameters which specify the **SHOC** code version to be used, and descriptive string for this run. The format is as shown below:

```
# This is the parameter file header. It usually describes the
# model application.
#
# The code header must be identical to the 'Version' string
# specified when SHOC is compiled (in version.c). This provides
# a check that the intended version of the model code is being
# used at run time.
CODEHEADER              SHOC default version

# A single line description of the model run. This string is
# written into all output files.
PARAMETERHEADER         NWS 20km rectangular grid, Run 1
```

4.2 Windows

SHOC is designed to operate in a distributed processing environment, where domain decomposition is performed on the grid to divide it into a number of partitions or 'windows', which are solved on different processors. The number of windows used is set via:

```
# Indicates the number of windows in the model domain.
   WINDOWS    2
```

Generally the number of windows is equal to the number of processors available. If **SHOC** is to operate on a single processor, the `WINDOWS = 1`. The domain decomposition be a striping or blocking method, or may be any arbitrary congregation of grid points. This allows total flexibility when decomposing geographically complex domains. The distributed processing procedure requires common information to be transferred between windows, hence by minimising the size of boundaries between windows (e.g. by utilizing the geography and placing window boundaries across narrow regions) the amount of data transferred is minimised and execution speed increases.

The window partitioning method is specified using the `WINDOW_TYPE`, where:

```
  WINDOW_TYPE     STRIPE_E1   # Stripe in the e1 direction (default).
  WINDOW_TYPE     STRIPE_E2   # Stripe in the e2 direction.
  WINDOW_TYPE     BLOCK_E1 n  # Blocking. n is an optional integer;
                              # when present the block is made
                              # rectangular in the e1 direction by n
                              # cells.
  WINDOW_TYPE     BLOCK_E2 n  # Same as BLOCK_E1, but rectangles
                              # are in the E2 direction.
  WINDOW_TYPE     EXPLICIT    # The user supplies the partitioning,
                              # see below.
```

The striping methods divides the wet domain into the number of specified windows, hence all 2D partitions contain the same number of cells (the last window may not if the total number of wet cells is not divisible by the number of windows). The blocking methods divide the total grid size into blocks of size `sqrt(nce1 x nce2)`. A block must contain at least 1 wet cell for it to be valid (i.e. blocks that contain all dry cells are ignored). This results in blocks containing quite different numbers of cells, depending on how many wet cells are encountered in each block. Consequently load balance may be poor. However, for large numbers of windows, it may be preferable, since the amount of information exchanged between windows decreases as windows increase with blocking, and the model load balance will be determined by blocks containing all wet cells (which will be more numerous as the number of windows increases).

For `STRIPE_E1` and `STRIPE_E2`, The window sizes may be set using the command:

```
# Sets the window sizes for n windows
WINDOW_SIZE             a1 a2. . . . an
or
WINDOW_SIZE             default
```

Where a_1 to a_n are fractions whose sum adds up to 1.0, or for `default`, a_1 to a_n = `1 / WINDOWS`. The surface of the domain is then partitioned into windows according to the specified fractions, e.g. if two windows are specified with sizes 0.5 and 0.5, then the surface is split into two equal windows. Note that the number of cells in a windows may not be equal if the surface is split into equal sizes, since windows with deeper water will contain more cells than windows with shallow water. When this option is used, the 'diag.txt' diagnostic file (section 4.32) will contain the amount of CPU time spent in each window. Also shown is the actual load balance used (i.e. the prescribed window sizes) and the predicted window sizes that are required to achieve equal amounts of CPU time in each window (i.e. an even load balance). This load balancing may be automated using:

```
# Resets window sizes to balance the CPU
WINDOW_RESET                  m
```

Where every m time steps the windows are automatically re-generated with sizes that attempt to balance the CPU load.

The window partitions may be explicitly defined for `WINDOWS – 1` windows using `WINDOW<n>_POINTS` where `<n>` is the window number. The number of points in the list should be specified, followed by a list of the (i,j) locations of the window cells, e.g:

```
# Define the first window to contain 2 cells
WINDOW1_POINTS          2
2 1
2 2
```

Note the 'Marked' facility in `jvismeco` is a useful tool for extracting (i,j) locations from a domain. The last window is created to consist of all cells not included in a list.

The window partitioning can be written to the output file using:

```
SHOW_WINDOWS      YES   # Creates a tracer 'window_partitions'
                        # containing window configuration.
```

This facility is switched off by default.
The window map may be written to netCDF file using:

```
DUMP_WIN_MAP      <mapfile.nc>
```

Where `<mapfile.nc>` is the name of the file the map is written to. This may then be subsequently read at runtime (rather than computed) using:

```
READ_WIN_MAP      <mapfile.nc>
```

Note that computing the sparse map for many windows on very large grids can take several hours; reading the window map from file provides a means of rapidly starting a simulation. `DUMP_WIN_MAP` will operate in the `–p` and `–g` modes, and `READ_WIN_MAP` operates in the `–p` mode.

When using multiple windows, the message passing library must also be specified, e.g.

```
DP_MODE     openmp      # Use the openMP libraries
            pthreads    # Use the pthreads library
```

Comparisons using 1 or multiple windows have shown identical results in simple test domains and a complicated real case study. However, not all functionality (advection schemes, mixing schemes, open boundaries etc) or combinations of bathymetry, geography and window partitions have been tested, hence it is possible that some combinations of the above do not result in identical solutions using 1 and multiple windows. It is known that if the model is subjected to SUB-STEP (Section 4.27) then at window boundaries values from different time levels are used resulting in solutions that differ. To avoid sub-stepping, the time-step should be reduced. When invoking extended functionality with multiple windows it is prudent to check results against a single window.

4.3 Time

Internally, the model represents time in seconds since some epoch date/time. These parameters allow the specification of that epoch, the period of the simulation, the ramp-up period for external forcing, and the model's internal (3-d) and external (2-d) time steps for integration.

```
# Defines the epoch for all time related parameters, as well as
# for all output files generated by the model. Currently, the
# units must be 'seconds since ...', but this may change in future
# versions. The epoch is specified in standard ISO date/time
# format, including a possible timezone specification. The
# timezone here is 8 hours ahead of UTC.
TIMEUNIT                seconds since 1990-01-01 00:00:00 +08

# Defines the base time unit that will be used for all
# timeseries and netCDF output files.
OUTPUT_TIMEUNIT         days since 1990-01-01 00:00:00 +08

# Define length units - this parameter is redundant and must
# always be metre!
LENUNIT                 metre

# Defines the start and stop time of the model simulation period,
# relative to the epoch defined above. Relative time
# specifications here and elsewhere in the parameter file can be
# specified in seconds, minutes, hours, or days. Here, the start
# time corresponds to 1995-02-10 00:00:00 +8, and the end time to
# 1995-03-13 00:00:00 +8
START_TIME              1866 days
STOP_TIME               1897 days

# Defines the period during which external forcing variables
# (wind, open boundary elevations and/or velocities) are smoothly
# ramped from 0 to their normally prescribed values.  This
# mechanism allows the suppression of start-up transients and
# shocks in the simulation.
# Prior to RAMPSTART, forcing is set to zero. After RAMPEND,
# forcing is applied normally. In between, forcing values are
# scaled by a raised cosine ramp.
RAMPSTART         1866 days
RAMPEND           1866.5 days

# Defines which variables are ramped in. Suppression of wind and
# boundary forcing (global tide, file or custom specification) are
# invoked by listing the processes subject to the ramp. All
# processes are suppressed by default. E.g. all processes are
# suppressed via;
```

```
RAMPVARS  WIND      # Ramp the wind
          TIDALH    # Tidal OBC η computed using TIDALH
          TIDALC    # Tidal OBC η using custom constituents
          TIDEBC    # Tidal OBC η using tidal synthesis
          FILEIN    # OBC η using FILEIN input
          CUSTOM    # OBC velocity using CUSTOM
          INV_BARO  # OBC inverse barometer contribution
          ETA_RELAX # Relaxation to eta
          FLUX_ADJUST # OBC local flux adjustment
          STOKES    # Stokes Coriolis and vortex forces

# Specifies the internal (3-d) time-step, and the number of times
# the external (2-d) code will be run per 3-d time-step.
# The external (2_d) time-step is thus DT divided by IRATIO.
DT               120 seconds
IRATIO           5
```

4.4 Computational settings and flags

A number of parameters change the way in which calculations are performed, as follows:

```
    # A flag which includes or excludes the non-linear terms in
    # both the momentum equations and the surface elevation.
    NONLINEAR         YES

    # A flag which enables the calculation of density at each time
    # step from the salinity and temperature of the water. If this
    # flag is turned on, then the model must include tracers called
    # salt and temp. If it is turned off, the density field used by
    # the model is as read from the input netCDF file, and doesn't
    # change over time, regardless of the behaviour of any tracers
    # in the model. If a valid tracer name is input for CALCDENS,
    # then the density used in the model is the distribution
    # represented by that tracer.
    CALCDENS          YES
or
    CALCDENS           density_tracer


    # The minimum layer thickness (m) value to be used when dividing
    # by the layer thickness in any of the momentum equations.
    # This prevents numerical problems, particularly in areas which
    # are drying. Usually set to ~7% of the surface layer.
    HMIN              0.01

     # Specification of the slip condition at solid horizontal
    # boundaries. This effectively specifies the tangential velocity
    # value at the land (or at any solid vertical face) used by the
    # horizontal momentum equations. Valid values are:
    #     1.0     Full slip condition - most commonly used
    #     0.0     Half-slip condition
    #    -1.0     No slip condition
    # Other values may be accepted by the model, but may give
    # unexpected or erroneous results.
    SLIP              1.0

    # Specification of what constitutes a simulation fatality. If ETA
    # is specified the model will exit if absolute sea level is
    # greater than ETAMAX. If VEL3D is specified exits occur if
```

```
# absolute 3D velocity is greater than VELMAX. If VEL2D is
# specified exits occur if 2D velocity is greater than VELMAX_2D.
# If T/S is present, temp. and salinity are checked for NaN.
# If NAN is present, exits occur if ETA, VEL3D or VEL2D assume
# the NaN value. The default is ETA NAN with ETAMAX = 10.
FATAL      ETA VEL3D VEL2D
ETAMAX     10
VELMAX     5
VELMAX_2D  3

# Specifies the quantity of messages / information written to the
# file ‘runlog’. Same as –l option (see Section 2.3). The levels
# supported may be a subset of the following:
log_levels    main,warn,info,debug,trace

  - main             # print information on major general events
  - info             # print information on minor general events
  - warn             # non-fatal warning information
  - debug            # print high level debug information
  - trace            # print low level debug information
  - metric           # information on time spent in routines,
                     # (for development only).

# Allows smoothing of various fields at initialisation. Currently
# valid fields are:
CD      # Bottom roughness
U1VH    # Horizontal viscosity in the e1 direction
U2VH    # Horizontal viscosity in the e2 direction
U1KH    # Horizontal diffusivity in the e1 direction
U1KH    # Horizontal diffusivity in the e2 direction
# The form of smoothing is:
SMOOTH_VARS    <name>:n
# where <name> is one of the names above, and n is the number of
# smoothing passes, e.g;
SMOOTH_VARS CD:2 U2VH:1
# will perform 2 smoothing passes on bottom drag, and one pass on
# e2 horizontal viscosity.

# Allows scaling of various fields at initialisation. Valid
# fields are the same as for SMOOTH_VARS. The form of scaling is:
SCALE_VARS    <name>:s
# where <name> is one of the names above, and s is a scaling
# fraction, e.g;
SCALE_VARS CD:1.2 U2VH:0.9
# will scale bottom drag by 1.2, and e2 horizontal viscosity by
# 0.9.

# Records a sequence of runs in the file ‘setup.txt’ and netCDF
# output files. The sequence is invoked via:
SEQUENCE      n
# The following field is then printed in the file setup.txt and
# as a global attribute in all output netCDF file:
Run # n
# If a setup.txt file is entered as the input to SEQUENCE, and
# the file contains ‘Run # n’, then the run identifier recorded
# in the setup.txt for the current run is:
Run # n+1

# Sets a unique identifier that is tagged in output. <n> is a
# floating point number (e.g. 1.1).
ID_NUMBER     <n>
```

```
    # Applies a Shapiro filter to selected tendencies.
    FILTERING    ADVECT  # 1st order Shapiro filter applied to
                         #  momentum advection tendencies.

    # Sets the model configuration to be V1562 with previous
    # versions of SHOC. Backwards incompatibility may be due to
    # bugfixes in the code, or implementation of improved numerics.
    # The backwards compatibility is currently defines as:
    COMPATIBLE  V1246  # Pre v1246: global boundary cells include
                       # R_EDGE and F_EDGE OUTSIDE cells.
                V1283  # Pre v1283: Numerous bugfixes for multiple
                       # windows are not included. Refer to Revision
                       # History Nov 16 2009, v1283-1331.
                V1562  # Pre v1562: swr added explicitly to the water
                       # column.
                V1598  # Pre v1598: wtop uses 2D detadt and low order
                       # approximations. U1 and u2 = 0 above the free
                       # surface for horizontal fluxes.
                V4201  # Run with 32 bit netCDF output (default is
                       # 64 bit).


    # Exclude certain points in the model domain from wave, tracer
    # statistic, sediment transport or biogeochemical computations.
    EXCLUDE_PROCESS_POINTS    <n>   # Number of points to exclude
    i1 j1  CODE1                    # i1 j1 are (i,j) locations of
    i2 j2  CODE2                    # the cell to exclude.
      .                             # CODE is a list of keywords:
      .                             # EX_WAVE to exclude waves
    in jn  CODEn                    # EX_TRST for tracer statistics
                                    # EX_SED for sediment transport
                                    # EX_BGC for biogeochemistry

    EXCLUDE_BGCSED                  # EX_SED & EX_BCG using blocks
      e.g.
EXCLUDE_BGCSED    3     # Set a series of rectangular regions to
(0,3)-(82,69)           # exclude BGC and sediments.
(184,3)-(248,69)
248 131

MOM_CONVERT  momgrid                # Convert the input file to a
                                    # MOM4 compatible grid_spec.nc
                                    # Output file is momgrid_spec.nc.


ROMS_CONVERT  romsgrid              # Convert the input file to a
                                    # ROMS compatible file. Output
                                    # file is romsgrid_roms.nc.
```

Physical constants

Values must be provided for a number of physical constants. Most are rarely changed far from the values shown below. An exception is the Coriolis parameter, which is latitude dependent.

```
# Acceleration due to gravity (m s-2)
G                       9.81

# Air density - note that it might be better to calculate this
# internally in the model code, based on the air temperature.
# For the moment, however, it is specified in the parameter file
# as a constant value (kg m-3).
AIRDENS                 1.225

# Specific heat of water. Again, the model could calculate this
# based on salinity, temperature, etc. For now, however, this
# is specified as a constant (J C-1 kg-1) - FIX - CHECK THIS
SPECHEAT                3990

# The Coriolis parameter value for the area of interest.
# This is an NCE1*NCE2 floating point array, so that it is
# possible to set a different value in every grid cell. However,
# for most applications where the grid geographical extent is not
# large, a uniform value can be used, as shown here, for a
# hypothetical 40*50.
# The CORIOLIS parameter will be automatically computed if not
# supplied, but the PROJECTION parameter is.
CORIOLIS          2000
-0.000019
```

4.5 Horizontal coordinate system

SHOC uses a sparse, or compressed, array configuration (Herzfeld, 2006) which represents a three dimensional region as a one dimensional vector in computer memory. One of the advantages of this approach is that all non-wet land cells may be omitted from the grid in memory. This means that when constructing a grid there is no computational penalty when large amounts of land are included in the grid. This approach requires, however, that **at least one land cell must be adjacent to wet cells at coastal boundaries** (i.e. a solid boundary is not allowed to be adjacent to a cell containing water; land cells only must be adjacent to wet cells).

A unique feature of **SHOC** is not only its ability to support a myriad of different horizontal grid geometries, but also its ability to handle different coordinate systems. Currently **SHOC** supports three coordinate systems:

- Arbitrary Cartesian
- Geographic - Latitude/Longitude
- Geographic - Map projected

The Cartesian system defines the coordinates on a rectangular plane with no physical association to real locations on the Earth. The geographic based coordinate systems however, map directly to real-world locations. For a Latitude/Longitude coordinate system all grid metrics are computed on the spheroid, while for the map projected coordinate system the metrics are computed on the projected plane.

The coordinate system is defined using the `PROJECTION` parameter and applies to ALL windows.

4.5.1 Defining a Cartesian coordinate system

An arbitrary Cartesian coordinate system can be specified by either leaving the `PROJECTION` blank, or by not specifying the parameter at all. Please note, it is assumed that the XY units are in metres, even though they have no real-world significance.

4.5.2 Defining a latitude/longitude coordinate system

The Latitude/Longitude coordinate system is specified as follows:

```
# The 'geographic' projections implies that all coordinates
# should be provided as decimal longitude and latitude.
PROJECTION geographic
```

Unfortunately at this time no mechanism is provided to specify the ellipsoid parameters, instead it is hard-coded as a sphere with a radius of 6370997.0m. It is hoped this restriction will be relaxed in a later version of **SHOC**.

4.5.3 Defining a map projected coordinate system

Of the three coordinate systems supported, defining the map projection is by far the most complicated, with a variety of map projections each with their own arguments.

The basic syntax is as follows:

```
PROJECTION proj=<projection-name> [<proj-param0>=<arg> […]]
```

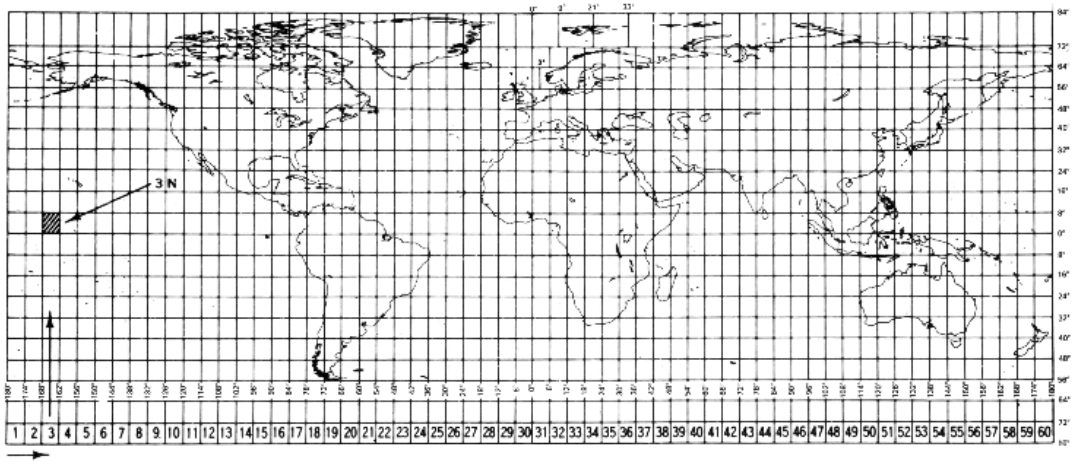
Standard projections
SHOC supports six standard projections. A description of each projection and their arguments are described below:

Transverse Mercator (Transverse Central Cylindrical)

The Transverse Mercator is a conformal cylindrical projection where the cylinder is rotated horizontally (transverse) across the ellipsoid.	
proj=tcc **lon_0**=<long> **k_0**=<number>	
lon_0	Central meridian.
k_0	Scale factor.

Universal Transverse Mercator (UTM)

The Universal Transverse Mercator (UTM) projection is based on the Transverse Mercator projection described above. However, the scale factor is fixed to 0.9996, and the central merdian is parameterised by zone. Each zone defines a 6 degree window in longitude around the Earth, making a total of 60 zones. Zone 1 is located at a 180W, with the zone number increasing in an easterly direction.



The default ellipsoid is clark66, and false eastings and northings are (500000E,10000000N) for the southern hemisphere and (500000E, 0N) for the northern hemisphere.

Defined by	**proj**=utm **zone**=<number> [**south**|**north**]	
	zone	UTM zone (1-60).
	south	Enabled if for southern hemisphere.
	north	Enabled if for northern hemisphere (default).

Australian Map Grid

A projection for the Australian region, based on the UTM projection, but using the gda66 ellipsoid.		
Defined by	**proj**=amg **zone**=<number>	
	zone	UTM zone (1-60).

Map Grid of Australia

A more recent projection for the Australian region, based on the UTM projection, but using the gda94 ellipsoid. This is the current Australian Standard Projection.		
Defined by	**proj**=mga **zone**=<number>	
	zone	UTM zone (1-60).

Lambert Conformal Conic

A conformal, conic projection, where parallels are unequally spaced arcs of concentric circles. Merdians are equally spaced radii of the same circles. The scale is true along two standard parallels. The default ellipsoid is wgs84, and false eastings and northings are (0E, 0N).		
Defined by	**proj**=lcc **lon_0**=< long> **lat_0**=<lat> **lat_1**=<lat> [**lat_2**=<lat>]	
	lon_0	Central meridian.
	lat_0	Central latitude.
	lat_1	First standard parallel latitude.
	lat_2	Second standard parallel latitude.

Mercator

The Mercator map projection is a cylindrical and conformal map projection, where the cylinder is aligned north/south. It has the properties that all meridians are equally spaced straight lines, parallels are unequally spaced (closer at the equator), and Rhumb lines are down as strait lines. The default ellipsoid is wgs84, and false eastings and northings are (0E, 0N).		
Defined by	**proj**=merc **lon_0**=<long>	
	lon_0	Central meridian.

Other projections

SHOC also supports a number of other projections if compiled and linked with the USGS PROJ 4 projection library. The list of projections supported by PROJ 4 are described below. For a full description of each projection and their arguments please consult the PROJ 4 manual (Evenden, 1995).

Projection	**Description**
aea	Albers Equal Area
aeqd	Azimuthal equidistant
alsk	Alaska Mod. Stereographic
apian	Apian Globular
bipc	Bipolar Conic
bonne	Bonne
cass	Cassini
cc	Central Cylindrical
cea	Cylindrical Equal Area
collg	Collignon
eck1	Eckert I
eck2	Eckert II
eck3	Eckert III
eck4	Eckert IV
eck5	Eckert V
eck6	Eckert VI
eqc	Equidistant Cylindrical
eqdc	Equidistant Conic
gall	Gall (Stereographic)
gnom	Gnomonic
gs50	50 State U.S. Mod. Stereographic
gs48	48 State U.S. Mod. Stereographic
hataea	Hatano Asymmetrical Equal Area
labrd	Laborde
laea	Lambert Azimuthal Equal Area
leac	Lambert Equal Area Conic
Projection	**Description**
lee_os	Lee Oblate Stereographics Pacific
loxim	Loximuthal
lsat	LANDSAT Space Oblique Mercator
mbtfpp	McBryde Thomas Flat Polar Parabolic
mbtfps	McBryde Thomas Flat Polar Sinusoidal
mbtfpq	McBryde Thomas Flat Polar Quartic
mill	Miller
mill_os	Miller Oblate Stereographics Euro-Africa
moll	Mollweides
nicol	Nicolosi Globular
nsper	General Vertical Persepective
nzmg	New Zealand Map Grid
ocea	Oblique Cylindrical Equal Area

omerc	Oblique Mercator
ortho	Orthographic
parab	Caster Parabolic
poly	Polyconic (American)
putp2	Putnins P2'
putp5	Putnins P5
quau	Quartic Authalic
robin	Robinson
sinu	Sinusoidal
stere	Stereographic
tcea	Transverse Cylindrical Equal Area
tpers	Tilted perspective
ups	Universal Polar Stereographic
vandg	Van der Grinten
wink1	Winkel I

Global parameters

In addition to the projection specific parameters, there are also a number of parameters supported by all projections.

Parameter	Description
ellps	Ellipsoid name (see Ellipsoid table below).
es	Eccentricity.
a	Major ellipsoid axis radius.
b	Minor ellipsoid axis radius.
rf	Reverse flattening.
x_0	False easting (automatically specified for the UTM projection).
y_0	False northing.

Ellipsoids

Supported ellipsoid include:

Ellipsoid	Parameters	Description
merit	a=6378137.0 rf=298.257	MERIT 1983.
grs80	a=6378137.0 rf=298.257222	GRS 1980 (IUGG, 1980).
iau76	a=6378140.0 rf=298.257	IAU 1976.
airy	a=6377563.396 b=6356256.910	Airy 1830.
mod_airy	a=6377340.189 b=6356036.143	Modified Airy.
aust_ntl	a=6378160.0 rf=298.25	Australian Natl, S. Amer., IAU 64.
grs67	a=6378160.0 rf=247.247167	GRS 67 (IUGG 1967).
bessel	a=6377397.155 rf=299.1528128	Bessel 1841.
bess_nam	a=6377483.865 rf=299.1528128	Bessel 1841 (Namibia).
clrk66	a=6378206.4 b=6356583.8	Clarke 1866.
clark66	a=6378206.4 b=6356583.8	Clarke 1866.
clrk80	a=6378249.145 rf=293.4663	Clarke 1880 mod.
everest	a=6377276.3452 b=6356075.4133	Everest 1830.
hough	a=6378270.0 b=6356794.343479	Hough.
intl	a=6378388.0 rf=297.	International 1909 (Hayford).
krass	a=6378245.0 rf=298.3	Krassovsky, 1942.
mercury	a=6378166.0 b=6356784.283666	Mercury 1960.
mod_ever	a=6377304.063 b=6356103.039	Modified Everest.
mod_merc	a=6378150.0 b=6356768.337303	Modified Merc 1968.
new_intl	a=6378157.5 b=6356772.2	New International 1967.
Seasia	a=6378155.0 b=6356773.3205	Southeast Asia.
walbeck	a=6376896.0 b=6355834.8467	Walbeck.
wgs66	a=6378145.0 b=6356759.769356	WGS 66.
wgs72	a=6378135.0 b=6356750.519915	WGS 72.
wgs84	a=6378137.0 rf=298.257223563	WGS 84.

Ellipsoid	Parameters	Description
agd66	a=6378160.0 rf=298.25	Same as aust_ntl.
agd84	a=6378160.0 rf=298.25	Same as aust_ntl.
gda94	a=6378137.0 rf=298.25722101	New Aust. ellip.
sphere	a=6370997.0 es=0.0	Sphere of 6370997 m.

An example definition of an AMG projection for Port Phillip Bay in Eastern Australia follows:

```
# Port Phillip Bay is located at Zone 55 of the UTM projection
PROJECTION proj=amg zone=55
```

4.6 Horizontal grid geometry

SHOC supports five orthogonal horizontal grid geometries - `rectangular`, `polar`, `geographic_rectangular`, `elliptic` and `numeric`. All internal grid metrics are stored in units of metres, although the coordinates maybe specified in either x/y or latitude/longitude units depending on how the `PROJECTION` parameter was specified.

All grid definitions share the following two parameters; `NCE1` and `NCE2`. `NEC1` and `NEC2` define the number of cells in the e1 (or i or x) and e2 (j or y) directions respectively.

4.6.1 Rectangular grid

Following is an example file fragment that describes all of the parameters required to define a rectangular grid:

```
# Type of grid
GRIDTYPE        RECTANGULAR

# Number of grid cells in the e1 (i) and e2 (j) directions
NCE1            57
NCE2            72

# Real-world coordinates of the lower left hand corner of
# the lower left-hand grid cell (i=0, j=0)
X00             257300
Y00             5770180

# Grid cell size in e1 (i) and e2 (j) directions
DX              1000
DY              1000

# Angle (in degrees) between e1 (i) direction and the real-world
# X axis (which is East in most reasonable projections).
# This represents a mathematical rotation, so that the value of
# 315 degrees would probably make the grid i axis run in a
# south-easterly direction.
ROTATION        315
```

The rectangular grid is defined as being 57 by 72 cells, with a 1000m resolution along both axes, rotated at 315 degrees, and an origin (the bottom left corner of cell (i = 0, j = 0)) at Easting 257300, Northing 5770180. If no `PROJECTION` parameter is specified, then it should the grid should only be used to model 'local' areas where the Earth's curvature is not

considered significant. This also true if a map projection is specified, but it's appropriateness depend on the region and projection.

4.6.2 Polar grid

Polar grids are specified is a similar way to rectangular grids, as shown below:

```
# Type of grid
GRIDTYPE  POLAR

# Number of cells in the e1, i, or azimuthal direction.
NCE1              5

# Number of cells in the e2, j, or radial direction.
NCE2              10

# Coordinates of polar origin
X00               250000
Y00               5770000

# Radial distance from origin to edge of first grid cell
# (metres).
R0                40

# Angle (in degrees) between e1=0 radial (i=0) direction and the
# real-world X axis (which is East in most reasonable
# projections).
# This represents a mathematical rotation (+ve anticlockwise).
ROTATION  20

# Angular extent of grid (degrees), running clockwise from the
# e1=0 (i=0) radial.
ARC               120
```

The above describes a polar grid with 5 by 10 cells, with a minimum radius of 40m and covering an angular range of 120°, from 110° to 230 ° with respect to true north. The grid polar origin is located at Easting 250000, Northing 5770000. The polar grids generated for the model have 'square' cells, in the sense that the size of any given cell is approximately equal in the azimuthal and radial directions. A brief analysis shows that this causes the cell size to increase exponentially in the radial direction (as j increases), so that the grid has higher resolution near the origin, and lower resolution further away. The origin itself cannot be part of the grid (ie, `R0` must be greater than zero), as the grid becomes singular at that point.

Like the rectangular grid, Polar grids are generally suitable for 'local' areas only, unless a Latitude/Longiutude `PROJECTION` is used.

4.6.3 Numerical grid

The numeric grid allows the specification of a general orthogonal curvilinear grid using the `XCOORDS` and `YCOORDS` parameters. The grid must include not only the cell corners, but also the position of the cell centre and the u1 and u2 positions. In effect the parameters define a grid twice the resolution of that being modelled. At this time there is no simple toolkit available for generating such grids, and grid generation is left to the reader.

4.6.4 Geographic rectangular grid

A Geographic rectangular differs from a normal rectangular grid, as it defines a grid that is orthogonal on a spheroid. A geographic rectangular grid can only be specified if the `PROJECTION` parameter is set to ‘geographic’.

SHOC supports three different ways of defining a geographic rectangular grid.

Auxiliary pole
The first method computes the grid metrics using an auxiliary coordinate system, defined by a false pole.

```
PROJECTION  geographic
GRIDTYPE    GEOGRAPHIC_RECTANGULAR
NCE1 10
NCE2 20
DLAMBDA 0.01      # Long. cell interval in aux. coords.
                  # (degrees)
DPHI 0.01         # Lat. cell interval in aux. coords.
                  # (degrees)
X00  144.3856     # Longitude of origin (degrees)
Y00  -38.2030     # Latitude of origin (degrees)
POLE_LONGITUDE 0  # Longitude of false pole (degrees).
POLE_LATITUDE  90 # Latitude of false pole (degrees).
```

Equally spaced grid in degrees
This is almost identical to the auxiliary pole definition, except that a rotation is used, instead on a false pole. The resulting cells are unequally spaced on the sphere, but equally spaced in degree space.

```
PROJECTION  geographic
GRIDTYPE    GEOGRAPHIC_RECTANGULAR
NCE1 10
NCE2 20
DLAMBDA 0.01      # Long. cell interval in aux. coords.
                  # (degrees)
DPHI 0.01         # Lat. cell interval in aux. coords.
                  # (degrees)
X00  144.3856     # Longitude of origin (degrees)
Y00  -38.2030     # Latitude of origin (degrees)
ROTATION 315      # Grid orientation.
```

Equally spaced grid over sphere
The third method requires that the grid cells preserve their distances over the sphere. The lat/long's of the grid are computed by projecting the interval (or multiple there of) along given a direction. This method does not always produce perfectly orthogonal grids, but the error is minimal.

```
PROJECTION  geographic
GRIDTYPE    GEOGRAPHIC_RECTANGULAR
NCE1 10
NCE2 20
DX   1000         # 1000m along i axis.
DY   1000         # 1000m along j axis.
ROTATION 315      # Grid orientation (degrees).
                  # This rotation is on the sphere.
X00  144.3856     # Longitude of origin (degrees)
Y00  -38.2030     # Latitude of origin (degrees)
FALSE_POLE YES    # Optional; if YES then a grid is constructed
                  # using a false pole where the equator lies
```

```
# through the grid's middle.
```

4.7 Vertical grid geometry

SHOC is a z or σ coordinate model. In the z coordinate system each layer height is the same across the whole grid domain. The layers are specified by giving the z-coordinate of their interfaces, relative to mean sea level. Because the model z-coordinate is positive up, with origin at mean sea level, this means that layer interface z-coordinates are usually negative (below the surface). For example, a model with 5 layers in the vertical, extending from 10m depth to the surface, and with uniform 2m vertical resolution, would be specified as follows:

```
# The z coordinates of the model layer interfaces.
LAYERFACES 6
-10.0
-8.0
-6.0
-4.0
-2.0
0.0
```

Layers need not all have the same thickness, but, for numerical reasons, care should be taken to avoid sudden large changes in layer thickness. The top layer need not be at mean sea-level. An example covering these points is shown below:

```
# A non-uniform vertical grid with 10 layers, covering from
# 15m depth to 5m above mean sea-level.
LAYERFACES 11
-15.0
-10.0
-6.0
-3.0
-1.0
 0.0
 1.0
 2.0
 3.0
 4.0
 5.0
```

The model includes drying and wetting algorithms, and the simulated water surface in the model is free to move up and down through the layers. The uppermost layer automatically grows thicker as required, to incorporate increases in surface elevation, up to some maximum height, specified as follows:

```
# Maximum allowable z-coordinate for water surface elevation.
# If the water surface ever exceeds this value, the model
# run stops and produces an error message.
#
# This value is also used by the grid generation program
# to decide whether the top layer is land or not (land if
# bathymetry above ETAMAX)
ETAMAX            10.0
```

The σ coordinate system scales the layer interfaces to the total water depth. This allows the bottom to be well resolved at any depth. If the sigma option is invoked (see section 4.25) then the σ levels are generated by **SHOC** such that a logarithmic distribution exists at the surface and bottom and a linear distribution in the interior. The user need only specify the number of layers to be used in this case.

```
# The number of σ coordinates for the model layer interfaces.
    LAYERFACES 6
```

NOTE: The vertical grid geometry described above is not used by the model when a run is initiated using the -p option. Layers are defined when the -g option is invoked (see section 8) to generate the model input netCDF file, which contains model initial values and geometric information. Any alteration to model vertical grid geometry must be accompanied by the creation of a new model input netCDF file, using the -g option.

4.8 Bathymetry

When a run is initiated using and existing parameter file and input netCDF file (i.e. using the -p option) the bathymetry used is read from the netCDF file. Any bathymetry data, and bathymetry manipulation options (e.g. bathymetry limits, smoothing etc.) present in the parameter file are ignored. This is because data for all the model variables read from the netCDF file is assumed to correspond to a particular layer configuration over a particular depth range, and changing the layer structure or bathymetry range will result in discrepancies between the data read from file and the assumed model geometry.
Using the -a or -g option (see section 5 and 8) the bathymetry of the area to be modelled is specified by providing a depth value for each horizontal grid cell. Thus, there are NCE1 * NCE2 bathymetry values (for each grid). They are specified as an array parameter, as follows.

```
# Example depth values for a 3 by 4 grid
BATHY 12
22.2
12.3
7.4
23.5
12.0
6.0
25.8
13.7
5.8
27.6
14.2
4.9
```

The values run in order from the bottom left corner of the grid (i=0, j=0), with i varying fastest. This means that for a single column bathymetry list (as in the above example) any cell (i,j) is located at position j x NCE1 + i + 1 in the list. Note that the values are depths, rather than z-coordinate values, and hence are usually positive. **Beware, as this can easily cause confusion**. Negative values are also allowed, and signify that the sea-bed is above mean sea-level. Where the sea-bed is above ETAMAX (see above), the cell is taken to be a land cell. Values which are deeper than the deepest model layer (see section 4.7) signify that the corresponding grid cell is outside the domain of computation of the model (denoted OUTSIDE cells). This mechanism allows open boundaries to be located at arbitrary positions within the grid.

Here is the above example again, but this time the right hand column of the model is land, and the top left cell is outside the computational domain:

```
# Example depth values for a 3 by 4 grid
BATHY 12
22.2
12.3
-99
23.5
12.0
```

```
-99
25.8
13.7
-99
9999
14.2
-99
```

For convenience, some parameters are provided which allow the specification of minimum and maximum depth values, as follows:

```
# All cells will be at least 20m deep
BATHYMIN          20

# No cell will be more than 2000m deep
BATHYMAX          2000
```

The BATHYMIN and BATHYMAX parameters are optional. If present, they override values in the BATHY array where necessary.

The bathymetry can be smoothed using a 9 point low pass convolution filter if required. This may be done several times by invoking:

```
#n is the number of smoothing passes performed
SMOOTHING   n       #
```

Alternatively, a maximum gradient threshold may be supplied, and if the local bathymetry gradient becomes greater than this threshold then the bathymetry is locally smoothed until the gradient becomes less than the threshold. This is accomplished by invoking:

```
# x is the gradient threshold, typically 0.07
MAXGRAD     x
```

Bathymetry smoothing may be performed over a discrete number of cells (with n smoothing passes) using:

```
SMOOTH_MASK       m     # m is the number of cells to smooth
1 1                     # List of (i,j) cell locations
2 1
```

Note that depth values need not correspond to layer interface positions. In each cell, the model implements a bottom layer which has a thickness which may be less than the full layer thickness, so that bathymetry is well resolved even in vertically coarse or single-layer (depth-averaged) grids. However, very thin bottom layers can cause numerical problems, so one final parameter prevents the creation of very thin layers, as follows:

```
# If the difference between a layer boundary and the bathymetry
# for a cell is too small, numerically instabilities can arise
# in the model. Specifying a minimum cell thickness ensures that
# no cell can get too thin.
# The value may be specified as a minimum thickness (in metres)
# or as a minimum percentage of the grid layer thickness, as
# shown below.
MIN_CELL_THICKNESS 15%
```

A sub-section of the bathymetry may be masked to a user defined value using the BATHY_MASK attribute. This consists of a list of (i,j) values whose bathymetry value in the grid is set to the value of BATHY_MASK_VAL, e.g;

```
# Set the bathymetry at points (1,1) and (2,1) equal to 5.0m.
```

```
BATHY_MASK_VAL   5.0     # Value to set bathymetry to.
BATHY_MASK       2       # Number of points in the list.
1 1
2 1
```

or

```
BATHY_MASK_VAL   5.0     # Value to set bathymetry to.
BATHY_MASK       1       # Number of blocksin the list.
(1,1)-(2,1)
```

The points list may be obtained using the 'Marked' facility in `jvismeco`. A linear gradient of bathymetry may also be applied to the masked sub-region in either the e1 or e2 direction (i or j direction) , e.g. to apply a linear bottom slope in the e1 direction from 5m to 10m:

```
# Set a linear bottom slope from 2m to 10m in the e1 direction
# from i=1 to i = 4. Any points in the list with i coordinates
# between the start and end coordinates are set to a linear
# interpolation of the start and end depths.
BATHY_MASK_IS    1    # Start i coordinate for gradient
BATHY_MASK_IE    4    # End i coordinate for gradient
BATHY_MASK_DS    2.0  # Depth at start i coordinate
BATHY_MASK_DE    10.0 # Depth at end i coordinate
BATHY_MASK       40   # Number of points in the list
```

Similarly this applies to `BATHY_MASK_JS` and `BATHY_MASK_JE` for the e2 direction.

Multiple blocks may be specified where a single bathymetry value only may be altered (i.e. no gradients of bathymetry) using:

```
BATHY_NBLOCKS     2       # Number of blocks
BATHY_MASK_VAL0   5.0     # Block 0 bathymetry value
BATHY_MASK0       1       # Block 0 blocks.
(1,1)-(2,1)
BATHY_MASK_VAL1   2.0     # Block 1 bathymetry value
BATHY_MASK1       2       # Block 1 blocks.
(10,1)-(20,10)
(50,1)-(50,20)
```

NOTE: The bathymetric parameters described above are not used by the model when a run is initiated using the `-p` option. They are used when the -g option is invoked (see section 8) to generate the model input netCDF file, which contains model initial values and geometric information. Any alteration to model bathymetry must be accompanied by the creation of a new model input netCDF file, using the `-g` option.

Cells can be changed to `OUTSIDE` or `LAND` status at runtime as a series of rectangular blocks e.g;

```
NOUTSIDE    3     # Set a series of rectangular regions to
(0,3)-(82,69)     # OUTSIDE.
(184,3)-(248,69)
(0,70)-(248,131)
```

Or

```
NLAND 4           # Set a list of points to LAND.
0 1
0 2
0 3
0 4
```

Bathymetry statistics can be generated using:

```
BATHY_STATS        <infile> e1i e2i
```

Here <infile> is a path and filename of a bathymetry database and e1i and e2i are decimations in the e1 and e2 directions respectively. Bathymetry statistics are generated by comparing the database bathymetry at its native resolution (with the decimation applied) with the interpolated bathymetry in a model grid. Statistics generated are:

- Maximum depth between the shallowest database depth in a grid cell and the model grid cell depth, stored in bathy_range_min,
- Maximum depth between the deepest database depth in a grid cell and the model grid cell depth, stored in bathy_range_max,
- The gradient of the model grid cell; $\sqrt{\left(\frac{\partial D}{\partial e_1}\right)^2 + \left(\frac{\partial D}{\partial e_2}\right)^2}$, stored in bathy_grad,
- The maximum gradient difference between the database gradient and the gradient in the grid cell, where the gradient is defined above, stored in bathy_grad_max.

4.9 Tracers (salinity, temperature, and others)

The model may include salinity and temperature as dynamic tracers which affect the density field via an equation of state. As well, some of the more complex vertical mixing schemes may use variables (like turbulent kinetic energy) which also essentially act as tracers as far as most of the model code is concerned. Finally, the model can include an arbitrary number of passive tracers, which are advected and diffused in the model grid, but which play no dynamic role.

The set of tracers included and their physical behaviour are defined as shown in the example below. The number of tracers included is specified using the parameter NTRACERS, and attributes for each tracer are prefixed by TRACER<M>, where <M> corresponds to the tracer number (starting at zero).

Tracers can be defined to exist in the water column (3D tracers), the benthos (2D tracers; these tracers may also represent vertically integrated 3D tracers or values at the air-water or water-sediment interfaces) or in the sediment (3D sediment tracers).

The following example shows the specification of three tracers - salinity, temperature and a passive dissolved contaminant. Detailed comments are provided for the salinity tracer.

```
NTRACERS 3                # Three tracers in this grid

# The following tracer attributes are mandatory, and must
# be present for each tracer
#
# Tracer name (must be 'salt' for dynamic salinity variable)
TRACER0.name salt

# A more descriptive name.
TRACER0.long_name Salinity

# Units string
TRACER0.units PSU         # Standard units


# Fill value for use with the –g option if no data is present
# (see below).
TRACER0.fill_value 35.0
```

```
# Range (minimum and maximum) of valid values
TRACER0.valid_range 0 40

#
# The following tracer attributes are optional
#
# The type of tracer. Options are WATER, WC3D or WC for 3D water
# column tracers, BENTHIC, INTER or WC2D for 2D tracers and
# SEDIMENT or SED for sediment tracers. Tracers are assumed to be
# 3D water column tracers by default.
TRACER0.type  WATER

# Allow the tracer to be advected (default is 1, or TRUE)
TRACER0.advect 1

# Allow the tracer to be diffused (default is 1, or TRUE)
TRACER0.diffuse 1

# Decay constant in seconds (default is 0.0, meaning no decay).
# This may also be the name of a tracer; in this case the values
# of that tracer (with units of that tracer; seconds, minutes,
# hours, days) will be used as the decay rate. This allows for
# spatially and temporally varying decay rates. Negative decay
# is equivalent to growth.
TRACER0.decay 0.0

# Settling velocity if required (m/s, -ve down) (default is 0.0)
TRACER0.svel 0.0
```

The `.data` attribute allows the specification of initial values for each tracer. This is of use when the initial values vary in space, or are obtained from observations.

```
# Data to initialize the tracer
TRACER0.data     <data_field>
```

The tracer data field, `<data_field>`, may be one of the following:

- The size of the grid, `nce1` x `nce2` x `nz` , followed by an array of values of size `nce1` x `nce2` x `nz`, listed in that order,
- a netCDF file on a regular grid, in which case the values will be bilinearly interpolated,
- a netCDF file on an irregular grid, in which case interpolation is performed using an inverse distance weighting scheme,
- an ascii file in column format with spatial information only (i.e. no time field, `lon` and `lat` must be present). In this case the tracer values are interpolated linearly by default, or as specified in the `.interp_type` field. This is useful for interpolating sparsely collected measurements onto the grid.

```
# Interpolation method for ascii data input
TRACER0.interp_type     cubic  # valid options are cubic, linear,
                               # average, nn_sibson or
                               # nn_non_sibson, where nn
                               # refers to Natural Neighbours.
```

- Tracers may be scaled to a normalized density profile that exists through the water column (i.e. at the deepest point in the domain). This ensures that the gradient of the tracer profile is some constant multiple of the density gradient, and therefore ensures that mixed layer depths are consistent between the tracer and density. This is invoked using:

  ```
  TRACER0.data      dens_scale file.nc v1 v2 <code>
  ```

  Where `v1` is the depth at which the tracer value is equal to that in `file.nc` at the same depth and `v2` is a scaling factor for the profile (if `v2` < 0 the profile is inverted).

Below depth v1 the profile in any layer k is determined by adding v2 x (density gradient) to the concentration in the layer k+1. This is iteratively computed down through the water column. Above depth v1 the profile in any layer k is determined by subtracting v2 x (density gradient) to the concentration in the layer k-1. This is iteratively computed up through the water column. If <code> = c then a copy of the values in file.nc is used for the profile below depth v1, and if <code> = t then the profile values are truncated to those in file.nc below the depth v1 if the profile values become greater than those in file.nc.
This formulation is the most general for density scaling and is supported by an equivalent scaling at open boundaries (see Section 4.10.18) – other methods may be used that are not supported by equivalent open boundary methods.

```
TRACER0.data      dens_scale v1 v2
```

Here, if v2 > 0 then v1 is the surface tracer concentration, and the profile in any layer k is determined by adding v2 x (density gradient) to the concentration in the layer k+1. This is iteratively computed down through the water column. If v2 < 0 then v1 is the bottom tracer concentration, and the profile in any layer k is determined by subtracting v2 x (density gradient) to the concentration in the layer k-1. This is iteratively computed up through the water column. A file (netCDF or ascii time series) may be used as the surface or bottom value in preference to v1, in this case use;

```
TRACER0.data      dens_scale file.nc v2
```

The tracer profile may be the inverse of the density profile if the following is specified:

```
TRACER0.data      dens_scale v1 v2 n
TRACER0.data      dens_scale file.nc v2 n
or
TRACER0.data      dens_scale v1 v2 inverse
TRACER0.data      dens_scale file.nc v2 inverse
```

- An alternative density scaling is possible where the normalized density profile is stretched between a surface value of v1 and bottom value of v2. This is invoked using:

```
TRACER0.data      dens_profile v1 v2
```

- Tracer values may be specified in regions using:

```
TRACER0.data      region region.bnc r1:v1 r2:v2  .... rn:vn
```

Where region.bnc is a region file (see Section 4.29.16). The vales in specified regions r1, r2 .... rn are then assigned the values v1, v2 .... vn respectively.

Tracer specification examples are:

```
# Temperature tracer - only mandatory attributes given here. The
# rest will assume their default values.
TRACER1.name temp
TRACER1.long_name Temperature
TRACER1.units degrees C
TRACER1.fill_value 20.0
TRACER1.valid_range 0 40


# Passive, dissolved contaminant tracer; specifying an
```

```
# initial distribution from a netCDF time-series file called
# profile.nc.  Note that the fill_value attribute must still
# be present (but isn't used).
TRACER2.name contam
TRACER2.long_name Contaminant
TRACER2.units kg m-3
TRACER2.fill_value 0.0
TRACER2.valid_range 0 2
TRACER2.data profile.nc
```

Note that the valid range attribute is a recommendation only and **SHOC** takes no action other than supplying a warning if these bounds are violated. The exception is, however, if the minimum range is zero and the model begins to produce negative results. In this case the tracer value is clipped to zero in **SHOC** to ensure positive-definiteness.

4.9.1 Tracer initialisation

When a run is initiated, the initial distribution for each tracer are read from the `INPUT_FILE`. This file may be generated using the `-g` option or be an output file from a previous run. If the `-g` option was used, then the `INPUT_FILE` will contain tracer distributions that reflect either the `.fill_value` or `.data` specified for that tracer (see above). However, if a run is initiated which has tracers in the tracer list that do not have corresponding distributions in the `INPUT_FILE` (i.e. new tracers are added) then the initial distributions for those tracers will be specified using any `.data` specified, or if this is absent then the `.fill_value`. Additionally, a netCDF file may be specified using;

```
# Specify a netCDF file to initialise any new tracers
TRACER_DATA       <data_file>
```

In this case, if the `.data` attribute is absent for any new tracers, SHOC will search the file `<data_file>` for the new tracer, and if found interpolate the initial tracer distribution from that in the file. This is done for 3D, 2D and sediment tracers.

4.9.2 Relaxation

Tracer values throughout the model domain can be relaxed towards some specified values (which may themselves vary in space and time). To enable relaxation for a particular tracer, three parameters are required: the relaxation data file (an ASCII or netCDF time-series file – see section 10), how often to perform the relaxation, and the relaxation time constant.

```
# Data file containing prescribed tracer values
TRACER0.relaxation_file         saltprof.nc

# How often to perform relaxation calculation
TRACER0.relaxation_input_dt     1 hour

# Relaxation time constant
TRACER0.relaxation_time_constant 20 days
```

Tracer relaxation may also be specified via a streamlined notation:

```
relax_trname      infile.nc dt.ts in units
```

where `trname` is the name of tracer, `infile.nc` is the file containing values to relax to, and `in units` is the `input_dt`; e.g. to relax salt to `saltprof.nc` with file input of 1 hour and relaxation constant set in `dt.ts`, then specify;

```
relax_salt  saltprof.nc dt.ts 1 hour
```

This specification is particularly useful with the automated `-a` or `-r` options, but will only operate if the relaxation time constant is input via file.

The relaxation_time_constant may be time dependent by specifying a netCDF or ascii filename. In this case the units for the time constant in the file must be a time unit, e.g.

```
# Ascii relaxation file where relaxation is 48 hours at day 0 and 2
# hours at day 10. Note 'Time' is converted to the model units
# specified by TIMEUNIT.
## COLUMNS  2
##
## COLUMN1.name               Time
## COLUMN1.long_name          Time
## COLUMN1.units              days since 1990-01-01 00:00:00 +8
## COLUMN1.missing_value      -999
## COLUMN1.fill_value         0.0
##
## COLUMN2.name               relaxation_time_constant
## COLUMN2.long_name          Relaxation time constant
## COLUMN2.units              hours
## COLUMN2.missing_value      -999
## COLUMN2.fill_value         0.0
##
0  48
10 2
```

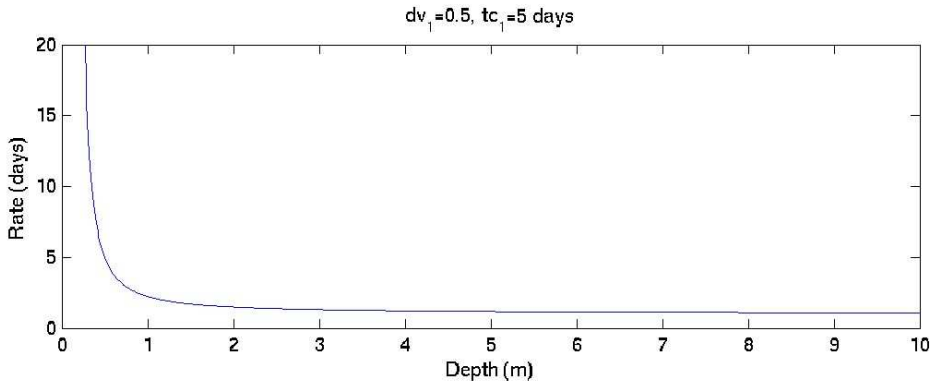
Adaptive relaxation can be invoked by specifying:

`TRACER0.relaxation_time_constant linear` dv_1 tc_1 $units_1$ dv_2 tc_2 $units_2$

In this case if the absolute difference between modelled tracer and that read from `infile.nc` is dv_1, then a relaxation constant of tc_1 $units_1$ is used and if the absolute difference is dv_2, then a relaxation constant of tc_2 $units_2$ is used, with linear interpolation for other values of the absolute difference. The relaxation constant will therefore vary spatially and temporally throughout the domain and simulation. For exponential relaxation:

`TRACER0.relaxation_time_constant exponential` dv_1 tc_1 $units_1$

In this case the relaxation constant is given by: $rate = \left[\exp(dv_1 \log(tc_1)/d)\right]^{-1}$ where d is the absolute difference in modelled tracer and that read from `infile.nc`, e.g. for dv_1 = 0.5 and tc_1 = 5 day;



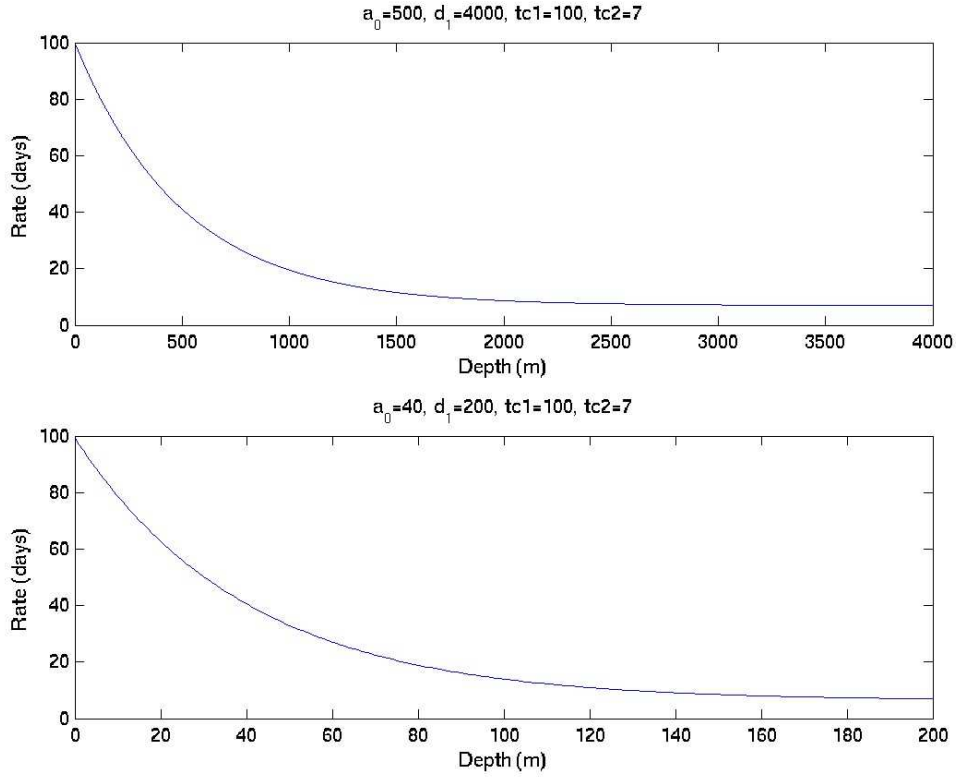
A depth scaled linear relaxation may be specified using:

`TRACER0.relaxation_time_constant depth` dv_1 tc_1 $units_1$ dv_2 tc_2 $units_2$

In this case if the depth is dv_1, then a relaxation constant of tc_1 $units_1$ is used and if the depth is dv_2, then a relaxation constant of tc_2 $units_2$ is used, with linear interpolation for other values of the depth. The relaxation constant will therefore vary spatially throughout the domain and simulation. Depths are truncated to the limits of dv_1 and dv_2. Note that all depths should be negative (i.e. dv_1 and $dv_2 < 0.0$).
An exponential depth dependent rate may be specified using:

`TRACER0.relaxation_time_constant exp_depth` a_0 tc_1 $units_1$ d_1 tc_2 $units_2$

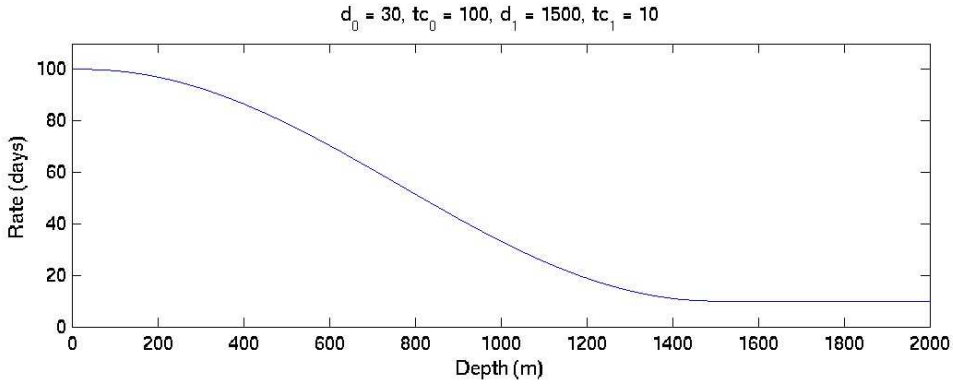
The relaxation rate is given by $rate = (\mathrm{tc}_2 - tc_1)\exp(-depth/a_0) + (tc_2 - tc)$ where $tc = tc_1 \exp(-d_1/a_0)$. Examples for different depths d_1 are shown below.



An cosine depth dependent rate may be specified using:

`TRACER0.relaxation_time_constant cos_depth` d_0 tc_1 $units_1$ d_1 tc_2 $units_2$

The relaxation rate is given by $rate = 0.5 * (tc_1 - tc_2)\cos(depth.PI/(d_1 - d_0) - d_1.PI/(d_1 - d_0)) + (tc_1 + tc_2)$. This formulation assumes $d_1 > d_2$. An example is shown below.



Relaxation rate linear in time may be specified using:

`TRACER0.relaxation_time_constant temporal` dv_1 tc_1 $units_1$ dv_2 tc_2 $units_2$

In this case the relaxation rate is tc_1 $units_1$ at dv_1 days (relative to the `TIMEUNIT`), changing linearly to tc_2 $units_2$ at dv_2 days, then thereafter capped at tc_2 $units_2$.

4.9.3 Resetting

Tracer values throughout the model domain can be reset to some specified distribution (which may vary in space and time). To enable resetting for a particular tracer, two parameters are required: the reset data file (an ASCII or netCDF time-series file – see section 10) and how often to perform the reset. Using this option allows the user to effectively force the model with supplied distributions of tracer.

```
# Data file containing prescribed tracer values
TRACER0.reset_file  saltprof.nc

# How often to reset the tracer
TRACER0.reset_dt    1 hour
```

4.9.4 Tracer Increments for State Variables

The value of a tracer subject to resetting may be added to a state variable. This procedure is an easy way to update state variables if the reset file is created from a data assimilation process offline. The state variable the tracer is added to is specified via:

```
# Add the tracer values to temperature
TRACER0.increment   TEMP
```

Valid values for state variable increments are:

```
TEMP        # 3D tracer value added to temperature
SALT        # 3D tracer value added to salinity
ETA         # 2D tracer value added to surface elevation
```

4.9.5 Scaling

The initial conditions specified for any tracer may be scaled by another tracer's values. This is useful for easily manipulating input data without creating a new initialisation files, for example when scaling is required to convert to the correct units for tracer input. The scaling may either be additive of multiplicative. To scale a given tracer, e.g. `tracer1.name = temp`, the scaling tracer, e.g. `tracer2`, must be set up and initialised, e.g;

```
TRACER2.name        scale
TRACER2.long_name   Scaling tracer
TRACER2.units       degrees C
TRACER2.scale_s     temp  # Add tracer2 values to tracer temp
TRACER2.fill_value  20.0
TRACER2.valid_range 0 40
TRACER2.advect      0
TRACER2.diffuse     0
TRACER2.diagn       0
TRACER2.data        scale_profile.nc # Initialisation for tracer2
```

In this case the tracer named '`temp`' is scaled additively by the data contained in the file `scale_profile.nc`. If the tracer were to be scaled multiplicatively, then use:

```
TRACER2.scale_p    temp  # Multiply tracer temp by tracer2 values
```

Alternatively, within the tracer attributes for the tracer desired to be scaled (e.g. `temp` in this case), the following attributes may be set:

```
TRACER1.name  temp
# Additively scale tracer 'temp' by the values in tracer 'scale'
TRACER1.tag   scale_s:scale

# Multiplicatively scale tracer 'temp' by the values of 'scale'
TRACER1.tag   scale_p:scale

# Additively scale tracer 'temp' by a constant (2 in this case)
TRACER1.tag   scale_s:2.0

# Multiplicatively scale tracer 'temp' by a constant (0.01)
TRACER1.tag   scale_p:0.01
```

Tracer scaling is invoked upon initialisation, and if any tracers are `reset` (Section 4.9.3).

A tracer scaling file may be generated from time series files of moored instrument data, or from profile measurements. To invoke this option set the `create_scale` attribute to a scaling map file, the format of which is described below, e.g:

```
TRACER2.create_scale      moor_temp.map
```

With the file `moor_temp.map` with the format:

```
VAR_NAME    temp              # name of the variable to scale
VAR_UNITS   Degrees_C         # Units of the variable
OUT_NAME    scale_temp_s      # Name of the scaling variable as
                              # it will appear in the output
                              # file.
OUT_FILE    scale_profile.nc  # Output file name.
FORCING     profile.nc        # The initialisation file for the
                              # variable VAR_NAME that requires
                              # scaling. May be a  multifile.
REF_VALUE   1                 # Optional reference value.
```

```
REF_DEPTH   -100              # Optional reference depth (m).
BOT_VALUE   temp_init.nc      # Optional bottom value.
nfiles      2
file0       moor1.ts 147.34 -43.05 -15.0 temp
file1       prof1.nc 147.34 -43.05 profile temp
```

In the above example it is assumed that there exist files `profile.nc`, `moor1.ts` and `prof1.nc` that contain the variable `temp` with units `Degrees_C`. The file `profile.nc` is the initialisation file for the variable `temp` used in the model, and this file is known to contain errors which are required to be corrected by scaling to measured data contained in data files `moor1.ts` and `prof1.nc` The geographic (longitude and latitude) locations and depth (depth < 0) for each mooring file are supplied (e.g. `file0`). Alternatively a profile at a geographic location may be used; in this case use `profile` instead of a numeric depth value (e.g. `file1`). The variable name used in the each mooring or profile file must also be supplied. Mooring files generally contain the variable as a function of time (`.ts` files), and profile files contain the variable at a specific time as a function of depth at a fixed geographic location (`.nc` files). The scaling routine will compute the difference between the measured data and the `FORCING` data, and store this as a spatially and temporally varying netCDF file, `OUT_FILE` (i.e. the sum of `OUT_FILE` and `FORCING` will equal the measured data). The scaling function is spatially interpolated over the model grid. Only an additive scaling function is available (i.e. product scaling is not supported). Additionally, an ascii file `OUT_NAME.ts` containing the raw data (`TIME`, `file#`, observed data `FORCING` data) is produced. This is useful for creating scatter plots of the observed vs `FORCING` data.

Additionally, the bottom value may be explicitly set to a particular value (temperature in this example) using the optional `BOT_VALUE`. This may be a number or a filename, whose value(s) are used in preference to those contained in the measured data files (`moor1.ts` and `prof1.nc`) at the sea bottom. For example, if the `BOT_VALUE` were the same data as used for the `FORCING` (i.e. `profile.nc`) then this would ensure that the scaling function would equal zero at the bottom. The scaling code actually adopts this approach by default for all depths greater than the deepest mooring at a particular geographic location.

The optional `REF_VALUE` and `REF_DEPTH` operate in a similar manner to the `BOT_VALUE`, except a particular value (temperature in this example) can be prescribed at the depth `REF_DEPTH` rather that at the bottom. In the absence of a `BOT_VALUE`, all values below the `REF_DEPTH` are set to the `REF_VALUE` in preference to those contained in the measured data files (`moor1.ts` and `prof1.nc`). The reference and bottom options are useful for prescribing the scaling function below depths where no measured data is available but the user has insight into what values are expected at those depths.

The scaling tracer may be initialised with the `OUT_FILE` created using the `create_scale` option, and if this file is also used as a `reset_file` then the scaling tracer may be used to scale the open boundary forcing in a time dependent manner (Section 4.11.18).

4.9.6 Surface fluxes

A 3D tracer defined in the tracer list may have a surface flux prescribed that acts as the upper boundary condition in the vertical diffusion equation (see Section 2.5, Science Manual). This implies that the tracer is allowed to be vertically diffused The flux tracer is introduced by specifying the name of a valid 2D tracer in the tracer list as follows (e.g. for tracer `passive`);

```
TRACER2.name        passive
TRACER2.long_name   Passive tracer
TRACER2.units       gm-3
TRACER2.fill_value  0.0
```

```
TRACER2.valid_range 0 100
TRACER2.advect      1
TRACER2.diffuse     1
TRACER2.diagn       0
TRACER2.tag         surf_flux:flux
```

This implies a 2D tracer flux must exist, which may vary in space and time using the reset function. The tracer may also be scaled to achieve the correct units:

```
TRACER3.name        flux
TRACER3.long_name   Surface flux
TRACER3.units       kgs-1
TRACER3.type        WC2D
TRACER3.fill_value  0.0
TRACER3.valid_range 0 100
TRACER3.advect      0
TRACER3.diffuse     0
TRACER3.diagn       0
TRACER3.tag         scale_p:0.001
TRACER3.data        flux_data.nc
TRACER3.reset_file  flux_data.nc
TRACER3.reset_dt    1 day
```

Note that a positive flux implies a flux out of the surface layer.

4.9.7 Tracer types

The following flags are currently supported by the `TRACER.type` flag:

```
WATER            The tracer is a 3D water column tracer
SEDIM            The tracer is a 3D sediment tracer
INTER            The tracer is a 2D tracer
HYDRO            The tracer is a hydrodynamic tracer
SEDIMENT         The tracer is a sediment transport tracer
ECOLOGY          The tracer is a biogeochemical tracer
WAVE             The tracer is a wave tracer
TRACERSTAT       The tracer is a tracer statistic tracer
PROGNOSTIC       The tracer is prognostic
DIAGNOSTIC       The tracer is diagnostic
PARAMETER        The tracer represents a parameter
FORCING          The tracer contains forcing data
```

These flags may be assigned to tracers explicitly in the parameter file, e.g;

```
TRACER1.type      WATER HYDRO PROGNOSTIC
```

The above defines a tracer as a 3D hydrodynamic prognostic tracer. For auto-tracers, these flags are set internally. The `type` flag may be interrogated within the code for various purposes. The list may also be expanded as required.

4.9.8 Tracer filling and filtering

It is common that coastlines and bathymetries do not align when interpolating tracers onto a grid from an external file. Sometimes the limits of the grid that are to be interpolated onto lie outside the geographic bounds of the file from which the data is interpolated. There exist data filling options to set no-gradient conditions over cells whose geographic location is outside the

bounds, or over cells that are associated with land, in the file from which data is interpolated. This can be done for 2D (including elevation), 3D or sediment tracers, and is invoked using:

```
TRACER_FILTER FILL    # Fill all tracers with a no-gradient
              FILL2D  # Fill only 2D tracers with a no gradient
              FILL3D  # Fill only 3D tracers with a no gradient
              FILLSED # Fill only sediment tracers with a no gradient
              SMOOTH  # Apply 9 point smoothing filter to filled data
              SHAPIRO # Apply Shapiro filter to filled data
              SHUMAN  # Apply Shuman filter to filled data
              MEDIAN  # Apply median filter to filled data
```

These keywords can be combined sequentially, e.g;

```
TRACER_FILTER FILL2D FILL3D SMOOTH SHUMAN MEDIAN
```

4.10 Open boundaries

Each open boundary (if there are any) is specified as a list of horizontal grid cell locations, together with parameters which define the nature and behaviour of the boundary. The cells in a single open boundary do not necessarily need to be adjacent to one another, but it is usually desirable to group boundary cells that are physically or logically related. For each open boundary it is usually necessary to define data files from which the boundary values (surface elevations, velocities or tracer concentrations) may be read. Constant values, or custom routines returning boundary values may also optionally be specified.

Open boundaries may be defined anywhere in the grid, however, if a boundary is defined in the domain interior (as opposed to the limits of the domain) then the boundary must lie adjacent to an 'OUTSIDE' cell.

Open boundaries require that velocities normal and tangential to the open boundary, elevation and tracer concentrations are specified. Velocities are specified at the outer edge(s) of open boundary cells while elevation and tracers are specified at the cell centers. This formulation allows for a suite of BULK open boundary conditions to be implemented (radiation, extrapolation, relaxation conditions) and facilitates the implementation of higher order advection schemes. These open boundaries are generally called velocity boundaries below. More specifically, they are called u1 boundaries if the left or right hand edge of the cell is open, or u2 boundaries if the back or front edge of the cell is open.

The orientation of the u1 or u2 velocity boundaries must be known so that the normal and tangential velocity components may be identified in the **SHOC** code. Flagging a boundary as u1 or u2 requires the user to make this decision. Alternatively, a boundary may be classified as a velocity boundary in which case **SHOC** will decompose the boundary cell into u1 and u2 boundaries on left, right, front or back faces. The cell location provided in the POINTS list for u1 and u2 boundaries corresponds to the cell face. This means that the cell locations of u1 boundaries on right faces and u2 boundaries on front faces are incremented by one, in the x and y directions respectively, from the interior cell center adjacent to the boundary. If the boundary is specified as a velocity boundary, then the boundary cell location corresponds to the cell center.

When specifying open boundaries in the parameter file, it is first necessary to indicate how many open boundaries the model grid has:

```
# This grid has 3 open boundaries
NBOUNDARIES 3
```

Then, each boundary is described by a number of parameters of the form BOUNDARY<M>.XXXX, where <M> is the boundary index. The parameters specify the boundary type, name, boundary condition type used, cell indices, and forcing data. Specification of a u1 boundary is shown below.

```
BOUNDARY0.TYPE            u1
BOUNDARY0.NAME            Offshore boundary
BOUNDARY0.DATA            offshore.nc
BOUNDARY0.BCOND_NOR       NOGRAD
BOUNDARY0.BCOND_TAN       CLAMPD
BOUNDARY0.BCOND_ELE       FILEIN
BOUNDARY0.BCOND_TRA_ALL   UPSTRM
BOUNDARY0.POINTS          3
4 7
4 8
4 9
```

Alternatively, if the BOUNDARY.POINTS are contiguous (e.g. not interrupted by land) then the BOUNDARY.RANGE specification may be used, e.g;

```
BOUNDARY0.RANGE    (4,7)-(4,9)
```

Generally this specification takes the form;

```
BOUNDARY0.RANGE    (is,js)-(ie,je)
```

where is and js are the start (i,j) coordinates and ie and je are the end (i,j) coordinates. Note that is=ie for u1 boundaries, and js=je for u2 boundaries. No white space is to be inserted in the syntax for this specification.
A specified zone of wet cells may be changed to OUTSIDE cells by specifying:

```
BOUNDARY0.OUTSIDE_ZONE  n      ! Set n wet cells into the
                               ! interior as OUTSIDE.
```

This must be performed using the both the -g and -p option. New boundary ranges are listed in the runlog file.

4.10.1 Boundary condition types

The boundary conditions available are based on a variety of approaches and are listed in Table 3.2.9.1. The name and keyword used as input to **SHOC** are listed, along with a reference to the original study if this exists. The variables the condition may be applied to are also included, where un = normal velocity, Un = depth averaged normal velocity, ut = tangential velocity, η = surface elevation and T = tracers.

Table 3.2.9.1 : SHOC Open Boundary Conditions

Condition name	Keyword	Reference	Variable
Clamped	CLAMPD	-	un,ut,η,T
Data prescription from file	FILEIN	-	un,ut,η,T
Custom data prescription	CUSTOM	-	un,ut,η,T
Tidal synthesis	TIDEBC	Bye (1977)	η
Global tide model	TIDALH	Cartwright and Ray (1990)	η
Custom tide constituents	TIDALC	-	η
3D vertical integral for 2D	VERTIN	-	un,ut
No-gradient	NOGRAD	-	un,ut,η,T
Linear least squares	LINEXT	-	un,ut,η,T
2nd order polynomial	POLEXT	-	un,ut,η,T
Cyclic	CYCLIC	-	un,ut,η,T
Linear calculation	LINEAR	-	un, ut
Gravity wave radiation	GRAVTY	Sommerfeld (1949)	un,ut,η
Orlanski	ORLANS	Orlanski (1976)	un,ut,η
Camerlengo and O'Brien	CAMOBR	Camerlengo & O'Brien (1980)	un,ut,η
Miller and Thorpe	MILLER	Miller and Thorpe (1981)	un,ut,η
Raymond and Kuo	RAYMND	Raymond and Kuo (1984)	un,ut,η
Flather	FLATHR	Flather (1976)	un
Upstream advection	UPSTRM	-	T
Tracer advection	TRCONC	-	T
Tracer flux	TRFLUX	-	T
Tracer flux using concentration	TRCONF	-	T
Statistical prescription	STATIS	-	T
Profile scaled to density	DEPROF	-	T
Idealised profile	PROFIL	-	T
Density gradient scaled	DESCAL	-	T

No condition imposed	NOTHIN	-	un,ut,η

Implementation of the open boundaries requires that a boundary condition type is assigned to normal and tangential velocity components, elevation and tracers for each open boundary via the use of the following keywords:

```
BCOND_NOR          for normal velocity components
BCOND_TAN          for tangential velocity components
BCOND_ELE          for elevation
BCOND_TRAn         for tracers where 0 ≤ n < number of tracers, or
BCOND_<tr_name>    where <tr_name> is the name of the tracer.
                   e.g.  BCOND_temp or BCOND_salt.
```

Different boundary conditions may be optionally set for the 2D components of velocity by defining the keywords:

`BCOND_NOR2D` for 2D normal velocity components
`BCOND_TAN2D` for 2D tangential velocity components

If these flags are absent then the 2D velocity components use the same open boundary condition as the 3D components specified by `BCOND_NOR` and `BCOND_TAN`.

The tracer boundary condition allows different conditions to be specified for each tracer. If all tracers are required to have the same boundary condition, the tracer flag used is:

`BCOND_TRA_ALL`

If this condition precedes a condition for individual tracers, then all the tracers are set to `BCOND_TRA_ALL` except the individually specified tracers. This is useful if only a few tracers out of many need a specific boundary condition.

4.10.2 Boundary Implementation (stagger)

The stencil for the open boundary stagger may use the outer face for normal velocity (the default, Fig. 4.1 Science Manual) or an inner stagger for normal velocity (Fig. 4.2 Science Manual). The outer stagger is generally more stable, and may use direct forcing (with or without relaxation to radiation conditions) for elevation forcing. The inner stagger must use a Flather condition if the model is to be forced with elevation. The stagger is imposed via:

```
BOUNDARY1.STAGGER       OUTFACE   # Outer stagger (default)
```

or

```
BOUNDARY1.STAGGER       INFACE    # Inner stagger
```

If the `STAGGER` keyword is absent an outer stagger is assumed.

4.10.3 Forcing Data

The open boundary condition example given above describes a `u1` boundary spanning 3 grid cells (i=4, j=7,8,9), where surface elevation values and tracer concentration values (if any) are found in the time series file `offshore.nc`. The surface elevation variable must be called `eta`, and the tracer variables must match the tracer names specified in the model parameter file (see section 4.9).

Unique among the input data forcing, the boundary `DATA` parameter supports the specification of multiple time-series data files. The files must all be defined on the same parameter line, and separated by white-space (spaces or tabs).

```
BOUNDARY1.DATA eta.ts salt.ts temp.ts
```

SHOC selects the first file that contains the requested variable and for which the current model time is within it's range. While overlap between files (in time) are permitted, care must be taken to ensure that there are no time gaps between files. The resulting extrapolation would be ill-defined. A path for all files included in the boundary specification (e.g. including custom velocity forcing files) for all boundaries may be specified using:

```
BDRY_PATH <file_path>  # e.g. <file_path> = /home/disk/project/model/
```

4.10.4 Flather Radiation

The Flather condition is most successful when using an inner stagger; `STAGGER = INFACE`. A uniform bathymetry gradient across the boundary assists stability (`BATHY_CON = 1`). This radiation condition requires data input for both normal depth averaged velocity and elevation. If depth averaged velocity and elevation are input as zero then the condition behaves in a passive manner. This scheme is invoked via:

```
BOUNDARY0.BCOND_NOR2D   FLATHR|<datain>
BOUNDARY0.BCOND_ELE     FLATHR|<datain>|<radiation>
```

Where `<datain>` is `FILEIN` if 2D velocity or elevation data is read from file, or `CUSTOM` if 2D velocity or elevation data is supplied by custom routines. `<datain>` = `TIDALH` or `TIDALC` may be used for elevation. For elevation, `<datain>` is the condition used to specify eta for the Flather OBC, and `<radiation>` may be any radiation condition, used to set the elevation OBC. A common specification is:

```
BOUNDARY0.BCOND_NOR2D   FLATHR|CUSTOM
BOUNDARY0.CUSTOM.u1av   uv_to_u1av  3D_velocity_data.nc
BOUNDARY0.BCOND_ELE     FLATHR|FILEIN|GRAVTY
BOUNDARY0.DATA          eta_data.nc
```

With additional conditions typically as:

```
BCOND_NOR          NOGRAD
BCOND_TAN          GRAVTY or NOGRAD
```

If normal depth averaged velocity and elevation data are unavailable, then a local solution (e.g. Palma and Matano (1998), p1340) may be used for velocity and elevation:

```
BOUNDARY0.BCOND_NOR2D   FLATHR|LOCALN
BOUNDARY0.BCOND_ELE     FLATHR|LOCALE
BOUNDARY0.BCOND_TAN     LOCALT
```

This condition may be improved by using a radiation condition on elevation rather than the solution to the 1-dimensional continuity equation, e.g.

```
BOUNDARY0.BCOND_NOR2D   FLATHR|LOCALN
BOUNDARY0.BCOND_ELE     FLATHR|GRAVTY
BOUNDARY0.BCOND_TAN     LOCALT
```

If elevation data only is available, a linearized local solution may be used, retaining the elevation forcing; e.g.

```
BOUNDARY0.BCOND_NOR     LINEAR
BOUNDARY0.BCOND_NOR2D   FLATHR|LINEAR
BOUNDARY0.BCOND_ELE     FLATHR|FILEIN
BOUNDARY0.DATA          eta_data.nc
```

If the velocity and elevation data are required to be zero, then this may be accomplished by creating a file with zero values and using the FILEIN specification above, or using the CLAMPD condition:

```
BOUNDARY0.BCOND_NOR2D    FLATHR|CLAMPD
BOUNDARY0.BCOND_ELE      FLATHR|CLAMPD
```

In this case elevation will use a zero value in the Flather computation for normal velocity, and a zero value for the elevation condition. Generally, radiation conditions may be used to approximate the elevation and velocity data <datain>, e.g:

```
BOUNDARY0.BCOND_NOR2D    FLATHR|NOGRAD
BOUNDARY0.BCOND_ELE      FLATHR|MILLER
```

4.10.5 Custom Routines

Another mechanism for associating data with an open boundary is the CUSTOM parameter. A CUSTOM parameter may be defined for any variable by appending the variable name to the keyword with a fullstop (see below). Following the parameter, on the same line, are a sequence of space separated arguments. If the first argument is a numeric value or the string default, then the variable will be set to that fixed value on the boundary (default corresponding to the fill value for a tracer, or zero for u1, or u2). If the first argument is the name of a standard or custom function supported by the **SHOC** code, then the responsibility for evaluating the variable boundary value will be passed on to that function, along with the remaining arguments. These parameters are optional, and additional to the DATA parameter described above. If present, they override the DATA parameter for the variable concerned. For example:

```
# Set salinity to a constant value of 35.5 on this boundary
BOUNDARY0.CUSTOM.salt 35.5

# Set the tracer called contam to its default value
BOUNDARY0.CUSTOM.contam default

# Set surface elevation by calling the etabdry routine, and
# passing it the argument string "data.ts 280000 5700000"
BOUNDARY0.CUSTOM.eta etabdry data.ts 280000 5700000
```

For a given open boundary, it is not necessary to specify a DATA parameter if a CUSTOM parameter has been specified for every tracer and the appropriate dynamic variable (u1, or u2). The CUSTOM mechanism allows a high degree of flexibility in boundary specification, particularly when combined with custom subroutines.

4.10.6 River Flow Custom Routines

There exist several standard custom routines that allow a parabolic velocity profile to be imposed as the normal open boundary condition. This type of boundary forcing is designed to emulate a river inflow. Velocities decrease in a parabolic fashion from a maximum value at the surface to zero at a pre-defined depth such that the flow rate over the entire open boundary corresponds to a user specified rate (given in cumecs : m^3s^{-1}). The syntax for this type of open boundary for a u1 boundary is as follows:

```
BOUNDARY0.BCOND_NOR      CUSTOM
BOUNDARY0.CUSTOM.u1      u1flowbdry
BOUNDARY0.U1_HC          -5.0
BOUNDARY0.U1_FLOW        <flowfile.ts> or flow_value
```

In this case a river flow boundary is set as the normal velocity condition on boundary0 and the parabolic profile exists from the surface to 5m depth. The flow rate can either be imposed in a time varying manner by specifying a time series file <flowfile.ts>, or can be set to a constant value by specifying the constant flow_value. The flow rate should always be positive regardless of the orientation of the open boundary. Similarly, a river flow for a u2 boundary is specified via;

```
BOUNDARY0.BCOND_NOR     CUSTOM
BOUNDARY0.CUSTOM.u2     u2flowbdry
BOUNDARY0.U2_HC         -5.0
BOUNDARY0.U2_FLOW       <flowfile.ts> or flow_value
```

A simplified specification for rivers is input as follows:

```
BOUNDARY0.NAME   River1
BOUNDARY0.TYPE   u1
BOUNDARY0.BCOND0 RIVER flowfile.ts data_1.ts data_2.ts .... data_n.ts
```

where;
data_<n>.ts = file containing temperature at the cell centre. Other tracer data is also required if the tracer OBC is active. There must be at least one of these files listed.
flowfile.ts = file containing river flow.
In this case the depth over which the flow profile is distributed is the mean depth of the boundary, and salinity is input with a value of zero. If this is used a diagnostic tracer flow is generated which records the flow used in that river.

The halocline depth generally has to be set a priori, and is typically used as a tuneable parameter. This may not be desirable if many rivers exist. A dynamic pycnocline depth may be dynamically prescribed using:

```
BOUNDARY0.bcond_salt    TRCONC|CUSTOM
BOUNDARY0.CUSTOM.salt   0.0
BOUNDARY0.OPTIONS       DYNAMIC_HC NO_HDIFF
```

This can be further enhanced by computing the baroclinic landward flow in the salt wedge, and adjusting boundary ‘ghost’ cells using an upstream advection algorithm accordingly.

```
BOUNDARY0.OPTIONS       DYNAMIC_HC NO_HDIFF GEOSTR UPSTRM
```

Note that the dynamic halocline depth is referenced to the free surface, and the absolute value will therefore change with the tide. Additional tracers are generated to report the depth the flow is distributed over (flow_depth) and the salinity of the flow (flow_salt).

If the salinity boundary condition is TRCONC|CUSTOM or TRCONF|CUSTOM, then a mass balance is performed to alter the salinity in the ‘ghost’ cell where;

```
salinity = [(river salt mass) + (landward mass flux)] /
           [(river flow) + (landward flow)]
```

If zero salinity is input to the river, then (river salt mass) is zero. This salt balance approximates mixing in a salt wedge estuary, where the up-estuary salt flux is entrained into the surface layer along the length of the salt wedge and mixed with the river outflow. For a tidally mixed estuary, an ‘effective’ river length can be specified, and the standing salt mass in the volume occupied by this river length is mixed with river inflow and landward salt wedge flow. A river length can be specified using:

```
BOUNDARY0.U1_LENGTH           10000.0
```
or
```
BOUNDARY0.U2_LENGTH           10000.0
```

Additional options are as follows:
NO_SALT : Do not adjust input 'ghost' cell salinity using the salt mass balance.
FULL_DEPTH : Use water depth rather than halocline to compute mean inflow velocity.
FRESH_FLOW : Surface density of 1000 is used in the internal wave speed calculation rather than actual surface density.
TRUNC_LAYER : Truncate halocline depth to next deepest layer.
SCALE_MULT : Use multiplicative scaling to inflow rather than additive scaling.
YANKOVSKY : Method of Yankovsky, A.E. (2000) The cyclonic turning and propagation of buoyant coastal discharge along the sheff. J. Mar. Res. 58, 585-607.
NO_OUTFLOW : River flow is delivered with the original unmodified parabolic profile.
MACREADY : Use the river mouth salinity approximation of MacCready and Geyer (2010) Annu. Rev. Mar. Sci., 2, 35-58, Eq. 19 and 16.

4.10.7 Forcing with Velocity

The standard custom routines may be used to force the open boundary with velocity profiles; e.g. saved from a coarser resolution simulation. Since this nesting approach usually uses large scale and fine scale grids having different orientation, any velocities saved on the coarse grid for nesting must first be rotated into east and north components (u & v). The point array (parray) netCDF output option will automatically do this. These east and north velocity components must be saved on both normal and tangential open boundary faces on the fine scale grid. The latitude and longitude of these faces must be supplied in the parray specification, and may be retrieved from utilities such as `jvismeco` or `plum` (matlab package). Once the normal and tangential (u,v) components are saved to file from the coarse scale grid, they may be re-read and rotated onto the fine scale boundaries using the custom routines, e.g. for a `u1` boundary;

```
BOUNDARY0.NAME          Offshore
BOUNDARY0.TYPE          u1
BOUNDARY0.BCOND_NOR     CUSTOM
BOUNDARY0.CUSTOM.u1     uv_to_u1  bdry_uv_nor.nc
BOUNDARY0.BCOND_TAN     CUSTOM
BOUNDARY0.CUSTOM.u2     uv_to_u2  bdry_uv_tan.nc
BOUNDARY0.ETA           NOTHIN
```

Forcing with velocity is often prone to boundary over-specification issues which may lead to instability. These are harder to control than when forcing with elevation, where partially passive conditions may be used (see Section 4.11.8). Also, when using velocities interpolated from a coarse grid to a fine grid, there is no guarantee that the flux through the open boundary in the coarse and fine grid are identical (e.g. due to differences in bathymetry resolution, hence cross sectional area of the open boundary). This may lead to a gradual filling or emptying of the domain over time. To avoid this, the flux prescribed at the normal boundary face that is required to achieve a target elevation via the flux divergence may be inversely computed and added to the normal boundary velocity. In practice normal velocities are relaxed to this value over a timescale. This flux adjustment is invoked by specifying an elevation value in the `.DATA` boundary specification (e.g. derived from a coarse scale model) in conjunction with the `FILEIN` attribute, and the time-scale of the adjustment in the boundary list, e.g:

```
BOUNDARY0.ETA           NOTHIN|FILEIN
BOUNDARY0.ADJUST_FLUX   60 seconds
BOUNDARY0.DATA          data_ets.nc
```

A 'default' timescale mat be specified by setting `ADJUST_FLUX < 0`; this default time-scale is given by (see Herzfeld and Andrewartha, 2011):

$$\tau_f = \frac{h_1}{\sqrt{gD_B}}$$

A dual time-scale may be implemented, where the tidal component is relaxed toward using a short time-scale, and the low frequency component using a longer time-scale. This is invoked using:

```
BOUNDARY0.ADJUST_FLUX   60 seconds  # Long time-scale
BOUNDARY0.ADJUST_TIDE   2 seconds   # Short time-scale
```

Often the short time-scale is that of the barotropic time-step, and the long time-scale is the default time-scale.

The velocity forced boundary conditions may specified in a simplified format;

```
BOUNDARY0.NAME   Offshore
BOUNDARY0.TYPE   u1
BOUNDARY0.BCOND0  NEST1WAY data_1.nc data_2.nc .... data_n.nc
                         bdry_uv_nor.nc bdry_uv_tan.nc
```

Where;

`data_<n>.nc` = file containing elevation, temperature and salinity data at the cell centre. Other tracer data is also required if the tracer OBC is active. There must be at least one of these files listed.
`bdry_uv_nor.nc` = file containing east and northward velocity components (u,v) at the normal velocity boundary face.
`bdry_uv_tan.nc` = file containing east and northward velocity components (u,v) at the tangential velocity boundary face.
In this case the 'default' flux adjustment is used, and the boundary condition for temperature and salinity is `TRCONC` (Section 4.10.17). Any other tracers must be individually specified.

Versions prior to v1670 input the elevation via the `eta relaxation` file. This input method is backwards compatible using:

```
eta_relaxation_file     bdry_eta.nc
eta_relaxation_input_dt 20 minutes
COMPATIBLE              V1670
```

Note that the time scaling applied to the velocity increment is `dt2d` / `dtr`, where `dt2d` is the 2D time step, and `dtr` is the relaxation time-scale above. Therefore, if it is required that the flux be adjusted so that at every 3D time-step the boundary elevation becomes that in the `eta_relaxation_file,` then set `dtr = dt`, where here `dt` is the 3D time-step (note that the adjustment is done on the 2D time-step and `dt = IRATIO x dt2d`). If `FLUX_ADJUST` is specified in `RAMPVARS`, then the time scaling decreases from 1 year at the start of the ramp to the `ADJUST_FLUX` value at the end of the ramp. If `SCALE_ETA` is specified for the boundary, (Section 4.11.24) then the relaxation value is adjusted by the scale value before the inverse calculation. Note that if `FILEIN` is included in `RAMPVARS` and the initial condition for sea level is non-zero, then the sea level for flux adjustment will start from zero over the ramp which may cause instability. The `RAMPVARS` for this forcing is generally:
`RAMPVARS    WIND CUSTOM TIDALH`

Using forcing with velocity can lead to discontinuities in elevation (and tracers) on corners where there is boundary overlap, and elevation is solely determined by the forcing velocity data with no option for self-adjustment via interior velocities. In some cases this can lead to a constant drift in sea level, ultimately causing instability. Hard relaxation is imposed at these locations to attempt to mitigate this, however, if this fails then elevation and tracers may be over-ridden with a corner mean value using:

```
BOUNDARY0.OPTIONS        CORNER_MEANS
```

4.10.8 Tracer Equation OBCs

The standard custom routine `use_eqn` may be used to create an open boundary value for a particular tracer from an equation that has valid tracers as arguments, e.g;

```
BOUNDARY0.BCOND_NO3   CUSTOM
BOUNDARY0.CUSTOM.NO3  use_eqn '14.01*(neg(127.8562) - (0.8621*temp) +
(4.0403*salt))'
```

Where `neg` is the unary negative operator and `temp` and `salt` are valid model tracers. There is no binary operator precedence so parentheses must be used to enforce this, otherwise the equation is evaluated left to right. The current list of operators is:

```
*     Multiply
+     Addition
-     Subtraction
^     Power
exp   Exponential (unary)
neg   Negative (unary)
```

The unary operators must be enclosed by parenthesis (as in the above example) and spaces are allowed anywhere in the equation. Division is not supported as yet (use multiplication of the reciprocal). Any keywords in the equation that are not valid unary operators will be considered as a model tracer. An error will occur if any specified tracers are not found in the model.

4.10.9 Relaxation to Forced Data

Boundary data specified from a file may be combined with a radiation condition so that the transient response of the domain is transmitted through the boundary while allowing the boundary to respond to the prescribed forcing. This is accomplished by or-ing an active data forcing condition (`FILEIN` or `CUSTOM`) with a passive boundary condition. The time scale of relaxation is input via the keyword `RELAX_TIME`, and must be supplied for the following boundary conditions:

```
ORLANS|FILEIN
CAMOBR|FILEIN
MILLER|FILEIN
GRAVTY|FILEIN
NOGRAD|FILEIN
CLAMPD|FILEIN
LINEXT|FILEIN
POLEXT|FILEIN
```

Specifying `RELAX_TIME` assumes that incoming and outgoing waves are relaxed equally. Alternatively, relaxation may differ for incoming and outgoing waves by specifying:

```
BOUNDARY0.RELAX_IN            1 hour
BOUNDARY0.RELAX_OUT           30 days
```

Long relaxation times are typically associated with outgoing waves so that the OBC behaves like a radiation condition, and short relaxation times are associated with incoming waves so that the OBC converges to the forcing data.

A boundary condition for relaxing surface elevation to observed data may appear as:

```
BOUNDARY0.TYPE u1
BOUNDARY0.NAME Offshore
BOUNDARY0.BCOND_NOR          NOGRAD
BOUNDARY0.BCOND_TAN          GRAVTY
BOUNDARY0.BCOND_ELE          ORLANS|FILEIN
BOUNDARY0.RELAX_TIME         1 hour
BOUNDARY0.BCOND_TRA0         UPSTRM
BOUNDARY0.BCOND_TRA1         CLAMPD
BOUNDARY0.DATA               offshore.nc
BOUNDARY0.RANGE              (4,7)-(4,9)
```

4.10.10 Boundary Relaxation

Elevation bay be relaxed throughout a user defined zone with differing relaxation times on the inner and outer limits of the zone. Elevation relaxation is invoked via:

```
BOUNDARY0.RELAX_ELE     r_width ts_b ts_i
```

where `r_width` is the number of cells into the interior the relaxation zone extends, `ts_b` is the relaxation time-scale on the boundary and `ts_i` is the relaxation time-scale at the interior limit of the zone. It is permissible for `ts_b = ts_i`. The values of `ts_b` and `ts_i` are relative to the 2D time-step; i.e. the actual time-scale used for relaxation is `ts_b` x Δt_{2D} and `ts_i` x Δt_{2D}, where Δt_{2D} is the 2D time-step. For example, if the 2D time-step is 60 seconds, and the relaxation zone is defined as:

```
BOUNDARY0.RELAX_ELE     8 1 100
```

then a relaxation zone for elevation is created 8 cells into the interior, with a relaxation time-scale of 60 seconds on the boundary and 6000 seconds at the inner limit of the zone. Note that this option also requires an accompanying relaxation file to be specified, e.g;

```
eta_relaxation_file          bdry_eta.nc
eta_relaxation_input_dt      20 minutes
```

4.10.11 Phase Speed Smoothing

The phase speed computed by the radiation schemes for elevation may be temporally smoothed using:

$$\tilde{c}^{t+1} = F\tilde{c}^{t} + (1-F)c^{t+1}$$

A typical value of F = 0.7. This smoothing assists in reducing numerical noise (e.g. MOM Users Guide). This smoothing is invoked using:

```
BOUNDARY0.SMOOTH_PHASE    0.7
```

4.10.12 Flow Relaxation Scheme

The flow relaxation scheme of Martinsen and Engedahl (1987) has been included to relax boundary data to interior data. This is accomplished over a region `NN` cells wide. The value of the prognostic values on the boundary (η, u1, u2 or tracers) are given by any of the conditions outlined in Table 3.2.9.1; whatever is specified on the boundary is relaxed to the model

integrated values over NN cells. If the prognostic variable at the boundary is equal to zero then this flow relaxation scheme acts as a sponge type condition. This condition is invoked by adding the following flags for normal velocities, tangential velocities and elevation respectively, where NN is the number of cells the relaxation method is to act over (typically NN=10):

```
BOUNDARY0.RELAX_ZONE_NOR       NN
BOUNDARY0.RELAX_ZONE_TAN       NN
BOUNDARY0.RELAX_ZONE_ELE       NN
```

For all tracers to have the same relaxation zone, include:

```
BOUNDARY0.RELAX_ZONE_ALL       NN
```

For individual tracers use:

```
BOUNDARY0.RELAX_ZONE_TRAn      NN
BOUNDARY0.RELAX_ZONE_name      NN
```

where n is the tracer number and name is the tracer name.

4.10.13 Linear Conditions

The advective and horizontal diffusive terms on the boundary may be omitted thus linearizing the boundary momentum balance. This is invoked via:

```
BOUNDARY0.BCOND_NOR      LINEAR  # Linear normal boundary velocity
BOUNDARY0.BCOND_TAN      LINEAR  # Linear tangential boundary velocity
```

For normal velocities on southern or western boundaries this is not particularly successful (see SHOC Science Manual, Section 4.5.6). A more successful linear strategy is to shift the stagger for normal velocities one cell into the interior and linearize the normal velocity at this location. This may be accomplished via:

```
BOUNDARY0.BCOND_NOR            NOGRAD
BOUNDARY0.LINEAR_ZONE_NOR      1
```

The linear zone make the momentum balance linear one cell into the interior of the model. This can be extended to any number of cells interior to the boundary, and may be applied to tangential components also;

```
BOUNDARY0.LINEAR_ZONE_NOR      n  # Linearize normal velocity n cells
                                  # into the model interior. Typically
                                  # n = 3.
BOUNDARY0.LINEAR_ZONE_TAN      n  # Linearize tangential velocity n
                                  # cells into the model interior.
```

4.10.14 No Action Taken : NOTHIN

The boundary condition NOTHIN will not alter the value of the prognostic value on the boundary. For example, if BCOND_ELE = NOTHIN the boundary value will assume that resulting from the solution to the continuity equation. This is useful if boundaries are forced with normal and tangential components of velocity, or the custom river OBC is imposed. The NOTHIN boundary condition may be combined with a radiation condition (e.g. BCOND_ELE = NOTHIN|GRAVTY), in which case the prognostic value on the boundary is relaxed to a radiation condition using the RELAX_TIME timescale. Alternatively, the prognostic value may be relaxed to data (NOTHIN|FILEIN) using the RELAX_TIME timescale.

4.10.15 Sponge Layers

As a simple way of damping high frequency noise in the model (and sometimes to aid numerical stability), it is possible to apply a region of greatly increased horizontal viscosity just inside any type of open boundary. This is done by defining the parameter NSPONGE_HORZ, followed by the number of cells in from the boundary that the sponge will occupy.

```
# Specifies that viscosity is greatly increased for 4 cells
# inside this open boundary.
BOUNDARY0.NSPONGE_HORZ 4
```

Within each sponge cell the horizontal viscosity is set near to the maximum numerically stable value for the particular grid and integration time step (default), or a multiple of the viscosity value at the boundary using, e.g;

```
# Set the maximum value of the sponge zone equal to 5 times the
boundary value.
BOUNDARY0.SPONGE_FACT   5
```

The alternate sponge formulation of Israeli and Orszag (1981) may be implemented where the coefficient of bottom friction is increased linearly to 4 times the interior value over a region NN cells wide. This sponge condition acts on 2D and 3D normal and tangential velocity components and is invoked by setting the following keyword for boundaries requiring a sponge:

```
BOUNDARY0.NSPONGE_VERT          NN
```

Where NN is the width of the sponge zone (typically NN=10).

The sponges are applied to only the normal component of velocity. To generate sponge zones for normal and tangential components use;

```
BOUNDARY0.options       ISO_SPONGE
```

4.10.16 Atmospheric Pressure

If atmospheric pressure is specified as a model forcing input (see section 4.14), then, by default, elevation boundary conditions include an additional increment for the eta variable which is proportional to the difference between the specified pressure and a background ambient atmospheric pressure (the inverse barometer effect). This behaviour can be turned off for a particular boundary as follows:

```
# Turn of the inverse barometer boundary calculation.
# This is necessary where the specified eta values
# on the boundary already incorporate the effects of
# atmospheric pressure differences (nested grids can
# be an example of this).
BOUNDARY0.INVERSE_BAROMETER FALSE
  or
BOUNDARY0.INV_BAR FALSE
```

4.10.17 Advection / flux conditions for tracers

A simple boundary condition for tracers is the upstream advection condition, UPSTRM. This condition is a 1-dimensional implementation of the upwind scheme discretized in advective form, and suffers the errors associated with this type of implementation, i.e. it is diffusive and non-conservative. Since the advective form only computes concentrations (as opposed to fluxes), it is uncertain as to what the actual flux of tracer entering the domain is when this

condition is used. It is, however, easily implemented. The UPSTRM condition must be used in conjunction with another viable condition, e.g:

```
UPSTRM|CLAMPD
UPSTRM|NOGRAD
UPSTRM|LINEXT
UPSTRM|POLEXT
UPSTRM|CYCLIC
UPSTRM|FILEIN
UPSTRM|CUSTOM
```

In this case the value derived from the additional boundary condition is used in the upstream equation as the boundary value when flow is into the domain. The UPSTRM|FILEIN condition is used as the default if no additional boundary condition is specified (e.g. BCOND_TRA_ALL=UPSTRM), and this requires the user to supply a data file containing boundary values. Note that the UPSTRM|CLAMPD condition sets the boundary value to the water column fill value specified for that tracer when flow is into the domain.

The UPSTRM method effectively solves a one dimensional advection equation (Eqn. 4.8.1 Science Manual) and the location in the grid of the velocity used in this equation may influence the results depending on the type of forcing in effect. For example if low river flow is used as a boundary condition in conjunction with large tides in the model interior, then using a velocity located at one cell into the interior to the boundary in the UPSTRM condition will drag tracer into the domain whenever the tide flows in an outward direction from the boundary. The result is that too much tracer enters the model domain. If the velocity at the boundary cell is used then (river) velocity is always directed into the domain and the tracer in the boundary cell will converge to the data forced value, thus will not be influenced by flow into the cell from the model interior due to the tide. Again too much tracer enters the domain. Clearly neither of these scenarios are optimum and ideally a combination (adaptive method) of the two would yield the best result. The user has the ability to choose which velocity location is used in the equation to best suit the forcing conditions via:

```
UPSTRM_METHOD     FACE     # Use the face centered velocity at the
                           # boundary location.
                  INTERIOR # Use the velocity one cell into the
                           # interior of the boundary.
                  CENTER   # Use the mean of the boundary and
                           # interior velocities.
                  ADAPTIVE # Use the FACE velocity if the CENTER
                           # velocity is away (outward) from the
                           # boundary, and the INTERIOR velocity if
                           # the CENTER velocity is toward the
                           # boundary.
```

The default is INTERIOR.

A better method of implementing the tracer OBC is to use the advection scheme nominated by the user (e.g. VANLEER, QUICKEST etc; see Section 4.12) to solve the advection equation on the boundary. Using these higher order schemes ensures diffusion and dispersion errors are minimised, and since the flux form of the equation is solved the solution is conservative. This method is denoted TRCONC, and similar to the UPSTRM scheme, an additional boundary condition must be used to specify the value in this cell (see above). The default is TRCONC|FILEIN, where the user must supply a data file containing boundary values. If no data are available, passive conditions may be specified using e.g. TRCONC|NOGRAD. Note that conservation is only achieved, and reasonable values computed, if the volume is conserved in the boundary cell. This requires the velocity forced OBCs to be used (Section 4.10.7).

If the total flux of tracer entering the domain at the open boundary is precisely known, then this may be specified using the TRFLUX condition. Here the prescribed flux is used directly on the boundary face in the solution of the advection equation, and all other faces use the nominated advection scheme. The specified flux is uniformly distributed over all boundary cells. This approach may not be appropriate if the boundary cell becomes dominated by interior processes (i.e. the boundary cell must behave in a passive manner). Again an additional boundary condition must be used to specify the boundary flux and the default condition is TRFLUX|FILEIN, where the user must supply a data file containing boundary fluxes. Note that a positive specified flux implies tracer import, regardless of the edge the open boundary occupies.

If a concentration is known, then the flux and input method analogous to TRFLUX may be specified using TRCONF. In this case the supplied concentration is multiplied by the volume flux to get the tracer flux that is applied to the face. This may be useful for river inputs, if the river flow and inflow concentration of a tracer are known. The result will be identical to that using TRFLUX with the flux = concentration x flow, and is provided as an option for convenience.

4.10.18 Profile Methods for Tracers

The profile methods for tracers allow a depth dependent profile to be constructed given a surface and bottom measurement. The surface measurement may be spatially variable, and the bottom measurement should correspond to the deepest location on the boundary. The DEPROF method scales these measurements to the actual density profile predicted by the model a certain number of cells into the model interior (currently hardwired to 5 cells), whereas the PROFIL method constructs a synthetic profile consisting of surface mixed layer, pycnocline and bottom mixed layer. This synthetic profile is made by matching two exponential profiles at an inflection corresponding to the mixed layer depth. The PROFIL method therefore requires MIX_LAYER = DENS_MIX to be set so that a mixed layer depth is available. These methods are useful for forcing the model with surface and bottom data collected using moored instruments.
Both these methods require a netCDF file to be provided to SHOC containing the measured data. The data must be input at the exact geographic coordinates of the cell centers of the open boundaries. The surface measurements (which may vary spatially across the boundary) must be input at the surface (i.e. 0m) and the bottom measurement must be input at the layer in which the bottom is located for each cell comprising the boundary (i.e. the layer in which the bottom lies must be found for each cell and the same bottom measurement must be written to the netCDF file for that layer and geographic coordinates corresponding to that cell). This arrangement of the netCDF input file is necessary so that the profile method knows where to find surface and bottom measurements for each boundary cell. This means that netCDF files used for the profile methods are layer configuration and boundary location dependent (i.e. if the layer configuration or location of the boundary changes a new file must be created).
Profile methods are specified using:

```
BOUNDARY0.BCOND_TRA<n>  UPSTRM|FILEIN|PROFIL  # Synthetic profile for
                                              # tracer <n>.
BOUNDARY0.BCOND_TRA<n>  UPSTRM|FILEIN|DEPROF  # Density profile for
                                              # tracer <n>.
BOUNDARY0.DATA          input_file.nc         # netCDF input file
                                              # containing measured
                                              # data for tracer <n>.
```

Tracers may also be scaled to a normalized density profile that exists through the water column (i.e. at the deepest point in the domain). This ensures that the gradient of the tracer profile is some constant multiple of the density gradient, and therefore ensures that mixed layer depths are consistent between the tracer and density. This is invoked using:

```
BOUNDARY0.BCOND_<trname>       FILEIN|DESCAL
BOUNDARY0.SCALE_D.<trname>     v1 v2 <code>
```

Where <trname> is the name of the tracer, v1 is the depth at which the tracer value is equal to that in input_file.nc at the same depth, and v2 is a scaling factor for the profile (if v2 < 0 the profile is inverted). Below depth v1 the profile in any layer k is determined by adding v2 x (density gradient) to the concentration in the layer k+1. This is iteratively computed down through the water column. Above depth v1 the profile in any layer k is determined by subtracting v2 x (density gradient) to the concentration in the layer k-1. This is iteratively computed up through the water column. If <code> = c then a copy of the values in input_file.nc is used for the profile below depth v1, and if <code> = t then the profile values are truncated to those in input_file.nc below the depth v1 if the profile values become greater than those in input_file.nc.

4.10.19 Tidal Synthesis for Elevation

The boundary condition TIDEBC will calculate the elevation on open boundaries from tidal constituent data supplied by the user. Data required are:

T_CONSTITUENTS	Number of tidal constituents to include
T_NAME	Name of the tidal constituent
T_XLOCATION	i_c : the x location of the supplied tidal amplitude and period (m)
T_YLOCATION	j_c : the y location of the supplied tidal amplitude and period (m)
T_AMP	A : the tidal amplitude at location (i_c,j_c) (m)
T_PERIOD	P : the tidal period at location (i_c,j_c) (hours)
T_MOD_AMP	α : the rate of modulation of tidal amplitude (cm/km)
T_DIR_AMP	θ : the direction towards which the tidal amplitude is progressing (i.e. direction of increasing α) (degrees T)
T_MOD_PSE	β : the rate of modulation of tidal phase (degrees/km)
T_DIR_PSE	ϕ : the direction towards which the tidal phase is progressing (i.e. direction of increasing β) (degrees T)

These data must be included for each tidal constituent on each boundary with the TIDEBC specification. An example of the domain forced with an M2 tide of amplitude 0.2m and an S1 tide of amplitude 0.1m is given below.

```
BOUNDARY0.T_CONSTITUENTS          2
BOUNDARY0.T_NAME                  M2
BOUNDARY0.T_XLOCATION             641300
BOUNDARY0.T_YLOCATION             341707
BOUNDARY0.T_AMPLITUDE             0.2
BOUNDARY0.T_PERIOD                12.0
BOUNDARY0.T_MOD_AMP               0.0
BOUNDARY0.T_DIR_AMP               0.0
BOUNDARY0.T_MOD_PSE               0.0
BOUNDARY0.T_DIR_PSE               0.0

BOUNDARY0.T_NAME                  S1
BOUNDARY0.T_XLOCATION             652000
BOUNDARY0.T_YLOCATION             341500
BOUNDARY0.T_AMPLITUDE             0.1
BOUNDARY0.T_PERIOD                24.0
BOUNDARY0.T_MOD_AMP               0.1
BOUNDARY0.T_DIR_AMP               350.0
BOUNDARY0.T_MOD_PSE               0.17
```

```
BOUNDARY0.T_DIR_PSE                 55.0
```

4.10.20 Global Tidal Model

The global tide model of Cartwright and Ray (1990) may be applied to the open boundaries using:

```
BOUNDARY0.BCOND_ELE      TIDALH
```

This condition is described in Section 4.11 of the Science Manual. The tide may be directly imposed on the boundary as above, or may be superimposed on some low frequency sea level signal using:

```
BOUNDARY0.BCOND_ELE      FILEIN|TIDALH
BOUNDARY0.DATA           low_frequency.nc  # netCDF file containing
                                           # low frequency sea level
                                           # data.
```

The global tide model requires paths to the orthotide functions and nodal corrections to be present, e.g:

```
TIDE_CSR_CON_DIR       /tide/nodal          # Path to nodal
                                            # correction directory.
TIDE_CSR_ORTHOWEIGHTS  /tide/ortho_csr_4.0 # Orthotide functions.
```

4.10.21 Custom Tidal Constituents

Tidal constituents' amplitude and phase may be specified via file input. This allows the model to be boundary forced with spatially variable tidal phases and amplitudes of the user's choice. File formats may be netCDF for spatially variable, or ascii time series for non-spatially variable constituents. The custom tidal constituent prescription is specified using:

```
BOUNDARY0.BCOND_ELE           TIDALC
BOUNDARY0.T_CONSTITUENTS      M2 S2 K1 O1  # List of constituents
```

The tide may be directly imposed on the boundary as above, or may be superimposed on some low frequency sea level signal using:

```
BOUNDARY0.BCOND_ELE       FILEIN|TIDALC
BOUNDARY0.T_CONSTITUENTS M2 S2 K1 O1      # List of constituents
BOUNDARY0.DATA           low_frequency.nc  # netCDF file containing
                                           # low frequency sea level
                                           # data.
```

The global tide model requires paths to the file specifying constituent phases and amplitudes and the nodal correction directory to be present, e.g:

```
TIDE_CSR_CON_DIR       /tide/nodal          # Path to nodal
                                            # correction directory.
TIDE_CONSTITUENTS      tide.nc              # Constituent file.
```

If any of the constituents listed in the `BOUNDARY0.T_CONSTITUENTS` list cannot be found in the `TIDE_CONSTITUENTS` file, SHOC will terminate with an error. The list of constituents

should be a subset of the following: if a constituent is not found in this subset it will be omitted from the forcing with an accompanying error.

Constituent Name	Doodson Number
long period	
LP	55.565
Sa	56.554
Ssa	57.555
TERa	58.554
Mm	65.455
Mf	75.555
TERm	85.455
93a	93.555
diurnal	
2Q1	125.755
Q1	135.655
O1	145.555
M1	155.655
P1	163.555
S1	164.556
K1	165.555
PHI1	167.555
J1	175.455
OO1	185.555
NU1	195.455
semi-diurnal	
227	227.655
2N2	235.755
MU2	237.555
N2	245.655
NU2	247.455
M2	255.555
L2	265.455
T2	272.556
S2	273.555
K2	275.555
285	285.455

Each constituent in the constituent file must be represented by an amplitude in '`metre`' with '`_amp`' appended to the constituent name from the table above, and a phase in '`degrees`' with '`_phase`' appended to the constituent name. A time stamp must also exist in the file for compatibility with the time-series file reading libraries, although this time value may be anything since it is not used in computations (however, this does allow time dependent amplitudes and phases if required). However, the amplitudes and phases must be relative to the local time zone, not GMT. Note that the spatial extent of the tidal netCDF file must completely encompass the region defined by all cell centres of the model grid. An example of a netCDF header for the M2 constituent is given below:

```
netcdf tide {
dimensions:
      t = UNLIMITED ; // (1 currently)
      i_centre = 20 ;
      j_centre = 20 ;
variables:
      double t(t) ;
```

```
            t:units = "seconds since 2000-01-01 00:00:00 +08" ;
            t:coordinate_type = "time" ;
      double x_centre(j_centre, i_centre) ;
            x_centre:long_name = "Longitude at cell centre" ;
            x_centre:coordinate_type = "longitude" ;
            x_centre:units = "degrees_east" ;
            x_centre:projection = "geographic" ;
      double y_centre(j_centre, i_centre) ;
            y_centre:long_name = "Latitude at cell centre" ;
            y_centre:coordinate_type = "latitude" ;
            y_centre:units = "degrees_north" ;
            y_centre:projection = "geographic" ;



}
```

4.10.22 Mixing coefficient boundary conditions

Open boundary conditions can be imposed on the vertical mixing coefficients Vz and Kz. The same boundary conditions applicable to tracers may also be applied to Vz and Kz with the exception of `FILEIN` and `CUSTOM`. If the boundary condition type for mixing coefficients is unspecified then the default condition of `NOTHIN` is imposed, which assigns the mixing values on the open boundaries via selected mixing scheme computations. Since these computations usually involve vertical velocity shear and density gradients on the open boundary, all of which use values derived from other open boundary conditions, it is possible that error is introduced into vertical mixing coefficients on the open boundary in this case. The velocity computations interior to the open boundary use the vertical viscosity on the open boundary hence it is possible for this error to propagate into the domain. Under these circumstances it is preferable to specify the mixing coefficients on the boundary via an open boundary condition.

4.10.23 Split conditions for tracers

A `NOGRAD` boundary condition may be applied above a certain depth for tracers and a `FILEIN` or `CUSTOM` condition below this depth. This is invoked by setting:

```
BOUNDARY0.BCOND_TRA<n>        FILEIN|NOGRAD  (or CUSTOM|NOGRAD)
BOUNDARY0.TRPC_TRA<n>         -50
```

Where <n> is the tracer number and in this case the depth above which the `NOGRAD` condition is applied is 50m. The depths should always be entered as a negative number.

4.10.24 Constant boundary bathymetry

Bathymetry may be specified as constant adjacent to an open boundary via;

```
BOUNDARY0.BATHY_CON   n # Specify bathymetry constant for n cells
                        # into the model interior.
```

This is performed by finding the bathymetry n cells into the interior and setting the bathymetry at all cells between the boundary and this n^{th} cell equal to this n^{th} cell bathymetry value. Note that the input file must be re-created when the bathymetry is altered using this option. Additionally, the boundary zone may be smoothed using:

```
BOUNDARY0.BATHY_SMOOTH   n # Specify bathymetry smoothing for n cells
                           # into the model interior.
```

4.10.25 Scaling

The values of the tracer values computed on the boundaries may be scaled by adding a constant or multiplying by a constant. Elevation values on the boundary may be scaled by adding a constant. This is useful for easily manipulating input data without creating a new input forcing file, for example when scaling is required to convert to the correct units for tracer input. The scaling may be either a constant specified value, or may be scaled by the value of a tracer existing in the tracer list. In the latter case the scaling may be temporally and spatially variable. To scale by a constant use:

```
# Add the value of one to the boundary value of eta
BOUNDARY0.SCALE_ETA      1
```

Multiplicative scaling on eta can be invoked using `'*'`, e.g, multiply by 1.5;

```
BOUNDARY0.SCALE_ETA      * 1.5
```

```
# Add the value of one to the boundary value of tracer with name <trname>
BOUNDARY0.SCALE_S.<trname>     1
```

```
# Multiply the boundary value of tracer with name <trname> by 0.9
BOUNDARY0.SCALE_P.<trname>     0.9
```

For example, to add 1^{o}C to the temperature boundary value, use:

```
BOUNDARY0.SCALE_S.temp         1
```

A tracer may be set up where its value is updated using the `reset` function (Section 4.10.2). The tracer should not be advected, diffused and should not be a diagnostic. This tracers value will therefore be updated with data from a specified file at a specified time interval. The values of this tracer on the open boundary can then be used to scale elevation or a different tracer's boundary values. First define the scaling tracer in the tracer list, e.g;

```
TRACER2.name         scale_p
TRACER2.long_name    Scaling tracer product
TRACER2.units        fraction
TRACER2.fill_value   0.0
TRACER2.valid_range  0 10
TRACER2.advect       0
TRACER.diffuse       0
TRACER2.diagn        0
TRACER2.reset_file   scale.nc
TRACER2.reset_dt     1 hour
```

The values of this tracer will assume spatially interpolated values from the file '`scale.nc`' at 1 hour intervals. The `reset_file` may be a netCDF or time-series file. Next, define different tracers to be scaled on each boundary by referencing to this tracer:

```
# Add the boundary values in tracer scale_p to the boundary value of eta
BOUNDARY0.SCALE_ETA            scale_p
```

```
# Add the boundary values in tracer scale_p to the boundary value of tracer with name
# <trname>.
BOUNDARY0.SCALE_S.<trname>     scale_p
```

```
# Multiply the boundary value of tracer with name <trname> by the boundary values in tracer
# scale_p,
BOUNDARY0.SCALE_P.<trname>     scale_p
```

For example, to add the boundary values in scale_p to the temperature boundary value, use:

```
BOUNDARY0.SCALE_S.temp         scale_p
```

4.10.26 Boundary geographic location

The latitude and longitude of the cell and face centres may be output to file using:

```
WRITE_BDRY          <bdry_file>
```

where `<bdry_file>` is the name of the file the information is written to. This file will contain the latitude and longitude of cell centres (for tracer / elevation), normal velocity face centres and tangential velocity face centres for every boundary present. The information is written in the point array output file format (Section 4.32.6), and may be directly pasted into a parameter file when outputting point array data for nested grids. The `WRITE_BDRY` option will only function when running the model under the `–p` or –g options.

4.10.27 Standard boundary conditions

A simplified format may be used to specify certain open boundary conditions. A list of these standard boundaries may be specified (currently the list size is 2) where boundaries may be re-configured to any in the list using run regulation (Section 4.31.1). The standard boundaries are specified using:

```
BCOND<n> type <data_1>....<data_n>
```

Where n is the list number (0 to 1), type is the `type` of the condition and `<data>` is a list of data required for the type. The `type` may be:

1. 1-way nesting (Section 4.10.7):

```
BOUNDARY0.BCOND0  NEST2WAY data_1.nc data_2.nc .... data_n.nc
  bdry_uv_nor.nc bdry_uv_tan.nc
```

where `data_<n>.nc` = file containing elevation, temperature and salinity data at the cell centre. Other tracer data is also required if the tracer OBC is active. There must be at least one of these files listed.
`bdry_uv_nor.nc` = file containing east and northward velocity components (u,v) at the normal velocity boundary face.
`bdry_uv_tan.nc` = file containing east and northward velocity components (u,v) at the tangential velocity boundary face.
In this case the ‘default’ flux adjustment is used, and the boundary condition for temperature and salinity is `TRCONC` (Section 4.10.17). Any other tracers must be individually specified.

2. 2-way nesting:

```
BOUNDARY0.BCOND0  NEST1WAY data_1.mpk data_2.mpk .... data_n.mpk
                           bdry_uv_nor.mpk bdry_uv_tan.mpk
```

where the format is the same as for 1-way nesting, except forcing files are memory packets.

3. Clamped nesting:

```
BOUNDARY0.BCOND0  NEST_CPD data_ets.mpk data_uv_nor.mpk
                           data_uv_tan.mpk
```

3D velocities are clamped, gravity wave radiation on sea level.

4. River boundaries (Section 4.10.6):

```
BOUNDARY0.BCOND0 RIVER flowfile.ts data_1.ts data_2.ts .... data_n.ts
```

Where `data_<n>.ts` = file containing temperature at the cell centre. Other tracer data is also required if the tracer OBC is active. There must be at least one of these files listed.
`flowfile.ts` = file containing river flow.
In this case the depth over which the flow profile is distributed is the mean depth of the boundary, and salinity is input with a value of zero.

5. No action taken:

```
BOUNDARY0.BCOND0 NOTHIN
```

Velocity, tracer and sea level open boundaries are set to `NOTHIN` (Section 4.10.14).

6. Emulate a solid wall:

```
BOUNDARY0.BCOND0 SOLID
```

This OBC is the same as No action taken, except normal velocities are clamped to zero such that a zero flux condition exists.

7. Flather radiation:

This OBC sets up a Flather radiation open boundary condition, and is invoked using:

```
BOUNDARY0.BCOND0 NEST_FLA ts.nc eta.nc uvav_nor.nc uvav_tan.nc
```

Where `ts.nc` is a file containing temperature and salinity data, `eta.ts` is a file containing sea level data, `uvav_nor.nc` is a file containing normal depth averaged velocity data and `uvav_tan.nc` is a file containing tangential depth averaged velocity data. The Flather OBC conforms to the following specification:

```
BOUNDARY0.BCOND_ELE     FLATHR|FILEIN|GRAVTY
BOUNDARY0.BCOND_NOR     NOGRAD
BOUNDARY0.BCOND_NOR2D   FLATHR|CUSTOM
BOUNDARY0.BCOND_TAN     GRAVTY
BOUNDARY0.salt          FILEIN
BOUNDARY0.temp          FILEIN
BOUNDARY0.STAGGER       INFACE
BOUNDARY0.custom.u1     uvav_to_u1av  uvav_nor.nc # or .u2
BOUNDARY0.DATA          ts.nc eta.nc
```

A standard open boundary configuration may appear as:

```
BOUNDARY0.NAME   Offshore
BOUNDARY0.TYPE   u1
BOUNDARY0.BCOND0 NEST1WAY data_1.nc bdry_uv_nor.nc bdry_uv_tan.nc
BOUNDARY0.BCOND1 RIVER flowfile.ts data.ts
```

Any additional boundary specification (e.g. INVERSE_BAROMETER, NSPONGE_HORZ) is also applied to the standard boundary.

4.11 Advection Schemes

The specification of the advection scheme for tracers is set via the flag TRA_SCHEME in the parameter file. Current options are:

```
ORDER1          # 1st order upwind flux form
VANLEER         # Van Leer's scheme
ORDER2          # 2nd order flux form
ORDER2_UW       # 2nd order upwind flux form (stable for Courant < 2)
ORDER4          # 4th order flux form
QUICKEST        # QUICKEST, flux form, variable grid
QUICKEST_AD     # QUICKEST scheme, advective form
QUICKEST_CO     # QUICKEST, flux form, constant grid formulation
LAGRANGE        # Semi-Lagrange scheme
```

For details of these advection schemes see section 5, Herzfeld (2002).
The ULTIMATE limiter (Leonard, 1991) is invoked on the chosen scheme by setting the flag UTLIMATE in the parameter file. This limiter eliminates non-monotonic behaviour in the solutions and is generally only successful on the higher order advection schemes (i.e. 2nd, 4th order and QUICKEST). The ULTIMATE limiter is not invoked by default.

```
e.g.
ULTIMATE    YES   # invoke the ultimate limiter
ULTIMATE    NO    # no ultimate limiting
```

A choice of advection scheme is also available for momentum. This is set via the flag MOM_SCHEME in the parameter file and the current options are:

```
ORDER1      # 1st order upwind scheme
ORDER2      # 2nd order scheme
VANLEER     # Van Leer's scheme
ANGULAR     # 2nd order flux form angular scheme for momentum
ANGULAR3D   # As for ANGULAR but applied to 3D momentum only
LAGRANGE    # Semi-Lagrange scheme
```

Several additional options may be appended to the MOM_SCHEME definition:

```
WIMPLICIT   # Implicit vertical advection
ADVECT_FORM # Horizontal advection solved in the advection form
WTOP_O2     # 2nd order approximation for surface vertical velocity
WTOP_O4     # 4th order approximation for surface vertical velocity
ZERO_DRYK   # Velocity=0 for horizontal terms above free surface
SHAPIRO     # Use 1st order Shapiro filter on advection tendencies
```

The default approximation for surface vertical velocity is 4th order. Velocities used in the horizontal fluxes are set to zero above the free surface using ZERO_DRYK, then set to a no-gradient for the vertical fluxes. The default is a no-gradient condition for horizontal and vertical fluxes. An example using these options may be:

```
MOM_SCHEME          ORDER2 ADVECT_FORM ZERO_DRYK
```

The semi-Lagrangian scheme can be used with 1st to 4th order interpolations using:

```
ORDER_SL            n      # Order of scheme; n = 1, 2, 3 or 4.
```

The default is first order using a tri-linear interpolation. The scheme is also unconditionally stable and can therefore be used with any time-step. However, this scheme is only suitable to use with multiple windows if the CFL condition is satisfied (in practice the stencil of the higher order schemes (n > 1) mean that insufficient partition transfers are available to provide an accurate solution). This allows the possibility to operate the tracers on a longer time-step than momentum, which is achieved by setting the flag;

```
TRATIO              n
```

where n is the multiple of the 3D time-step the tracers are to operate on, e.g. if n=4 and dt=50 seconds then the tracers are updated every fourth 3D time step (every 200 seconds). Note that the Semi-Lagrangian scheme has conservation and numerical diffusion characteristics inferior to some of the other schemes available (semi-Lagrange characteristics improve with increasing Courant number), but if many tracers exist and speed is a priority, then this scheme may be attractive. Note that the effective upper limit of TRATIO may be determined by other events in the time scheduler's control, i.e. the routine cgrid_step() may be called with a stop time less than the tracer time-step. For this reason ideally the TRATIO time-step must be less than any other time IO interval used for output dumps, output timeseries or forcing data input.

In transport mode, TRATIO may be 0 <TRATIO < 1. This effectively reduces the time-step used with the transport model, and may be useful using the FFSL scheme if the DT time-step violates the stability criterion (Lipschitz stability – i.e. streamlines cannot cross). In this case a constant flux and linear elevation change is assumed over the interval DT, and at each substep TRATIO x DT the velocity profile is reconstructed according to these assumptions.

Due to the undesirable characteristics of the LAGRANGE scheme, it is possible to advect tracers temp and sal with a higher order scheme (VANLEER) and all remaining tracers with LAGRANGE using:

```
TRA_SCHEME          LAGRANGE|VANLEER  # T/S = VANLEER,
                                      # other tracers = LAGRANGE
```

The TRATIO facility may be used in conjunction with these split schemes.

4.12 Surface elevation and velocity

The initial condition for the surface elevation may be specified by input from file (netCDF or timeseries) or by direct input in the parameter file. The latter consists of specifying an NCE1*NCE2 floating point array, so that it is possible to set a different value in every grid cell. However, for most applications where the grid geographical extent is not large, a uniform value can be used. Examples of surface initialisation are given below:

```
SURFACE     surface.nc   # Input eta from netCDF or timeseries file.

SURFACE     2000         # Elevation set uniformly to 1m for a
1.0                      # hypothetical domain of size 40*50.

SURFACE     4            # Elevation set at each cell for a domain of
0.1 0.2                  # size 2*2.
0.2 0.3
```

If file input is used for surface initialisation and this file doesn't contain an elevation dump at the time corresponding to the model start time, then linear interpolation of elevation to the start time is performed. Surface elevation initialisation using the above methods generates a surface field that is written to the input netCDF file, hence if any changes are made to the surface initialisation then a new input netCDF file must be generated using the –g option (see section 8). Changes to surface initialisation have no effect when running the model using the –p option.

The surface elevation may be explicitly overwritten at a number of arbitrary cells using the SURACE_POINTS list. This option is useful for quickly initialising barotropic relaxation experiments (e.g. tsunami modelling). The format is as follows:

```
SURFACE_POINTS n          # n = number of points in the list
i1 j1 val1                # (i,j) location and value for point 1
i2 j2 val2                # (i,j) location and value for point 2
.
.
in jn valn
```

Similarly, the surface velocity initial condition may be specified using:

```
VELOCITY     velocity.nc   # Input velocity from netCDF file.
```

The initial velocity field can be set to the geostrophic flow using:

```
VELOCITY     GEOSTROPHIC
```

4.12.1 Elevation (and velocity) relaxation

Surface elevation may be relaxed to a surface field supplied via a time series or netCDF file using:

```
eta_relaxation file           infile.nc # η field to relax towards
eta_relaxation_input_dt       1 hour    # Time interval elevation is
                                        # read from file.
eta_relaxation_time_constant            # elevation relaxation time
                                       # constant.
```

The elevation to relax towards is read from the file infile.nc at the time interval eta_relaxation_input_dt. Every 2D time-step the actual elevation is relaxed towards this value using a relaxation time constant of eta_relaxation_time_constant. The relaxation time constant is the time it takes for the elevation to converge to the elevation field

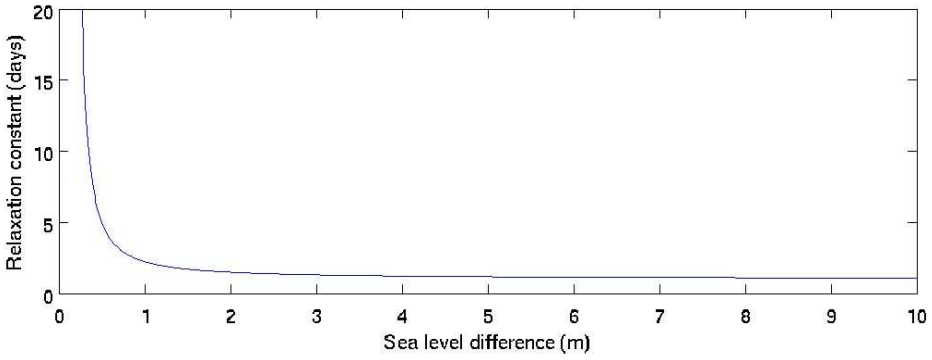
in `infile.nc`, i.e. if the time constant is equivalent to the 2D time-step then elevation is reset to that found in `infile.nc` every 2D step.
If the `eta_relaxation_time_constant` is the name of a file (netCDF or ascii) then the units for the time constant in the file must be a date unit, e.g.

```
# Ascii relaxation file where relaxation is 48 hours at day 0 and 2
# hours at day 10. Note 'Time' is converted to the model units
# specified by TIMEUNIT.
## COLUMNS  2
##
## COLUMN1.name               Time
## COLUMN2.long_name          Time
## COLUMN1.units              days since 1990-01-01 00:00:00 +8
## COLUMN1.missing_value      -999
## COLUMN1.fill_value         0.0
##
## COLUMN1.name               eta_relaxation_time_constant
## COLUMN2.long_name          Eta relaxation time constant
## COLUMN1.units              hours
## COLUMN1.missing_value      -999
## COLUMN1.fill_value         0.0
##
0  48
10 2
```

Adaptive relaxation can be invoked by specifying:

`eta_relaxation_time_constant linear` dv_1 tc_1 $units_1$ dv_2 tc_2 $units_2$
`eta_relaxation_time_constant exponential` dv_1 tc_1 $units_1$

In the linear case, if the absolute difference between modelled eta and that read from `infile.nc` is dv_1, then a relaxation constant of tc_1 $units_1$ is used and if the absolute difference is dv_2, then a relaxation constant of tc_2 $units_2$ is used, with linear interpolation for other values of the absolute difference. For the exponential case, a function $rate = \exp(\alpha / |dv|)$ is used where *dv* is the difference between modelled eta and that read from `infile.nc` and $\alpha = dv_1 \ln(tc_1)$. The relaxation constant will therefore vary spatially and temporally throughout the domain and simulation. An example is included below, where dv_1=0.5 m and tc_1 = 5 days.



A relaxation rate linear in time may be specified using:

`eta_relaxation_time_constant temporal` dv_1 tc_1 $units_1$ dv_2 tc_2 $units_2$

In this case the relaxation rate is tc_1 $units_1$ at dv_1 days (relative to the `TIMEUNIT`), changing linearly to tc_2 $units_2$ at dv_2 days, then thereafter capped at tc_2 $units_2$.

Depth based relaxation methods analogous to tracer relaxation (see Section 4.9.2) are also available. In these cases the sea level increment is saved to a 2D tracer `eta_inc`. These methods are invoked using:

```
eta_relaxation_time_constant depth dv1 tc1 units1 dv2 tc2 units2

eta_relaxation_time_constant exp_depth a0 tc1 units1 d1 tc2 units2
:
eta_relaxation_time_constant cos_depth d0 tc1 units1 d1 tc2 units2
```

Often the relaxation elevation does not contain tidal variation. If the model includes tidal forcing, this must be removed before relaxation can occur. This may be invoked using:

```
TIDAL_REMOVAL CSR   # Removal using tide computed from the CSR tide
                    # model.
              MEAN  # Use the long term eta mean as an approximation
                    # to the relaxation elevation. ETA must be
                    # included as a MEAN diagnostic (see Section
                    # 4.30.2) for this to operate, with a MEAN_DT
                    # equal to the length of the run.
```

Velocity relaxation may be achieved with the same functionality as for elevation. In this case any '`eta_`' is replaced with '`vel_`' in the relaxation specification. Relaxation is performed every 3D time-step for the 3D mode, and 2D time-step for the 2D mode.

4.13 Wind

Wind forcing is specified by number of parameters which define an input time series of wind velocity components, and drag law coefficients. The model implements a general piece-wise linear surface drag coefficient (see, for example, Large and Pond, 1981). It has the form:

$$C_d = \begin{cases} C_{d0} & V \le V_0 \\ C_{d0} + (C_{d1} - C_{d0})\dfrac{(V - V_0)}{(V_1 - V_0)} & V_0 < V < V_1 \\ C_{d1} & V \ge V_1 \end{cases}$$

where C_d is the surface drag coefficient, V is the wind speed and C_{d0}, C_{d1}, V_0 and V_1 are specified parameters (described below). The surface stress $\vec{\tau}_{top}$ is then calculated as follows:

$$\vec{\tau}_{top} = \rho_{air} C_d \vec{V} \left| \vec{V} \right|$$

where ρ_{air} is the air density (see section 0), and $\vec{V}$ is the wind velocity vector. Note that the above formulation for C_d implies that the surface stress varies roughly as the cube of the wind speed for speeds between V_0 and V_1. As a result, in some applications the model results can be very sensitive to the wind input data.

The drag parameterization may be alternatively specified using the following:

```
WIND_STRESS_FCTN  L&P   # Large and Pond (1982) scheme,(Eqn 21)
                  K/W   # Kitaigorodskii et al (1973) scheme
                  B     # Bunker (1976) scheme
                  Ko    # Kondo (1975) scheme
```

These alternative schemes also require a reference height in metres to be supplied, corresponding to the height where measurements were made, e.g;

```
WIND_STRESS_REFH        10    # Reference height in (m)
```

For Ko the option exists to use the drag coefficient for neutral conditions:

```
WIND_STRESS_NEUTRAL     YES   # neutral drag coefficient
```

At the start of a model run, wind forcing may be smoothly ramped up from zero over some specified period (see RAMPSTART and RAMPEND in section 4.3). This may help to avoid shocks or start-up transients in the model.

Wind inputs are specified as follows:

```
# A time series file containing wind East and North
# velocity components, which must be called 'u'; and 'v'
# respectively, and have units of ms-1.
WIND_TS                 cyc_bobby95.nc
# How often to read data from the wind file and update
# the wind field in the model.
WIND_INPUT_DT           10 minutes
# Scale factor applied to the wind speed. This makes it
# easy to do experiments with different wind strengths
# without having to generate a new wind time series file.
WIND_SPEED_SCALE        1.0

# Drag law coefficients. Here they are as used by
# Large and Pond, (1981). V0 and V1 have units of m/s.
DRAG_LAW_V0             10.0
DRAG_LAW_V1             26.0
DRAG_LAW_CD0            0.00114
DRAG_LAW_CD1            0.00218
```

The wind speed components in the north and east directions must bear the names ‘u’ and ‘v’ in the wind input file (see Section 4.29). These wind components are then rotated onto the grid to conform to the grid e1 and e2 directions. If the wind components already conform to the grid orientation they may be directly applied without rotation by specifying the names ‘wind_e1’ and ‘wind_e2’ in the wind input file.
Wind stress may be directly applied to the grid by using the WIND_TYPE flag, eg.;

```
# Wind input file contains wind speed (ms-1) (used by default)
WIND_TYPE               SPEED
# Wind input file contains wind stress (Nm-2)
WIND_TYPE               STRESS
```

If the WIND_TYPE flag is absent the wind input file is assumed to contain wind speeds.

4.13.1 Generic Storm Systems

Wind stress may be applied to the domain corresponding to the passage of generic cyclonic or anticyclonic synoptic weather systems. This is useful for performing idealized experiments or prescribing a realistic time and space dependent wind-field in the absence of measured data. These systems are defined by their (i,j) location in the grid relative to the grid origin, maximum pressure gradient, rotation to a latitude circle and eccentricity. Any number of these systems may be defined corresponding to certain times, and SHOC piecewise interpolates the defined systems to produce a wind pattern at any particular time during the simulation. The (i,j) location need not be defined within the dimensions of the domain but may assume any value ($-\infty < i < \infty, -\infty < j < \infty$). For this reason the locations must be supplied in

terms of (i,j) rather than geographic coordinates, since there only exists a map between geographic coordinates and (i,j) locations within the confines of the domain. Generally the user must perform some type of extrapolation if the storm center is to be defined beyond the confines of the domain; this may not be trivial for curvilinear grids and some trial and error may be necessary. The storm systems are defined via:

```
NSTORM            n            # Number of storm systems to define
STORM_INPUT_DT    ? day        # Interval wind stress is updated
ST0.stime         ? days       # Time this system is defined at
ST0.stype         HIPR or LOPR # High pressure or low pressure
systems
ST0.sp            ?            # Maximum pressure gradient (HPa/km)
ST0.ss            ?            # Radius (km)
ST0.si            i            # i location of system center
ST0.sj            j            # j location of system center
ST0.se            ?            # Eccentricity (0<e<1)
ST0.sr            ?            # Rotation (0<0<360)
```

An example of a propagating storm system is given below:

```
NSTORM            3
STORM_INPUT_DT    1 day
ST0.stime         0 days
ST0.stype         HIPR
ST0.sp            7e-4
ST0.ss            3000
ST0.si            -20
ST0.sj            20
ST0.se            0
ST0.sr            0



ST0.stime         5 days
ST0.stype         HIPR
ST0.sp            1e-5
ST0.ss            2000
ST0.si            20
ST0.sj            20
ST0.se            .8
ST0.sr            90


ST0.stime         10 days
ST0.stype         HIPR
ST0.sp            7e-4
ST0.ss            3000
ST0.si            40
ST0.sj            20
ST0.se            0
ST0.sr            180
```

This system propagates through the domain along the ξ_1 axis, centered on ξ_2=20. At day 0 it assumes the form of a circular anticyclone, at day 5 it strengthens, contracts in size and becomes elliptic with the major axis aligned in the north-south direction. By day 10 it has weakened and become larger again with a circular shape. The wind stress field is updated according to this progression at daily intervals.
If a wind file is specified in conjunction with the storm system specification then the wind and storm components are added to produce the wind stress vector.

4.14 Atmospheric pressure

A mandatory parameter sets the background air pressure, as follows:

```
# Background air pressure, in Pa
AMBIENT_AIR_PRESSURE   101000
```

This value sets the air pressure throughout the model domain. Because this value is uniform, it is not dynamically significant unless time and space varying pressure forcing is also specified, as outlined below.

Models covering larger domains (or including phenomema such as severe storms) may require such atmospheric pressure inputs. These are specified by the following optional parameters:

```
# A time-series file containing the variable 'pressure' with
# units of Pa.
PRESSURE               cyc_bobby95.nc
# How often to read the file and update the pressure
# field in the model.
PRESSURE_INPUT_DT      10 minutes     # Update every 10 minutes.
```

In this case, horizontal gradients in atmospheric pressure are dynamically included in the model, and any difference between the pressure specified in the PRESSURE data file and the AMBIENT_AIR_PRESSURE value may cause an inverse barometer effect at elevation open boundaries (see section 4.10.16).

4.15 Rainfall

Rainfall can be included as a model forcing input by using the following optional parameters:

```
# A time-series file containing the variable 'precipitation'
# with units mm day-1 (the SI unit would be m s-1, but this
# results in ridiculously small values).
PRECIPITATION          rain.nc

# How often to read the precipitation data.
PRECIPITATION_INPUT_DT  10 minutes
```

Rainfall is assumed to be fresh (zero salinity), at ambient air temperature (see section 4.17), and have zero concentration of all other tracers. Rainfall increases the volume of water in the model, and so may directly affect the model surface elevation.

4.16 Evaporation

Evaporation can be included as a model forcing input by using the following optional parameters:

```
# A time-series file containing the variable 'evaporation'
# with units mm day-1.
EVAPORATION            evap.nc

# How often to read the evaporation data.
EVAPORATION_INPUT_DT    10 minutes
```

Evaporation removes fresh water from the model. Evaporation can cause numerical problems in the model if the surface layer is very thin, as tracer concentrations can increase without

bound as the surface layer evaporates and the thickness approaches zero. This problem will be addressed in future model versions, but can usually be avoided by judicious choice of vertical grid geometry.

Note that evaporation rates are specified in an input time series file. This implies that the rates must be obtained by calculation or observation prior to the model run, so that the water temperature simulated by the run itself is not directly used as an input to the estimates of evaporation.

4.17 Surface heat flux

SHOC includes a variety of explicit heat flux parameterizations. The options for defining a heat flux are:

```
HEATFLUX    NONE         # No heat flux included
HEATFLUX    BULK         # Computed using bulk method
HEATFLUX    NET_HEAT     # Net heat flux supplied via timeseries
HEATFLUX    SURF_RELAX   # Surface layer temperature relaxation
HEATFLUX    INVERSE      # Heat flux calculated inversely
HEATFLUX    COMP_HEAT    # Heat flux from RAMS components
HEATFLUX    COMP_HEAT_MOM # Heat flux from MOM4 components
```

The least complex (and least realistic) surface heat flux mechanism is implemented by relaxation of the surface layer temperature to some prescribed, possibly time varying field using the SURF_RELAX option as follows:

```
# Time-series file specifying surface temperatures, containing
# the variable 'heatflux_temp' with units 'Degrees C'.
HEATFLUX_TEMP           temp.nc
HEATFLUX_TEMP_DT        1 day
# Relaxation time constant
HEATFLUX_TC             20 days
```

This mechanism is similar to the more general tracer relaxation mechanism described in section 4.9, except that it only operates on the surface layer of the model, rather than throughout the model.

The BULK heat flux formulation uses a more complex bulk formulation and long wave parameterisation, in addition to calculating the short wave component rather than supplying a time-series file (see Herzfeld et al (2002), section 9.2). A number of input data sets are required, all of which are optional, as described below.

Sensible heat flux requires the specification of the air temperature (as well as wind inputs - see section 0). Air temperatures are specified as follows:

```
# Time-series file containing the variable 'air_temp' with
# units 'Degrees C'.
AIRTEMP                 airtemp.nc

How often to read the air temperature file.
AIRTEMP_INPUT_DT        10 minutes
```

The sensible heat flux is proportional to the product of the wind speed and the difference between the model surface layer temperature and the air temperature. The latent heat flux requires data to calculate specific humidity:

```
# Time-series file containing the variable 'wet_bulb' with
# units 'Degrees C'.
```

```
WET_BULB                wetbulb.nc
WET_BULB_INPUT_DT       10 minutes
```

In the absence of wet bulb measurements, the dew point temperature may be substituted;

```
# Time-series file containing the variable ‘dew_point’ with
# units 'degrees C'.
WET_BULB                dewpoint.nc
WET_BULB_INPUT_DT       10 minutes
```

If available, a file containing short wave radiation may be supplied directly as below.

```
# Time-series file containing the variable 'swr' with
# units 'W m-2'.
RADIATION               swr.nc

# How often to read the solar radiation data
RADIATION_INPUT_DT      10 minutes

# Albedo of the surface
ALBEDO                  0.2
```

If `-1 < ALBEDO < 0` then the albedo is computed as a function of cloud amount and hour angle (sect 9.1.1 Science Manual). In the absence of a `CLOUD` file, clear skies are assumed. There are five bulk schemes available to specify latent and sensible heat fluxes. These are specified via;

```
# Specify the bulk method
BULK_SCHEME         L&P   # Large and Pond (1982) scheme
                    Ko    # Kondo (1975) scheme
                    B     # Bunker (1976) scheme
                    K/W   # Kitaigorodskii et al (1973) scheme
                    M     # Masagutov (1981) scheme
```

These schemes are compared in Blanc (1985). The default is the scheme of Kondo (1975).

A ramp may be applied to the heatflux, where zero heatflux is applied before the time specified, e.g.

```
# Do not apply a heatflux before 10 days, relative to the TIMEUNIT
HEATFLUX_RAMP       10 days
```

It is possible to distribute the short wave radiation throughout the water column by specifying an attenuation coefficient, `SWR_ATTENUATION`; if this is absent all short wave radiation is included in the surface boundary condition. It is possible to partition a fraction of the short wave radiation to be input as the surface boundary condition with the remainder distributed throughout the water column according to the attenuation coefficient. This is achieved by specifying a transmission coefficient, `SWR_TRANSMISSION`; if this is absent it is assumed all short wave radiation is depth distributed..

```
# Specify short wave radiation attenuation and transmission
# parameters.
SWR_ATTENUATION     0.2  # Attenuation
SWR_TRANSMISSION    0.5  # Fraction for depth distributed swr
```

Attenuation and transmission may be set to standard water classes according to Mellor (1992), e.g;

```
# Set the water type to Type II water
WATER_TYPE          TYPE_II
```

Attenuation and transmission are set according to the table below:

Water Type	Attenuation	Transmission
I	0.037	0.32
IA	0.042	0.31
IB	0.056	0.29
II	0.073	0.26
III	0.127	0.24

Note that SWR_TRANSMISSION = 1 means that all shortwave radiation is depth distributed. Alternatively the dual extinction parameterization may be used where separate extinction coefficients are used for the surface and deeper layers. A fraction determines the partitioning between surface and deep attenuation.

```
# Specify dual short wave radiation attenuation parameters.
SWR_ATTENUATION           2.8  # Surface attenuation
SWR_ATTENUATION_DEEP      0.04 # Deep attenuation
SWR_FRACTION              0.58 # Fraction for surface attenuation
```

Where short wave radiation penetrates to the bottom, it is assumed that all surplus radiation below the sea floor is absorbed into the sea bed with no additional heating of the bottom layer. This may be altered using the SWR_BOT_ABSORB flag, where a (default) value of 1 assumes the above, while a value of 0 assumes all surplus short wave radiation is input into the bottom layer. The reality is that bottom reflectance would supply some heat to the bottom layer and the value SWR_BOT_ABSORB of would be somewhere between 0 and 1. This flag may be used as a tuning parameter, e.g.

```
# Specify fraction of surplus radiation input into bottom layer.
SWR_BOT_ABSORB            0.5  # Bottom absorbtion
```

The may be input as a 2-D spatially varying field by supplying a netCDF file as input, e.g.

```
SWR_BOT_ABSORB            babs.nc  # 2D varying bottom absorbtion
```

Or a list of ascii values in the parameter file, e.g. for a 2 x 2 grid:

```
SWR_BOT_ABSORB            4  # 2 x 2 = 4 values
  0.9 0.8 0.0 0.5            # List of values.
```

If measurements of shortwave radiation are not available, then this parameter may be calculated. This requires the specification cloud cover as follows:

```
# Time-series file containing the ‘cloud' with units 'oktas'.
CLOUD                   cloudiness.nc
CLOUD_INPUT_DT          10 minutes
```

ALBEDO must not be present if short wave radiation is to be computed by the model.
Note that if the ecology module is invoked then short wave radiation is input via the LIGHT and ALBEDO_LIGHT parameters which differ from the RADIATION parameters in that the ecology module requires a daily mean short wave radiation, which is inadequate for the heat flux calculation.

The bulk parameters are usually specified at a standard height of 10m. If the wet and dry bulb temperatures (and wind) are not measured at this standard height, then the bulk parameters must be scaled from the standard height to the reference height the measurements were taken at. The user should therefore supply the reference height of measurements via:

```
# Reference height of meteorological measurements, units ‘m’.
      HEATFLUX_REFH           5.0
```

If the reference height is absent a height of 10m is assumed. A larger reference height results in larger bulk fluxes.

The sensible heat flux uses a gradient between the air temperature and SST. The SST used in this calculation is that predicted by the model. The user may submit an alternate file (e.g. of field measured SST) from which the sensible heat is computed. In this case a HEATFLUX_TEMP file (see above) containing sea surface temperature must be supplied.
Correcting air temperature and humidity for advection effects (see section 9.3 Herzfeld et al 2002) is invoked via:

```
# Include the correction to air temperature and humidity due to
# advective effects.

      HEATFLUX_ADVECT          YES
```

Note that the advection correction uses a calculation of fetch from 8 compass points; if all these directions are not required then the array `mask[]` in `init_fetch()` in the module `forcings/heatflux.c` may be modified (zero values omit the corresponding wind directions in the advection calculation).

The NET_HEAT option imposes a net heat flux directly from time-series input as the surface boundary condition for temperature and requires the following:

```
    # Time-series file containing the variable 'heatflux' with
    # units 'W m-2'.
    HEATFLUX_FILE                heatflux.nc
    HEATFLUX_DT                  1 day
```

Note that a positive flux indicates heat input into the ocean. Short wave radiation may be input separately and distributed with depth as per the BULK option above. In this case the net heat flux corresponds to the sum of long wave radiation, sensible and latent heat fluxes.

Finally the INVERSE option calculates a heat flux inversely based on a time-series of surface water temperatures (see Herzfeld et al 2002, section 9.4 for details). In the absence of any heat flux information this constitutes a helpful first estimate of heat input. This option requires a timeseries of SST observation, input in the same manner as relaxation to the surface; i.e.

```
    # Time-series file specifying surface temperatures, containing
    # the variable 'heatflux_temp' with units 'Degrees C'.
    HEATFLUX_TEMP           temp.nc

    # Time constant
    HEATFLUX_TC             20 days
```

In this case the time constant determines the time-scale over which the SST will change due to the applied heatflux, i.e. the shorter the time constant the larger the estimated fluxes. Generally the time constant should be of the order of the frequency of observations.

The heat flux generated with the BULK and INVERSE methods (and heat flux components) are saved as tracers which may be viewed in the model output. If the BULK option is invoked, the heat flux components are written to the time series files.

The atmospheric model RAMS (Pielke et. al., 1992) can output heatflux components that may be assembled to generate a net heat flux comprising of sensible, latent and longwave fluxes, and a short wave component that is depth distributed as above. Note that this formulation the longwave radiation is replaced with analytical blackbody outgoing radiation and clear sky longwave input, since this seems to generate heatfluxes that balance (i.e. do not excessively heat or cool the ocean) in the long term, hence producing better results. Also, RAMS may

produce latent heat > 0 when it is raining, hence the latent heat imposed using this option has a maximum of zero. This option is invoked, for example, via:

```
# Impose RAMS heat flux components
HEATFLUX          COMP_HEAT
HEATFLUX_FILE     RAMS.nc
HEATFLUX_DT       30 minutes
```

In this case the file `RAMS.nc` must contain variables with names `swr` (short wave radiation), `lwr_in` (downward long wave radiation), `lwr` (outward long wave radiation), `sensible` (sensible heat flux) and `latent` (latent heat flux). See Section 7 for more detail on `COMP_HEAT`.

Heatflux components used in the global ocean model MOM4 may also be assembled in a similar manner. In this case the short wave radiation is provided as a mean over some fraction of a day defined by `HEATFLUX_DT`. The daily profile is reconstructed from these means using the methodology of Schiller and Godfrey, 2003. Also, latent heat is provided as an evaporation rate in units of $kgm^{-2}s^{-1}$, which is converted to Wm^{-2} by multiplication by the latent heat of evaporation ($Lv = 2.5x10^{6}$). This option is invoked, for example, via:

```
# Impose MOM4 heat flux components
HEATFLUX          COMP_HEAT_MOM
HEATFLUX_FILE     MOM.nc
HEATFLUX_DT       30 minutes
```

In this case the file `MOM.nc` must contain variables with names `swr` (short wave radiation), `lwr` (outward long wave radiation), `sensible` (sensible heat flux) and `latent` (latent heat flux). These variables usually require the use of variable substitution, since they typically have the following MOM names:

```
swr = sw_flux
lwr = lw_flux
sensible = t_flux
latent = q_flux
```

4.18 Surface salt flux

A surface salt (or freshwater) flux may be included to account for the effect of water fluxes on salinity. This can be specified via the flag:

```
SALTFLUX    NONE        # No salt flux included
SALTFLUX    BULK  # BULK salt flux
SALTFLUX    BULK        # Salt flux partially determined using bulk
                        # schemes.
```

The `BULK` method requires `PRECIPITATION` and `EVAPORATION` time-series files to be defined (sections 4.15 and 4.16) from which the surface salt flux is calculated and applied as a surface boundary condition for the vertical diffusion of salinity (see Herzfeld et al (2002), section 9.4). Evaporation is difficult to measure over water, and the latent heat of evaporation may be used to estimate this parameter (Herzfeld et al (2002), section 9.4) when the `BULK` method is invoked. Since this bulk flux is used, the `BULK` method will only function if the `HEATFLUX` flag is set to `BULK` so that latent heat of evaporation is calculated. If a `PRECIPITATION` time-series file is present then the effect of rain is added to the calculated evaporation.

4.19 Bottom friction

Bottom friction in the model is implemented as a combination of a linear and quadratic drag law. The bottom stress $\vec{\tau}_{bot}$ is calculated as follows:

$$\vec{\tau}_{bot} = \rho C_d \vec{U} \max\left(\left|\vec{U}\right|, U_f\right)$$

where ρ is the water density, $\vec{U}$ is the bottom velocity, and U_f is a small background friction velocity, below which the friction law changes from quadratic to linear (with an effective drag coefficient of $C_d U_f$.

The bottom drag coefficient C_d is calculated using a bottom roughness length z_o (which may vary spatially), as follows:

$$C_d = \max\left(\sqrt{\frac{1}{\kappa}\ln\left(\frac{z+z_0}{x_0}\right)}, C_{d\min}\right)$$

Here, κ is the von Karman constant (0.4), and z is the height of the nearest velocity point above the sea bed. $C_{d\min}$ is a parameter, typically between 0.002 and 0.003, which places a lower limit on the value of C_d when the velocity point is a long way from the bottom.

The model parameters associated with the formulations described above are specified as follows:

```
# Minimum bottom drag coefficient. If QBFC < 0, then this value is
# used directly for the bottom drag.
QBFC              0.0025

# Background friction velocity (ms-1)
UF                0.01

# Bottom roughness (values in metres).
Z0                0.001
```

4.20 Waves

Waves are primarily used in SHOC in conjunction with sediment transport libraries so that bottom friction may be enhanced by wave action to result in increased resuspension. This requires that wave period, wave amplitude, wave direction and orbital velocity are supplied or computed. These quantities may be supplied via file input using:

```
WAVE_VARS           wave.nc     # Wave time series file
WAVE_VARS_INPUT_DT  2 hours     # How often to read the wave data
```

Alternatively, the wave variables may be created by SHOC and provided with values via the wave library (see below) using:

```
WAVE_VARS           YES
```

If a WAVE_VARS = YES or a file is specified, then SHOC will automatically create 2D tracers for the wave variables. This is done even if the input file does not contain data for the wave variables (e.g. an empty file). The wave variables created by SHOC are (see Section 4.31.15):

Tracer name	Variable name in input file	Description
wave_amp	amplitude	wave amplitude (m)
wave_period	period	wave period (s)
wave_dir	direction	wave direction (deg T)
wave_ub	ub	bottom orbital velocity (ms^{-1})
ustrcw	-	wave current friction
wave_Fx	force_x / force_e1	x Radiation stress (Nm^{-2})
wave_Fy	force_y / force_e2	y Radiation stress (Nm^{-2})
wave_ste1	stokes_x / stokes_e1	x Stokes drift velocity (ms^{-1})
wave_ste2	stokes_y / stokes_e2	y Stokes drift velocity (ms^{-1})

The influence of wave action on the hydrodynamics is controlled by the parameter WAVES. Currently, feedback of wave enhanced bottom friction to the hydrodynamics and the influence of waves on currents due to radiation stresses is supported. The wave options are invoked by listing the following:

```
WAVES       BOT_STRESS        # Allow feedback of wave bottom
                              # friction.
            TAN_RADIATION     # Include tangential radiation
                              # stresses.
            WAVE_FORCING      # Include 2D wave forcing using
                              # radiation stresses read from
                              # file.
            STOKES            # Include Stokes drift velocity.
            VERT_MIX          # Wave amplitude used for surface
                              # length scale in vertical
                              # mixing.
            NONE              # No wave options invoked.
```

The default is NONE. Note that multiple options may be invoked in the list, e.g:

```
# Allow wave enhanced bottom friction and radiation stresses
WAVES       BOT_STRESS TAN_RADIATION
```

SHOC will automatically create the following 2D tracers if these conditions are invoked:

```
wave_Cd           # Wave enhanced bottom drag for BOT_STRESS
wave_Sxy          # Tangential radiation stresses (m2s-2) for
wave_Syx          # TAN_RADIATION.
wave_Fx, wave_Fy  # Radiation stresses (Nm-2) for WAVE_FORCING.
wave_ste1, wave_ste2 # Stokes drift velocity (ms-1) for STOKES.
```

If wave enhanced mixing is invoked, several methods are available for the k-ε and k-ω mixing schemes only:

MIX_JONES : The method outlined in Jones, N.L. and Monismith , S.G. (2008). Modelling the influence of wave-enhanced turbulence in a shallow tide- and wind-driven water column. JGR, 113, C03009. This method allows for the constant α to be altered via WAVE_ALPHA (default is 100).
MIX_WOM : The wave orbital method, Babanin and Haus, (2009), On the existence of water turbulence induced by non-breaking surface waves JPO, Notes and Correspondence, 39, 2675 – 2679. This method allows for the constant b1 to be altered via WAVE_B1 (default is 0.0014).
MIX_BVM : The wave induced mixing coefficient, Bv method for monochromatic waves, Qiao, F., Yuan, Y., Ezer, T., Xia, C., Yang, Y., Lu, X., Song, Z., (2010) A three dimensional surface wave-ocean circulation coupled model and its initial testing, Ocean Dynamics, 60, 1339 – 1355. This method allows for the constant α to be altered via WAVE_ALPHA (default is 100 as per the MIX_JONES method, and should be changed to 1 or 4.).

The radiation stresses are applied to the 2D mode following the implementation of Bye (1977a). If the MOM_TEND flag is true, then tangential radiation stress tendencies (ms^{-1}) are added to the tracer list. Alternatively, if radiation stresses may be read from file, as provided by a wave model. These variables may be aligned with the grid or east/north, and have units of Nm^{-2}. In this case the depth averaged velocity is augmented to reflect the forcing due to these radiation stresses. To invoke this forcing, the WAVE_FORCING keyword should be specified.

The stokes drift velocity may be aligned with the grid or east/north, and have units of ms^{-1}. In this case the drift velocity is added to the 3D and 2D Coriolis terms. To invoke this forcing, the STOKES keyword should be specified. The Stokes Coriolis and vortex forces are applied according to Moon (2005), Eq. 14.

A wave library exists which is responsible for the calculation of wave variables (period, amplitude, direction, orbital velocity, bottom stress, enhanced bottom drag and tangential radiation stresses). If this library is to be invoked, then the following parameters are set:

```
DO_WAVES    YES         # Invoke the waves library
WAVES_DT    1 hour      # Time interval which waves are invoked
```

The wave variables are computed according to the amount of information supplied in the WAVE_VARS file. If WAVE_VARS = YES, or the WAVE_VARS file doesn't contain any of the wave variables, then the waves are assumed to be wind waves and are estimated using Eqns. 10.9, 10.11 and 10.14 in the Science Manual. Wave direction is assumed to be the same as the wind direction. Alternatively, Eqns. 10.12 and 10.13 may be used to estimate wave amplitude and period. This choice is controlled by the flag:

```
WIND_WAVE   TOBA  # Use eqns. 10.9 and 10.11
            USAC  # Use eqns. 10.12 and 10.13
```

The fetch is required when estimating wind waves using these methods. This is automatically created by SHOC when using DO_WAVES. The fetch at the limits of the model domain (open boundaries) may be specified via spatially variable netCDF of spatially constant .ts file input:

```
FETCH       fetch_OBC.nc      # Boundary values for fetch
```

If the wave period only is supplied in the WAVE_VARS file, then wind wave amplitudes are estimated using the simpler formulation of Eqn. 10.8 (Science Manual) which does not use the fetch. If all the wave variables are included in the WAVE_VARS file, then waves are assumed to be swell waves and the values retrieved from file are used for wave amplitude, period and direction.

A Grant-Madsen style bottom boundary layer (see Grant and Madsen, 1986 or Madsen,1994) is used to compute wave enhanced bottom friction. In this case, the bottom roughness, Z0, is replaced by a time and space varying apparent bottom roughness, calculated according to specified wave input data. The bottom friction model parameters are still required, with Z0 becoming the bottom roughness value in the absence of waves.

4.21 Vertical mixing

SHOC currently supports seven vertical mixing schemes, one of which must be specified for any model run. For more details on these mixing scheme formulations, see section 6, Herzfeld et al (2002). Mixing schemes can be specified by one of the following:

```
# Mixing scheme types
MIXING_SCHEME      constant
MIXING_SCHEME      csanady
```

```
MIXING_SCHEME       mellor_yamada_2_0
MIXING_SCHEME       mellor_yamada_2_0_estuarine
MIXING_SCHEME       mellor_yamada_2_5
MIXING_SCHEME       k-e
MIXING_SCHEME       k-w
MIXING_SCHEME       W88
```

4.21.1 Constant

The first scheme simply specifies constant values for the vertical diffusivities for momentum and mass, as follows:

```
# Use the constant mixing scheme
MIXING_SCHEME         constant

# Vertical eddy diffusivity
VZ0                   0.001

# Vertical diffusivity for tracers
KZ0                   0.001
```

4.21.2 Csanady

The vertical momentum diffusion coefficient V_z and vertical tracer diffusion coefficient K_z are calculated using a formulation along the lines described in Csanady (1982), equation 6.22b, with modification due to stratification as described by Bowden and Hamilton (1975):

$$V_z = V_{z0} + \alpha_V \mu_* H \left(1 + 10 R_i\right)^{-\frac{1}{2}}$$

$$K_z = K_{z0} + \alpha_K \mu_* H \left(1 + 3.33 R_i\right)^{-\frac{3}{2}}$$

where μ_* is the maximum of the surface and bottom friction velocities (to account for both tidal and wind mixing), H is the depth of water, V_{z0}, K_{z0}, α_V and α_K are constants, and R_i is a Richardson number, dependent on the vertical stratification and vertical velocity shear. The constants V_{z0} and K_{z0} specify small background mixing values. This scheme is specified as follows:

```
# Use the Csanady mixing scheme
MIXING_SCHEME   csanady
VZ0             0.00001 # Background viscosity (m^2s^-1)
VZ_ALPHA        0.0625  # Viscosity coefficient
KZ0             0.00001 # Background diffusivity (m^2s^-1)
KZ_ALPHA        0.03    # Diffusivity coefficient
```

Csanady (1982) suggests a value of 1/16 (0.0625) for α_V.

4.21.3 Mellor-Yamada 2.0

The Mellor/Yamada level 2 scheme is described (Mellor and Yamada, 1982). This is specified as follows:

```
# Use the Mellor-Yamada level 2 scheme
MIXING_SCHEME         mellor_yamada_2_0
VZ0                   1e-5     # Background viscosity
KZ0                   1e-5     # Background diffusivity
ZS                    0.3      # Surface length scale
```

The Richardson number criterion in this scheme can create grid point noise when background mixing coefficients are imposed due to the flux Richardson number being greater than the critical Richardson number. This can create grid point noise in the temperature solution if a heatflux is imposed. A Shuman filter may be applied to the mixing coefficients to remove this noise by setting:

```
# Smooth Vz and Kz using a Shuman filter
SMOOTH_VzKz       YES
```

4.21.4 Mellor-Yamada 2.0 Estuarine

This scheme uses an alternate mixing length parameterisation for the Mellor-Yamada 2.0 mixing scheme (Burchard et al, 1999; Eifler and Schrimpf, 1992; Demirov et al., 1998). This is based on a three layer system where surface and bottom mixed layers are intersected by a stably stratified interior layer.
Required parameters to invoke this mixing scheme are given below.

```
# Use the modified Mellor-Yamada level 2 scheme
MIXING_SCHEME  mellor_yamada_2_0_estuarine  # scheme type
ZS             0.6            # surface length offset
LMIN           0.01           # Minimum stratified length scale
E              1              # Mixed layer tuning parameter
VZ0            0.001          # Background viscosity
KZ0            0.000001       # Background diffusivity
```

This type of scheme displays better results than Mellor-Yamada-2.0 or k-ε for estuarine applications where a three layer system commonly exists. A large degree of flexibility exists in tuning this mixing model, where changes to `ZS, LMIN, E, VZ0, KZ0` and density gradient threshold (hardwired as variable `thr` in routine `mld()` in `MY2-0.c`) may affect the solution. The bottom roughness, `Z0`, also influences the mixing length scale in the bottom mixed layer (ZS is analogous to Z0 for the surface layer). Solutions may be particularly sensitive to the background viscosity and diffusivity. If the mixed layer interfaces are required to be identified using turbulent kinetic energy rather than the density gradient, then the routine `mld()` must be changed to `mldk()` in `MY2_VzKz_mod()` in `mixing/MY2-0.c`. The threshold is given by the variable `thr` in `mldk()` in the same module. Finally, the mixing length scale may be modified by the local turbulent kinetic energy in the mixed layers (Blackadar, 1962) via the flag lof in the routine `get_Lscale()` in `mixing/MY2-0.c`. This option is switch off by default (`lof=0`) and can be included by hardwiring `lof=1`. Accounting for local turbulent kinetic energy in the mixed layers generally decreases the mixing length scale in those regions. These hardwire options can generally be left unaltered unless complex tuning of the mixing scheme is required.

4.21.5 Mellor-Yamada 2.5

Finally the Mellor-Yamada 2.5 (or kkl) scheme (Mellor and Yamada, 1982) includes the transport of turbulence kinetic intensity and turbulence length, and requires four additional tracers. Note length scale and turbulence mixing are diagnostic tracers and do not undergo advection and diffusion.

```
# Use the Mellor-Yamada 2.5 scheme
MIXING_SCHEME         mellor_yamada_2_5
```

```
VZ0                   1e-5     # Background viscosity
KZ0                   1e-5     # Background diffusivity
ZS                    0.3      # Surface length scale
MIN_TKE               1e-8     # Optional – minimum TKE
MIN_DISS              1e-12    # Optional – minimum dissipation
LMIN                  0.17     # Optional - minimum length scale
```

This scheme requires four additional tracers corresponding to turbulent kinetic intensity (tki), turbulent kinetic intensity length scale (tki_l), turbulence length scale (lscale) and turbulence diffusion (Kq). These tracers are automatically generated by **SHOC** when the `mellor_yamada_2_5 scheme` is chosen, but may be over-ridden by manually specifying the following tracers in the parameter file:

```
# Q2 tracer
TRACER2.name        tki
TRACER2.long_name   Turbulent Kinetic Intensity
TRACER2.units       m2s-2
TRACER2.fill_value  2.0e-8
TRACER2.valid_range 0 1

# Q2L tracer
TRACER3.name        tki_l
TRACER3.long_name   Turbulent Kinetic Intensity Length Scale
TRACER3.units       m2s-1
TRACER3.fill_value  3.4e-9
TRACER3.valid_range 0 1

# Length scale tracer
TRACER4.name        lscale
TRACER4.long_name   Turbulence length scale
TRACER4.units       m
TRACER4.fill_value  0.17
TRACER4.valid_range 0 1e4
TRACER4.advect      0
TRACER4.diffuse     0
TRACER4.diagn       1

# Turbulence mixing tracer
TRACER5.name        Kq
TRACER5.long_name   Turbulence Mixing
TRACER5.units       m2s-1
TRACER5.fill_value  1e-5
TRACER5.valid_range 0 1
TRACER5.advect      0
TRACER5.diffuse     0
TRACER5.diagn       1
```

4.21.6 k-ε

The k-ε scheme is described by Burchard *et al.* (1998). The specification for this scheme is shown below.

```
# Use the k-e scheme
MIXING_SCHEME         k-e      # scheme type
VZ0                   1e-5     # Background viscosity
KZ0                   1e-5     # Background diffusivity
MIN_TKE               7.6e-6   # Optional – minimum TKE
MIN_DISS              5.0e-10  # Optional – minimum dissipation
WAVE_ALPHA            100      # Optional – wave a parameter,
```

```
                                    # Craig & Banner (1994).
```

This scheme requires two additional tracers corresponding to turbulent kinetic energy (tke) and dissipation (diss). These tracers are automatically generated by **SHOC** when the `k-e` scheme is chosen, but may be over-ridden by manually specifying the following tracers (e.g. to change fill values or valid ranges) in the parameter file:

```
# tke tracer
TRACER2.name        tke
TRACER2.long_name   Turbulent Kinetic Energy
TRACER2.units       m2s-2
TRACER2.fill_value  7.6e-6
TRACER2.valid_range 0 1

# diss tracer
TRACER3.name        diss
TRACER3.long_name   Dissipation
TRACER3.units       m2s-3
TRACER3.fill_value  5e-10
TRACER3.valid_range 0 1
```

4.21.7 k-ω

The k-ω scheme is similar to k-ε except it solves for turbulence frequency rather than dissipation (Umlauf et al 2003).

```
# Use the k-w scheme
    MIXING_SCHEME         k-w
    VZ0                   1e-5     # Background viscosity
    KZ0                   1e-5     # Background diffusivity
    ZS                    0.3      # Surface length scale
    MIN_TKE               7.6e-6   # Optional – minimum TKE
    MIN_DISS              7.27e-19 # Optional – minimum dissipation
```

This scheme requires two additional tracers corresponding to turbulent kinetic energy (tke) and turbulence frequency (omega). These tracers are automatically generated by **SHOC** when the `k-w scheme` is chosen, but may be over-ridden by manually specifying the following tracers in the parameter file:

```
# tke tracer
TRACER2.name        tke
TRACER2.long_name   Turbulent Kinetic Energy
TRACER2.units       m2s-2
TRACER2.fill_value  7.6e-6
TRACER2.valid_range 0 1

# diss tracer
TRACER3.name        omega
TRACER3.long_name   Turbulence frequency
TRACER3.units       s-1
TRACER3.fill_value  1.0e-12
TRACER3.valid_range 0 1
```

4.21.8 W88

The W88 model of Wilcox (1988) is the same as the k-ω model, but using $f_{c\mu} = f_{c\omega} = 1.0$.

```
# Use the k-w scheme
    MIXING_SCHEME         W88
```

Additional parameters required for the W88 scheme are identical to the k-w scheme.

4.21.9 Stability functions.

The stability function used in the turbulence closure schemes for k-ε, k-ω and MY2.5 may be specified using STABILITY_FUNC. The stability functions available are:

```
      STABILITY_FUNC   CANUTO_A  # Canuto et. al. (2001) model A
      STABILITY_FUNC   CANUTO_B  # Canuto et. al. (2001) model B
      STABILITY_FUNC   GALPERIN  # Galperin et. al. (1988)
      STABILITY_FUNC   KANTHA&CLAYSON  # Kantha and Clayson (1994)
      STABILITY_FUNC   POM       # Mellor (1992)
      STABILITY_FUNC   MUNK&ANDERSON    # Munk and Anderson (1948)
      STABILITY_FUNC   EIFLER&SCHRIMPF  # Eifler and Schrimpf (1992)
      STABILITY_FUNC   SCHUMANN&GERZ    # Schumann and Gerz (1995)
```

4.21.10 Waves

The effects of waves can be included in the k-ε, k-ω and W88 models. This requires the DO_WAVES flag to be invoked (see Section 4.23) with feedback to vertical mixing, i.e;

```
WAVES       VERT_MIX          # Wave amplitude used for surface
                              # length scale in vertical
```

The impact of waves on vertical mixing of momentum follows the Craig and Banner (1994) approach, where the constant α and scaling factor for significant wave height are set according to:

```
WAVE_ALPHA        100   # Wave factor α

WAVE_HEIGHT_FACT  1     # Scaling for significant wave height
```

The default values are those listed above. See Jones and Monosmith (2008) for alternative values.

4.22 Horizontal mixing

SHOC includes horizontal mixing of momentum and tracers, by specifying a viscosity and diffusivity value respectively. This term is usually included in the momentum equations for stability reasons. The parameters are specified as follows:

```
    # Horizontal viscosities are specified separately for the u1
    # and u2 momentum equations, but except under special
    # circumstances, both values should be the same.
    #
    # Horizontal viscosity in u1 equation
    U1VH              1.0

    # Horizontal viscosity in u2 equation
    U2VH              1.0
```

Horizontal diffusion for tracers is also included and is invoked by specifying the diffusivities in the x and y directions in the parameter file via:

```
# Horizontal diffusivity in the x direction (m2s-1)
U1KH    100
# Horizontal diffusivity in the y direction (m2s-1)
U2KH    100
```

The horizontal mixing coefficients may be scaled according to the grid size at each cell. This allows reasonable values to be specified for curvilinear grids which encompass a large range of resolutions. Scaling of horizontal mixing coefficients is specified by the parameter `DIFF_SCALE` and may take on the following forms, where Δx is the grid size and Δx_m is the mean grid size :

```
DIFF_SCALE        NONE        # No scaling performed
DIFF_SCALE        LINEAR      # Linear scaling by Δx / Δxm
DIFF_SCALE        NONLIN      # Non-linear scaling by (Δx)2 / (Δxm)2
DIFF_SCALE        AUTO        # Grid optimized: mixing = 0.1 Δx2 / Δt
DIFF_SCALE        SMAG        # Sets smagorinsky = 0.1 (see below)
```

The default scaling is `DIFF_SCALE = LINEAR`. If scaling is performed, the value set in the parameter file is relative to the mean grid spacing in the e1 and e2 directions (mean grid spacing is output in the file `setup.txt`).

The Smagorinsky diffusion coefficients can be independently invoked on any component of viscosity or diffusivity by setting:

```
SMAGORINSKY       c
```

Where c is the value of the constant above (typically `c=0.1`), and any combination of `U1VH, U2VH, U1KH, U2KH` is negative. For example, if the y compoment of horizontal diffusivity is to be calculated using Smagorinsky diffusion then set;

```
SMAGORINSKY       0.1
U2KH              -100.0
```

If `DIFF_SCALE = SMAG` then Smagorinsky diffusion is set for all horizontal mixing coefficients using a constant `smagorinsky = 0.1`. This constant may be over-ridden if the `SMAGORINSKY` constant is explicitly defined.
If Smagorinsky diffusion is to be used, then an extra tracer is required, which stores the value of the diffusion coefficient. This tracers is automatically generated by SHOC when the smagorinsky diffusion is invoked, but may be over-ridden by manually specifying the following in the parameter file:

```
TRACERn.name            smag
TRACERn.long_name       Smagorinsky
TRACERn.units           m2s-1
TRACERn.diagn           1
TRACERn.advect          0
TRACERn.diffuse         0
TRACERn.decay           0.0
TRACERn.svel            0.0
TRACERn.fill_value      0.0
TRACERn.valid_range     0 10000
```

The Smagorinsky distribution can be smoothed prior to use any number of times, n, using:

```
SMAG_SMOOTH       n
```

Note that the horizontal mixing of momentum in **SHOC** follows the full formulation (Herzfeld et al, 2002, section 2.4). A simple formulation exists (e.g. Apel, 1987, p99, Eqn (3.61)) where metric terms are omitted and incompressibility assumptions are made; these can be controlled by the VISC_METHOD flag:

```
VISC_METHOD       NONE        # No horizontal viscosity
                  LAPLACIAN   # Full formulation (default)
                  SIMPLE      # Simple formulation
```

The horizontal viscosity routine executed is controlled by function pointers, allowing relatively straightforward inclusion of biharmonic viscosity if required.

4.23 Point sources/sinks

A **SHOC** implementation can include an arbitrary number of point sources (or sinks) of water and tracers. These allow the representation of minor inputs of fresh water, or perhaps nutrients, for example. Associated with each point source (or sink) is a time series file (see section 11.1) which specifies inputs in one of two ways. If flows of water are associated with the point source, then the file must specify time varying flow rates (m^3 s^{-1}), and tracer concentrations (kg m^{-3}). If no water is associated with the point source, then the file specifies tracer input rates (i.e loads or fluxes in kg s^{-1}) only. The file need not specify concentrations or fluxes for all model tracers. Values for those tracers not mentioned in the file are assumed to be zero; the exception is temperature and salinity which are assumed to be equal to the receiving water values if not specified.

Sources of momentum may also be directly input as the source/sink; in this case the u1 or u2 velocity (in ms^{-1}) is directly read from file. If flows of water are associated with the point source (i.e. flow rates are specified in the time series file), then the rate of momentum input is:

$$P_t = \rho_i Q v / \rho V \qquad (ms^{-2})$$

where ρ_i = density of the inflow (kg m^{-3}); if temperature and salinity are associated with the source in the time series file, then the inflow density is computed using the equation of state. If no temperature and salinity are specified, the inflow density is assumed to be equal to the receiving water. Q is the flow rate (m^3s^{-1}) and v is the velocity associated with the inflow (u1 or u2 velocity in ms^{-1}), both specified in the time series file. ρ is the density of the receiving water and V is the cell volume, where the vertical depth distribution of the source is used to compute this volume if specified (see below).

Point source/sinks are specified as follows:

```
# Number of point source/sinks
npointss     2

# Parameters for each point source/sink
pss0.name       Nasty stuff           # Point source/sink name
pss0.location   447174 5442668 0      # Location (X Y Z)
pss.reference   surface               # reference level
pss0.data       nasty.ts              # Time-series file

pss1.name   Nice stuff
pss1.location 450477 5446628 -10
pss1.data   nice.ts
```

The z location (i.e. depth) of the source/sink input may encompass a depth range, with the deepest limit entered first and depths below the surface entered as negative. The tracer input

values are equally distributed over the depth range, e.g. for tracers to be distributed between -5m and -10m;

```
pss0.location 147.31 -43.06 -10 -5  # Source between -10 and -5m
```

The (X Y Z) locations may be entered as a time series file and be allowed to vary with time. In this case `pss0.location` contains the name of the time series file and the file must contain the variables X (or x), Y (or y), z_low and z_high, e.g:

```
pss0.location input_location.ts     # Time dependent input
```

The time series file has variables:

```
## COLUMNS 5
##
## COLUMN1.name time
## COLUMN1.long_name Time
## COLUMN1.units days since 1990-01-01 00:00:00 +10
## COLUMN1.missing_value -99999999
##
## COLUMN2.name X
## COLUMN2.long_name Longitude
## COLUMN2.units Degrees
##
## COLUMN3.name Y
## COLUMN3.long_name Latitude
## COLUMN3.units Degrees
##
## COLUMN4.name z_low
## COLUMN4.long_name Lower depth range
## COLUMN4.units m
##
## COLUMN5.name z_high
## COLUMN5.long_name Upper depth range
## COLUMN5.units m
4382 147.31 -43.06 -10 -5
4392 147.31 -43.06 -20 -15
```

The source/sink may be distributed over multiple cells horizontally and a depth range using:

```
pss0.location   -200 -100      # Depth range
pss.ncells      3              # Number of entries
12 25                          #1: (i,j) location
(2,5)-(10,11)                  #2: (i,j) range
24 27                          #3: (i,j) location
```

If a range is given, SHOC will determine only those cells within the range that are wet. Therefore, for example, if a flux were to be input in the bottom layer over the whole domain (approximating a groundwater flux) then (assuming the grid size is 100x100) one would use;

```
pss.reference   bottom
pss0.location   -1 0
pss.ncells      1
(0,0)-(100,100)
```

The source/sink may also be distributed over multiple cells horizontally and a depth range using a region file (see Section 4.29.16), where the flux can be specified over one or multiple regions:

```
pss0.location   -200 -100              # Depth range
```

```
pss.region      region.bnc 3 4 ... n   # Region file and numbers
```

The flux may be scaled according to:

```
pss0.flag   AREA_WEIGHTED     # Input flux scaled by cell area
pss0.flag   VOL_WEIGHTED      # Input flux scaled by volume of the
                              # cell mass is delivered into.
```

The reference level is determined by the following (`msl` by default):

```
pss0.reference  surface       # referenced to the free surface
pss0.reference  msl           # referenced to mean sea level
pss0.reference  bottom        # referenced to the bottom
```

Major inflows or outflows of water (which carry significant momentum) should not be specified in this way, as the point source/sink code ignores momentum input considerations. Such inputs can be specified at open boundaries (see section 4.9.6).

Sometimes the mapping of the point source location from geographic space (lat, long) to index space (i, j) is unsuccessful for the slaves. This is because sometimes custom curvilinear grids have land or outside cells that are not associated with valid coordinate values in the parameter file, and cannot be assigned geographic locations. Also, the precision of the inverse tetragonal bilinear texture map that performs this mapping is sometimes not sufficient to discriminate cell indices for point sources close to cell faces. If the code exits with the warning `'Mismatch between point sourcesinks on master and slave'` then refer to the runlog to identify the point source that could not be successfully mapped and redefine its geographic location. Placing point source locations at the cell centre, and avoiding open boundary locations will rectify this problem.

4.23.1 Steady State Approximation

The steady state concentration resulting from a point source input into a grid cell is dependent on the grid size, and can be approximated via the following. Assume a flux F_{in} (gs^{-1}) is input into a cell with dimensions ($\Delta x,\Delta y,\Delta z$) in the ($e_1,e_2,z$) directions. The e_1 direction only is considered, it is assumed that a constant e_1 velocity of u (ms^{-1}) exists, and the horizontal diffusion is A_H (m^2s^{-1}). The concentration of tracer, c (kgm^{-3}), at time t+1 can be written in terms of mass as:

$Vc^{t+1}=Vc^{t}+$(`source input`)$-$(`mass advected out`)$+$(`mass advected in`)$-$(`mass diffused out`)

where $V=\Delta x\Delta y\Delta z$. Over a time-step Δt, this is equivalent to:

$$c^{t+1}V = c^{t}V + F_{in}\Delta t - c^{t+1}\Delta y\Delta z u\Delta t + 0.\Delta y\Delta z u\Delta t - \Delta y\Delta z A_H \frac{c_i^{t+1} - c_{i-1}^{t+1}}{\Delta x}\Delta t$$

It is assumed that the concentration of tracer advected in (c_{i-1}^{t}) is zero, and that a zero gradient of tracer exists down-current from the source ($c_{i+1}^{t} = c_i^{t}$). This is simplified to:

$$V\frac{c^{t+1} - c^{t}}{\Delta t} = V\frac{\partial c}{\partial t} = +F_{in} - c^{t+1}\Delta y\Delta z u - \frac{\Delta y\Delta z}{\Delta x}A_H c_i^{t+1}$$

At steady state, $\partial c/\partial t = 0$, thus steady state concentration, c_s, is;

$$F_{in} = c_s \Delta y \Delta z u + \frac{\Delta y \Delta z}{\Delta x} A_H c_s$$

or;

$$c_s = \frac{F_{in}}{\Delta y \Delta z u + \Delta y \Delta z A_H / \Delta x}$$

For uniform grid size (Δx=Δy), this reduces to:

$$c_s = \frac{F_{in}}{\Delta z(\Delta y u + A_H)}$$

Therefore, as the horizontal grid size decreases, then the steady state concentration will increase to a limit where horizontal diffusive process dominate.

4.24 2D Mode

SHOC can be operated in the capacity of a 2D depth integrated model. This is achieved by setting:

```
2D-MODE        YES
```

The default is `2D-MODE=NO`. The 3D currents are not calculated in this case, resulting in large increases in execution time. The initial tracer distribution is vertically averaged and tracers are subsequently advected using the 2D current (i.e. the water column is assumed to be well mixed).

4.25 Sigma vertical coordinates

SHOC can be configured to use sigma coordinates in the vertical. The formulation follows that of Blumberg and Herring (1987), for curvilinear coordinates. Sigma coordinates are invoked by setting the flag:

```
SIGMA          YES
```

The default value is `SIGMA = NO`. In the sigma case, the value of `LAYERFACES` is equal to the number of sigma levels the model uses, and the distribution of these layers is generated by **SHOC** such that a logarithmic distribution exists at the surface and bottom and a linear distribution in the interior. The input netCDF file for sigma coordinates is the same as that used for 'z' coordinates. **SHOC** linearly interpolates the initial condition for tracers onto the sigma grid (then also applies a smoothing filter in the vertical). The bathymetry is checked to ensure no extreme gradients are encountered; if the bottom slope becomes greater than 0.07 then the bathymetry is smoothed (up to a maximum of 5 passes) until the gradient becomes less than 0.07. The bathymetry may be optionally smoothed n times by setting the flag:

```
SMOOTHING      n
```

The sigma layers converge at the coast, and this can lead to small vertical grid spacing, which in turn may lead to vertical velocity stability violations. To avoid program termination due to this violation, the sigma system should always be used with `STABILITY = SUB-STEP` or

STABILITY = SUB-STEP-TRACER. Note also that the minimum depth at the coast may need to be increased to maintain stability when using sigma coordinates.

It is reccomended to use Smagorinsky diffusivity when using the sigma system so that mixing along sigma surfaces over steep bathymetry does not lead to cross-isobaric exchange in the absence of any motion.

4.26 Stability sub-stepping

SHOC can invoke several methods to ensure the model remains stable if there exist local violations of the advection scheme stability criteria (which may occur, for example, if the forcing becomes locally large for a short period of time). The advective terms (for 2D, 3D momentum and tracers) are calculated using a sub-timestep based on the maximum Courant number in the grid, and the remaining terms in the model equations are calculated using the original time-step. Note that the original time-step must still obey the CFL condition so as fast moving gravity and internal waves are adequately resolved.

To invoke the sub-time stepping the parameter STABILITY is set in the parameter file as follows;

```
STABILITY  SUB-STEP          # Sub-stepping stability adjustment
STABILITY  SUB-STEP-NOSURF   # As for SUB-STEP but excluding
                             # the surface layer.
STABILITY  SUB-STEP-TRACER   # Only sub-step for tracers
STABILITY  NONE              # No stability compensation
```

The default option is NONE.
If STABILITY = SUB-STEP-NOSURF then the vertical velocity in the surface layer is not included in the maximum sub-step calculation. This is consistent with the original MECO formulation. This option avoids sub-stepping when the surface elevation is only slightly greater than a layer level (the surface layer is thin) and moderately large vertical velocities exist. This condition may occur often and increase the run time ratio due to frequent sub-stepping. However, the model may go unstable in the surface layer in this case, and HMIN may need to be increased to maintain stability in the surface layer.

4.27 Thin layers

In order to maintain stability when layers become very thin, an option exists whereby if a layer becomes thinner than the parameter HMIN, then that layer is merged with the layer below prior to the calculation of the advective terms. The velocity of the merged layer is set to the layer weighted mean of the two layers merged. It is assumed that the velocity is uniform throughout the merged layer, and subsequent to the calculation of the advective terms the merged layer is split back to the original thin layer and associated layer beneath and the thin layer is assigned the updated velocity. This option is initiated via the flag;

```
# Invoke thin layer merging
MERGE_THIN        YES
HMIN              0.05
```

The default is MERGE_THIN = NO. The implementation of the thin layer code effectively decreases the k coordinate of the surface and resets the velocity of the layer to the mean when thin layers are encountered. The optimum value of HMIN generally needs to be derived on a trial and error basis, but generally 2–3% of the surface layer thickness is a good initial estimation.

4.28 Particle tracking

Particle tracking is currently supported in **SHOC.** If an input particle file is specified, then the domain will be seeded with an initial distribution of particles. Particles will be advected and diffused according to parameters defined below. Particles maybe reset to their initial locations periodically if requested. If desired, particles can also display a specific vertical movement prescribed on a time series. The time series file should contain the vertical velocity as a function of time and space. This allows implementing particle 'swimming behaviour'. Mortality or the loss of a percentage of the remaining particles at every time step can be prescribed with a time series file. Output files will contain the variable '`ptconc`' if particle tracking is invoked; this variable indicates the concentration of particles (kgm^3) for each cell over time. For `ptconc` to be computed the particle mass has to be given as non-zero.

Particle tracking will only occur if an input file is specified. Following is an example particle tracking specification:

```
# Defines the input particle input file. This is a netCDF
# time-series containing the variables 't', 'x', 'y' and 'z'
# for a specified number of particles ('n').
PT_InputFile      pt/pt50000.nc # 50000 particle file.
PT_InputRecord    0             # Dump number to use for initial
                                # particle distribution.

# The output file where the position of all active particles
# will be written.
PT_OutputFile     pt.nc

PT_StartTime      1580 days  # Start time for PT.
PT_StopTime       1612 days  # Stop time.
PT_OutputStep     1 hours    # Output interval.
PT_TimeStep       10 minutes # Update period for recalc.
                             # particle positions.
PT_ResetStep      100 days   # How often to reset particles
                             # to the original locations.
PT_KH             1          # Horizontal diffusion coeff.
PT_KZ_MULT        1          # Vertical diffusion coeff.
                             # multiplier
PT_Mass           1          # Particle mass (kg).
PT_Restart        yes        # Interpolate particle positions
                             # from the InputFile onto the grid.

# If true then the particles are not lost when they move
# outside the model domain, instead they 'stick' to the
# boundary and are released when the current changes direction.
PT_StickyBoundary TRUE

# A continuous source of particles along a line is specified
# by a rate of release and the start/end positions of the line.
# These parameters are not mandatory, and multiple sources
# are permitted.
PT_NSource 1
PT_Source0.Rate           20   # Number of particles/second.
PT_Source0.ColourBit      2    # The bit to set in the flag
                               # array when the particle is
                               # seeded. Valid range 2-15.
PT_Source0.StartLocation  280000 7000000 -15 # XYZ of start
                                             # position.
PT_Source0.EndLocation    280000 7020000 -25 # XYZ of start
                                             # position.
```

4.28.1 Particle Status

The status of a particle may be active / inactive and unlost / lost. Active, unlost particles are the particles that appear in the domain. If a particle exits through an non-sticky boundary then it becomes lost and returns to the inactive pool of particles available to be released at each source. A particle may become lost by moving through an open boundary, or by failing to reach a solid boundary within a certain number of sub-steps (currently hardwired to 110). The latter case arises if a large velocity, v, is normal to a solid boundary which advects the particle into the boundary. The model will attempt to calculate the particles position at a future time by adding the distance, s, the particle moves over a time interval Δt where $s = v\Delta t$. If v is large then the model successively reduces Δt to resolve the particles position near the boundary. If the position cannot be resolved after 110 reductions of Δt it is assumed the particle has moved through the boundary and becomes lost. An example of this may be a particle settling into the sediments. If settling of a particle is invoked and a particle is attempted to be advected through the bottom, then the vertical diffusion is modified to counteract such effect. Consequently these particles are not lost but remain close to the bottom.

4.28.2 Source Colour

Individual sources can be identified by the `ColourBit` parameter, with valid ranges between 2 and 15 (the colourbit values 0 and 1 are used to flag inactive and lost particles). These data are written to the output file making it possible to display particles from multiple sources and identify each individual source by colour.

4.28.3 Age

The age of each particle since the release time may be computed. When a particle becomes lost the age is reset to zero. In order to minimise output file size the age of particles are stored as unsigned bytes with values ranging from 0 to 255. The actual age in floating point precision is scaled to this output range via the parameter `AgeLimit`, e.g:

```
PT_AgeLimit           20 days
```

If the `AgeLimit` parameter is present then the age is calculated and scaled age is included in the output file. Scaling is performed linearly such that an age of 0 is scaled to zero, and an age of `AgeLimit` is scaled to 255. Typically `AgeLimit` is the flushing time of the water body. Particles older than `AgeLimit` remain scaled to 255. These scaled ages may be plotted as a colour spectrum for all sources.
A histogram of the distribution of ages in bin sizes of 1 day can be produced. This is in the form of a time series file named ‘part_hist.ts’, with the histogram output at a specified interval, e.g;

```
PT_Histogram_DT          1 hour  # Output the histogram at 1
                                 # hour intervals to the file
                                 # part_hist.ts.
```

A region file (see Section 4.29.16) may be used to specify a subsection of the domain within which the mean age of partices is reported:

```
PT_age_region     region.bnc 3
```

In the above case the mean age region will comprise regions `3` of the region file `region.bnc`.

4.28.4 Size

A size of particles released from each source may be prescribed using;

```
PT_Source0.Size     1e-4  # Size in m
```

A growth or decay rate may also be specified for the source and the particle will decay to zero or double in size on this timescale, e.g;

```
PT_Source0.Decay    10 days  # Size decreases to zero in 10 days
PT_Source0.Growth   10 days  # Size doubles in 10 days
```

When a particle becomes lost the size is reset to `PT_Source0.Size`. A particle threshold size of 10^{-10} is hardwired so that if particles decay to sizes less than this threshold they are flagged as lost. In order to minimise output file size the age of particles are stored as unsigned bytes with values ranging from 0 to 255. The actual size in floating point precision is scaled to this output range via the parameter `SizeLimit`, e.g:

```
PT_SizeLimit           1e-3
```

If the `SizeLimit` parameter is present then the size is calculated and scaled size is included in the output file. For decaying particles scaling is performed linearly such that a size of `SizeLimit` is scaled to 255, and a size of `zero` is scaled to zero. For growing particles a size of `PT_Source0.Size` is scaled to zero, and a size of `SizeLimit` is scaled to 255. These scaled sizes may be plotted as a colour spectrum for all sources.
Particle sizes are only invoked if `SizeLimit` is present, regardless if sizes are set for individual sources. If `SizeLimit` is present and sizes for individual sources are not, then the particle size for each source defaults to zero. In this case all particles will always be flagged as lost, since the particle size is below the threshold of 10^{-10} (see above).

4.28.5 Settling

Particles may be prescribed setting velocities as a function of the source, or as a function of position when an initial particle distribution is prescribed (i.e. no sources). For the former, different types of settling behaviour for particles released from each source may be prescribed using:

```
PT_Source0.Stype  NONE      # No settling imposed
                  CONSTANT  # Particles from this source settle with
                            # a constant settling velocity.
                  STOKES    # The stokes settling formula is used to
                            # compute the settling velocity. This is
                            # a function of particle size, density
                            # and water density.
                  DIURNAL   # A periodic settling velocity is used
                            # where the amplitude and period are
                            # prescribed.
                  FILEIN    # Velocity is read from file.
```

For all particles, a negative settling velocity means the particle will sink and a positive velocity will result in a buoyant particle. The `CONSTANT` settling velocity for particles released from each source may is prescribed using;

```
PT_Source0.Svel  1e-3       # velocity in ms-1
```

The `STOKES` settling velocity may be computes using Stokes settling formula:

$$v = \frac{g(\rho_w - \rho_p)d^2}{18\mu} \quad 3.27.1$$

where g = 9.81 (m^2s^{-1}) is the acceleration due to gravity, ρ_w (kgm^{-3}) is the density of surrounding water, ρ_p (kgm^{-3}) is the density of the particle, d (m) is the particle diameter (size in this case) and m = 1.4e-3 ($kgm^{-1}s^{-1}$) is the viscosity of water at 20^{o}C. This settling velocity is calculated and applied to each particle if the particle size is set (see Section 4.28.4) and the particle density is prescribed:

```
PT_Source0.Dens     1030  # Density in kgm-3
```

Hence if a growth rate is also prescribed, then as the particle grows its diameter increases and therefore settles faster.

The `DIURNAL` settling velocity is computed using the formula:

$$v = -svel.\cos(2\Pi(t/sper - floor(t/sper))) \quad 3.27.2$$

where `svel` is the maximum vertical velocity (ms^{-1}) at which the particle will move, `t` is time and `sper` is the periodicity of the cosine function, e.g.

```
PT_Source0.Svel  1e-3   # Velocity in ms-1
PT_Source0.Sper  1 day  # Periodicity
```

The `FILEIN` settling velocity is prescribed using an ASCII or netCDF time series file.

```
PT_Source0.File svel.ts       # Time series file containing
                              # variable and 'wpt'(ms-1).
```

The settling velocity variable in the file must be named '`wpt`'. The settling velocity in the file may be a function of time or space (or both). The spatial coordinates of the source (i.e. `StartLocation` and `EndLocation`) are used to interpolate from the file onto the source location if spatial information is contained in the file.

Additionally, particles released from an initial distribution (i.e. without sources specified) may undergo settling as a function of their position in time and space as read from file. This is specified using:

```
PT_w_file   svel.nc     # File containing settling variable 'wpt'.
```

The settling velocity variable in the file must be named '`wpt`', and the velocity may be a function of time, space or both. Spatially dependent velocities interpolate the settling velocity onto cell centres of the grid, and all particles within a particular cell will adopt that corresponding settling velocity.

NOTE: The differences between invoking `PT_Source0.Svel` settling velocity type and the `PT_w_file` are that the former is used for particles released from sources; in which case a continuous source of particles along a line is specified by a rate of release and the start/end positions of the line. Each source must have their own time series file. The second from is used for a release of particles determined with the particle input file, in which case the domain is seeded with an initial distribution of particles. In this case, the settling velocity can vary as a function of time t and space .

4.28.6 Swimming

Similar to the settling for particles released from an initial distribution, particles may be assigned horizontal swimming velocities applicable to an initial release. This swimming is read from netCDF file as a function of time and space and is specified via:

```
PT_uv_file  vel.nc      # File containing settling variable 'upt'
                        # for swimming in the x (east-west)
                        # direction and 'vpt' for swimming in the y
                        # (north-south) direction.
```

Note that `upt` and `vpt` are velocities are relative to the east-west / north-south axis rather than the numerical grid, and must generally undergo rotation (within the particle tracking code) to be transformed onto the grid.

4.28.7 Mortality

Mortality, or the loss of particles expressed as a percentage of active, unlost, particles at every time step, can be prescribed with a time series file (note: this input is not spatially dependent), e.g:

```
PT_mortality_file   mp.ts   # mortality percentage file
```

The mortality percentage variable in the file must be named '`mpt`'.

4.29 Grid Refinement

Grid refinement, or two-way nesting, allows a fine resolution grid (FRG) to be embedded within a coarse resolution grid (CRG) so that increased resolution is achievable in a sub-region of the whole domain. Although the time-step for the simulation is determined by the smallest grid, savings in computer time is generally achieved by not highly resolving the whole domain. The method used for grid refinement is detailed in Section 14 of the Science Manual.
There must exist at least 2 windows for grid refinement to operate. A grid must be constructed where the number of fine grid cells that comprise one coarse grid cell (i.e. the zoom factor, zf) is an odd number so that cell faces and centers in the coarse grid are coincident with fine grid locations at the coarse-fine boundary. The user must therefore choose a zoom factor and provide a list of the (I,j) locations of the centers of the coarse grid. An example of invoking grid refinement is given below.

```
WINDOWS           2    # At least 2 windows are necessary
GRID_REFINEMENT   YES  # Turn on grid refinement
ZOOM_FACTOR       3    # Use a zoom factor of 3 so that 3 x 3
                       # = 9 fine grids comprise 1 coarse grid.
ZOOM_POINTS       28   # List the (i,j) locations of the cell
17 9                   # centers of the coarse grid. There are
20 9                   # 28 (i,j) locations in the list.
23 9
26 9
29 9
32 9
35 9
17 12
20 12
23 12
26 12
29 12
```

```
32 12
35 12
17 15
20 15
23 15
26 15
29 15
32 15
35 15
17 18
20 18
23 18
26 18
29 18
32 18
35 18
```

The resulting grid for a closed basin test domain is illustrated in Figure 4.29.1.

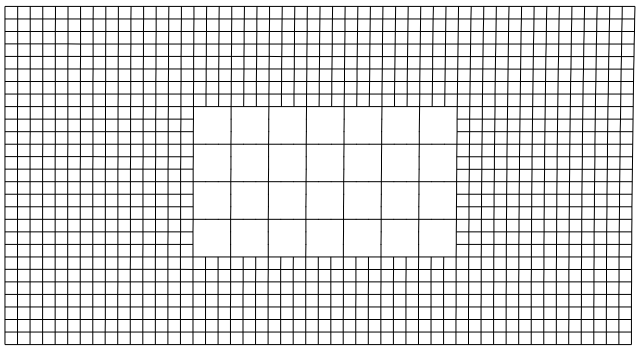


Figure 4.29.1 : Grid refinement example

A section of the grid can be retained at high resolution, or a coarse resolution section can be created using:

```
ZOOM_HR_ZONE      (17,9)-(35,18)    # Set a high resolution zone
or
ZOOM_CR_ZONE      (17,9)-(35,18)    # Set a coarse resolution zone
```

Grid refinement may be turned off using `GRID_REFINEMENT NO`. The default is for no grid refinement. Note that the bathymetry is averaged over the coarse grid cells, hence a new netcdf input file must be created when grid refinement is invoked.
Anisotropic grid refinement may be invoked using:

```
ZOOM_FACTOR_E1          3    # Use a zoom factor of 3 in the e1
                             # direction only.
or

ZOOM_FACTOR_E2          5    # Use a zoom factor of 5 in the e2
                             # direction only.
```

It is possible to construct a grid which has refinement in one direction, e.g. Figure 4.29.2 has a refinement of factor 3 in the e1 direction. This grid may be reverted to a uniform grid using the `PRECONDITIONED` grid refinement option;

```
GRID_REFINEMENT   YES PRECONDITIONED
ZOOM_FACTOR_E1    3
```

This option is useful for reverting a portion of the grid to a uniform grid, while increasing the resolution of another part of the grid (e.g. an upstream river section). In the example below the river section that is three cells wide may be retained at this resolution while the remainder reverted to uniform. Note that the ZOOM_POINTS of the cell centres required to be reverted must also be supplied.

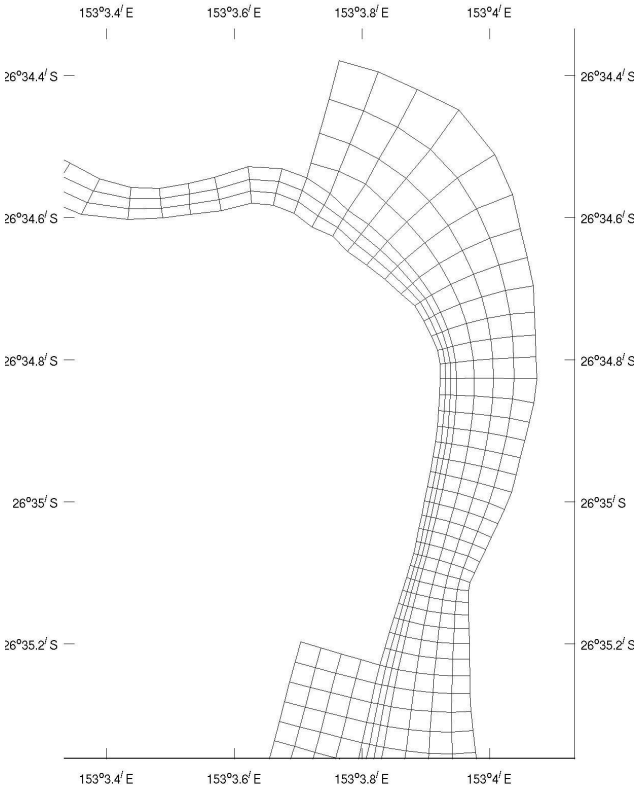


Figure 4.29.2. Grid example with refinement of factor 3 through the river section in the e1 direction.

Usually time-steps are compromised when resolution is increased laterally in a river section of the grid. A grid section where variables are linearly blended can be useful to overcome this. In the case of a river, if variables are blended laterally across the entire width of the river then there will be no transverse flow since the lateral boundary conditions prohibit flow through the solid boundaries. This makes flow along-river only, and the cross-river direction is irrelevant in terms of determining the time-steps for stability. The river effectively consists of a number of independent channels stacked side by side. Tracer exchange between the channels may exist via horizontal mixing. Such a configuration has the benefit of allowing increased resolution of the bathymetric cross section of the river, and aids in constructing river branches. Blending is invoked using:

```
NE1_BLEND   1             # Number of blend areas in the e1 direction
E1_BLEND0   e1s  e1e e2s e2e   # Start & end e1 coordinates (e1s and
                               # e1e) and start & end e2 coordinates
                               # (e2s and e2e) for blend area 0.
```

Or

```
NE2_BLEND   1             # Number of blend areas in the e2 direction
E2_BLEND0   e2s  e2e e1s e1e   # Start & end e2 coordinates (e2s and
                               # e2e) and start & end e1 coordinates
                               # (e1s and e1e) for blend area 0.
```

Examples may be:

```
NE1_BLEND   2
E1_BLEND0   45 47 241 255
```

```
E1_BLEND1   45 47 260 298

NE2_BLEND   1
E2_BLEND0   18 22 100 110
```

4.30 Tracer diagnostics

There exist several options for SHOC to generate diagnostics of interest which are subsequently saved to 2D or 3D tracers. These tracers then appear in any specified netCDF output files or timeseries files. Currently these diagnostic tracers include mixed layer depth, heat flux (described in section 4.17), steric height, vorticity, mixing length scale, flushing time, CFL time-steps, tracer fluxes, mean velocity or mean tracer flux and tendencies in the momentum balance. Specification of these diagnostics is described below.

4.30.1 Tracer Fluxes

The advective and vertical diffusive flux of a specified tracer may be calculated. The flux calculation of a tracer is invoked by specifying a tracer name, e.g;

```
CALC_FLUXES             salt   # Name of tracer for flux calculation
```

To disable the flux diagnostic, set the flux diagnostic to `NONE`. This diagnostic requires the specification of tracers representing the advective fluxes in e1, e2 and z directions, and a diffusive flux in the z direction. These tracers are automatically generated by SHOC when the `CALC_FLUXES` flag is invoked, but may be over-ridden by manually specifying any of the following tracers in the parameter file:

```
TRACER?.name            flux_e1
TRACER?.long_name       Advective flux e1
TRACER?.units           kgs-1
TRACER?.diagn           1

TRACER?.name            flux_e2
TRACER?.long_name       Advective flux e2
TRACER?.units           kgs-1
TRACER?.diagn           1

TRACER?.name            flux_w
TRACER?.long_name       Vertical advective flux
TRACER?.units           kgs-1
TRACER?.diagn           1

TRACER?.name            flux_kz
TRACER?.long_name       Vertical diffusive flux
TRACER?.units           kgs-1
TRACER?.diagn           1
```

Fluxes are calculated at each grid cell via:

$$flux\_e1 = u_1 T \Delta h_2 \Delta z$$
$$flux\_e2 = u_2 T \Delta h_1 \Delta z$$
$$flux\_w = wT \Delta h_1 \Delta h_2$$
$$flux\_kz = K_z \frac{\partial T}{\partial z} \Delta h_1 \Delta h_2$$

where u_1 and u_2 are the velocities in the e_1 and e_2 directions respectively, T is the tracer concentration at the cell face, Δh_1 and Δh_2 are the grid metrics at the cell faces and Δz is the layer thickness.

4.30.2 Means

The mean of certain variables may be calculated via the flag MEAN. Options are:

```
MEAN        NONE        # No mean velocity calculation
MEAN        VEL3D       # Mean 3D velocity calculation
MEAN        VEL2D       # Mean 2D velocity calculation
MEAN        ETA         # Mean sea level calculation
MEAN        TS          # Mean temperature and salt
MEAN        KZ          # Mean vertical diffusivity calculation
MEAN        WIND        # Mean wind calculation
MEAN        VOLFLUX     # Mean volume flux calculation
MEAN        TENDENCY    # Mean momentum tendencies
MEAN        FLUX        # Mean tracer flux calculation
MEAN        TIDAL       # Means calculated over a tidal cycle
MEAN        TRANSPORT   # Tracers advected with mean velocities
MEAN_DT     1 day       # Averaging period
```

A MEAN_DT value of SEASONAL or MONTHLY is also supported for seasonal or monthly means respectively. These quantities may be written to file using the SEASONAL or MONTHLY netCDF file output time increments (see Section 4.32.6); here the mean dumped at the start of the season corresponds to the mean computed over the previous season (ditto for months, e.g. output on 1 March corresponds to a mean computed over the previous summer for SEASONAL means and means computed over February for MONTHLY means). Additionally, if SEASONAL or MONTHLY means are written to netCDF file at the same interval as MEAN_DT (e.g. file0.tinc = SEASONAL with MEAN_DT = SEASONAL) then the mean will be cumulative over the season for successive years (e.g. for a multi-year run, the mean dumped to file on 1 March will be that of all previous summers for SEASONAL means and that of all previous Februaries for MONTHLY means). If the mean is not desired to be cumulative in this fashion, then the mean for each season of each year should be saved using MONTHLY dumps for SEASONAL means.

The means computed are running means, where the value present in the output file is the mean from the start of the computation period to that point in time. When the MEAN_DT time is reached, the mean values are reset to zero and the running mean begins again. If a restart is performed, the running mean values are correctly populated from the restart file but the time counter for the means is reset to zero. This may result in inaccurate means when restarting, and can be avoided by explicitly setting the time counter to its correct value since the last re-setting of the means using:

```
MEANS_OFFSET      <time>      # e.g. <time> = 10 days is the time
                              # since the last reset occurred.
```

The default is no calculation of mean quantities. If the VEL3D flag is invoked, then three additional tracers corresponding to the mean 3D velocity in the e_1, e_2 and z directions must exist. These tracers are automatically generated by SHOC when the MEAN flag is invoked, but may be over-ridden by manually specifying any of the following tracers in the parameter file:

```
TRACER?.name            u1mean
TRACER?.long_name       Mean u1 velocity
TRACER?.units           ms-1
TRACER?.diagn           0

TRACER?.name            u2mean
TRACER?.long_name       Mean u2 velocity
TRACER?.units           ms-1
TRACER?.diagn           0

TRACER?.name            wmean
```

```
TRACER?.long_name       Mean w velocity
TRACER?.units           ms-1
TRACER?.diagn           0
```

If the FLUX flag is invoked then the mean values of the tracer fluxes (section 4.30.1) are calculated for the respective flux tracers, hence additional flux tracers must also be specified. If the TENDENCY flag is set then the contributions to the momentum balance are averaged for the respective tendency tracers (see section 4.30.10). The VEL2D and WIND flags generate means of the 2D velocity and wind-field respectively. These averages are stored in 2D tracer arrays which are automatically created by SHOC when these flags are invoked.

If the TIDAL flag is present then the mean values are calculated over a tidal period. To do this SHOC attempts to find the maximum sea level in a 24 hour period at each point in the grid, then proceeds to average until the next maximum sea level is encountered at that point. Note that this may result in the exact averaging period differing throughout the grid (e.g. if a modulation of tidal phase exists across the grid). After each output dump event the mean arrays are reset. When invoking this option, the file output interval should be set to around 3 times the dominant tidal period (i.e. 3 days for diurnal tides) since **SHOC** may require up to 1 tidal period to locate the start of the averaging period, 1 tidal period to calculate the mean and 1 tidal period for safety to avoid any overlap of the tidal averaging into the next cycle.

The TRANSPORT flag allows tracers to be advected using the mean 3D velocity field. If the averaging period is set so as to filter out higher frequency oscillation (e.g. the tide) then these velocities represent the residual current field which may be much smaller than the instantaneous current. In these cases the time-step for tracers may be dramatically increased, resulting in an improvement in execution speed.

The mean fields appear in the output file and time-series files as an additional tracer. Note that if tracers are set as diagnostic tracers (`TRACER?.diagn = 1`) then SHOC initializes the tracer to zero every time the tracer is dumped to file. Since mean tracers sum contributions over the averaging period, always set `TRACER?.diagn = 0` when manually defining mean tracers.

4.30.3 Mixed Layer Depth

The mixed layer depth may be computed using a threshold on the vertical density profile (currently hardwired to –0.01 kgm^{-2} in the routine mld()) or threshold on the turbulent kinetic energy (hardwired to 10^{-5} Wkg^{-1} in the routine mldk(); see Burchard et al (1999), p26). Obviously the latter will only function if the mixing scheme calculates TKE (e.g. Mellor-Yamada 2.5, k-ε, k-ω). Finally, the mixed layer may be computed as the level where water temperature attains a value of 0.1 x SST. The mixed layer option is invoked by setting the flag:

```
MIX_LAYER   NONE        # Default : no mixed layer calculation
MIX_LAYER   DENS_MIX    # Density gradient computation
MIX_LAYER   TKE_MIX     # TKE threshold computation
MIX_LAYER   TEMP_MIX    # Temperature (0.1 x SST) computation
```

The default is no mixed layer calculation. If this flag is invoked, then a 2D tracer is automatically created to store the mixed layer depth in units of metres.

4.30.4 Flushing Time

The time required to flush a sub-region of the model domain may be calculated using the flushing diagnostic. The flushing time is defined as the time for the total mass in the sub-region to decrease by a factor of 1/e (~38%, i.e. the e-folding time). This representation of the

flushing time assumes that tracer is well mixed in the sub-region and the total mass is assumed to decrease exponentially according to:

$$M(t) = M_0 e^{-t/\tau}$$

where M_0 is the initial mass and τ is the flushing time scale (Tartinville et al, 1997). When M = M_0/e then t = τ, hence the flushing time can be recovered. This diagnostic is invoked by specifying the tracer number of a flushing tracer, e.g.

```
FLUSHING_TR             YES         # Invoke flushing diagnostic
FLUSHING_DT             30 minutes  # Output interval.
FLUSHING_PTS            3           # Grid cells defining the
15    5                             # flushing region.
16    5
17    6
```

The flushing region may also be distributed over multiple cells horizontally using blocks:

```
FLUSHING_BLOCKS      3          # Number of entries
12 25                           #1: (i,j) location
(2,5)-(10,11)                   #2: (i,j) range
24 27                           #3: (i,j) location
```

If a range is given, SHOC will determine only those cells within the range that are wet.
A region file (see Section 4.29.16) may also be used to specify the flushing region:

```
FLUSHING_REGION      region.bnc 3 4 ... n   # Region file and numbers
```

Invoking the flushing tracer diagnostic will automatically create a tracer named ‘flush’ with the following attributes:

```
TRACER5.name            flush
TRACER5.long_name       Flushing tracer
TRACER5.units           mgL-1
TRACER5.fill_value      0.0
TRACER5.valid_range     0 1
TRACER5.diagn           0
TRACER5.advect          1
TRACER5.diffuse         1
```

The flushing tracer concentration is automatically initialised to 1.0 within the flushing region and zero elsewhere during startup. The flushing region is defined by listing a series of (i,j) locations, whose total number is `FLUSHING_PTS`. The (i,j) locations of any sub-region of the domain may be retrieved using the ‘marked’ facility in `jvismeco`. The total mass in the flushing region is printed to the time-series file ‘flushing.ts’ at the time interval `FLUSHING_DT`. This time-series file contains the total mass in the flushing region, the normalised mass (i.e. the ratio of total mass : total initial mass) and the flushing time. The flushing (e-folding) time can be calculated from this output, i.e. the time when the normalised mass falls below 1/e. When this occurs the flushing time variable in the time-series file will assume this time value. Subsequent to this flushing time being reached, the initial concentration is re-set after a further two flushing times.

4.30.5 Age tracer

An age tracer may be specified, where the value of the age tracer is indicative of the time the tracer has spent in a defined region. The region may be defined using a list of points, blocks or a region. If the tracer lies within the specified region, it is incremented at a rate of 1 day^{-1},

and outside the specified region it is not incremented. To specify the region using a list of points use:

```
AGE_TR            3     # Number of points in the list
18    5                 # Points list.
19    5
20    6
```

Blocks can also be used to specify the region, e.g;

```
AGE_TR            3     # Number of points in the list
12 25                   #1: (i,j) location
(2,5)-(10,11)           #2: (i,j) range
24 27                   #3: (i,j) location
```

To specify the region using a region file (see Section 4.29.16);

```
AGE_TR   region.bnc 3 4 ... n   # Region file and numbers
```

In the above case the age region will comprise regions `3 4 ... n` of the region file `region.bnc`.

A depth range for the age region may be specified using:

```
AGE_RANGE   top_depth  bot_depth
```

If this is absent, the region encompasses the whole water column. The age tracer is named 'age' in output files and is generated automatically. Alternatively the age tracer may be manually specified in the tracer list.

4.30.6 Steric Height

The steric height within a domain can be calculated by specifying the flag:

```
STERIC_HEIGHT            lnm   # Level of no motion
```

Where *lnm* is a number corresponding to the level of no motion used in the steric height calculation. If this flag is set, a 2D tracer is automatically created to store the steric height output with units of metres. Steric height is defined as the geopotential anomaly divided by the acceleration due to gravity (e.g. Godfrey and Ridgeway, 1985). Geopotential anomaly is defined as:

$$\Delta\Phi = \int_{p1}^{p2} \delta dp$$

where $p_1 > p_2$ are any pressure levels and δ is the anomaly of specific volume where:

$$\delta = \alpha(S,T,p) - \alpha(35{,}0,p)$$

with $\alpha=1/\rho$ = the specific volume, S=salinity, T=temperature and p=pressure. For the steric height diagnostic the pressure p_1 is taken as the pressure at the level of no motion (*lnm* where it is assumed velocity=0) and p_2 is taken as the sea surface.

The geostrophic current relative to the level of no motion in the e_1 direction is then given by:

$$u_g = \frac{g}{f}\frac{\partial s_h}{\partial e_1}$$

where s_h is the steric height (m) and f is the Coriolis parameter. The gradient of steric height in the e_2 direction gives geostrophic velocity in the e_2 direction. If `lnm` =0 then the steric height diagnostic is not calculated.

4.30.7 Vorticity

The vorticity may be calculated and stored in 2-D tracer diagnostic variables by invoking the flag:

```
VORTICITY          <string>
```

Where `<string>` is a string containing `ABSOLUTE`, `RELATIVE`, `POTENTIAL`, `TENDENCY` or `NONE`, with;

```
ABSOLUTE    # absolute vorticity saved to tracer 'abs_vor' (s-1)
RELATIVE    # relative vorticity saved to tracer 'rel_vor' (s-1)
POTENTIAL   # potential vorticity saved to tracer 'pot_vor' (m-1s-1)
TENDENCY    # barotropic tendency terms saved to tracers (see below)
NONE        # no vorticity calculations performed
```

Relative vorticity is defined as:

$$\zeta = \frac{1}{h_1}\frac{\partial u_2}{\partial e_1} - \frac{1}{h_2}\frac{\partial u_1}{\partial e_2}$$

and absolute vorticity = ζ+f where f is the Coriolis parameter (equivalent to planetary vorticity). Potential vorticity is then defined as (Gill, 1982, p232):

$$\Pi = \frac{f+\zeta}{H+\eta} = cons\tan t$$

i.e. potential vorticity is equal to absolute vorticity divided by water depth and is conserved following the flow. Relative vorticity is calculated using the depth averaged velocity to provide a 2-dimensional vorticity diagnostics which are saved to the 2D tracers abs_vor, rel_vor and pot_vor.
The 2D relative vorticity equation is described in the SHOC Science Manual. The contributing terms to this balance are automatically generated and saved as 2D tracers if `TENDENCY` is specified. These tracers have the following attributes:

rv_drvdt	Temporal rate of change of relative vorticity (production of relative vorticity) (s^{-2}).
rv_nonlin	Nonlinear contribution to relative vorticity. Includes advection, metric terms and diffusion (s^{-2}).
rv_beta	Transport across contours of constant planetary vorticity (s^{-2}).
rv_strch	Vortex stretching, i.e. transport across f/H contours (s^{-2}).
rv_jebar	Joint Effect of Baroclinicity And Relief ; the contribution of the mass field to vorticity production (s^{-2}).
rv_wsc	Production of vorticity due to wind stress curl and the interaction of the wind stress with the gradient of topography (s^{-2}).
rv_bsc	Dissipation of vorticity due to bottom stress curl and the interaction of the bottom stress with the gradient of topography (s^{-2}).

4.30.8 Mixing Length Scale

The mixing length scale is saved to the diagnostic tracer `lscale` if this tracer is defined, e.g. if :

```
TRACER?.name            lscale
TRACER?.long_name       Mixing length scale
TRACER?.units           m
TRACER?.fill_value      0.0
TRACER?.valid_range     0 100
TRACER?.diagn           1
TRACER?.advect          0
TRACER?.diffuse         0
```

is defined then this tracer will be populated with the mixing length scale calculated in the Mellor-Yamada 2.0 k-ε or k-ω mixing schemes.

4.30.9 CFL Time-steps

The Courant-Friedrichs-Levy stability time-step (see section 2.7 Herzfeld et al, 2002) for barotropic and baroclinic modes, the Courant and Lipschitz stability criterion and horizontal diffusion stability limit may be calculated at every grid point and time-step. The CFL time-steps are saved to 2D diagnostic tracers in units of seconds. This is useful to precisely set the time-steps used by the model. An option exists to include the vertical advection Courant constraint (i.e. $w\Delta t/\Delta z < 1$) The minimum time-step for the simulation is printed to the diagnostic file 'diag.txt' (section 4.32). Options exist to adaptively alter the time-step used by the model to the CFL condition. This process is performed for a user defined time period. The CFL diagnostics are invoked via:

```
CFL   PASSIVE           # CFL calculated and output to tracers

      ACTIVE            # 2D and 3D time-steps are set to the minimum
      CFL_DT <x> days   # CFL time-steps at x days

      ACTIVE3D          # 3D time-step is set to CFL step whenever
      CFL_DT <x> days   # the CFL step becomes less than the 3D step
                        # and the simulation time is less than x
                        # days.
      |WVEL             # By or-ing WVEL to the above flags the
                        # vertical advection stability constraint
                        # (i.e. Courant number < 1) is included in
                        # the stability calculation.
```

An example of the CFL stability diagnostic is:

```
CFL         AVTIVE3D|WVEL
CFL_DT      20 days
```

Tracer names in output files for these stability limits are:

```
cfl2d       # 2D CFL stability time-step
cfl3d       # 2D CFL stability time-step
courant     # Courant stability time-step
lipschitz   # Lipschitz stability time-step
diffstab    # Horizontal diffusion stability time-step
```

4.30.9.1 Heat Flux Diagnostics

If the heat flux is calculated (see section 4.17) then the components of the heat flux are automatically written to 2D diagnostic tracers. The attributes of these tracers are listed below.

Heat Flux Diagnostic Attributes

2D Tracer Name	Description	Units
swr	Short wave radiation	Wm^{-2}
lwr	Long wave radiation	Wm^{-2}
shf	Sensible heat flux	Wm^{-2}
lhf	Latent heat flux	Wm^{-2}
nhf	Net heat flux	Wm^{-2}

4.30.10 Momentum Balance Tendencies

The contribution to each of the terms in the 3D momentum balance may be saved to 3D diagnostic tracers. These variables will then appear in any specified output netCDF and time-series files. These diagnostics are invoked by invoking the flag:

```
MOM_TEND            YES
```

This diagnostic automatically generates the following tracers (with units ms^{-1}) representing the momentum tendencies when the `MOM_TEND` flag is invoked

```
u1_adv      u1 advective tendency
u1_hdif     u1 horizontal diffusion tendency
u1_vdif     u1 vertical diffusion tendency
u1_btp      u1 barotropic pressure gradient tendency
u1_bcp      u1 baroclinic pressure gradient tendency
u1_cor      u1 Coriolis tendency
u1_sto      u1 Stokes Coriolis and vortex forces

u2_adv      u2 advective tendency
u2_hdif     u2 horizontal diffusion tendency
u2_vdif     u2 vertical diffusion tendency
u2_btp      u2 barotropic pressure gradient tendency
u2_bcp      u2 baroclinic pressure gradient tendency
u2_cor      u2 Coriolis tendency
u2_sto      u1 Stokes Coriolis and vortex forces
```

The Stokes tendencies are only generated for `waves = STOKES` (see Section 4.20).

```
mom_balance A code representing the maximum term in the momentum
            balance, where the code:
            1 = advection
            2 = horizontal diffusion
            4 = vertical diffusion
            8 = Coriolis
            16 = barotropic pressure
            32 = baroclinic pressure
```

The sum of the momentum diagnostic tracers for u1 or u2 velocity is equal to the total change in velocity over the time-step. If the MOM_TEND flag is set to NO but any of the above tracers are included in the parameter file, then the momentum tendency corresponding to just that tracer will be calculated. This diagnostic will not work in the 2D mode.

4.30.11 Tracer Tendencies

Tracer tendencies can be saved to 3D diagnostic tracers using:

```
TRA_TEND     <tr_name>
```

where <tr_name> is the name of a tracer in the tracer list for which the tendencies are to be computed. The units of the tendencies are the same as that of the nominated tracer, and the following diagnostic tracers are automatically generated;

```
<tr_name>_adv          advective and horizontal diffusive tendency
<tr_name>_vdif         vertical diffusive tendency
<tr_name>_ncon         non-conservative tendency
```

4.30.12 Selective Momentum Calculations

The terms in the 2D and 3D momentum balance (i.e. advection, horizontal diffusion, vertical diffusion, barotropic pressure gradients, baroclinic pressure gradients and Coriolis) may be selectively omitted from the momentum calculation via the flags:

```
U1_OMIT     <string>
U2_OMIT     <string>
U1AV_OMIT   <string>
U2AV_OMIT   <string>
```

Where <string> is a string containing ADVECT, HDIFF, VDIFF, PRESS_BT, PRESS_BC or CORIOLIS. This facility is useful for diagnosing the source of instability in the model. The baroclinic contribution is only omitted from the 2D mode if it is also omitted from the 3D mode.

4.30.13 Diagnostic numbers

A variety of diagnostic numbers can be computed at every time-step. These are invoked via the NUMBERS diagnostic as follows:

```
NUMBERS      <string>
```

Where <string> is a string containing BRUNT, INT_WAVE, RICHARDSON_GR, RICHARDSON_FL, REYNOLDS, FROUDE, ROSSBY_IN, ROSSBY_EX, SOUND, SHEAR_V, BUOY_PROD, SHEAR_PROD, SPEED_2D, SPEED_3D, SPEED_SQ, SIGMA_T, UNIT or ALL_NUMBERS. These diagnostics are computed as follows:

BRUNT : Brunt-Vaisala (buoyancy) frequency (s^{-1}), N, where;

$$N^2 = -\frac{g}{\rho_o}\frac{\partial \rho_o}{\partial z}$$ (Gill, 1982, eqn 6.4.9).

INT_WAVE : Internal wave speed (ms^{-1}). For constant N the n^{th} mode long wave phase speed is approximated by:

$$c_n = \frac{NH}{n\pi}$$ (Gill, 1982, eqn 6.11.1)

where H is the water depth. Mode 1 internal waves are produced as this diagnostic.

RICHARDSON_GR : Gradient Richardson number (dimensionless), where;

$$Ri = \frac{N^2}{\left(\partial u / \partial z\right)^2} \qquad \text{(Dyer, 1997, eqn 4.2)}$$

If Ri > 0 flow is stable
Ri = 0 flow is neutral
Ri < 0 flow is unstable

RICHARDSON_FL : Flux Richardson number (dimensionless), where;

$$Rf = \frac{K_z Ri}{V_z} \qquad \text{(Dyer, 1997, p54)}$$

REYNOLDS : Reynolds number (dimensionless), where;

$$\mathrm{Re} = \frac{uD}{\upsilon} \qquad \text{(Dyer, 1997, eqn 4.1)}$$

The diagnostic produced uses layer thickness for D and vertical eddy viscosity, V_z, for the kinematic viscosity, υ.

FROUDE : Interfacial Froude number (dimensionless) where;

$$Fr^2 = \frac{u^2}{c_n^2} \qquad \text{(Dyer, 1997, p42)}$$

The internal wave speed used is that from the INT_WAVE diagnostic.
If Fr < 1 flow is sub-critical
Fr = 1 flow is critical
Fr > 1 flow is super-critical.
Note, Dyer (1997, p43) states critical flow occurs at Fr = 0.33 for continuous stratification.

ROSSBY_IN : Internal Rossby radius (m), where:

$$Ro_i = \frac{c_n}{|f|} \qquad \text{n = 1,2,3… (Gill, 1982, eqn 7.5.4)}$$

The mode 1 internal Rossby radius is supplied as the diagnostic.

ROSSBY_EX : External Rossby radius (m), where:

$$Ro_i = \frac{\sqrt{gH}}{|f|} \qquad \text{(Gill, 1982, p 207)}$$

SOUND : Speed of sound given by:

$$c = c(S,T,Z) = c_o + \alpha_o(T-10) + \beta_o(T-10)^2 + \gamma_o(T-18)^2 + \delta_o(S-35) + \varepsilon_o(T-18)(S-35) + \zeta_o|z| \qquad \text{(Apel, 1887, eqn 7.19)}$$

where c_o=1493.0, α_o=3.0, β_o=-0.006, γ_o=-0.04, δ_o=1.2, ε_o=-0.01 and ζ_o=0.0164. This equation is believed to be accurate to within $\pm$0.2 ms^{-1}. Sound channels are defined as the depth

where a change of sign in the sound speed gradient occurs, i.e. where the curvature of the sound profile is equal to zero. The vertical representation of all variables in SHOC occupies discrete vertical layers arranged at variable depths, usually with higher resolution at the surface (and being dependent on maximum water depth). Therefore, the speed of sound is also only provided at discrete depths. In SHOC the sound channels are simply computed from a linear interpolation between two layers where the gradient of sound speed changes. The gradient of sound speed is computed with a 4th order approximation:

$$\frac{\partial c}{\partial t} \sim dcdk_k = \frac{4}{3}\frac{c^t_{k+1} - c^t_{k-1}}{2h} - \frac{1}{3}\frac{c^t_{k+2} - c^t_{k-2}}{4h}$$

Where *C* is the sound speed, *k* is the vertical index and *h* is the layer thickness. Layers *k* and *k-1* are identified where $dcdk_k / dcdk_{k-1} < 0$, and the sound channel depth, D_k, is then given by:

$$D_k = d_k - dcdk_k (d_{k-1} - d_k) / (dcdk_{k-1} - dcdk_k)$$

where d_k is the depth of layer *k*. Sonic depth and sound channel depths are provided along with the speed of sound when this diagnostic is invoked.

SHEAR_V : The vertical velocity shear magnitude (s^{-1}), defined by:

$$\left|\frac{\partial \vec{v}}{\partial z}\right| = \sqrt{(\partial u_1 / \partial z)^2 + (\partial u_2 / \partial z)^2}$$

BUOY_PROD and SHEAR_PROD : These diagnostics are assigned from the closure scheme used, where buoyancy production, B (m^2s^{-2}), and shear production, P (m^2s^{-2}), are defined by (e.g. Burchard et al, 1998, eqn. 9):

$$P = V_z \left[(\partial u_1 / \partial z)^2 + (\partial u_2 / \partial z)^2\right]$$

$$B = K_z N^2$$

where N^2 is the Brunt-Vaisala frequency (see above). Note that these diagnostics are extracted directly from the mixing scheme used, and may differ for different schemes (e.g. some schemes add a correction for internal wave shear to P).

SPEED_2D : Depth averaged current speed (ms^{-1}) , given by:

$$|U| = \sqrt{U_1 * U_1 + U_2 * U_2}$$

SPEED_3D : Three dimensional current speed (ms^{-1}) , given by:

$$|u| = \sqrt{u_1 * u_1 + v_2 * v_2}$$

SPEED_SQ : Three dimensional current speed squared (m^2s^{-2}) , given by:

$$u^2 = u_1 * u_1 + v_2 * v_2$$

WIND_CD : The momentum drag coefficient given by the function in Section 4.14.

OBC_PHASE : Open boundary phase speed for elevation, as given by radiation conditions in Science Manual Section 4.6. The phase speed is bounded by the CFL condition

($0 \leq phase \leq 1$); if waves are incoming then the phase is negative, hence bounded to zero. Out-going waves have the phase > 0.

SIGMA_T : σ_T (kgm^{-3}) is output as dens_0 – 1000.

ENERGY : Mechanical energy (Jm^{-3}) given by (Kowalik and Murty (1993), eqn. 1.24):

$$E_T = E_k + E_p = \tfrac{1}{2}\rho(u_1^2 + u_2^2 + w^2) + \rho g \eta$$

KINETIC : Kinetic energy (Jm^{-3}) given by (Kowalik and Murty (1993), eqn. 1.24):

$$E_k = \tfrac{1}{2}\rho(u_1^2 + u_2^2 + w^2)$$

SLOPE : Computes the surface slope in the e1 and e2 directions, stored in surf_slope_x and surf_slope_y respectively.

SURF_LAYER : The k index of the surface layer is stored in the 2d array surf_layer.

BOTSTRESS : Bottom stress in e_1 and e_2 directions, and bottom stress magnitude.

WET_CELLS : A diagnostic to show wet and dry cells. Water columns are assigned the percentage of water they contain relative to being dry; i.e. a dry water columns is assigned 100%, cell with sea level at msl is assigned 0 and when sea level rises the percent dry is negative. If sea level falls to half the water depth, the cell is 50% dry. Note that a cell is considered dry when the water falls below DRY_FRAC * HMIN, where DRY_FRAC is currently hardwired to 0.05 and HMIN is defined in Section 4.4; e.g. if HMIN = 0.07 m, then cells dry when the sea level gets within 3.5 mm of the bottom.

UNIT : A passive tracer with an initial value of 1. Good for testing the constancy condition in transport models.

DUMMIES : Three generic 3D dummy variables (dum1, dum2 and dum3) are created for hardwiring debugging diagnostics internally in the code.

ALL_NUMBERS Invokes all the diagnostic numbers.

4.30.14 Tracer percentiles

The tracer percentile diagnostic calculates the spatial distributions of percentiles of a snapshot of a given tracer distribution, i.e. it shows the spatial position of the percentile values of a given tracer at a particular time. This diagnostic is useful for determining the position in a domain where e.g. a median, 95 %ile or 5%ile tracer concentration may be found. This diagnostic is time dependent, but if a mean is created using the tracerstats library, then the position in the domain where the average of a particular percentile (e.g. average median over a simulation) may be determined. The percentile calculation of tracer is invoked by specifying a tracer name, e.g;

```
CALC_PERCS          salt    # Name of tracer for percentile calculation
```

A 3D tracer containing the specified tracer percentiles is automatically created with the tracer name appended to 'percentile_' e.g. in this case 'percentile_salt'.

4.30.15 Alerts

The alert diagnostic attempts to detect early signs of instability by monitoring maximum absolute velocities, divergences and, if invoked, maximum absolute momentum tendencies. These maximums are written to an alert diagnostic file every time-step, along with the maximums encountered during the whole simulation. A time series file containing the history of the maximum values is also created. To invoke alert tracking in passive mode:

```
ALERT       PASSIVE <alert_file>
ALERT_DT    1 hour
```

Where `<alert_file>` is an optional filename to write the maximum value information to. This file name is appended with '`.txt`'. If `<alert_file>` is absent then output is written to the file '`alert.txt`' by default. If `ALERT_DT` is present then a time series file is created with the alert filename appended with '`.ts`', and maximum values are output at the specified time interval. The maximum values printed to file are absolute maximum values. Note that maximum tendencies are only printed if the `MOM_TEND` flag is invoked. The mechanical energy, excess mass (mean sea level) and boundary energy flux are defined according to Palma and Matano (1998) and are useful for diagnosing the stability of a domain;

$$\text{Mechanical Energy} = \frac{1}{A}\left[\int_A \rho g \eta^2 dA + \int_A 0.5\rho D(U_1^2 + U_2^2)dA\right] \quad (\text{Jm}^{-2})$$

$$\text{Excess Mass} = \frac{1}{A}\int_A \eta dA \quad (\text{m})$$

$$\text{OBC Energy Flux} = \frac{1}{W}\int_W DU_1(g\eta + 0.5U_2^2)\Delta y \quad (\text{m}^4\text{s}^{-3})$$

Where A = domain area, W = OBC width (the energy flux is for a `u1` boundary in this case, see Section 3.11). Note that ρ(OBC Energy Flux) has units Wm^{-1}.

Alert tracking may be made active using the following:

```
ALERT       ACTIVE <alert_file>
```

Using the `ACTIVE` alert mode, when a maximum value exceeds defined thresholds then specific action is taken. This action falls into three categories:

`LEVEL1` : 2D or 3D velocities exceed the `VELMAX` parameter. Horizontal diffusion is increased to the value $\Delta x^2/4\Delta t$ which most effectively damps the shortest waves possible in the grid (Kowalik and Murty, 1993, eqn. 3.141). Velocity thresholds may be defined using the following parameters:

```
VELMAX     2      # Maximum horizontal velocity (ms-1)
WMAX       1e-3   # Maximum vertical velocity (ms-1)
```

`LEVEL2` : 2D divergence = $\partial\eta/\partial t$, or 3D divergence = $\partial w/\partial z$ exceed a (hardwired) threshold. The Shapiro (1970) smoothing filter is applied to the relevant velocity field (Kowalik and Murty, 1993, eqn. 3.136)

`LEVEL3` : momentum tendencies exceed (hardwired) thresholds. The relevant process is omitted during the next time-step.

Individual alert actions can be turned on or off by prescribing `0` or `1` for each individual action::

```
            eta vel2d vel3d w tend 2d_div 3d_div cfl ts shear hdiff
ALERT_CODE  1     1     1   0   0    0       0    0   0  1      1
```

Alert information written to file has the following format (note: indexes in brackets are in Cartesian coordinates, outside the brackets are sparse coordinates);

```
Simulation time = 10.000000 (days)

Maximum absolute sea level :
elevation :  0.248644 at 26 (25 1 22)

Maximum absolute velocity :
u1 3D     :  0.203112 at 1226 (1 25 22)
u1 2D     :  0.093261 at 1066 (45 21 22)
u2 3D     :  0.093234 at 1225 (0 25 22)
u2 2D     :  0.001336 at 1023 (2 21 22)
w         :  0.000044 at 12290 (49 25 14)
Div 3D    :  0.000004 at 1249 (24 25 22)
Div 2D    :  0.000000 at 767 (1 16 22)

Maximum absolute tendencies :
u1 velocity
u2 velocity

Area averaged energy :
Mechanical energy  : 231.513328 (J/m2)
Excess mass        : -0.003424 (m)
Energy flux (W/m2) :
    Boundary 0 (West) : 2.276448
    Boundary 1 (East) : 2.272259

---------------------------------------
Simulation maximum absolutes

eta      : 0.248644
u1 3D    : 0.203115
u1 2D    : 0.093282
u2 3D    : 0.121123
u2 2D    : 0.006932
w        : 5.72e-05
div 3D   : 5.20e-06
div 2D   : 3.60e-06
```

4.30.16 Total mass, volume, heat and salt

The total mass, volume, heat and salt in the domain, useful for diagnosing conservation properties, may be output in time series format. The totals are output to the time-series file ‘totals.ts’ . If `OutputPath` is set, then the totals file will reside in this directory. To invoke the totals diagnostic use:

```
      TOTALS            YES     # Invoke totals diagnostic
      TOTALS_DT         1 hour  # Interval to print totals.
                                # The default is 1 hour.
```

The default is for no totals to be calculated. The output timeseries file consists of the following:

```
## COLUMNS 5
##
## COLUMN1.name  Time
## COLUMN1.long_name  Time
## COLUMN1.units  days since 1990-01-01 00:00:00 +10
```

```
## COLUMN1.missing_value -999
##
## COLUMN2.name  Total mass
## COLUMN2.long_name  Total mass
## COLUMN2.units  kg
## COLUMN2.missing_value  0.000000
##
## COLUMN3.name  Total volume
## COLUMN3.long_name  Total volume
## COLUMN3.units  m3
## COLUMN3.missing_value  0.000000
##
## COLUMN4.name  Total heat
## COLUMN4.long_name  Total heat
## COLUMN4.units  deg C m3
## COLUMN4.missing_value  0.000000
##
## COLUMN5.name  Total salt
## COLUMN5.long_name  Total salt
## COLUMN5.units    psu m3
## COLUMN5.missing_value  0.000000
##
```

Additional tracer totals may be computed by appending the tracer name to the `TOTALS` diagnostic, e.g;

```
# Include ‘silt’ and ‘Chla’ in totals diagnostic
TOTALS            YES silt Chla
```

The additional tracer totals will then appear in the time series. Note that `temp` and `salt` are always included. If a tracer included a sediment component, then the total mass is the sum of mass in the water column and the sediment. If the tracer is a 2D tracer, then the areal mean is reported.

Finally the volume flux through each open boundary, in m^3s^{-1}, is computed.

4.30.17 De-correlation length scales

The de-correlation length scales in the `e1` and `e2` directions can be computed and stored in `decorr_e1` and `decorr_e2` respectively. This is computed according to Romanou et al, 2006. The length scale is calculated on a sub-set of the grid, where the user specifies the length scale of the sub-set, `sz`. The de-correlation length scale is invoked using;

```
DECORR_LENGTH     <variable> sz <scale>
```

where `<variable>` may be;

```
<variable>        eta   # Sea level de-correlation length scale
                  u1    # u1 velocity
                  u2    # u2 velocity
                  any valid 3D tracer name (e.g. temp, salt)
```

`<scale>` is a scaling factor for `sz`; e.g. if `<scale>` = `km` then the sub-set size `sz` is assumed to be in kilometres, and output length scales will also be in km. The default is metres if `<scale>` is absent; e.g;

```
DECORR_LENGTH     temp 1000   # Temperature de-correlation length
                              # scale using sub-set size of 1000m.
```

4.30.18 Mass Budgets

The model domain can be arbitrarily divided into a number of regions for which mass and volume budgets can be computed over a predefined period. A netCDF file containing the region partitions (usually appended with '.bnc') must first exist. These files can be created using the 'BOX CREATION' option in PLUM. Instructions for creating regions in PLUM are as follows:

1. Enter PLUM in Matlab.
2. Click on GRID CREATION and then Read NETCDF File to read in the Shoc grid information.
3. Click on Draw/Erase Grid to remove the grid line detail, leaving just the bathymetry.
4. Return to Main Menu and click on BOX CREATION, and then Create New Boxes to draw required boxes over the bathymetry. Note that instructions are provided in the matlab window.
5. Click on Edit Boxes to optimize the regions.
6. Click on Partition SHOC to partition all of the water cells into the 2D regions.
7. Click on Assign Box Layers as many times as there are regions that are required to be a function of depth; e.g. enter a vector such as [4 0 -20 -40 -100] to create 3 layers in Box 4 with layer faces at 0, -20, -40 and -100m. A maximum of 5 layers can only be assigned to any box. The depth slider can be used to scan layers and observe the different 3D regions.
8. The output is saved to a '.bnc' file. This can be read back via Read netcdf File at a later date to make more changes by repeating the above procedure.

Any '.bnc' file that SHOC attempts to read must contain the variable 'boxnos', and have the dimensions 'i_centre', 'j_centre' and 'k_centre' to specify the grid size in x,y and z directions respectively. **Note:** *be sure that .bnc files are created for the input file you wish to use.* If the variable regionid in the output file shows values of -9999 as region numbers, then this is probably not the case and region exchanges may be incorrect. A warning is only issued if the grid dimensions in the .bnc and input file differ (# wet cells are not compared).

To invoke the budgets over the regions, use:

```
REGION      path/name.bnc  # Path and filename of the .bnc region
                           # file.
REGION_DT   10 days        # The time interval over which the
                           # budgets are computed.
REGION_VARS passive        # Tracers for which the budgets are
                           # computed.
```

The variables 'salt' and 'temp' are always computed by default (i.e. these variables do not need to be specified in REGION_VARS. A volume budget is also created by default. The keywords MONTHLY, SEASONAL and YEARLY may be input as REGION_DT, and ALL, TRACERS_WC and TRACERS_DIAGN_WC may be used for REGION_VARS.

Output is created for each region in the ascii file region*.ts where * is the region number. If OutputPath is present, the files will be written to this directory. These files contain the mass at the start of the interval REGION_DT for each variable, mass at the end of the interval, the mean mass and standard deviation over the interval, the mass fluxes through segments connecting regions or through open boundaries (i.e. mass transfers from region to region, or across open boundaries) and the mass budget of the region, where:

```
mass budget = start mass + mass fluxes – end mass
```

Note that the mass fluxes are positive if mass is imported into the region, and negative if mass exits the region. If the budget is not approximately zero, then this means that there has been net import of mass into (positive budget) or export from (negative budget) the region. This may be due to a point-source/sink delivering mass into the region over the interval, fluxes through the surface or sediment or non-conservative processes associated with the tracer. The mean concentration in the region can be computed using mean mass divided by mean volume.

The mass fluxes in the hydrodynamic model are computed using the same fluxes as are used to update tracer advection, which are basically the (tracer concentration at a cell face) x (velocity through the face) x (area of the face) x (model time-step). The transport model computes fluxes by multiplying any interpolation weights that lie outside the region by the mass of the destination cell. Both these methods are inaccurate near open boundaries; the hydrodynamic model because conservation is not respected in the boundary cell, and the transport model because a source cell for outflow may be a destination cell beyond the domain grid. These issues can be overcome by effectively migrating the open boundary location into the domain or creating extra 'boundary' regions for which it is acknowledged that the mass budget will be inaccurate. To migrate a boundary into the interior, use;

```
REGION_MODE       OBC_BDRY    # Migrate OBC into the interior
REGION_OBC_ZONE   1           # Number of cells to migrate the OBC
```

For the hydrodynamic model it is sufficient to migrate the boundary only 1 cell, and this is recommended (a warning is displayed if this is not the case). To create new regions adjacent to open boundaries, use;

```
REGION_MODE       OBC_AREA    # Migrate OBC into the interior
REGION_OBC_ZONE   5           # Cell width of the OBC regions
```

Regions may be used with multiple windows for the hydrodynamic model, but must be used with one window with the transport model. When `REGION` is used, the region partitions are written to the variable `regionid`, which is written to the output files.

For the transport model the update rule for tracer concentration c_i^t in destination cell *i* is:

$$c_i^t = \sum_j a_{ij} c_j^{t-1}$$

where c_j^{t-1} is the tracer concentration in source cell j at time *t-1*. The mass at time *t* in destination cell *i* is $c_i^t V_i^t$, therefore $a_{ij} c_j^{t-1} V_i^t$ can be regarded as a mass transfer from cell *j* to cell *i*. This is the basis of our mass conservation analysis. It follows that $a_{ij} c_j^{t-1} V_i^t$ is also a mass transfer from region r_j to r_i. If the total mass fluxes between regions is to be computed, then all these mass transfers are required to be cumulated. For the transport model, the mass budget is represented as:

```
start mass + mass fluxes + mass error + global fill = end mass
```

and as above, denoting the budget as:

```
mass budget = start mass + mass fluxes – end mass
```

then:

```
mass budget + mass error + global fill = 0
```

Here `mass error` is the mass conservation error for source cells in a region, and global fill is the mass change in the region due to the global filling algorithm. The former errors arise from using the non-conservative semi-Lagrangian advection scheme and an underlying flow field that is non-conservative (see Section 9.3). These errors are rectified globally using the global

fill (i.e. mass is conserved over the whole domain), but this manifests as an input or removal of mass within a region, which is represented by `global fill`. If global filling is not invoked, then this error is zero.

If `ALL_TRANSFERS` is included in `REGION_MODE` when using the transport model, then mass or volume transfers from all defined regions are reported (as opposed to only those that share common boundaries).

The residence time for each region is output in each time-series file, and as a tracer in netCDF output having the name `residence`. This time is computed over the interval `REGION_DT`. The residence time in this case is the time it takes for the volume in each region to be turned over (i.e. replaced with water from other regions) due to volume fluxes through the region perimeters or open boundaries. Note that this must be considered in the context of the time and space scales of dynamics in play, and the size and location of the region. For example, a small region in an area of large tidal flow will have a small residence time, which may not be informative for, e.g. the time it takes fresh water deposited in the region to become saline again (since the tidal current may have a large instantaneous flux but a small residual). This residence time is also listed in the region output timeseries files. Additionally, the residence time computed using the net flow through the region perimeters (i.e. the sum of incoming and outgoing fluxes) is listed in this file under `residence_time_net`. This is the time it would take the residual flow to turn the volume within the region over.

4.30.19 Diagnostic tracer names

The following table lists the tracer names (2D and 3D) associated with each diagnostic. These names must be used when attempting to output the relevant diagnostic to file.

Diagnostic name	Purpose	Tracer names
CALC_FLUXES	Tracer flux calculation	flux_e1, flux_e2, flux_w, flux_kz
MEAN VEL3D	3D mean velocity (ms^{-1})	u1mean, u2mean, wmean
MEAN VEL2D	2D mean velocity (ms^{-1})	u1av_mean, u2av_mean
MEAN ETA	Mean sea level (m)	eta_mean
MEAN KZ	Mean vertical diffusivity (m^2s^{-1})	Kzmean
MEAN WIND	Mean wind (Nm^{-2} or ms^{-1})	w1mean, w2mean
MEAN VOLFLUX	3D mean volume flux (m^3s^{-1})	u1vmean, u2vmean
MEAN TS	Mean temperature and salinity	temp_mean, salt_mean
MIX_LAYER	Mixed layer depth (m)	mixed_layer
FLUSHING_TR	Flushing tracer	flush
STERIC_HEIGHT	Steric height (m)	steric
VORTICITY ABSOLUTE	Absolute vorticity (s^{-1})	abs_vor
VORTICITY RELATIVE	Relative vorticity (s^{-1})	rel_vor
VORTICITY POTENTIAL	Potential vorticity ($m^{-1}s^{-1}$)	pot_vor
VORTICITY TENDENCY	Vorticity tendencies (s^{-2})	rv_drvdt, rv_nonlin, rv_beta, rv_strch, rv_jebar, rv_wsc, rv_bsc
MIXING_SCHEME	Mixing length scale (m)	lscale
CFL	CFL stability criterion (s)	cfl2d, cfl3d
MOM_TEND	Momentum tendencies (ms^{-1})	u1_adv, u1_hdif, u1_vdif, u1_btp, u1_bcp, u1_cor u2_adv, u2_hdif, u2_vdif, u2_btp, u2_bcp, u2_cor
HEATFLUX	Heat flux components (Wm^{-2})	swr, lwr, shf, lhf, nhf
WAVE_VARS	Wave variables	wave_amp, wave_period wave_dir, wave_ub, ustrcw
WAVES	Wave bottom drag Wave radiation stress	wave_Cd wave_Sxy, wave_Syx
BRUNT	Brunt-Vaisala frequency (s^{-1})	brunt_vaisala
INT_WAVE	Internal wave speed (ms^{-1})	int_wave_speed
RICHARDSON_GR	Gradient Richardson number	richardson_gr
RICHARDSON_FL	Flux Richardson number	richardson_fl
REYNOLDS	Reynolds number	reynolds
FROUDE	Interfacial Froude number	froude
ROSSBY_EX	External Rossby radius (m)	rossby_external
ROSSBY_IN	Internal Rossby radius (m)	rossby_internal
SIGMA_T	Sigma_t, σ_t (kgm^{-3})	sigma_t
SOUND	Speed of sound (ms^{-1})	sound
	Sonic layer depth (m)	sonic
	Sound channels (m)	sound_channel
SHEAR_V	Vertical shear (s^{-1})	shear_vert
BUOY_PROD	Buoyancy production (m^2s^{-2})	buoy_prod
SHEAR_PROD	Shear production (m^2s^{-2})	shear_prod
SPEED_2D	2D Current Speed (ms^{-1})	current_speed_2d

ENERGY	Mechanical energy (Jm^{-3})	energy
KINETIC	Kinetic energy (Jm^{-3})	kenergy
SPEED_3D	3D Current Speed (ms^{-1})	current_speed_3d
SPEED_SQ	3D Current Squared (m^2s^{-2})	speed_sq
WIND_CD	Momentum drag coefficient	wind_Cd
UNIT	Unit passive tracer	unit
OBC_PHASE	OBC phase speed (ms^{-1})	obc_phase
CALC_PERCS	Tracer percentiles (%)	percentile_<tr name>
ALERTS	Alert information	alerts_actual alerts_cumulative
SHOW_WINDOWS	Window partitions	windows
WET_CELLS	Wet cell diagnostic	wet_cells
SHOW_LAYERS	Layer thickness (m)	layer_thick
BOTSTRESS	Bottom stress	tau_be1, tau_be2, tau_bm
SURF_LAYER	k index of surface layer	surf_layer
SLOPE	Surface slope (mm^{-1})	surf_slope_x, surf_slope_y
REGION	Region budgets	regionid
AGE	Age tracer	age
DECORR_LENGTH	De-correlation length scale	decorr_e1, decorr_e2
Particle tracking invoked	Particle concentration	ptconc

4.31 Data variables and input time-series files

There are a variety of parameters in SHOC for specifying input time-series datafiles (e.g. `WIND_TS john.hunter@utas.edu.au, BOUNDARY?.DATA`). It is expected that:

- The datafile specified be either a NetCDF or ASCII time-series datafiles
- The files conform to the coordinate conventions described in section 10.
- The files contain the necessary variables name(s) for the parameter.

Following is a list of the parameters names and the variables that each parameter expects to find in the datafile:

Parameter name	***Expected variable names in datafile***	***Substitution names***
`AIRTEMP`	air_temp	air_temp
`BOUNDARY?.DATA (elevation)`	eta	eta
`BOUNDARY?.DATA (u1)`	u1 or u and v	u1 or u and v
`BOUNDARY?.DATA (u2)`	u2 or u and v	u2 or u and v
`BOUNDARY?.DATA (tracers)`	tracer-name	tracer-name
`CLOUD`	cloud	cloud
`ETA_RELAXATION_FILE`	eta	eta
`EVAPORATION`	evaporation	evaporation
`HUMIDITY`	humidity	humidity
`ORBITAL_VEL`	ub	ub
`WAVE AMPLITUDE`	amplitude	amplitude
`WAVE PERIOD`	period	period
`WAVE DIRECTION`	direction	direction
`PRESSURE`	pressure	pressure
`PRECIPITATION`	precipitation	precipitation
`WET_BULB`	wet_bulb	wet_bulb
`RADIATION`	swr	swr
`TRACER?.RELAXATION_FILE`	tracer-name	tracer-name
`TRACER?.DATA`	tracer-name	tracer-name
`WIND_TS`	u, v	wind_u, wind_v

4.31.1 Variable substitution

Since it is not always possible to supply datafiles with exactly the required variables names, **SHOC** permits the expected variable name to be substituted for an alternate name. This is done by assigning (=) the new variable name to the default expected variable name. Multiple assignments are separated by commas . The assignments are enclosed within parentheses. No whitespace is permitted.

For example, for a standard file assignment such as:

```
WIND_TS windfile.ts
```

SHOC would search for the variables `u` and `v` within `windfile.ts`. If these variables were not present then **SHOC** would quit with an error. If however, there were two variables called `wu` and `wv` then the following substitution could be used.

```
WIND_TS windfile.ts(wind_u=wu,wind_v=wv)
```

4.31.2 Multiple datafiles

At this time the specification of multiple datafiles is only permitted when defining boundary inputs, wind files, relation and resetting. Following is an example of how to substitute variable names and specify multiple time-series files for a boundary parameter:

```
BOUNDARY1.DATA t1.nc(salt=salinity) t2.nc(temp=tmp)
```

A list of files may be included in a separate text file, to which the boundary (or wind etc) specification may define, e.g. a multi-file-netcdf text file, `boundary.mnc` may be generated having the following format:

```
multi-netcdf-version 1.0
nfiles 2
file0.filename   t1.nc
file1.filename   t2.nc
```

Boundary data may then be defined via (with variable substitution included):

```
BOUNDARY1.DATA boundary.mnc(salt=salinity)(temp=tmp)
```

This is a convenient method of specifying a long list of files as input.

4.31.3 Model variable initialisation

At the start of a model run, the model variables are initialised for each grid using a netCDF input file which is either generated from the parameter file using the `-g` option, or obtained from the output of a previous run. This initialisation input file for each grid is specified as follows:

```
INPUT_FILE  in.nc
```

The input file may contain more than one record, the record is selected based on the `START_TIME` parameter for this run. The time in the datafile must match **exactly**.

4.31.4 Model variable output

SHOC provides two mechanisms for recording its results: ASCII time-series of values as computed for particular locations and as an n-dimensional netCDF datafiles.

4.31.5 ASCII time-series

ASCII time-series output files contain values for significant model variables at specific locations. A time series file is created for each location in the model domain and records are written at a pre-determined interval. Currently the output variables include time, surface elevation, current components (2D and 3D), and tracers. Non-time dependent geometry information is also provided (cell centre, bottom depth, etc.) in the header. Time series output in **SHOC** are referenced to the free surface, mean sea level or the bottom.

ASCII time-series are convenient for comparisons with point observations (such as tide gauges or current meters).

```
# Number of time-series outputs.
TSPOINTS 2

# Parameters for each time-series point.
TS0.pname       MP1.ts                  # Filename prefix
TS0.location    319672.69 5758871.98 -4 # Location (X Y Z)
TS0.dt          1800 seconds            # Output interval.
TS0.reference   surface                 # reference level
TS0.vars        salt temp               # Tracer variables output
TS0.type        simple                  # Velocity output type

TS1.pname       MP2.ts
TS1.location    319672.69 5758871.98 -12.75
TS1.dt          0.5 hour
TS0.reference   bottom
```

The reference level is determined by the following:

```
TS0.reference  surface        # referenced to the free surface
TS0.reference  msl            # referenced to mean sea level
TS0.reference  bottom         # referenced to the bottom
```

An output type of `simple` will cell centre the velocity variables and rotate them onto the east-west / north-south axis. A `standard` type will print the velocity at the cell face relative to the e_1/e_2 grid orientation (i.e. as they are used by the model). The `simple type` is the default.

The default value is `reference = msl`. If the reference level is `surface`, then output will always occur at the specified depth below the free surface and if the free surface is fluctuating may not always be in the same cell. If the reference level is `msl` then output will be the specified depth below the undisturbed sea surface and will always be in the same cell if it is wet. Note that the depth below the free surface may change in this case. If the reference level is `bottom` then output is the specified depth above the bottom. This will always occupy the same cell providing the cell is wet. For the surface and bottom cases, the sign of the depth may be positive or negative.

If the `vars` field is absent then all tracers are included in the time series file.

Time series files are ASCII files, with a header containing information about the data in the files, and data in columns. Their format is described in section 11.1.

4.31.6 NetCDF dump files

More than one netCDF output dump file maybe specified in the **SHOC** parameter file. Each output file contains the grid geometry, times and selected model variables.

The number of output files are specified by the parameter `OutputFiles`. The parameters for each output are specified with the prefix `file<N>` where `<N>` is the output file number.

Four netCDF output conventions are supported by **SHOC**, the standard dumpfile output (as used when hot-starting a run), a simple format, a point array output or a sparse array output.

1. The `standard` output contains up to four staggered grid geometries, based on a Arakawa C-Grid.
2. The `simple` format contains only one grid geometry, with all data variables interpolated on to the cell centre. Velocity components are therefore represented as eastward and northward components, rather than components relative to the grid

used (i.e. e_1 and e_2 directions which may be spatially variable for curvilinear grids). Vector variables can be stored as vector components, or speed and direction.

3. The point array, `parray`, is essentially a standard output on user defined cells, therefore generally using significantly less disk space than other file formats. This is useful for outputting open boundaries for nesting purposes. Velocities are represented as eastward and northward components.
4. The `sparse` output contains a dump of the sparse format used internally in **SHOC**, i.e. a one dimensional vector of *only* the wet cells in the grid. If a large amount of the model grid contains land, the sparse format can therefore use significantly less disk space than standard formats, and is an extremely useful format to use in conjunction with the transport (-t) mode. Note that the sparse format cannot be sub-sectioned, i.e. the whole array must be dumped for 3D or 2D variables. The exception to this is that the surface only may be dumped if the filename is appended with '_surf'.
   (n.b. The sparse netCDF format does contain geographic information in the file and mappings from sparse position to Cartesian (i,j,k) locations. This information may be used to visualize a sparse format file directly. If a sparse format is to be read back into the model then it must be un-packed using the routine 'unpack_sparse()' to scatter the file data to wet cell locations).

```
# Specifying two output files for a grid.
OutputFiles              2

# Specify the path for output files. Time series files are also
# output to this path. If the SEQUENCE flag is invoked (Section
# 4.4) then /run<n> is appended to the path, where <n> is the
# run sequence number.
OutputPath               /home/data/output

OutputTransport          <tag>
# Output transport files. Files are created for each month with
# the name tag_trans_mmmyyyy.nc where 'tag' is the tag specified
# above, mmm is the month (e.g. 'jan') and yyyy is the year.
# Files are output in 'sparse' format. Variables output are:
# eta, u1mean, u2mean, wmean, temp, salt, Kzmean

# Output file 0
# The tag ALL for the vars parameter means the following
# variables are save to the output dump file.
# eta, u1, u2, w, u1av, u2av, topz, wtop, wind1, wind2, patm,
# dens, dens_0, Kz, Vz, Cd, u1bot, u2bot, u1vh, u2vh, flag
# all the tracers and ptconc if particle tracking is enabled.
# This is in addition to the coordinate variables.
#
# The following fields are manadatory.
file0.name               out.nc      # Output prefix.
file0.type               standard    # Standard dumpfile.
file0.tstart             0 days      # Output start time.
file0.tinc               1 day       # Output interval.
file0.tstop              44 days     # Output stop time.
file0.bytespervalue      4           # 2 – shorts
                                     # 4 - floats.
                                     # 8 - doubles
file0.vars               ALL         # ALL variables.

# Output file 1
# A spatial subset of the grid (possible for use in nesting).
# Notice only a subset of the variables are being output.
file1.name               nested_smp.nc
file0.type               simple      # simple output.
file0.tstart             0 days      # Output start time.
file1.tinc               1 hour      # Output interval.
```

```
    file1.tstop               44 days     # Output stop time.
    file1.bytespervalue       2           # Output as shorts.
    file1.vars                eta salt temp # Limited variables

    # These fields are optional, if they any are not specified
    # then the full range is used for that dimension.
    file1.i_range             60 70  # Cells 60 to 70 along I.
    file1.j_range             13 18  # Cells 13 to 18 along J.
    file1.k_range             0 45   # Half water column.
```

If the file name is appended with '`_surf.nc`', then only the topmost layer of the grid dumped to file (e.g. equivalent to `<file?.k_range 20 20>` for a 20 layer model). If `tstart` and `tstop` are absent, then these values assume the specified `START_TIME` and `STOP_TIME` respectively.

The following output intervals are also supported:

```
file0.tinc   YEARLY   # Output occurs on 1 Jan every year
file0.tinc   SEASONAL # Output occurs on 1 March for summer
                      #                  1 June for autumn
                      #                  1 September for winter
                      #                  1 December for spring
file0.tinc   MONTHLY  # Output occurs on 1st day of the month
```

An option exists to automatically **chunk** netcdf output `DAILY`, `MONTHLY` or `YEARLY` as follows:

```
file1.name  out.nc
file1.chunk DAILY    # or MONTHLY or YEARLY
```

In the above case there will be multiple output files created with the date stamp as a suffix

```
out_2011-02-01.nc
out_2011-02-02.nc
...
```

Note that there may not necessarily be one file per day, it depends on the file increment. The option merely enforces *at most one days (months or years)* worth in each file. For `MONTHLY` only the year and month suffix is added and for `YEARLY`, only the year. This applies to standard, simple, simple_cf, parray and sparse output netcdf formats.

A sparse or standard formatted files may have the additional `modulo` attribute which may take the value `year, month, week, day, hour, minute` or `second`, e.g;

```
    file0.modulo              year        # yearly modulo
```

When these sparse formatted files are input via tracer resets or in the transport mode, then the model time is converted relative to the defined modulo. For example, if a `year` modulo is specified then all model times are converted to times within the range 0 to 365, and an input file of length 1 year may be used to cycle through a simulation of many years length. When dumping, the modulo is relative to the `tstart` time specified for the output file (e.g. for `year` modulo, set `tstart` to be 1 Jan for a particular year).

A filling algorithm may be applied to the output variables prior to dumping which re-assigns values over land, e.g;

```
file0.fill_rule   default          # eta = 0 and 3D tracers = NaN at
                                   # land cells.
file0.fill_rule   no_fill          # No filling applied
file0.fill_rule   zero_fill        # eta = 0 and 2D & 3D tracers = 0
                                   # at land cells.
```

```
file0.fill_rule   cascade_search    # Land cells filled with the
                                    # nearest wet cell for eta, 2D
                                    # and 3D tracers.
```

Output may be filtered before being dumped by using:

```
file0.filter      avarge3     # 9 point convolution smoothing filter
                  average5    # 25 point smoothing filter
                  weighted3   # 9 point Shapiro filter
                  shapiro3    # 9 point Shapiro filter
                  weighted5   # 25 point weighted filter
                  shuman3     # 9 point Shuman filter
                  highpass3   # 9 point high pass Laplacian filter
```

Filtering is useful for the update of coarse resolution grids when using 2-way nesting.

4.31.7 Multi-dumpfiles

Dump files may be specified using a system analogous to the multi-netcdf input specification (Section 4.30.2); in this case a valid text file is specified for `OutputFiles` with the following format:

```
OutputFiles       df.txt      # Name of the multi-dumpfile text file
```

With `df.txt` containing, for example:

```
multi-dumpfile-version 1.0
nfiles      2
file0       standard.txt
file1       simple.txt
```

Each of the text files `standard.txt` and `simple.txt` then contains a list of output files as described in Section 4.30.6, e.g;

In `standard.txt`:

```
OutputFiles               2
file0.name                out.nc
file0.type                standard
file0.tstart              0 days
file0.tinc                1 day
file0.tstop               44 days
file0.bytespervalue       4
file0.vars                ALL

file1.name                out_surf.nc
file1.type                standard
file1.tstart              0 days
file1.tinc                1 day
file1.tstop               44 days
file1.bytespervalue       4
file1.vars                eta temp salt u1 u2
```

In `simple.txt`:

```
OutputFiles               1
file0.name                out.nc
file0.type                simple
file0.tstart              0 days
file0.tinc                1 day
file0.tstop               44 days
```

```
file0.bytespervalue       4
file0.vars                ALL
```

4.31.8 Customised parameters

As discussed in section **Error! Reference source not found.**, **SHOC** source code may be customised to suit special circumstances that the standard model does not support. The customised source may well define its own parameters and read them from the parameter file. In such cases please consult the code directly.

4.31.9 Coastlines

If using the utility `jvismeco`, you will probably need to specify coastline data (unless you are modelling simple test cases, or a completely open patch of water). These are specified in ASCII files containing 2 columns (x and y). A file may contain more than one coastline section (several islands, for example). It is preferable that each coastline section forms a closed polygon which does not contain any self-intersections. Coastline sections are separated by a blank line (and/or usually one or more comment lines as well). An example coastline file is shown below:

```
# This is an optional comment line.
    # This is another comment line.
    0 0
    0 1
    1 1
    1 0
    0 0


# A second coastline section
    1 0
    1 1
    2 1
    2 0
    1 0
```

You can have as many coastlines as you like, in as many files as you like, but it is usually convenient to keep all the data in one file.

4.31.10 Bathymetric data

In order to define the area to be modelled, you need to specify the bathymetry of the area. To do this, you need an ASCII file containing bathymetric data in 3 columns (x y and depth, free format). An example file is as follows:

```
    # This is an optional comment line.
    # This is another comment line.
    # The 3 columns are x, y and depth
    1000 1000 20
    2020.2 1354 10
    1520 7322 15
    # You can even have comments in the middle of the data
    7261 6123 8
    8761 7991 5
```

The data does not need to be on any sort of regular grid - they may be randomly scattered in x and y. This data can be read with `jvismeco`, and the the interpolated model bathymetry saved as a text file, suitable for inclusion in a **SHOC** parameter file.

4.32 Diagnostic files

A summary of the simulation is always printed to the file `setup.txt` upon execution of **SHOC**. This file is written to the path specified by `OuputPath` and the directory **SHOC** is run from. Typically this summary contains the following information:

```
SHOC Simulation Summary
Version : v1.0
Input file = open.prm
Open channel test domain
Grid description : Coarse open channel (120:1)

Simulation start time :  Mon Jul 31 16:02:58 2006

Operating in 3D mode
3D time step = 40.000
2D time step = 5.000
Tracer time step = 40.000
Sub-stepping stability compensation; excluding surface layer
Thin layer adjustment implemented
Exit on fatal eta instabilities when |eta| >  10.00
Exit when above variables = NaN

Grid dimension : 212 x 52 x 25
Vertical structure
  Vertical coordinate system = 'z'
-40.0 -30.0 -25.0 -21.0 -18.0 -15.0 -13.0 -11.0 -9.0 -8.0 -7.5 -7.0 -
6.5 -6.0 -5.5 -5.0 -4.5 -4.0 -3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5

2nd order momentum advection scheme.
QUICKEST (flux form : variable grid) tracer advection scheme.
Ultimate filter invoked.

Free slip condition.
Horizontal diffusion (x direction) = 2.000
Horizontal diffusion (y direction) = 2.000
Horizontal viscosity (x direction) = 20.000
Horizontal viscosity (y direction) = 20.000
Mean horizontal grid spacing : e1 =   275.01, e2 =   228.49

Vertical mixing scheme : mellor_yamada_2_0
  Surface roughness length scale =  0.100
  Background diffusivity = 1.000e-07
  Background viscosity = 5.000e-07
Bottom roughness length scale = 0.000100

Number of tracers = 2
  Tracer #0 : salt [0.00e+00 : 4.00e+01]
  Tracer #1 : temp [0.00e+00 : 4.00e+01]

Number of open boundaries = 2
Boundary #0 : west
  Normal velocity = NOGRAD
```

```
  Tangential velocity = CLAMPD
  Elevation = FILEIN|MILLER
  Tracer #0 (salt) = FILEIN|UPSTRM
  Tracer #1 (temp) = FILEIN|UPSTRM
    Relaxation constant =  0.008 (hours)
    Boundary data file #0 : /home/mgs/dent/c2/west_ets.nc

Boundary #1 : east
  Normal velocity = NOGRAD
  Tangential velocity = CLAMPD
  Elevation = FILEIN
  Tracer #0 (salt) = FILEIN|UPSTRM
  Tracer #1 (temp) = FILEIN|UPSTRM
    Boundary data file #0 : /home/mgproja/derwent/st_meco/east_ets.nc

Wind forcing from file /home/mgproja/dent/wind/wind_grid.nc
  Wind speed scale =  1.00
  Wind speed threshold #1 = 10.00
  Wind speed threshold #2 = 26.00
  Surface drag coefficient #1 =  0.00114
  Surface drag coefficient #2 =  0.00218

Heat flux calculated
Heat flux calculated : bulk formulation
  Bulk scheme = Kondo (1975)
  Reference height for air temperature/humidity =  4.00

  Air temperature file : /home/mgproja/dent/heat_obs/airport_3hr.ts
  Wet bulb temperature file :
/home/mgproja/dent/heat_obs/airport_3hr.ts
  Cloud cover file : /home/mgproja/dent/heat_obs/airport_3hr.ts
  Atmospheric pressure file :
/home/mgproja/dent/press_meco/press_grid2.nc

No salt flux specified

Number of output file dumps = 6
Output file #0 : /home/swirl1/test1/test_all
Output file #1 : /home/swirl1/test1/test_sur
```

At every time step the simulation progress is written to file `diag.txt` which is useful to estimate the time remaining for the simulation. This file contains the following information:

```
Simulation start =    0.0000 (days) : 1990-01-01 00:00:00
Simulation stop  =  400.0000 (days) : 1991-02-05 00:00:00
Simulation time  =  400.0000 (days) : 1991-02-05 00:00:00

CPU time used this iteration = 0.000 (sec)
Mean CPU time used / iteration = 0.000 (sec)
CPU run time ratio = 1236051.502146
Elapsed time = 0 day(s) 00:08:22
Total time ratio = 68844.621514
Time to completion = 0 day(s) 00:00:00
Percent complete = 100.0%
Running…
```

Information useful for debugging model crashes may be generated using:

```
DEBUG_LOC   i j k
```

where i, j and k are integers specifying the (i,j,k) location in the grid information is desired to be generated at. Note the k index for the surface layer is given by LAYERFACES – 2. At present the debug information relates mostly to the 2D mode, providing velocity values at the debug location after each term in the equations is computed, for each step of the 2D mode. Maximum velocities in the window containing the debug location are listed. Elevation flux divergence details and elevation at the forward time-step are also provided. The debugging information is written to the file 'debug.txt' at the current time-step. If a history of debugging information is required, use:

```
DEBUG_LOC   i j k append
```

Note that these files can then become quite large. The debugging information may be written after n days (or hours, minutes, seconds etc.) of simulation using:

```
DEBUG_LOC   i j k append after 2 days
```

The debugging can print the position in the computational flow of control (i.e. what numerical algorithm the code is currently computing) using:

```
DEBUG_LOC   i j k step
```

4.32.1 Run regulation

The user may interactively control various aspects of the simulation using the REGULATE_FILE command. By defining a valid filename with this command, the user can enter commands in real-time to stop, pause, resume and re-configure various aspects of the run. This functionality is invoked via a scheduled function that reads the nominated file at a user defined interval. The run regulation is invoked via:

```
REGULATE_FILE     filename.txt      # Name of the file that contains
                                    # run regulation commands.
REGULATE_DT       1 hour            # Time interval that the file is
                                    # read.
```

Note that the REGULATE_FILE may be the parameter file. Any run regulation commands may begin with the keyword REGULATE. Valid commands are:

```
REGULATE STOP           # Stop the simulation. Output is dumped prior
                        # to quitting.
REGULATE PAUSE          # The run is suspended.
REGULATE RESUME         # A paused run is resumed.
REGULATE DUMP_REINIT    # A new dump file specification is invoked.
                        # Any existing files are appended. Dump
                        # specification should be listed in the
                        # input parameter file.
REGULATE TS_REINIT      # A new ascii time-series file specification
                        # is invoked. Any existing files are
                        # appended.
REGULATE WIN_REINIT     # A new window partitioning is invoked.
                        # Window information should be listed in the
                        # input parameter file.
REGULATE OBC_REINIT <obc_name> <obc_type> # A the boundary condition
                        # <obc_type> is applied to open boundary
                        # <obc_name>. Valid types are:
            NEST1WAY    # 1 way nesting (Section 4.10.7)
```

```
            NEST2WAY    # 2 way nesting
            RIVER       # River OBCs (Section 4.10.6)
            NOTHIN      # No OBCs (Section 4.10.14)
            SOLID       # The OBC emulates a solid boundary.
REGULATE DT_REINIT      # Re-initialises the time-step to that
                        # specified in the input parameter file.
                        # Horizontal mixing is also adjusted.
REGULATE HVISC_REINIT   # Re-initialises the horizontal viscosity to
                        # a constant value (i.e. non Smagorinsky).
REGULATE PSS_REINIT     # Re-initialises the point source/sink
                        # specification.
```

The run regulation may be invoked at a specific time, by using `@ n days` where n is a valid day number relative to the timestamp, e.g:

```
REGULATE OBC_REINIT West NEST1WAY @ 10 days
```
or
```
REGULATE PAUSE @ 0.5 days
```

4.33 Explicit mapping

SHOC operates on a sparse coordinate system internally, where all cell locations are aggregated in a one-dimensional vector and each cell's position in space is determined by the location in the vector of its neighbours. Ordinarily every cell is mapped to its immediate neighbour in three-dimensional space, but with the sparse system this does not need be the case. Cells can be made to have 'neighbours' which are nowhere near the cells geographic position. This explicit mapping method can be useful, for example, for connecting two ends of a channel if the channel cannot be resolved by the models discretization. Furthermore, a range of vertical cells may be specified which are subjected to this explicit mapping. This makes it possible to simulate flow beneath solid structures floating on the surface.
Explicit maps can be specified in either the e1 or e2 directions. The (i,j) cell locations listed for the maps must correspond to the cell centers. For the e1 direction, one of the cells must be adjacent to a solid boundary on the left edge, and the other a solid boundary on the right edge. The cell with the right edge will then map through the solid boundary to access water properties in the cell with the solid left edge, and vice versa. For the e2 direction, one of the cells must be adjacent to a solid boundary on the back edge, and the other a solid boundary on the front edge. Explicit maps through the whole water column are specified using the following:

```
MAP_POINTS_E1 2   # Maps cell (2,4) to cell (4,4), and cell
2 4 : 4 4         # (2,5) to (4,5) in the e1 direction. The
2 5 : 4 5         # reverse maps are also implied.

MAP_POINTS_E2 2   # Maps cell (9,12) to cell (9,14), and cell
9 12 : 9 14       # (10,12) to (10,14) in the e2 direction. The
10 12 : 10 14     # reverse maps are also implied.
```

If the source and destination cells have different depths the mapping is performed through the water column until the bottom of shallower of the cells is reached. A vertical range of the map can be specified by appending the upper and lower k level the maps are operate within after the number of mapping points, e.g.

```
# Map the first cells in the list between layer 22 and layer
# 10. The upper-most layer (closest to the surface) is always
# listed first. The second cells in the list are mapped through
# the whole water column.
MAP_POINTS_E1  2
```

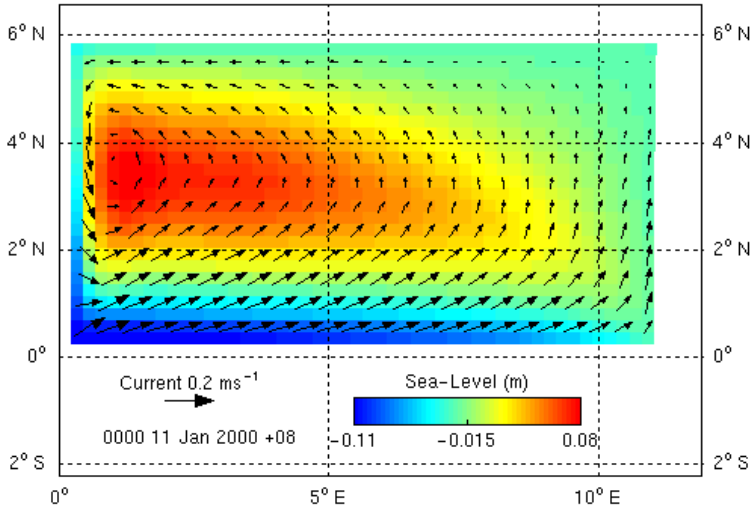
```
2 4 : 4 4 : 22 10
2 5 : 4 5
```

The explicit mapping list may contain any combination of cells mapped only between certain layers and cells mapped through the whole water column, i.e. any combination of the formats:

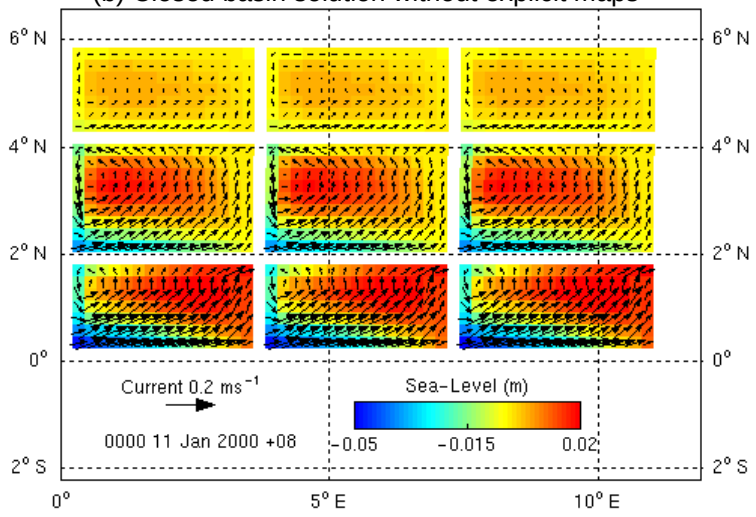
```
is ie : js je
is ie : js je : kt kb
```

Using the auxiliary program `jvismeco` is generally helpful when determining the map lists. An example of a domain using 2 explicit maps in the e1 and e2 directions is illustrated in Figure 4.31.1. The domain is divided into 9 sub-sections separated by land, but the explicit maps make the domain behave as if it were one connected region.
The explicit mapping function only works with ‘z’ coordinates.

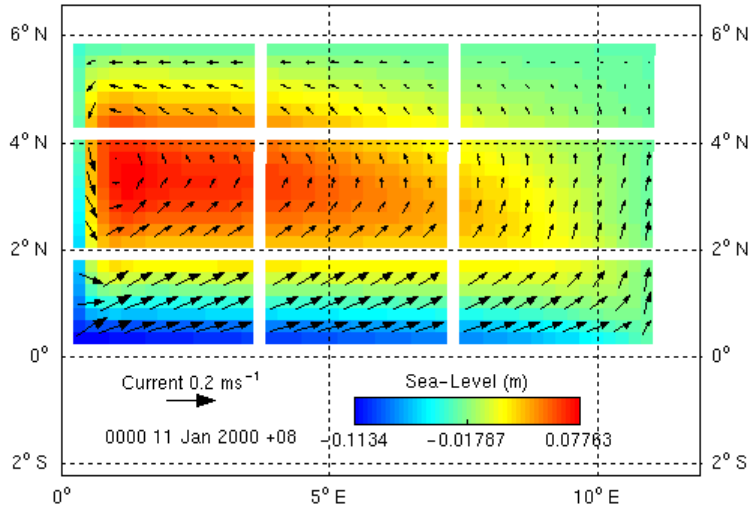
Figure 4.31.1 :
(a) Un-partitioned closed basin solution



(b) Closed basin solution without explicit maps



(b) Closed basin solution with explicit maps across the partitions



Note : Fig 4.31.1 (a) and (c) utilize slightly different bathymetry, i.e. Fig 4.31.1 is 2 cells narrower in either direction since the ‘walls’ are not recognized as part of the domain, and bathymetry has a step across these ‘walls’, hence any slight differences in solutions between (a) and (c); the general dynamics are the same however.

5 Automatic setup (-a option)

As mentioned in section 3, the parameters outlined in this section may be automatically generated using the –a option in **SHOC**. In this case the parameter file must contain the following information:

```
# The start and stop time of the model simulation period,
# relative to the epoch (01/01/1990 00:00:00+8 by default).
# Relative time specifications here and elsewhere in the parameter
# file can be specified in seconds, minutes, hours, or days.
# Here, the start time corresponds to 1995-02-10 00:00:00 +8
#, and the end time to 1995-03-13 00:00:00 +8.
START_TIME              1866 days
STOP_TIME               1897 days

# The name of the input and parameter output files. The input
# netCDF file will have ‘.nc’ appended to this name (i.e. test.nc)
# and the input parameter file will have ‘.prm’ appended (i.e.
# test.prm).
INPUT_FILE          test

# Grid information (see section 4.6) defining the grid layout is
# mandatory. An example is included below:
PROJECTION     geographic
GRIDTYPE       GEOGRAPHIC_RECTANGULAR
NCE1           10
NCE2           20
DLAMBDA        0.01  # Long. cell interval in aux. coords.
                     # (degrees)
DPHI           0.01  # Lat. cell interval in aux. coords.
                     # (degrees)
X00            144.3856    # Longitude of origin (degrees)
Y00            -38.2030    # Latitude of origin (degrees)
POLE_LONGITUDE 0     # Longitude of false pole (degrees).
POLE_LATITUDE  90    # Latitude of false pole (degrees).

# Bathymetry : example depth values for a 3 by 4 grid
 BATHY 12
 22.2
 12.3
 7.4
 23.5
 12.0
 6.0
 25.8
 13.7
 5.8
 27.6
 14.2
 4.9
```

The parameter file may then contain optional fields specifying the forcing and initialization of the model, i.e;

```
# Information regarding any forcing data to be read (e.g. wind,
# pressure).
# A time series file containing wind East and North
# velocity components, which must be called 'u'; and 'v'
# respectively, and have units of ms-1.
```

```
WIND_TS                 cyc_bobby95.nc
# How often to read data from the wind file and update
# the wind field in the model.
WIND_INPUT_DT           10 minutes

# A time-series file containing the variable 'pressure' with
# units of Pa.
PRESSURE                cyc_bobby95.nc
# How often to read the file and update the pressure
# field in the model.
PRESSURE_INPUT_DT       10 minutes     # Update every 10 minutes.

# Information regarding any initialization data for tracers temp
# and salt.
TRACER0.data profile.nc
TRACER1.data profile.nc
```

The open boundaries are automatically generated by **SHOC** on the basis that any wet cell at the grid extremes or any cell in the grid interior adjacent to an `OUTSIDE` flagged cell are set to open boundary cells. The grid is searched for these occurrences in the following order:

1. `u1` boundaries on the left hand (i=0 or west) grid extremities
2. `u1` boundaries on the right hand (i=`NCE1` or east) grid extremities
3. `u2` boundaries on the bottom (j=0 or south) grid extremities
4. `u2` boundaries on the top (j=`NCE2` or north) grid extremities
5. Interior `u1` boundaries from i=0 to i= `NCE1`
6. Interior `u2` boundaries from j=0 to j= `NCE2`

If elevation boundary data is present in the parameter file, the corresponding boundary is set to be elevation forced, otherwise the boundary is set to be passive, e.g;

```
# Set the first 3 boundaries found to be elevation forced
 BOUNDARY0.DATA eta_west.ts
 BOUNDARY1.DATA eta_south.ts
 BOUNDARY2.DATA eta_north.ts
```

River inputs may be specified at a location using;

```
RIVER#  <name> <lon> <lat> <flowfile>
```

Where # is the number of the river in a consecutive list, `<lon>` is the longitude of the river, `<lat>` is the latitude of the river and `<flowfile>` is the name of a file containing the river flow. The river will be located at the nearest coastal location in the model grid to `<lon>,<lat>`. A `u1` or `u2` custom river open boundary is created for each river specified. If `<lon>,<lat>` lies outside the footprint of minimum & maximum longitude and latitude for the grid, it is ignored. An example is;

```
RIVER0 river1 137.9 -33.4 flow1.ts
RIVER1 river2 137.8 -33.5 flow2.ts
```

Alternatively, a full boundary specification may be included, giving the user exclusive control over the open boundaries. Often this is best performed using a two step approach, where a grid is first created with all boundaries closed, i.e. by specifying;

```
# Set all boundaries closed
NBOUNDARIES    0
```

Then boundaries are defined in `jvismeco` and pasted back into the parameter file.

Various parameters automatically generated by **SHOC** using the –a option may be over-ridden by specifying that parameter in the input parameter file. Parameters which fall into this category are:

```
# Open boundaries (see above)

# The epoch for all time related parameters, as well as
# for all output files generated by the model. Currently, the
# units must be 'seconds since ...', but this may change in future
# versions. The epoch is specified in standard ISO date/time
# format, including a possible timezone specification. The
# timezone here is 8 hours ahead of UTC.
TIMEUNIT                seconds since 1990-01-01 00:00:00 +08



# The base time unit that will be used for all
# timeseries and netCDF output files.
OUTPUT_TIMEUNIT         days since 1990-01-01 00:00:00 +08

# A single line description of the model run. This string is
# written into all output files.
PARAMETERHEADER         NWS 20km rectangular grid, Run 1

# The internal (3-d) time-step, and the number of times
# the external (2-d) code will be run per 3-d time-step.
# The external (2_d) time-step is thus DT divided by IRATIO.
DT                 120 seconds
IRATIO             5

# Vertical geometry; z coordinates of the model layer interfaces.
LAYERFACES 5
 -10.0
 -8.0
 -4.0
 -2.0
 0.0

# Bathymetry limits
# All cells will be at least 20m deep
BATHYMIN           20

# No cell will be more than 2000m deep
BATHYMAX           2000

# Invoke thin layer merging
HMIN                  0.05

# Bottom roughness (values in metres).
Z0                 0.001

# Mixing scheme
mellor_yamada_2_0
ZS       0.2

# Horizontal viscosity in u1 equation
U1VH               1.0
# Horizontal viscosity in u2 equation
U2VH               1.0
# Horizontal diffusivity in the x direction (m2s-1)
U1KH     100
```

```
# Horizontal diffusivity in the y direction (m2s-1)
U2KH     100

# Sigma
SIGMA    YES

# Tracer relaxation
TRACER0.relaxation_file saltprof.nc
# How often to perform relaxation calculation
TRACER0.relaxation_input_dt 1 hour
# Relaxation time constant
TRACER0.relaxation_time_constant 20 days

# Full tracer specification
NTRACERS 2
TRACER0.name salt
TRACER0.long_name Salinity
TRACER0.units psu
TRACER0.fill_value 35.0
TRACER0.valid_range 0 40
TRACER1.name temp
TRACER1.long_name Temperature
TRACER1.units degrees C
TRACER1.fill_value 20.0
TRACER1.valid_range 0 40

 # Output files for a grid.
 OutputFiles               1
 file0.name                out.nc      # Output prefix.
 file0.gridtype            standard    # Standard dumpfile.
 file0.tstart              0 days      # Output start time.
 file0.tinc                1 day       # Output interval.
 file0.tstop               44 days     # Output stop time.
 file0.bytespervalue       4           # 2 – shorts
                                       # 4 - floats.
                                       # 8 - doubles
 file0.vars                ALL         # ALL variables.
```

Executing **SHOC** with the –a option will result in the generation of an input netCDF file (having a name of the INPUT_FILE name with '.nc' appended) and an input prm file template (having a name of the INPUT_FILE name with '.prm' appended) which may be subsequently modified and executed using the –p option (see section 2). **SHOC** will then proceed to run using the automatically generated parameter specification.

6 Restarts

6.1 Basic restarts

The model may be restarted using any standard format netCDF output file (see Section 4.31.6) containing ALL variables as the INPUT_FILE. In this case the model START_TIME must correspond to one of the dump times in the netCDF file. A warning is issued if this is not the case.

6.2 Restarts using restart file (-restart option)

Alternatively, a restart facility exits to allow the model to be seamlessly hot-started. Firstly, when initially running the model a restart_dt must be specified which defines an output interval that a special restart file, named restart.nc, is dumped at (in standard format, containing ALL variables), e.g;

```
restart_dt          2 days      # Create a restart.nc file every 2 days
```

This restart file is overwritten at the interval restart_dt. A path and restart filename may be specified using:

```
restart_name       <path>/<name>  # Restart path and name, e.g.
                                  # <path> = /home/data
                                  # <name> = restart_1.nc
```

Once this file is written, the model may be terminated, or may crash, and can be restarted using the restart.nc file, e.g;

```
shoc –p  test.prm –restart
```

Using this restart method the model will read the appropriate START_TIME from the restart.nc file, and will append subsequent data generated to existing netCDF and time-series output files defined in the .prm parameter file (in the above example test.prm).

Note that restarts generally do not produce bit-exact solutions if output dumps are saved in floating point precision (bytespervalue = 4).

6.3 Near real-time restarts (-nrt option)

A near real-time operation mode may be invoked capitalising on restarts. This allows simulations to be repetitively started daily without having to manually alter the parameter file; this mode is invoked using:

```
shoc –p  test.prm –nrt
```

In this case, the START_TIME for the simulation is read from the netCDF file specified as the INPUT_FILE, the stop time for the simulation is this START_TIME + STOP_TIME specified in the parameter file (i.e. the STOP_TIME is an increment rather than an absolute value), both the RAMSTART and RAMPEND are set equal to the START_TIME (i.e. no ramping is performed) and the output file tstart and tstop are set to the start and stop simulation times. This means that the START_TIME, RAMSTART, RAMPEND, tstart and tstop are not required to be set in the parameter file. Furthermore, if a restart file is overwritten to the same location, then this may be used as the INPUT_FILE. Additionally, the SEQUENCE option may be used

to store model output in a unique directory, requiring that the only manual tasks to initiate repetitive simulations are the creation of the directory and commencement of the simulation, both of which are easily scripted. A near real-time parameter file for daily simulations may therefore appear as:

```
STOP_TIME         1 day                    # Run length
INPUT_FILE        /home/data/restart.nc    # Input file
restart_dt        1 day                    # Restart interval
restart_name      /home/data/restart.nc    # Restart file name
OutputPath        /home/data/              # Path for output
SEQUENCE          setup.txt                # Sequence set from file

OutputFiles             1                  # Output files
file0.name              out.nc
file0.filetype          standard
file0.tinc              1 hour
file0.bytespervalue     4
file0.vars              ALL
```

Then to run:

```
mkdir /home/data/run<n>       # <n> is the current run
shoc –p test.prm –nrt
```

6.4 Crash recovery (-cr option)

Often when a model fails, the strategy to maintain stability is to reduce the time-step, modify time dependent parameterisations (e.g. horizontal mixing coefficients) and restart the model before the failure occurred. This process can be automated using the '`-cr`' option, e.g;

```
shoc –p  test.prm  -cr
```

A restart file (Section 6.2) must be specified for this option to operate. If the model fails when this option is invoked (e.g. due to sea level rising above `ETAMAX`) then the time-step is progressively reduced (currently by a factor of 5), horizontal mixing is adjusted and the prognostic fields are re-initialised from the last restart file dump. The model then progresses using the smaller time-step to the next restart dump event, whereupon the time-step and mixing are reset to original values. If the model fails during the restart, the time-step is further reduced and the process repeated. Output to netCDF and timeseries files are over-written during the period the time-step is reduced. If the time-step is reduced more than 5 times, then the model will exit, on the assumption that it cannot recover by simply reducing the time-step. In this case, the instability may have to be diagnosed and rectified by other means (e.g. alternative OBCs, better forcing etc).

7 ROAM (-r option)

SHOC may be configured to operate in the ROAM (Relocatable Ocean and Atmospheric Model) environment. The ROAM configuration is essentially the same as the `-a` option configuration with a number of alternative parameterisations. The ROAM configuration is invoked using the '`-r`' option. The same mandatory information as used in the `-a` option is requited (start/stop time, grid information, bathymetry). The ROAM option is designed to nest SHOC within a global ocean model and use information from this larger scale model for initial and boundary conditions. It is assumed that global model output exists covering the region of interest containing output dumps at approximately 1 day intervals. Temperature, salinity and sea level are required to be present in this output.
Currently the global model is a derivative of the GFDL MOM3 (Modular Ocean Model) model termed OFAM (Ocean Forecasting Australia Model). Using the `-r` option, these global model data are specified using:

```
OFAM_DATA          EAC_200401.nc     # OFAM input filename
```

These data will then be used for T, S and η initial and boundary conditions. Whenever an open boundary is located, the information found in the global model file is used to prescribe T, S and η OBC's. The sea level contained in the OFAM data represents the low frequency component only, and the ROAM configuration will prescribe these values on the open boundary with a tide superimposed using the global tide model of Cartwright and Ray (1990), (see Section 4.11, Science Manual). This model requires paths to the orthotide functions and nodal corrections to be present, e.g:

```
TIDE_CSR_CON_DIR       /home/tide/nodal  # Path to nodal
                                         # correction directory.
TIDE_CSR_ORTHOWEIGHTS  /home/tide/ortho_csr_4.0 # Orthotide functions
```

Temperature and salinity are prescribed on the open boundary using an upstream advection open boundary condition. Normal velocity uses a no-gradient condition and tangential velocity is clamped to zero. A horizontal sponge zone 8 cells wide is also imposed on the open boundaries.

It is possible to prescribe initial conditions for T, S and η which are different to the open boundary data defined in `OFAM_DATA` by using:

```
INIT_DATA          EAC_2004_init.nc  # T,S,η Initialisation data file
```

Furthermore, each stream of T, S and h may be defined independently using:

```
TEMP_DATA          EAC_temp.nc      # Input temperature filename
SALT_DATA          EAC_salt.nc      # Input salinity filename
ETA_DATA           EAC_eta.nc       # Input sea level filename
```

If only these specifications are present, then the data contained in these files is also used for open boundary forcing. However, if `OFAM_DATA` is present then the data contained in this file is used for T, S and η boundary forcing.

The ROAM configuration may be restarted from a previous run using the '`-rs`' option. In this case a restart file must be supplied:

```
RESTART_FILE       run1_all.nc      # Restart filename
```

The restart may be configured to commence using the temperature and salinity initial conditions from OFAM using the '`-rso`' option. The '`-rg`' option will terminate after the input and parameter files have been created (i.e. the setup is complete but the simulation does not commence).

Bathymetry may be specified in the ROAM configuration using a bathymetric database rather than supplying the bathymetry list via BATHY, e.g. by specifying;

```
BATHYFILE    /home/bathy/ga2002_tiled.bth
```

the bathymetry will be interpolated onto the grid using the information contained in the bathymetric database 'ga2002_tiled.bth'. This file has a unique format and lists all the tiled netCDF bathymetry files that comprise the database.

ROAM is designed to use surface fluxes from a relocatable atmospheric model (currently RAMS - Relocatable Atmospheric Model). The wind and pressure inputs may be the same as for the –a option. Alternatively, if wind and pressure are present in the same file, then use:

```
RAMS_DATA          /home/atmos/EAC_rams.nc  # Atmospheric forcing file
```

If the RAMS_DATA file contains heatflux data, e.g.

- incident flux of shortwave radiation (W m-2)
- incident flux of longwave radiation (W m-2)
- upward flux of longwave radiation (W m-2)
- surface sensible heat flux (W m-2)
- surface latent heat flux (W m-2)

then a heat flux may be imposed using:

```
HEATFLUX           COMP_HEAT   # Create net heatflux from components
```

This formulation of the heatflux will create a net heat flux from the longwave, sensible and latent fluxes, truncating the latent heat flux to zero to omit contributions from condensation. The shortwave flux is depth distributed according to the SWR_TRANSMISSION and SWR_ATTENUATION parameters (note defaults are 0.42 and 0.2 respectively).
All atmospheric data are read in with a time interval of 10 minutes. Wind and pressure may have an alternative input time specified.

The ROAM configuration was designed for robust simulation (at the expense of accuracy) and therefore various defaults differ in comparison to the –a configuration, vis;

- The Mellor-Yamada 2.0 mixing scheme is used.
- Smagorinsky horizontal diffusion is used with a constant of 0.1.
- One bathymetry smoothing pass is performed (SMOOTHING 1) and a maximum bathymetry gradient of 0.05 is specified (MAXGRAD 0.05).
- Minimum bathymetry is 1m. If maximum bathymetry is > 200m and minimum bathymetry < 4m then minimum bathymetry = 4m.
- The time-step is far more conservative by at least one half.
- Relaxation of T and S to OFAM data is performed using a 20 day relaxation time.
- OFAM temperature and salinity are present as tracers 'otemp' and 'osalt' respectively, read in on a daily time interval.
- RAMPVARS WIND TIDALH is used.
- Active alerts are implemented on 2D & 3D velocity and eta (ALERT ACTIVE). The eta relaxation file is taken to be the global model data; i.e. SHOC sea level is relaxed back to the low frequency sea level if the difference between the mean ROAM sea level (tidally averaged) and OFAM sea level exceeds the prescribed threshold.
- Thresholds for ACTIVE ALERTS are:
    - VELMAX = 3.51 ms^{-1}
    - VELMAX_2D = 2.40 ms^{-1}
    - ETA_DIFF = 0.26 m
- Mean sea level is computed for the active eta alerts (MEAN ETA).

The robustness of ROAM may be altered using the parameter ROBUST which is assigned from 1 (least robust) to 10 (most robust). The ROBUST levels 1 to 5 linearly increase the Smagorinsky coefficient from 0.1 to 0.5. For ROBUST > 2 the horizontal diffusion distribution is smoothed using a 9 point convolution filter, and mixing coefficients have an upper limit corresponding to the computed constant mixing coefficients. For ROBUST > 5 constant mixing coefficients are used and the time-step is linearly decreased from its computed value using ROBUST = 6 to half its computed value with ROBUST = 10. The model starts from an initial velocity distribution at rest for ROBUST > 6. The default value is ROBUST = 6. Note that more robust parameterisations are generally less accurate.

These configurations are applicable for the default ROAM version #4 (ROAMv 4). An additional set of configurations can be invoked using ROAMv flag:

```
ROAMv   CPD     # Standard ROAM, clamped open boundaries.
ROAMv   RMD     # Standard ROAM, RAYMND radiation OBCs.
ROAMv   FLA     # Standard ROAM, FLATHR OBCs.
ROAMv   ROAMv1  # Standard ROAM, velocity forced OBCs.
ROAMv   ROAMv2  # ROAMv1 with alternative ROBUST parameterisation.
ROAMv   RECOMv1 # Standard RECOM, no ROBUST.
ROAMv   RECOMv2 # RECOM with ROBUST parameterisations.

ROAMv   1       # Same as CPD
ROAMv   2       # Same as RMD
ROAMv   3       # Same as FLA
ROAMv   4       # Same as ROAMv1
ROAMv   5       # Same as ROAMv2
ROAMv   6       # Same as RECOMv1
ROAMv   7       # Same as RECOMv2
```

The default ROAM should use ROAMv = ROAMv2 which sets robustness according to:

```
ROBUST=1: OFAM currents + Smagorinsky = 0.1
ROBUST=2: OFAM currents + Smagorinsky = 0.2
ROBUST=3: Geostrophic currents + Smagorinsky = 0.1
ROBUST=4: Start from rest + hard T/S relaxation + Smagorinsky = 0.1
ROBUST=5: Start from rest + Smagorinsky = 0.1
ROBUST=6: Start from rest + Smagorinsky = 0.2
ROBUST=7: OFAM currents + constant horizontal viscosity
ROBUST=8: Geostrophic currents + constant horizontal viscosity
ROBUST=9: Start from rest + constant horizontal viscosity
ROBUST=10: As for ROBUST=9 with reduced time-step
```

A ROBUST 0 flag has been implemented that will use a more optimized configuration that one may typically use for a case study. While this configuration may have higher accuracy than standard ROAM configurations, it is also more prone to instability. This option is recommended only for more experienced modellers. The configuration is as follows:

- The model starts from rest,
- The k-ω mixing scheme is used,
- Smagorinsky horizontal diffusion is used with a constant of 0.1, with 2 smoothing passes,
- The ULTIMATE QUICKEST tracer advection is used,
- Boundary sponges of 8 cells ramp to 5 times the interior value,
- No active alerts,
- Flux adjusted open boundaries using the default timescale.

Using ROAMv = RECOMv2 sets the ROBUST parameterisation as:

```
ROBUST=1: Same as ROBUST 0 above, Smagorinsky, no alerts
ROBUST=2: Same as ROBUST 0 above, constant viscosity, no alerts
ROBUST=3: Same as ROBUST 1, active alerts
ROBUST=4: Same as ROBUST 2, active alerts
ROBUST=5: Standard ROAM parameteristion, Smag = 0.1, rest start
ROBUST=6: Standard ROAM parameteristion, Smag = 0.1, OFAM start
ROBUST=7: Rest + hard T/S ramp relaxation + Smagorinsky = 0.1
ROBUST=8: Rest + hard T/S ramp relaxation + Smagorinsky = 0.1
ROBUST=9: OFAM currents + constant horizontal viscosity
ROBUST=10: Start from rest + constant horizontal viscosity
```

As mentioned, the time-step parameterisation using the `-r` option is very conservative. Speed may be increased using the `SPEED` parameter which is assigned from 1 to 10. The speed is controlled by altering the 'safety factor' applied to the CFL condition. The ROAM 'safety factor' is assigned a value 0.4 (note; 0.8 is used for `-a` option), and further decreases depending on the maximum depth. If `SPEED = 1` then the safety factor is unchanged. For `SPEED > 1` the safety factor linearly scales to 0.9 for `SPEED = 10`. Using `SPEED = 10` will generally double the time-step used, and still satisfy the CFL condition.

8 Input file generation (-g option)

The input netCDF file containing initial values for the model variables over the model grid and the model geometry / bathymetry required to run SHOC using the –p option may be generated from any parameter file using the –g option, i.e.

```
shoc –g prmname infile.nc
```

where `prmname` is the name of the model parameter file and `infile.nc` is the name for the generated input netCDF file. Note that whenever initialization data is changed (e.g. `TRACER?.data`), model geometry is changed (e.g. number of `LAYERFACES`) or the bathymetry is changed a new input netCDF file must be generated.

9 Transport mode (-t option)

The transport option invokes the tracer transport only in **SHOC**, using offline velocities and vertical diffusivities read from file. All tracer diagnostics, including sediment transport, biogeochemistry, tracer statistics, source/sinks and particle tracking will function in the transport mode. The advection scheme used in this mode is the unconditionally stable semi-Lagrangian scheme, allowing increased time-steps (e.g. 1 hour) to be used which dramatically increases run time ratios. This scheme is, however, quite diffusive and does not possess as good conservation characteristics as other schemes available in **SHOC**, hence some accuracy is forfeited at the expense of speed. The semi-Lagrangian scheme is unconditionally stable because it traces streamlines back in space from the point of origin (e.g. cell centres) using velocity information, then interpolates tracers using the origin location.

The concept of using offline velocities to drive a transport model is not new, however, in practice it is rarely used due to the enormous amounts of disk space required to run for extended periods. This problem is circumvented by generating the offline velocity/diffusivity files with a sparse file format (Section 4.31.6) which eliminates land from the dumpfile and can lead to large saving in disk space (savings up to 90% are possible). I/O overhead can be reduced if the sparse format file is read into SHOC without interpolation, i.e. the dumpfile contains information on ***exactly*** the same grid as the transport model is using for *exactly* the times required.

The transport option requires a standard input file for initialization, from which model initial conditions, grid, layer structure and bathymetry are defined. A forcing file containing the variables `eta, u1, u2, w, Kz must also be supplied`. If the grid definition is incompatible with the forcing file the model will terminate with an error. The variables `temp, salt` may optionally be included in the forcing file if the `advect` and `diffuse` attributes are false for these variables in the tracer list. A transport mode is also defined to specify the format of the offline file, which has consequences for the speed at which I/O is performed. To define input and offline data a transport parameter file is created which defines:

```
INPUT_FILE        in.nc       # Initialisation file

TRANS_DATA        offline.nc  # File containing eta, u1, u2, w and Kz
                              # This may be a multifile using
                              # variable substitution.

TRANS_MODE        SP_EXACT    # The TRANS_DATA file is expected to
                              # be in sparse format, with time
                              # records corresponding exactly to the
                              # input intervals required by the model
                              # (determined by the start time and
                              # time-step).
                  SP_INTERP   # TRANS_DATA is in sparse format
                              # (contains information on exactly the
                              # same grid as the transport model) but
                              # may be at different times to the
                              # input interval (interpolation in time
                              # is performed which slows I/O).
                  XYZ_INTERP  # TRANS_DATA is in standard format and
                              # may be spatially and temporally
                              # different to the grid. Interpolation
                              # in space and time is performed on
                              # input. The slowest method using the
                              # most disk space.
                  NONE        # No reading of forcing data and no
                              # advection is performed. Useful for
                              # format conversion using tracer reset
```

```
                # capability in conjunction with
                # different forms of file output.
SP_CHECK        # Used to check transport data files
                # for NaN values or values greater than
                # specified limits (etamax & velmax).
                # Set TRANS_DATA to the file required
                # to be checked when using this mode.
TR_CHECK        # Checks the input data for NaN and
                # values greater than specified limits,
                # and checks valid source cells &
                # interpolation weights (>0 and <1)
                # are computed.
GLOBAL          # Reads BRAN or OceanMAPS global data
                # and reads eta_t, T/S, u and  v into
                # the model variables. Velocities are
                # rotated onto the grid.
```

Monthly transport files in sparse format can be automatically generated using:

```
TRANS_OUTPUT            YES
TRANS_DT                1 hour      # optional dump increment
```

In this case the transport files will be created for each month with the name `prmname_trans_mmmyyyy.nc` where `'prmname'` is the name of the parameter file, `mmm` is the month (e.g. '`jan`') and `yyyy` is the year. An alternative to `prmname` can be generated using `OutputTransport` (Section 4.31.6). Files are output in `'sparse'` format. Variables output are `eta, u1mean, u2mean, wmean, temp, salt` and `Kzmean` (`swr` is also output if present). The mean variables required for output are automatically invoked. The default dump increment is `1 hour`, unless specified using `TRANS_DT`. Note that `TRANS_OUTPUT` may be used in transport mode when wishing to dump multi-grid output (for the `STREAMLINE` mode; see below). In this case output variables are `eta, u1, u2, temp, salt, Kz, origin, p, q` and `r`.

Note that if a list of tracers is generated for the transport mode then the tracers must have unique names, e.g. if `eta, u1, u2` or `w` are used as tracer names then these will be in conflict with the prognostic variables of those names, and output may not be correctly generated (`u1` and `u2` will not output to `standard` files, `u` and `v` will not output to `simple` files). This is especially relevant when using `TRANS_MODE = NONE`.

Additionally the following attributes are mandatory in the transport parameter file (see Section 4 for a description of these parameters):

```
CODEHEADER          SHOC default version    # Code version
PARAMETERHEADER     Transport model         # Header text
TIMEUNIT            seconds since 1990-01-01 00:00:00 +08
OUTPUT_TIMEUNIT     days since 1990-01-01 00:00:00 +08
LENUNIT             metre
START_TIME          1866 days
STOP_TIME           1897 days
DT                  1 hour      # Transport timestep
HMIN                0.02        # The minimum layer thickness
Z0                  0.002       # Bottom roughness – optional :
                                # required for sediment transport only.
NAME                            # Comments (optional)
```

A tracer list (Section 4.10) and the definition of the open boundaries (Section 4.11) is also required. The latter is required so that the open boundary conditions for any additional tracers may be defined. Open boundary conditions for `temp` and `salt` are best created offline and

stored in a point array file, in conjunction with the FILEIN open boundary condition. The UPSTRM open boundary condition is reconfigured for the transport mode to use the characteristic for outward flowing velocity.

Additionally, any diagnostics (e.g. source / sink, particle tracking, mixed layer, diagnostic numbers, flushing times, steric height, conservation diagnostics, tracer statistics) and any surface forcing (e.g. HEATLUX for temp, SALTFLUX for salt : these may require additional atmospheric input) may be specified in the transport parameter file.

Additional tracers may exist in the forcing file, and these may be reset in the transport mode by listing the names of these variables using the TRANS_VARS attribute, e.g;

```
TRANS_VARS          NO3 Chl_a sand silt
```

A transport parameter file may be generated from a full parameter file when using the –g or –p option by including TRANS_DATA in the parameter file. In this case the transport file will adopt the name specified by the INPUT_FILE appended with .tran, e.g;

```
TRANS_DATA          dummy.txt
```

If the time-step does not violate stability criteria, alternative advection schemes may be used. The ULTIMATE and STABILITY options may be used in conjunction with this. Often the velocity fields read into the transport model (snapshots or means) are not conservative in the sense that the divergence of the depth averaged velocity does not always equal the change in elevation over the time-step. This can lead to conservation errors using advection schemes solved using the flux method. Conservation may be forced locally in time by computing the change in elevation over the time-step and vertical velocity from the specified velocity distributions. This maintains conservation for tracers using non semi-Lagrangian advection schemes, and is invoked using:

```
CONSERVATION        YES   # Force volume conservation
```

The sea level may be re-initialized to that in the transport file or left to evolve over time by using;

```
CONSERVATION        RE_INITIALIZE     # Force volume conservation with
                                      # eta re-initialization.
CONSERVATION        NO_INITIALIZE     # Force volume conservation with
                                      # no eta re-initialization.
```

Additionally only vertical velocity or sea level may be forced to conserve by adding W or ETA to the CONSERVATION specification, e.g;

```
CONSERVATION        NO_INITIALIZE ETA
CONSERVATION        RE_INITIALIZE W
```

The default is CONSERVATION = RE_INITIALIZE W ETA.

For the FFSL scheme, vertical velocity may be only recomputed in the water columb if the new vertical velocity does not violate the Lipschitz condition using WSTAB instead of W.

Note that the semi-Lagrangian scheme is not compatible with multi-processing, hence the transport model will only operate on one window unless an alternate advection scheme is specified. The order of the semi-Lagrange advection scheme may be specified using:

```
ORDER_SL    0     # Original tri-linear formulation.
            1     # 1st order tri-linear (same as ORDER_SL = 1)
            2     # 2nd order tri-quadratic
            3     # 3rd order tri-cubic
```

```
4      # 4th order tri-quartic
```

The default is ORDER_SL = 0. The higher order schemes are non-monotonic and require a monotonicity constraint to be applied. The higher the order, the slower the scheme.

Speed is reduced if IO is excessive, hence any variables read into the model from file should have an INPUT_DT at least as much as the timestep used (e.g. don't input a variable at INPUT_DT=10 minute intervals, or output data with tinc = 10 minutes if the timestep DT=1 hour). Additionally, if file input or output is less than the time-step, then the model will effectively run using the smaller time-step; this may cause the semi-Lagrangian scheme to become stuck in an infinite loop.

The transport model may be used with input fields derived from other models (e.g. MOM). Sometimes these models do not account for leap years in their simulation; to account for this specify:

```
NO_LEAP_YEARS      YES   # Always use 365 days per year
```

A transport file can be created from a standard .prm file by specifying TRANS_DATA in the .prm file. The name of the transport file in this case is <INPUT_FILE>.tran; e.g. if the input file in the .prm file is 'infile.nc', then the transport filename will be 'infile.tran'.

When the transport mode is invoked using semi-Lagrangian advection, a tracer Vi with long name 'Volume error' is created which contains the volume conservation error (in m^3) for each cell resulting from the use of the semi-Lagrange scheme.

9.1 Multiple grids

It is possible to perform transport on a subset of the grid used to save the transport files. In this case, the streamline origin is computed on the source grid, which is defined as the grid on which the TRANS_DATA were created, and the values of tracer variables are interpolated on a different target grid. All output is performed on the target grid. The target grid must lie completely within the source grid, and will conform to one of the following:

1. The target grid may be an exact duplicate of the source grid. This may be for a smaller subset of the source grid. In this case the target grid is defined as having an EXACT relationship to the source grid, and resolution of source and target grids are the same.
2. The target grid may be a decimation of the source grid, i.e. 4, 9, 16 etc. source cells may be grouped to form a target cell, so that the target grid has coarser resolution than the source grid. In this case the target grid is defined as a SUBSET of the source grid.
3. The target grid is completely different to the source grid. An example of this may be a target grid created at higher resolution than the source grid. These grids are defined as a SUPERSET.

To perform transport on multiple grids, a SOURCE_GRID must be defined in the parameter file. This is simply an input file containing the grid configuration one wishes to use as the source grid. The TRANS_DATA files must also be created on the source grid. The target grid is assumed to be defined as the grid nominated by the INPUT_FILE in the parameter file. These files must be created using the -g option. An example is as follows:

```
INPUT_FILE        in.nc       # Target grid
SOURCE_GRID       source.nc   # Source grid
```

The transport model will compare these grids to determine if the relationship is EXACT, SUBSET or INEXACT, and handle them accordingly. From a users perspective, the

differences are that EXACT grids operate the fastest and INEXACT the slowest, owing to the amount of interpolation involved between grids.

9.2 STREAMLINE mode

An intermediate step may be performed to create transport files that contain information regarding the streamline origin, rather than velocities used to calculate the streamline. This approach may increase execution speed since the streamline origin is no longer required to be calculated. If multiple grids are used, then potentially slow input of velocity information for the source grid may also be avoided.

The STREAMLINE data files may be created when running the transport mode normally and dumping the variables origin, p, q, and r to SPARSE formatted files (Section 4.32.6). This file is then used to specify the TRANS_DATA, using the STREAMLINE option. Note that these TRANS_DATA input files to the STREAMLINE option cannot be interpolated in space and time, and must be read in exactly as written, hence the use of the SPARSE data format. Note also that this means that if STREAMLINE data files are created, the user is locked into using the time-step corresponding to that for which the files were created.

When using the STREAMLINE option, the input of data from file and transport computation are out of sync, necessitating reading TRANS_DATA information one time-step in advance. For this reason, when creating STREAMLINE data files, the stop time should be at least one time-step longer than the STREAMLINE transport is to run for.

Open boundary input is required if global MONOTONIC fills are used, so mass flux through open boundaries can be calculated. This information may be saved to file under normal operation of the transport mode, and re-read using the open boundary specification. Alternatively, complete u1 and u2 velocity fields may be saved to the STREAMLINE data files, which may be used in the global filling. This approach will be automatically invoked if BCOND_NOR = NOTHIN for all open boundaries. Note that when files are read into SHOC interpolation is always performed, even if the input file geometry and model grid are exactly the same; this can lead to slightly different numerical values entering the code compared to the values in the file. SPARSE formats do not suffer this problem, since no interpolation in space occurs when they are read into SHOC.

The STREAMLINE mode is invoked via:

```
TRANS_MODE          STREAMLINE
```

9.3 Conservation

The transport model is non-conservative for two reasons:

1. The semi-Lagrange scheme is cast in advective form and is non-conservative.
2. Continuity is not achieved when using snapshots or temporal averages of velocity and surface elevation fields. For a snapshot this is obvious; continuity is only achieved if the velocity is constant over the transport time-step. For temporal means, the elevation change over a time-step, $\Delta\eta$, is *not* equal to the horizontal divergence of depth averaged mean velocity multiplied by mean total depth, i.e.
$$\Delta\eta = \int_{t1}^{t2} \eta dt \neq \nabla_H \int_{t1}^{t2} D dt \int_{t1}^{t2} \vec{u} dt$$
hence continuity is also not achieved.

The global filling attempts to compensate for these effects, and an option exists to impose a global fill on the tracer solutions to ensure conservation. This method computes the mass

before advection, and the mass after advection accounting for input of mass through the open boundaries and due to source/sinks. If the scheme is conservative then mass before and after should equal. If not, then the excess or shortage of mass is distributed over all cells equally. This excess/shortage mass is usually results in very small (multiplicative) adjustments to the concentrations in each cell. Furthermore, the mass adjustment may be computed so that resulting tracer values remain monotonic, i.e. the adjusted concentrations are not greater or less than the local maximum or minimum concentrations.

```
FILL_METHOD       NONE        # No conservation adjustment
                  GLOBAL      # Global filling
                  MONOTONIC   # Global filling ensuring monotonicity
```

The default method is `FILL_METHOD = MONOTONIC`.

Continuity dictates that total volume in the whole domain at the end of the time-step is equal to total volume at the start of the time-step plus volume fluxes into the domain. Volume is not subject to errors from 1) above, so ideally (assuming volume fluxes are due to *n* open boundaries only):

$$V^t + \sum_n OBC_n = V^{t+1}$$

Any error from 2) can be compensated by adjusting the boundary fluxes by some factor *f;*

$$f = \frac{V^{t+1} - V^t}{\sum_n OBC_n}$$

This factor may then be applied to mass fluxes for tracers in the transport model, so that the global fill factor is adjusted to reflect extra mass that would need to be added (or subtracted) if volume conservation were achieved in the domain. In practice continuity is not achieved in the 3D model at open boundary locations since velocity and elevation are prescribed independently via OBCs, and these OBCs rarely honour continuity (e.g. a radiation condition on elevation is often used with a no-gradient condition on normal velocity and zero tangential flow, leading to zero divergence but non-zero change in elevation). This can corrupt the above computation, therefore *f* is computed excluding open boundary cells, with boundary fluxes computed at the first interior location to open boundaries. The open boundary adjustment is invoked by including `OBC_ADJUST` in the `FILL_METHOD`, e.g. for `MONOTONIC` filling:

```
FILL_METHOD       MONOTONIC OBC_ADJUST
```

If the `MONOTONIC` transport mode is invoked, then a 2D diagnostic variable `vol_cons` is written to the output files which contains the volume error of each water column expressed as a percentage of total volume in each water column. This volume error is the difference between the volume at the end of a time-step and the sum of volume at the start of the time-step and volume flux divergence into the water column.

If `DIAGNOSE` is included in the `FILL_METHOD`, then a time series file containing the mass that must be added (or subtracted) to the domain for each tracer to achieve mass conservation, and the corresponding multiplicative fill factor is created. This also contains the total domain volume error and open boundary scaling factor.

9.4 Flux form semi-Lagrange

The flux form semi-Lagrange (FFSL) advection scheme, developed by Leonard et al. (1996) and Lin and Rood (1996), is a conservative advection scheme that can be used with the transport model. While not unconditionally stable, the scheme is constrained by the less

restrictive Lipschitz condition, that basically ensures that streamlines cannot cross. The advantage of the FFSL scheme lies in that it is locally conservative. It is based on the 3rd order scheme of Van Leer, hence is more accurate than the 1st order semi-Lagrangian scheme. The FFSL scheme may be used in fully coupled mode, or in transport mode. For the latter, the average volume fluxes through cell faces must be additionally saved to the transport files. To invoke this when running shoc using the `-p` option, use:

```
TRANS_MODE      SP_FFSL  # Save volume fluxes to transport files.
```

When running the transport model with the FFSL scheme, use:

```
TRANS_MODE          SP_FFSL             # Use FFSL transport mode
FILL_METHOD         NONE                # No fill method
TRA_SCHEME          FFSL                # FFSL advection
STABILITY           SUB-STEP-NOSURF     # Enable sub-stepping
MERGE_THIN          YES                 # Merge thin layers
CONSERVATION        ETA W               # Conservation options
```

Since vertical velocity is a diagnosed quantity, computed from the volume fluxes (which are accessible in the FFSL transport mode), it is possible to reconstruct the vertical velocity distribution. This is the recommended approach and is achieved by using:

```
CONSERVATION        W             # Enforce w conservation
```

The vertical velocity may be recomputed only if it does not violate the Lipschitz condition by using:

```
CONSERVATION        W WSTAB       # Enforce stable w conservation
```

If this occurs, then the tracer `vol_cons` will be assigned the value 1 at that water column. Sea level may be similarly recomputed; in this case sea level is updated to the computed value if that value and the value in the transport files differ by some threshold (currently $1x10^{-5}$ m). This is invoked using:

```
CONSERVATION        ETA                 # Enforce η conservation
```

If this occurs, then the tracer `vol_cons` will be assigned the value 2 at that water column. If vertical velocity or sea level are re-computed (enforcing conservation), then any water fluxes input via point sources or sinks must be accounted for. These cannot be read in during the transport simulation in exactly the same manner as during the hydrodynamic simulation due to differences in time stepping, and are therefore also saved to the transport file during the hydrodynamic simulation. To minimize file size, these volume fluxes are saved to the vertical velocity variable in the transport file if point sources are specified in the hydrodynamic simulation with volume fluxes (i.e. hydrodynamic point source files contain `flow`), and copied to the point source volume flux variables when re-read in the transport mode. This only occurs if the point sources are also specified in the transport simulation with volume fluxes (i.e. transport point source files contain `flow`). To override this transfer of vertical velocity to volume fluxes in transport mode, use:

```
CONSERVATION        NO_PSS_FLOW   # No volume flux transfer
```

A no-gradient condition can be enforced for each tracer before entering the FFSL advection scheme by using:

```
CONSERVATION        NOGRAD   # Enforce no gradient conditions
```

This can assist in ensuring the transverse terms do not contain spurious data, however, should only be used if severe non-conservation is observed as this option has been known to degrade the solution in some applications.

If the transport files contain unreasonable data due to the hydrodynamic model tending toward instability, then this may be mitigated in the surface layer by merging volume fluxes and velocities using:

```
CONSERVATION          MERGED   # Merge surface layer volume fluxes
```

This should be a last resort option when trying to ensure conservation in the FFSL model.

To ensure that consistency (and hence conservation) occurs between hydrodynamic transport files and transport simulations***, ALWAYS USE THE SAME POINT SOURCE CONFIGURATION IN THE TRANSPORT MODE AS THAT SPECIFIED IN THE HYDRODYNAMIC SIMULATION.*** If volume fluxes are used in the hydrodynamic simulation, then those same point sources in the transport mode must also use volume fluxes. If no volume fluxes are present in the hydrodynamic simulation, then do not specify volume fluxes for point sources in the transport mode.

The FFSL advection scheme is not as diffuse as the semi-Lagrangian scheme, and it may be desirable to explicitly include horizontal mixing, e.g;

```
DIFF_SCALE            LINEAR
U1KH                  -0.455
U2KH                  -0.940
SMAGORINSKY           0.1
```

Note that if the `DYNAMIC` river open boundary is used in the hydrodynamic model (Section 4.10.6), then there will be inflow and outflow at the river open boundary in the transport model. If a `TRCONF` tracer open boundary condition is used, then the value supplied with the `TRCONF` OBC rather than the cell interior value will be multiplied by any outflow through the boundary face to get the boundary flux. This may result in negative boundary cell tracer concentrations.

10 Percentile computations (-ps option)

SHOC can compute the percentile distributions, i.e. order statistics of temporal records (in increments of 5%-iles), of a time series file using:

```
shoc –ps prmname
```

The keywords required in the parameter file are:

```
P_IFILE     # Input file. This may be ASCII, netCDF, multi-netcdf or
            # sparse format (including multiple datafiles (Section
            # 4.32.2) sparse files.
P_OFILE     # Output file. If OutputPath is specified, the file is
            # placed in this directory.
P_VARS      # Variable names to compute percentiles.
P_STIME     # Start time of the computations relative to TIMEUNIT
P_ETIME     # End time of the computations relative to TIMEUNIT
P_DT        # Processing interval; subsamples the input file.
```

An example is as follows.

```
TIMEUNIT    seconds since 2000-01-01 00:00:00 +08
OutputPath  /home/work/

P_IFILE     inut.txt
P_OFILE     perc.nc
P_VARS      temp salt
P_STIME     10 days
P_ETIME     20 days
P_DT        12 hours
```

With `input.txt` containing:

```
multi-netcdf-version 1.0
nfiles 2
file0.filename   t1.nc
file0.filename   t2.nc
```

the files `t1.nc` and `t2.nc` may be sparse formatted files. Every record in the input file is read and included in the computations unless `P_DT` is specified, when every *n* record is included where *n* = (`P_DT` in seconds) / (output interval of `P_IFILE` in seconds).

11 File formats

SHOC uses two file formats for input and output data exchange. An ASCII time series column format and a multi-dimensional netCDF format. Both of these files support multiple variables, an unlimited number of time records, and the association of geometry with variables.

Typically ASCII time series files are used when a time series of multiple variables is required for a specific location, and netCDF files for input/output of time varying grid or multi-point data.

11.1 ASCII time series

An ASCII time-series file contains data formatted into columns and a header describing the number of columns, their names, units, missing values, etc. Typically the first column contains the time (which must monotonically increase) and the remaining columns the data and coordinate variables.

Following is a schematic represenation of a time series file:

```
# Comments
## COLUMNS n
##
## COLUMN1.name time
## COLUMN1.long_name Time
## COLUMN1.units days since 1990-01-01 00:00:00 +10
## COLUMN1.missing_value -99999999
##
## COLUMN2.name XXXX
## COLUMN2.long_name XXXX
## COLUMN2.units XXXX
## COLUMN2.missing_value XXXX
##
      .
      .
      .
##
v   v   v   v   ...
v   v   v   v   ...
v   v   v   v   ...
      .
      .
      .
```

11.1.1 Units

The units for each variables should follow the standard **udunits** conventions, however at this stage, other than time, no interpretation of the units is made by **SHOC**. Since **SHOC** uses SI units internally it is suggested that these units be adopted for all input variables.

An ISO date/time format has been adopted in for time units, it has the following syntax:

```
[units since ]yyyy-MM-dd [hh[:mm[:ss[.sss]]][ +|-hh[:ss]]]
 |---- 1 ----|  |-- 2 ---|  |----- 3 -----|     |-- 4 --|
1 - The scaling units (e.g. days, hours, seconds, ms, us, etc.)
2 - Date (year, month, day_of_month).
3 - Time of day (hours, minutes, seconds, milliseconds).
4 - Time zone relative to UTC (+ or - UTC, hours, seconds).
```

All text enclosed within square brackets is optional.

11.1.2 Utilities

The time series format is well suited for use with standard plotting packages such as gnuplot or Matlab. Two Matlab scripts (`tsheader` and `tsread` have been installed in the Matlab software repository directory `/home/software/matlab`).

- `tsheader` reads the header from a time series file and returns a vector of structures each containing the time series file attributes as fields of the structure.
- `tsread` reads the header into a structure and returns a column vector of time's, and a matrix of the data records.

11.2 NetCDF time series

The netCDF file format is commonly used by many research organizations for the storage of time varying gridded data in a manner that it is plaform independent. NetCDF also permits the association of attributes with any variable, this feature is extensively used by **SHOC** to describe the units, missing values, coordinate conventions, etc. The netCDF library was written by Unidata (http://www.unidata.ucar.edu/), and can be download from ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf.tar.Z. **SHOC** requires version 3 or higher.

All **SHOC** input/output dumpfiles are stored using netCDF.

11.2.1 Units

Units for netCDF variables are handled the same as for ASCII time series files.

11.2.1.1 Coordinate conventions

The netCDF library provides a frame work for reading and writing blocks of data, but it does not provide any implicit mechanism by which coordinate information is associated with data variables. This association needs to be explicitly made by the software reading the netCDF file.

To assist in automating this association, **SHOC** has adopted it's own coordinate convention for binding data variables and coordinate variables. The convention requires the specification of special attributes for both data and coordinate variables. Data variables contain a **coordinates** attribute which defines a list of coordinate variables associated with it. The coordinate variables contain an attribute **coordinate_type** that describes the spatial coordinate this dimension corresponds to. Following is an example NetCDF CDL snippet:

```
netcdf file {
   dimensions:
     nrecord = UNLIMITED;
     ni = 10;
     nj = 20;
     nk = 5;

   variables:
      // Time coordinate variable.
      double t(nrecords);
        t:units="seconds since 1990-01-01 00:00:00 +10";
        t:coordinate_type="TIME";
```

```
      // X coordinate variable of a 2d rectangular grid.
      double x(nj, ni);
        x:units="m";
        x:coordinate_type="X";
        x:analytic="rectangular 0 0 10 20 0 0 1000 1000 0";

      // Y coordinate variable of a 2d rectangular grid.
      double y(nj, ni);
        y:units="m";
        y:coordinate_type="Y";
        y:analytic="rectangular 0 0 10 20 0 0 1000 1000 0";

      // Z coordinate variable.
      double z(nj, ni);
        z:units="m";
        z:coordinate_type="Z";

      // Each record, and dimension has a unique T, X, Y and Z
      // coordinate associated with it. The coordinates are stored
      // in units of m.
      double salt(nrecords, nk, nj, ni);
        salt:units="practical salinity units";
        salt:long_name=”Salinity”;
        salt:coordinates="t, x, y, z";
};
```

In the above example, the salinity variable represents a four dimensional gridded data object. The **coordinates** variable associates with this the t, x, y, and z coordinate information. Note that all dimensions used in the salnity variable are collectively found in the coordinate variables, and there are no additional dimensions.

The optional **analytic** attribute should be specified for coordinate systems where a simple analytically defintion is possible (e.g. rectangular grids). The inclusion of an **analytic** attribute permits faster and more accurate conversion between coordinate and indice space. **SHOC** currently understands both rotated rectangular and polar grids. The attribute should be associated with each coordinate variable.

To define an analytic attribute for a rectangular grid, use the following syntax:

```
   var:analytic = "rectangular ioff joff ni nj x0 y0 dx dy rot";
   ioff - I offset within the grid 0 is grid edge 0.5 is centre.
   joff - J offset within the grid 0 is grid edge 0.5 is centre.
   ni - number of grid points along i dimension (one more than number
of cells).
   nj - number of grid points along j dimension (one more than number
of cells).
   x0 - X coordinate origin.
   y0 - Y coordinate origin.
   dx - Width of cell in X direction.
   dy - Height of cell in Y direction.
   rot - Mathematically defined angle of rotation of grid.
```

To define an analytic attribute for a polar grid, use the following syntax:

```
   var:analytic = "polar ioff joff ni nj x0 y0 rmin arc";
   ioff - I offset within the grid 0 is grid edge 0.5 is centre.
   joff - J offset within the grid 0 is grid edge 0.5 is centre.
   ni - number of grid points along i dimension (one more than
        number of cells).
   nj - number of grid points along j dimension (one more than
        number of cells).
```

```
   x0 - X coordinate origin.
   y0 - Y coordinate origin.
   rmin = Minimum radius.
   arc = Angular width of cell.
```

This example netCDF CDL snippet defines a geographic grid. If a `PROJECTION` parameter was specified as the default coordinate system, then SHOC will automatically convert from geographic coordinates to the map projection (if necessary), when reading the data file.

```
netcdf file {
   dimensions:
     nrecord = UNLIMITED;
     ni = 10;
     nj = 20;
     nk = 5;

   variables:
      // Time coordinate variable.
      double t(nrecords);
        t:units="seconds since 1990-01-01 00:00:00 +10";
        t:coordinate_type="TIME";

      // Latitude coordinate variable of a 2d rectangular grid.
      double lat(nj, ni);
        lat:units="degrees_east";
        lat:coordinate_type="latitude";

      // Longitude coordinate variable of a 2d rectangular grid.
      double lon(nj, ni);
        lon:units="degrees_east";
        lon:coordinate_type="longitude";

      // Z coordinate variable.
      double z(nj, ni);
        z:units="m";
        z:coordinate_type="Z";

      // Each record, and dimension has a unique T, X, Y and Z
      // coordinate associated with it. The coordinates are stored
      // in lat/lon units.
      double salt(nrecords, nk, nj, ni);
        salt:units="practical salinity units";
        salt:long_name=”Salinity”;
        salt:coordinates="t, lon, lat, z";
};
```

This a snippet demonstrate how to define a 3d grid with a map projection (Australian Map Grid):

```
netcdf file {
   dimensions:
     nrecord = UNLIMITED;
     ni = 10;
     nj = 20;
     nk = 5;

   variables:
      // Time coordinate variable.
      double t(nrecords);
        t:units="seconds since 1990-01-01 00:00:00 +10";
```

```
        t:coordinate_type="TIME";

      // X coordinate variable of a 2d rectangular grid.
      double x(nj, ni);
        x:units="m";
        x:coordinate_type="X";
        x:projection="proj=amg zone=55”;

      // Y coordinate variable of a 2d rectangular grid.
      double y(nj, ni);
        y:units="m";
        y:coordinate_type="Y";
        y:projection="proj=amg zone=55”;

      // Z coordinate variable.
      double z(nj, ni);
        z:units="m";
        z:coordinate_type="Z";

      // Each record, and dimension has a unique T, X, Y and Z
      // coordinate associated with it. The coordinates are stored
      // in AMG units.
      double salt(nrecords, nk, nj, ni);
        salt:units="practical salinity units";
        salt:long_name=”Salinity”;
        salt:coordinates="t, x, y, z";
};
```

Finally if the data is not stored on a grid but as a series of discrete points then an evalatuion at an arbitary point will use an inverse weighted interpolation scheme (1/r). Of course this assumes the **coordinates** and **coordinate_type** attributes have been specified.

```
netcdf file {
   dimensions:
     nrecord = UNLIMITED;
     np = 1000;

   variables:
      // Time coordinate variable.
      double t(nrecords);
        t:units="seconds since 1990-01-01 00:00:00 +10";
        t:coordinate_type="TIME";

      // X coordinate variable of a 2d rectangular grid.
      double x(np);
        x:units="m";
        x:coordinate_type="X";

      // Y coordinate variable of a 2d rectangular grid.
      double y(np);
        y:units="m";
        y:coordinate_type="Y";

      // Z coordinate variable.
      double z(np);
        z:units="m";
        z:coordinate_type="Z";

      // Each record and point has a unique T, X, Y and Z
      // coordinate associated with it.
      double salt(nrecords, np);
```

```
        salt:units="practical salinity units";
        salt:long_name=”Salinity”;
        salt:coordinates="t, x, y, z";
};
```

11.2.1.2 Utilities

The simplest way to view the contents of a netCDF file is to use the standard netCDF utility `ncdump`.

To view the file header, use:

```
ncdump -h filename
```

or to view the entire file, use:

```
ncdump filename
```

This gets impractical for large output files, and doesn't produce graphical output, this is particularly true for model dumpfile. Another way to view the netCDF dumpfiles is to use `jvismeco`, which can read these files and display the values of most variable. This technique is useful for examining the model in detail, to find the cause of an instability, for example. However, it still doesn't allow you to save any sort of graphical output (yet).

Modules to read and write netCDF files have been added to the commercial application Matlab (commonly used in the scientific community). Matlab is a good tool for analysing the model dumpfiles. A number of supplementary Matlab scripts (`mecoread2d`, `mecoread3d` and `ncinfo`) have been installed in the Matlab software repository directory `/home/software/matlab` for reading **SHOC** netCDF dumpfiles.

- `mecoread2d` reads a two dimensional variable and associated geometry from a **SHOC** file. Following is an example of how to use `mecoread2d`:
  ```
  [xl,yl,u1av] = mecoread2d('out.nc','u1av',10);
  ```
- `mecoread3d` reads a three dimensional variable and associated geometry from a **SHOC** file. The data is returned as a 3d volume unless a specific layer is specified. Following is an example of how to use `mecoread3d`:

```
[xc,yc,eta] = mecoread3d('out.nc','salt',44);
```

or

```
[xl,yl,u1av] = mecoread3d('out.nc','u1',10, 151);
```

- ncinfo provides summary information bout all variables within a netCDF file, and their dimensions.

```
ncinfo('out.nc');
```

12 Tests

A suite of tests has been collected for this model. These tests are used to validate the model against analytic solutions or other known, simply understood situations. They are particularly useful to check the correct operation of the model after modifications to the model code.

12.1 No forcing

Test 1 is an extremely simple, null case, test, where no forcing is applied to a closed model domain. The purpose is to demonstrate that no model variables deviate from their initial values. A rectangular grid is used with a horizontal grid of 5 by 10 cells, and 5 layers in the vertical having 1m vertical spacing. The bathymetry varies and the water is initially vertically stratified. Vertical diffusion of salt and heat is turned off in this case to avoid diffusive changes. Each run consists of a 1000 second integration with no externally applied forcing. The initial variable values (zero elevation, zero velocity, salinity and temperature) should remain unchanged for the duration of the integration.

12.2 Ekman Spiral

A wind of constant stress and direction is blown over a homogeneous open ocean of constant depth. The model uses cyclic open boundaries reflect the open ocean condition, and utilizes constant vertical viscosity and linear bottom friction for simplicity. According to Kowalik and Murty (1993, p27) the linear resistance coefficient is related to the bottom drag coefficient via:

$$r = \rho C_d |v| \qquad 12.2.1$$

where C_d is the drag coefficient, v is the bottom current speed and ρ is the density. Given a constant eddy viscosity, the Ekman depth, D_E, is given by (Pond and Pickard, 1983, p108):

$$D_E = \pi\sqrt{2V_z/|f|} \qquad 12.2.2$$

where V_z is the eddy viscosity and f is the Coriolis parameter. The surface current speed, V_o, is then given by (Pond and Pickard, 1983, eqn 9.10):

$$V_o = \frac{\sqrt{2}\pi\tau_s}{D_E\rho|f|} \qquad 12.2.3$$

where τ_s is the wind stress, and the current speed, V_b, at the Ekman layer depth is (Pond and Pickard, 1983, p108):

$$V_b = V_o \exp(-\pi) \sim 0.04V_o \qquad 12.2.4$$

Therefore, using a wind stress of 0.01Nm^{-2} on and f-plane with f = 1e^{-4}, and V_z = 0.0507 m^{2}s^{-1}, the Ekman layer depth D_E = 100m. Furthermore, using 12.2.3 with ρ = 1025 kgm^{-3} gives V_o = 4.33x10^{-3} ms^{-1} and V_b = 1.87x10^{-4} ms^{-1}. Using the bottom velocity in 12.2.1 and a nominal drag coefficient of C_d = 0.003 gives a resistance coefficient of r = 0.00058. Linear friction is achieved by setting the parameter `UF` to a large value and `Z0` to a low value. The value of `Z0` below which bottom drag is set to the parameter `QBFC` is given by:

$$Z0 < \frac{0.5\Delta z_{bot}}{\exp(\kappa.sqrt(1/QBFC)-1)} \qquad 12.2.5$$

Using the value of QBFC quoted above, Z0 < 7.7x10^{-8}. Using these values with UF = 1.0 provides linear bottom friction with the required resistance coefficient. Using the above configuration, model results should show an Ekman spiral with velocities rotating clockwise with depth, surface current speed ~ 0.0043 ms^{-1} and bottom current speed ~ 0.00019 ms^{-1}. Surface elevation should be equal to zero.

12.3 Constant wind stress – closed basin

This test examines the set-up due to a steady wind applied to a 1-layer (depth-averaged) model domain. If a constant wind is applied to a homogeneous closed basin of constant depth then depth averaged velocities are equal to zero in the steady state. For a linear model and constant wind stress in the x direction the surface slope should balance the applied wind stress, and the equations of motion reduce to an expression for the sea level gradient in the x direction:

$$\frac{\partial \eta}{\partial x} = -\frac{\tau_s}{\rho g D} \qquad 12.3.1$$

where D is the water depth. If a wind stress of 1Nm^{-2} is applied to a homogeneous ocean of temperature 20^{o}C and salinity 35 psu so ρ = 1024.76 kgm^{-3}, then the slope in a 10m deep basin is equal to 9.958x10^{-6}, and the depth averaged velocities should be near zero.

12.4 Constant wind stress – alongshore open channel

An analytical solution exists for a linear model of constant wind stress applied in a longshore direction along an infinitely long coast. Assuming cross-shelf transport and alongshore sea level gradient are small, then along shelf transport, U, is given by (Chapman, 1985, eqn 4.5):

$$U = \frac{D\tau_s}{\rho r}\left(1 - \exp(-tr/D)\right) \qquad 12.4.1$$

with a steady state velocity ($t = \infty$) given by:

$$U = \frac{D\tau_s}{\rho r} \qquad 12.4.2$$

Note U is the transport, hence velocity u = U/D.
The sea surface slope is given by (Chapman, 1985, eqn 4.6):

$$\frac{\partial \eta}{\partial y} = -\frac{fU}{gD} = -\frac{f\tau_s}{\rho g r}\left(1 - \exp(-tr/D)\right) \qquad 12.4.3$$

with steady state sea level given by:

$$\eta(y) = -\frac{f\tau_s}{\rho g r}\left(\tfrac{L}{2} - y\right) \qquad 12.4.4$$

where L is the width of the channel and it is assumed $\eta = 0$ at y = -L/2.

Cyclic open boundaries are used to represent an infinite coastline. Using a wind stress of 0.1 Nm^{-2} in a channel 500km wide (the dimensions of this domain are the same as the test

domain used by Palma and Matano (1998) except the Southern hemisphere is considered) with linear resistance coefficient r = 0.0005, Coriolis = -1.028e^{-4} and ρ = 1024.76 kgm^{-3}, the along-shore depth averaged velocity is 0.195 ms^{-1}, the cross-shore depth averaged velocity is zero and elevation at the coast is 0.49 m (slope of 2.05x10^{-6}. Note the first elevation cell center is found at y = 10km). This result assumes a linear depth averaged model is used, and a non-linear 3-D model with quadratic bottom friction is expected to give different results.

12.5 Constant wind stress – cross-shore open domain

A wind applied perpendicular to an infinitely long coastline (on the southern boundary in this case) will result in an elevation setup against the coast with zero depth averaged currents everywhere. The on-shore wind stress drives depth averaged flow to the west (east) in the northern (southern) hemisphere, and the sea level gradient resulting from setup at the coast drives this flow to the east (west). In a perfect situation the sea level gradient and wind stress forces balance resulting in no flow. Boundary effects and numerical error may make one of these forces dominate, leading to non-zero flow in the east (west) direction in the northern (southern) hemisphere if the sea level pressure gradient dominates, and vice versa if wind stress dominates. Assuming a linear model with linear bottom friction, the analytical solution for sea level profile is given by (Chapman, 1985, eqn 4.13a):

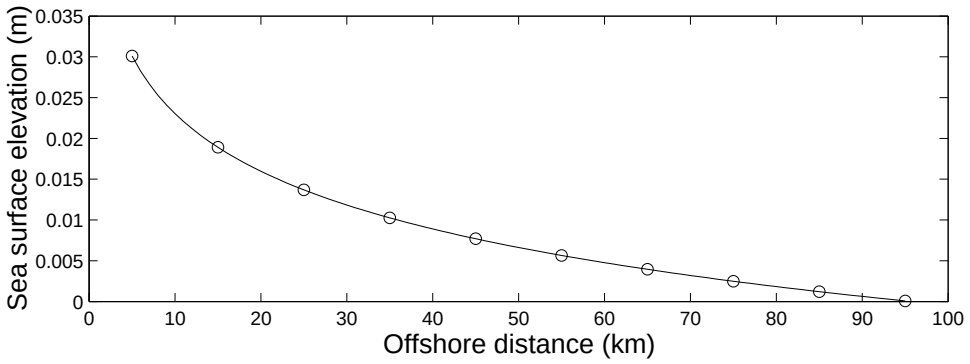
$$\frac{\partial^2 \eta}{\partial y^2} = -\frac{\tau_s}{\rho g D^2}\frac{\partial D}{\partial y} \qquad 12.5.1$$

Using a domain with two cyclic cross-shelf open boundaries and one offshore boundary with elevation clamped to zero, and the linear depth profile used by Chapman (1985, eqn 4.1), then the sea level profile is given by Chapman (1985, eqn 4.14) and shown in Figure 12.5.1 and Table 12.5.1. The boundary conditions of eqn. 12.5.1. for this domain are:

$$\frac{\partial D}{\partial y} = -D_o \text{ at y} = 0 \;\; \therefore \;\; \frac{\partial \eta}{\partial y} = \frac{\tau_s}{\rho g D_o} \;\; \text{and} \; \eta = 0 \text{ at y} = \text{L} \qquad 12.5.2$$

where L is the distance to the offshore boundary.

Figure 12.5.1 : Sea level profile for onshore wind stress.



Offshore distance (km)	*Surface elevation (m)*
5	***0.0301***
15	***0.0189***
25	***0.0137***
35	***0.0103***
45	***0.0077***
55	***0.0057***
65	***0.0039***
75	***0.0025***
85	***0.0012***
95	***0.0001***

Table 12.5.1 : Sea level profile for onshore wind stress.

Again, a non-linear 3-D model with quadratic bottom friction is expected to give different results, and bottom friction is generally required to be increased for solutions to match theory. Specifically, adequate solutions were obtained using the `CONSTANT` mixing scheme with background vertical viscosity `VZ0` = 0.0507 (see Test2) and minimum bottom drag coefficient of `QBFC` = 0.003 (`UF` = `Z0` =1e-8). Horizontal viscosity of `U1VH` = `U2VH` = 800 is also required for stability.

12.6 Propagation of a bore

This test simulates a wetting bore propagating along an initially dry channel. The model domain represents a channel 2km wide and 100km long with uniform (flat) bathymetry. A constant velocity of 1 ms^{-1} is applied at one end of the initially dry channel. A bore propagates along the channel, with a parabolic shape (surface elevation profile) determined by a balance between the quadratic bottom friction and surface slope. The length of the bore is related to the depth at the inflow via:

$$L = \frac{gD^2}{2C_d U^2} \qquad 12.6.1$$

12.7 Wind stress curl – closed basin

Wind stress possessing curl applied to a closed basin with a gradient of f/D results in the formation of a gyre due to conservation of potential vorticity which is biased to the east if f/D < 0 and biased to the west if f/D > 0 (e.g. Herzfeld and Tomczak, 1999). The gradient of f/D may result from a gradient of f (β effect) or a change in topography. This test consists of a closed basin in the southern hemisphere with constant depth in the east – west direction, 50m depth at the southern coast and 100m depth at the northern coast. Wind stress in the e1 direction is applied, with 0.1 Nm^{-2} at the southern boundary and 0 at the northern boundary, hence this stress possesses negative curl. The gradient of f/D is positive in this case, thus an anticyclonic gyre biased to the west is expected, generated by topographically induced conservation of potential vorticity. Theory predicts that:

- A negative gradient of f/D (i.e. `CORIOLIS = 1.0e-4`) results in an eastward biased gyre.
- A flat bottom (`BATHYMAX = 50`) results in an unbiased gyre.
- Wind stress with positive curl (`WIND_SPEED SCALE = -1`) results in a cyclonic gyre with unaltered bias.

13 Tracer Statistics

A library named tracerstats exists in the directory ems/model/lib (see Figure 2.1) which allows various operations to be performed on existing tracers in the model. This includes sediment transport and ecological tracers if they exist. The tracerstats library offers a convenient way to perform processing on the fly rather than post-processing an output file. The advantage of using processing while the model is running is that statistics are computed at every time-step, rather than at the times data is dumped in an output file. Note that the tracerstats library must be present when the code is configured for the user to access this functionality.
The statistics available to be performed on 2D or 3D tracers are:

```
fluxe1      # Flux of 3D tracer in the e1 direction
            usage:      TRACER<n>.tracerstat  fluxe1(<3Dtracer>)
fluxe2      # Flux of 3D tracer in the e2 direction
            usage:     TRACER<n>.tracerstat   fluxe2(<3Dtracer>)
fluxw       # Flux of 3D tracer in the vertical direction
            usage:     TRACER<n>.tracerstat   fluxw(<3Dtracer>)
meanfluxe1  # Mean flux of 3D tracer in the e1 direction
            usage:     TRACER<n>.tracerstat   meanfluxe1(<3Dtracer>)
            optional:  TRACER<n>.dt           <m> days
meanfluxe2  # Mean flux of 3D tracer in the e2 direction
            usage:     TRACER<n>.tracerstat   meanfluxe2(<3Dtracer>)
            optional:  TRACER<n>.dt           <m> days
meanfluxw   # Mean flux of 3D tracer in the vertical direction
            usage:     TRACER<n>.tracerstat   meanfluxw(<3Dtracer>)
            optional:  TRACER<n>.dt           <m> days
mean        # Mean of 2D or 3D tracer
            usage:   TRACER<n>.tracerstat     mean(<tracer>)
            optional:  TRACER<n>.dt           <m> days
variance    # Variance of 2D or 3D tracer
            usage:   TRACER<n>.tracerstat     variance(<tracer>)
stdev       # Standard deviation of 2D or 3D tracer
            usage:   TRACER<n>.tracerstat     stdev(<tracer>)
corr        # Correlation coefficient of two 2D or 3D tracers
            usage:   TRACER<n>.tracerstat     corr(<tracer>:<tracer>)
cov         # Covariance of two 2D or 3D tracers
            usage:   TRACER<n>.tracerstat     cov(<tracer>:<tracer>)
sum         # Sum of 2D or 3D tracers
            usage:   TRACER<n>.tracerstat sum(<tr1>,<tr2>...
)
diff        # Difference of two 2D or 3D tracers
            usage:   TRACER<n>.tracerstat     diff(<tracer>:<tracer>)
max         # Maximum tracer value over a given time period
min         # Minimum tracer value over a given time period
vmax        # Maximum water column value of a 3D tracer
vmin        # Minimum water column value of a 3D tracer
vint        # Vertical integral of 3D tracer
            usage:   TRACER<n>.tracerstat     vint(<3Dtracer>)
vmean       # Vertical mean of 3D tracer
            usage:   TRACER<n>.tracerstat     vmean(<3Dtracer>)
vdiff       # The ratio of a series of layers of a 3d tracer
            usage:   TRACER<n>.tracerstat
                                vdiff(<3Dtracer>:<toprange>:<botrange>(strict))
copy        # Copy of a tracer
            usage:   TRACER<n>.tracerstat     copy(<tracer>)
sectionflux # integrate the flux over a defined area and time
            usage:   RTSTAT<n>.name   section(<3Dtracer>:<direction>)

rmse        # Compute the RMS error between two tracers
```

```
            usage:   TRACER<n>.tracerstat     rmse(<tracer1>:<tracer2>)

exposure    # Exposure time of a tracer above/below a threshold
            usage:      Tracer<n>.tracerstat
      exposure(<3Dtracer>:<threshold>:<expose_time>)
            optional:  TRACER<n>.dt           <m> days
            optional:  TRACER<n>.start        <m> days
            optional:  TRACER<n>.scale_factor <m> days
```

where:

`<3Dtracer>` is a 3-dimentional tracer
`<tracer>` is a 3-dimensional or 2-dimensional tracer

To initiate a tracerstat operation, an additional attribute `TRACER?.tracerstat` in the tracer list must be specified. The form of this attribute is of the type `operation(tracer_name)`, where `operation` is the statistic from the list above, and `tracer_name` is the name of the tracer to operate on. For example, to specify the flux in the `e1` direction of a tracer named `temp`, and output to a tracer called `flux_temp`, the following tracer is specified;

```
TRACER?.name            flux_temp
TRACER?.long_name       Temp flux in e1 direction
TRACER?.tracerstat      fluxe1(temp)
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

Note that these tracers are diagnostic and are not to be advected or diffused. Also, the `diagn` flag is turned off so that these tracers are not re-initialized to zero at every dump step. If a mean of tracer temp is required at 12 hourly intervals, use;

```
TRACER?.name            mean_temp
TRACER?.long_name       Average temp
TRACER?.tracerstat      mean(temp)
TRACER?.dt              12 hours
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

If the attribute `TRACER?.dt` is absent the mean for the whole simulation is calculated.
For statistics involving multiple tracers, the tracer names are separated by a colon in the `tracerstat` attribute. For example, to calculate the covariance of tracers `passive1` and `passive2` use;

```
TRACER?.name            covariance
TRACER?.long_name       Covariance of passive1 and passive2
TRACER?.tracerstat      cov(passive1:passive2)
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

The variance, standard deviation and covariance statistics for any tracers also require that that tracer's mean be specified. The correlation coefficient of two tracers requires that those tracers' means and standard deviations are specified. The vertical integral, mean or

difference of a 3D tracer is placed in a 2D tracer, e.g. to specify the vertical integral of a tracer `chl_a` use;

```
TRACER?.name            vint_chla
TRACER?.long_name       Vertical integral of chl_a
TRACER?.type            WC2D
TRACER?.tracerstat      vint(chl_a)
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

The vertical difference tracer statistic calculates the difference between the sums of various layers, e.g.

$$vdiff = \sum toprange - \sum botrange$$

where `toprange` and `botrange` are a list of individual layer numbers or layer ranges in the format `<from>_<to>`, separated by commas, e.g.

```
TRACER?.tracerstat      vdiff(salt:2,6,9_12:15_17,20)
```

will result in the sum of salinity concentration in layers 15,16,17 and 20 subtracted from the sum of salinity concentration of layers 2,6,9,10,11 and 12. The variable `strict` is given as 0 or 1 (with 0 used as the default). If `strict = 1` then the difference is given as zero if any of the layers in the `toprange` or `botrange` are not present, e.g. if one or more layers happens to lie below the sea bed.

The tracer statistics are computed in the order of the operation list provided above, hence it is possible to compute a statistic of a statistic if the order permits this. For example a vertical integral of a mean may be computed, but a mean of a vertical integral will result in operations performed at different time levels.
In addition to the tracers in the tracer list, it is possible to compute tracers on the following 2D and 3D hydrodynamic variables;

```
eta   # sea level, 2D
Kz    # Verical diffusivity, 3D
Vz    # Vertical viscosity, 3D
u1vh  # Horizontal viscosity in the e1 direction
u2vh  # Horizontal viscosity in the e1 direction
u1kh  # Horizontal diffusion in the e1 direction
u2kh  # Horizontal diffusion in the e1 direction
```

For example, the mean sea level may be calculated using:

```
TRACER?.name            mean_eta
TRACER?.long_name       Mean sea level
TRACER?.type            WC2D
TRACER?.tracerstat      mean(eta)
TRACER?.dt              12 hours
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

The `exposure` tracerstat computes the time a nominated tracer's value is above or below a given threshold. The units of the exposure are the nominated tracer's units multiplied by days. To change the units, use the `scale_factor` (e.g. `7 days` for units of <tracer units>.< weeks>). This tracerstat is effectively the integral of the tracer when its value is above/below

the threshold. The optional dt provided is a time period that the tracer must be below/above the threshold in order for the exposure time to be reset to zero. The <exposue_time> is the name of a tracer in the list that is used to keep track of how many days in the interval dt the tracer is below/above the threshold. This tracer is required primarily for housekeeping purposes. The start time is the time in model days that the exposure computation begins (the START_TIME is used as the default if this is absent). This allows the exposure tracerstat to operate with restarts. The <threshold> can be either a number or a tracer in the tracer list. The latter option allows a temporally and spatially varying threshold to be supplied. The threshold is the value the nominated tracer must be greater than by default; if this threshold is prefixed with '+' then the tracer must also be greater this threshold, if prefixed with '-' the tracer must be less than the threshold for the exposure to be incremented. For example, if an exposure is to be set up for salinity where the model salinity is integrated below values of 10 psu starting in summer 1990 (1 Dec 1990) using the tracer salt_ex_time as the exposure time, then use:

```
TRACER?.name            salt_exposure
TRACER?.long_name       Salinity exposure
TRACER?.units           psu days
TRACER?.tracerstat      exposure(salt:-10:salt_ex_time)
TRACER?.dt              1 day
TRACER?.start           334 days
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0

TRACER?.name            salt_ex_time
TRACER?.long_name       Salinity exposure time
TRACER?.units           days
TRACER?.fill_value_wc   0
TRACER?.valid_range     -1e-10 1e10
TRACER?.advect          0
TRACER?.diffuse         0
TRACER?.diagn           0
```

In this case the salinity must be greater than 10 psu for 1 day at a location before the salinity exposure is reset to zero at that location. Note that salt_exposure may be integrated for periods greater than 1 day; the dt used only sets a time period for when salt_exposure is reset to zero. The salinity exposure time (salt_ex_time) contains the accumulated time (days) within the period dt that the salinity is actually below 10 psu; i.e. if salinity is below 10 psu for a full day then salt_ex_time will contain 1. If, for example, dt were 1 hour and salinity was below 10 psu for 36 minutes (0.6 hour) then salt_ex_time would contain 0.025 days. Although not the primary array of interest, the exposure time is required by this tracerstat to keep track of the instances when the exposure is reset to zero. The salt_ex_time must be zero for a period dt for the exposure to be reset to zero.

The sectionflux statistic is designed to calculate the integral of the flux of a tracer over a defined spatial area and time interval. The spatial area may be a vertical 'curtain' in the e1-z or e2-z plane, or a horizontal layer in the e1-e2 plane. The spatial area is defined by a list of (i,j) coordinates input via ascii file, with an optional top and bottom layer included. If the top and bottom layer are not present, the section is integrated over the entire water column. The user must specify in which direction the flux is to be calculated (e.g. u1, u2 or w); it is the users responsibility to ensure this direction is perpendicular to the plane of the section (e.g. a flux in the u1 direction must have a section defined in the vertical e2-z plane, or a flux in the w direction must have a section defined in the horizontal e1-e2 plane). Note that the section must be defined along constant e1, e2 or z coordinates; if the section is defined across e1, e2 or z planes then the spatial integral will nor be conservative.

The file containing a list of <i j> locations (or optionally <i j topk botk>) defining the section is specified using the data attribute. Again, if the direction is u1, then this list should contain constant i coordinates, etc.
The section is integrated in time over a timescale defined by the dt attribute, and subsequently output to an ascii file specified by the output attribute. Note that the integrating timescale may not be exactly the specified dt, since if dt is not an integral number of model time-steps output will be written to file at the next larger time-step. The output file contains the time and value of integrated flux over the section and interval dt.
A start time may be optionally defined by the startt attribute. The default is the model start time. The default time unit in the output file is that defined by OUTPUT_TIMEUNIT in the parameter file. This may be scaled by supplying optional attributes tscale and tunit, where output time format is OUTPUT_TIMEUNIT / tscale (tunit). Similarly the units of the calculated flux may be optionally scaled using the attributes outscale and outunit, where integrated fluxes are written to the output file in units of (3D tracer unit) / outscale (outunit).
This form of tracer statistic computes one number for each section which is written to a time series file, i.e. the result of the calculation is not a 2-D or 3-D field and is therefore not sensible to output to a 2-D or 3-D tracer. The syntax for the specification of sectionfluxes is therefore different. An example is given below, where the prefix RTSTAT refers to 'run time statistic'.

```
NRTSTAT   1
RTSTAT.name    sectionflux(salt:u1) # type of run time statistic
RTSTAT.data    bay_mouth.sect       # file containing (i,j) list
RTSTAT.dt      6 hours              # time interval to write output
RSTAT.startt   3182 days            # (optional); start time for the
                                    # section integration. Default is
                                    # the model start time.
RTSTAT.tscale  6 hours              # (optional) time interval to
                                    # write output.
RTSTAT.tunit   minutes              # time interval to write output
RTSTAT.outscale 1000                # (optional) scaling factor for
                                    # output flux.
RTSTAT.outunit kg                   # (optional)output flux units.
```

The user may submit any number of individual sections.

A step attribute may be specified to compute tracerstats at a particular point in the sequence of computations within a time-step. This is invoked by prescribing:

```
TRACER?.step            n
```

Where the computational sequence is:

n = 1 : After computation of mixed layer depth, vorticity balance, flushing times, tracer percentiles, steric height and numbers.
n = 2 : After tracer decay, relaxation, increments and computation of totals.
n = 6 : After the wave library is called.
n = 3 : After the sediment library is called.
n = 4 : After the biogeochemistry library is called.
n = 5 : After the tracerstats library is called (i.e. statistics of statistics can be computed using step = 5).

Alternatively, these steps may be invoked via keywords, where:

PRE_DECAY	or POST_DIAG	corresponds to n=1
PRE_WAVE	or POST_DECAY	corresponds to n=2
PRE_SED	or POST_WAVE	corresponds to n=6

PRE_ECO	or POST_SED	corresponds to n=3
PRE_RTSTAT	or POST_ECO	corresponds to n=4
POST_RTSTAT		corresponds to n=5

For example, if `tracerstats` were to be invoked before the ecology library is called, then set:

```
TRACER?.step              PRE_ECO
```

or

```
TRACER?.step              POST_SED
```

If no step is specified, the standard `tracerstats` library call is between `step 4` and 5.

The tracerstats library may be easily expanded to provide functionality suited to a user's specific needs.

14 Getting Started

The steps required to compile SHOC, run on a simple test case and generate a custom application are detailed below. Note that visualisation and grid generation requires the matlab based software package PLUM.

14.1 Compile SHOC

Install the source code depicted by the directory structure Figure 2.1. Configure the code making sure any netCDF library paths are correctly specified (Section 2.2);
`./conf/configure`
Make the executable;
`make`
The SHOC executable now resides in `ems/src/model/hd`.
The version number is retrieved using:
`shoc –v`

14.2 Run a test case

Test cases are located in;
`ems/src/model/tests/hd`
A useful first test case is test 7, where a wind with positive curl is blown over a closed basin with sloping bathymetry (Section 12.7). To run this test:

Make an input file (Section 2.3 and 8):
```
shoc –g test7.prm in7.nc
```
Make sure no output files exist:
```
rm out7_z.nc
```
Run the model:
```
shoc –p test7.prm
```
View the output.

14.3 Generate a custom grid

The generation of custom grids requires the matlab based package PLUM (john.andrewartha@csiro.au for details) with the executables `gridgen` and `gridbathy` installed. The executable `gridbathy` is located in `ems/utilities/grid/`, however `gridgen` is currently not a member of `ems`. Refer to the README documentation supplied with PLUM for installation. Note that dedicated bathymetry and coastline databases may be required for custom grid generation of certain areas. Default databases are supplied with PLUM.

1. Invoke matlab and PLUM, for unix/linux;
```
matlab –nodesktop –nosplash -nojvm
>> plum
```

2. Generate a grid, in this case a geographic rectangular grid. This is a spherical grid where the spheroid is rotated so that the equator passes through the centre of the grid (Section 4.6.4). On the main PLUM menu, click on ‘GRID GENERATION’ and the following is displayed;

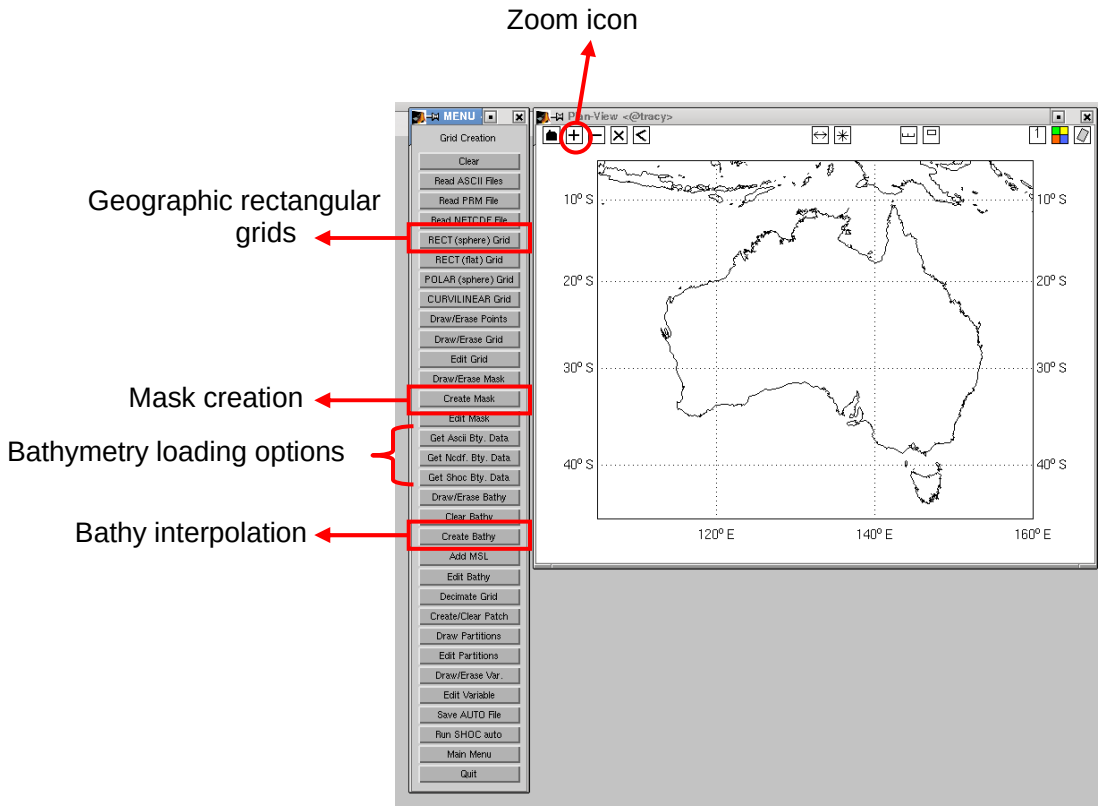


Figure 14.3.1. PLUM grid generation menu.

Zoom in on the location the grid is to be constructed for using the '+' icon at the top-left of the Plan-View screen. Click on 'RECT (sphere) Grid' to generate a spherical geographic rectangular grid. Other options are a non-geographic grid, polar grid or orthogonal curvilinear grid. Follow the instructions in the matlab window (i.e. click on the grid centre, left and right bottom corners). A grid is then created, e.g. Figure 14.3.2. The grid can be rotated, relocated or scaled by clicking and dragging the blue dots. The number of cells in the x-direction is specified by entering 'x' followed by the number of cells in the matlab window, and similarly for cells in the y-direction. Right-click the mouse to exit and define the grid, or click 'RECT (sphere) Grid' again for further definition of the grid. An example of the final grid is shown in Figure 14.3.3, in this case focussed on the South Australian Gulfs. Note the '+', 'x' and '-' icons in the Plan-View pane can be used to zoom in, centre and zoom out around the image while creating the grid (right click to exit from 'x').

3. Create a land mask. Click on the 'Create Mask' button (see Figure 14.3.1). The land in the domain is coloured green. Land, water or outside cells (Section 4.8) can be manually reset using the 'Edit Mask' button. The resulting masked image is shown in Figure 14.3.4. The number of 2D wet cells is displayed in the matlab window.

4. Load the bathymetry from a database. Bathymetry can be loaded from pre-existing ascii or netCDF databases, or can be loaded from a SHOC output file. In this case bathymetry is loaded from the AGSO 2002 database by clicking 'Get Ncdf. Bty. Data' and choosing the appropriate database. Bathymetry is loaded onto the image as depicted in Figure 14.3.5 (a). Return to the 'GRID CREATION' menu and click on 'Get Ncdf. Bty. Data' again. A decimation value for the bathymetry dataset may be then entered (enter 0 for default), and the bathymetry is truncated to the grid domain size (Figure 14.3.5 (b)).

5. Interpolate the bathymetry onto the grid. Click on 'Create Bathy' (Figure 14.3.1); a list of interpolation methods is listed in the matlab window. Enter the interpolation method required. In this case a '(7) for weighted area' is used. It is possible that the interpolation scheme will not fill all the cells in the domain. In this case click on 'Create Bathy' again and use '(6) for inverse distance (fill-in)'. This may be required to be performed several times. The

resulting interpolated bathymetry is displayed in Figure 14.3.6. Sometimes the interpolation scheme may fail, and no cells are interpolated. In this case try another interpolation method. Bathymetry cells may be manually edited by using the 'Edit Bathy' button.

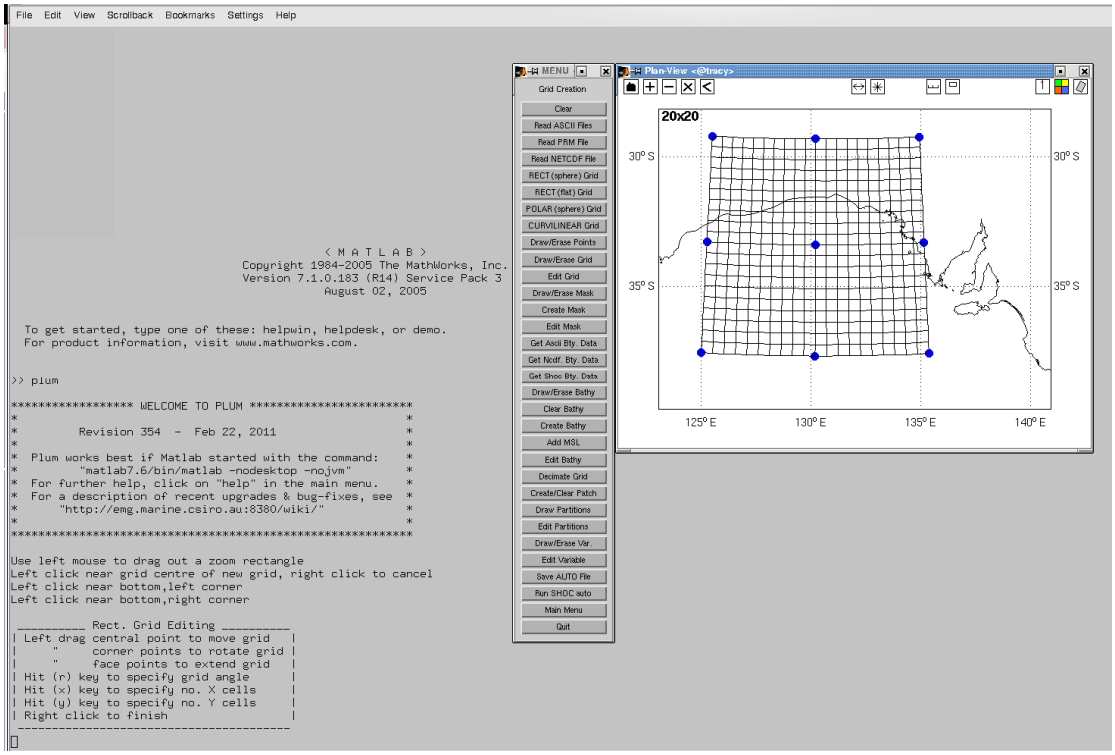


Figure 14.3.2. Geographic rectangular grid of the Great Australian Bight.

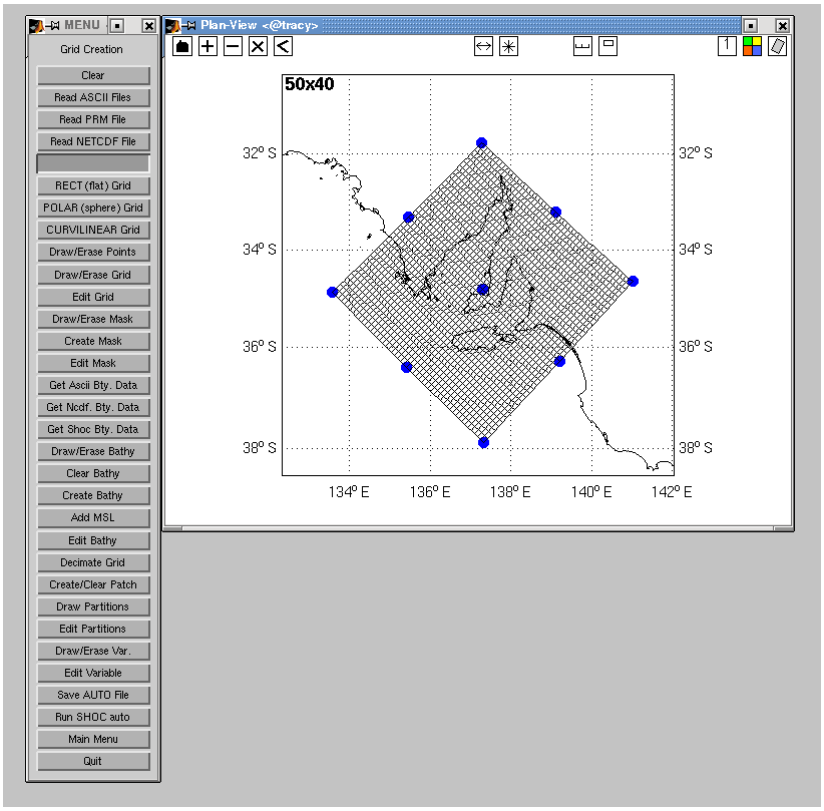


Figure 14.3.3. Geographic rectangular grid of the South Australian Gulfs.

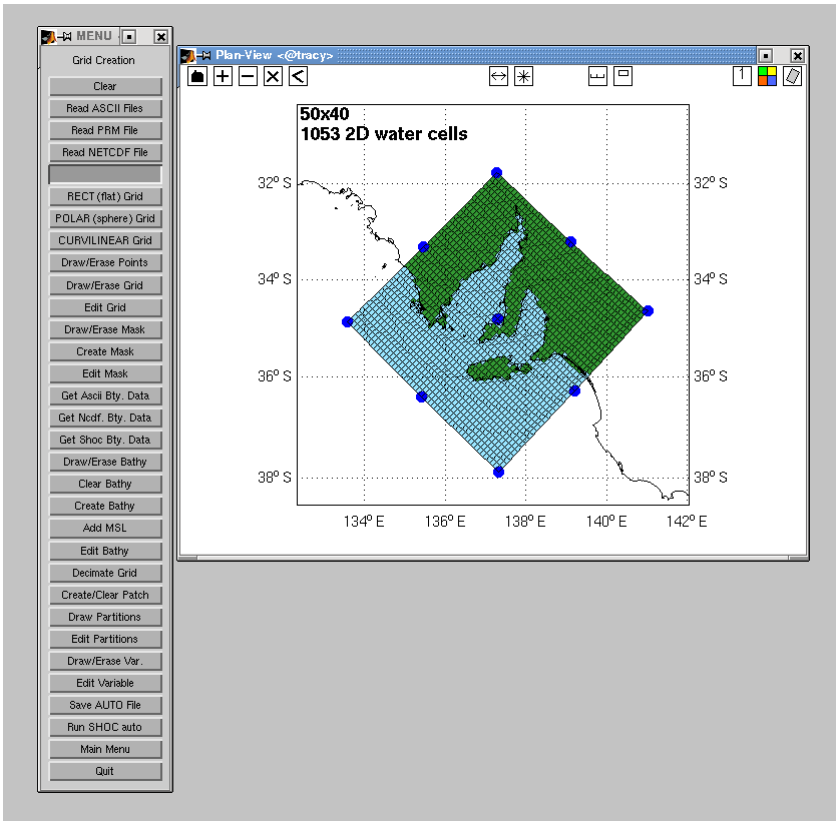
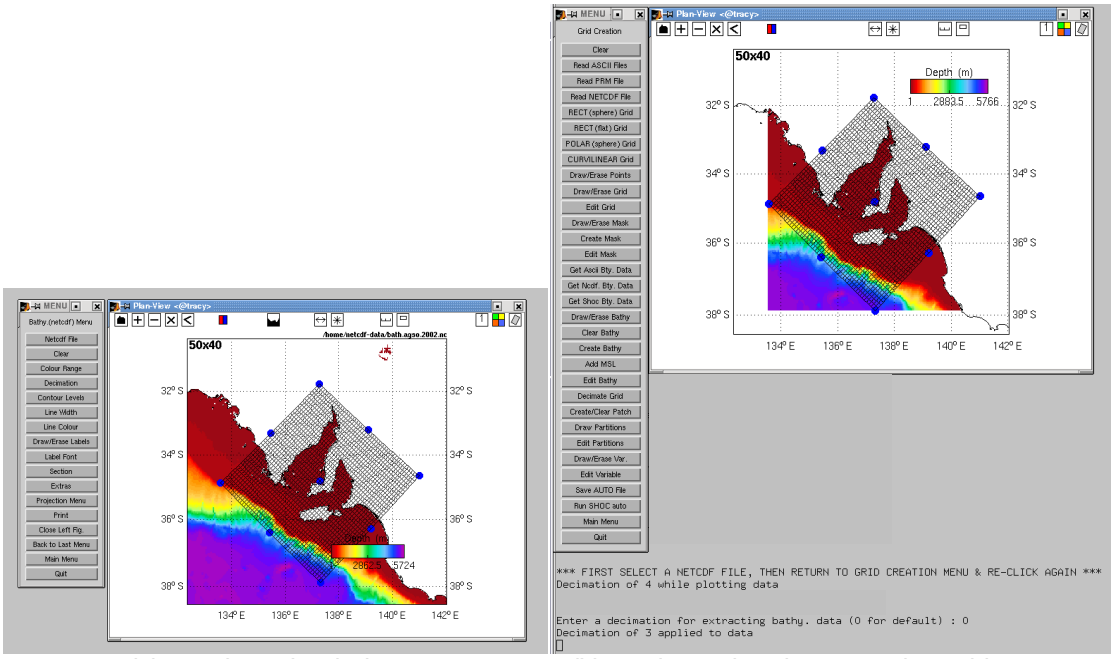


Figure 14.3.4. Masked image of the South Australian Gulfs.



(a) Database loaded (b) Decimated and truncated to grid

Figure 14.3.5. Bathymetry loaded onto the South Australian Gulfs.

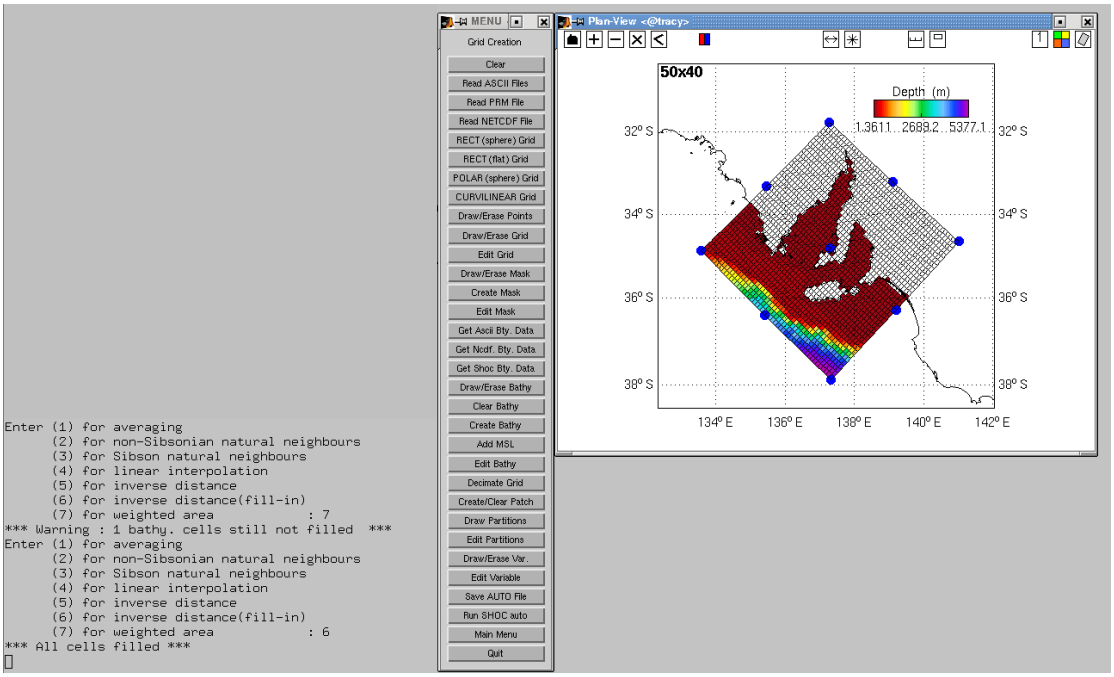
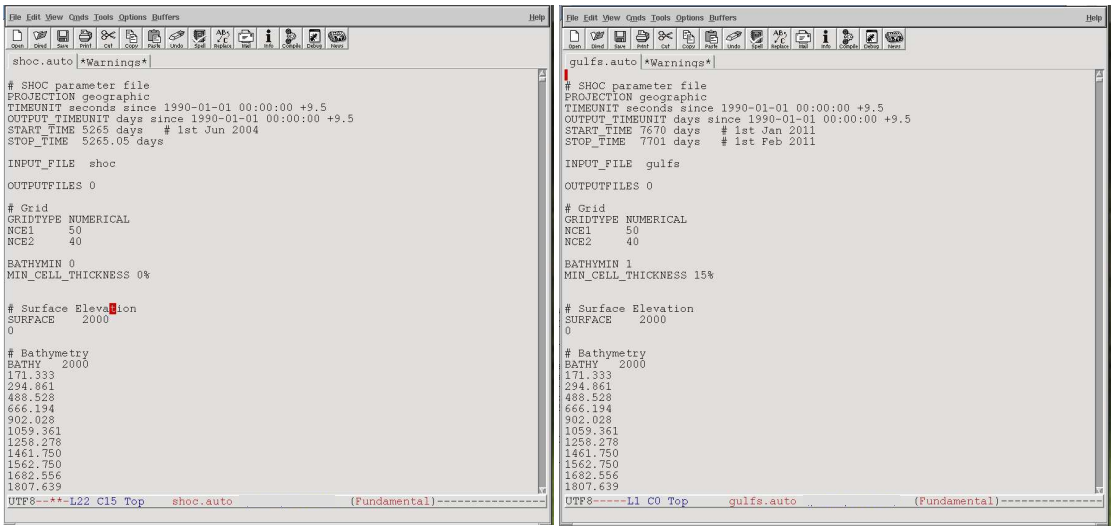


Figure 14.3.6. Bathymetry interpolated onto the South Australian Gulfs.

6. Create a SHOC auto file. Click on 'Save AUTO file' to create an auto file (Section 5) suitable for generating a full parameter file and netCDF input file. The auto file will be saved to `shoc.auto`. This file should be edited before invoking the `-a` option to modify the `START_TIME` and `STOP_TIME` to the start and end times desired, `INPUT_FILE` should be changed to a unique name and `BATHYMIN` and `MIN_CELL_THICKNESS` should be set to desired values. The original shoc.auto is shown in Figure 14.3.7 (a), and the modified file in 14.3.7 (b), now renamed to `gulfs.auto`. Additionally, any optional parameterisations outlined in Section 5 may be added at this stage, e.g. if the model forcing, initial conditions or boundary data are known, they may be included and will be propagated into the parameter file generated by the `-a` option. Alternatively, this generated parameter file may be edited to include forcing and initial conditions. The parameter file (`gulfs.prm`) and input file (`gulfs.nc`) may then be generated using:

```
shoc -ag gulfs.auto
```



(a) Original file from PLUM (b) Modified file

Figure 14.3.6. Parameter files for the South Australian Gulfs.

7. Edit the parameter file `gulfs.prm`. This generally includes initial condition data for temperature, salinity and surface elevation, surface fluxes (wind, pressure, heatflux and saltflux) and specification of open boundary conditions. For example, if BLUElink data were available where the file `jan2011_ets.nc` contained the variables `temp`, `salt` and `eta`, the file jan2011_uv.nc contained 3D velocities u and v and ACCESS-A data `jan2011_met.nc` were available containing variables `pressure`, u and v, then `gulfs.prm` may be modified thus:

In the tracer list add (see Section 4.9);

```
TRACER0.data            jan2011_ets.nc
and
TRACER1.data            jan2011_ets.nc
```

Surface initial condition (see Section 4.12);

```
SURFACE           jan2011_ets.nc
```

Wind and pressure forcing (see Section 4.13 & 4.14);

```
WIND_TS           jan2011_met.nc
WIND_INPUT_DT     10 minutes
WIND_SPEED_SCALE  1.0
DRAG_LAW_V0       10.0
DRAG_LAW_V1       26.0
DRAG_LAW_CD0      0.00114
DRAG_LAW_CD1      0.00218

PRESSURE          jan2011_met.nc
PRESSURE_INPUT_DT 10 minutes
```

Open boundary forcing (see Section 4.10.7 & 4.10.17);

```
NBOUNDARIES             3

BOUNDARY0.NAME          West
BOUNDARY0.TYPE          u1
BOUNDARY0.BCOND_NOR     CUSTOM
BOUNDARY0.CUSTOM.u1     uv_to_u1  jan2011_uv.nc
BOUNDARY0.BCOND_TAN     CUSTOM
BOUNDARY0.CUSTOM.u2     uv_to_u2  jan2011_uv.nc
BOUNDARY0.BCOND_ELE     NOTHIN|FILEIN
BOUNDARY0.BCOND_salt    UPSTRM
BOUNDARY0.BCOND_temp    UPSTRM
BOUNDARY0.ADJUST_FLUX   200 seconds     # ~ 0.2 x DT
BOUNDARY0.DATA          jan2011_ets.nc
BOUNDARY0.RANGE         (0,0)-(0,14)

BOUNDARY1.NAME          East
BOUNDARY1.TYPE          u1
BOUNDARY1.BCOND_NOR     CUSTOM
BOUNDARY1.CUSTOM.u1     uv_to_u1  jan2011_uv.nc
BOUNDARY1.BCOND_TAN     CUSTOM
BOUNDARY1.CUSTOM.u2     uv_to_u2  jan2011_uv.nc
BOUNDARY1.BCOND_ELE     NOTHIN|FILEIN
BOUNDARY1.BCOND_salt    UPSTRM
BOUNDARY1.BCOND_temp    UPSTRM
BOUNDARY1.ADJUST_FLUX   200 second
BOUNDARY1.DATA          jan2011_ets.nc
BOUNDARY1.RANGE         (50,0)-(50,23)
```

```
BOUNDARY2.NAME          Offshore
BOUNDARY2.TYPE          u2
BOUNDARY2.BCOND_NOR     CUSTOM
BOUNDARY2.CUSTOM.u1     uv_to_u1  jan2011_uv.nc
BOUNDARY2.BCOND_TAN     CUSTOM
BOUNDARY2.CUSTOM.u2     uv_to_u2  jan2011_uv.nc
BOUNDARY2.BCOND_ELE     NOTHIN|FILEIN
BOUNDARY2.BCOND_salt    UPSTRM
BOUNDARY2.BCOND_temp    UPSTRM
BOUNDARY2.ADJUST_FLUX   200 seconds
BOUNDARY2.DATA          jan2011_ets.nc
BOUNDARY2.RANGE         (0,0)-(49,0)
```

If a tide is required to be included using the CSR tide model, then set `TIDE_CSR_CON_DIR` to the nodal correction directory, and `TIDE_CSR_ORTHOWEIGHTS` to the orthoweight database (see Section 4.10.20) and use the elevation boundary condition:

```
BOUNDARY0.BCOND_ELE     NOTHIN|FILEIN|TIDALH
```

Numerous other parameters may be edited in the file gulfs.prm to suit the application (e.g. `PARAMETERHEADER`, `DESCRIPTION`, `NAME`, netCDF output files (Section 4.31.6), time series output (Section 4.31.5), `WINDOWS` (Section 4.2), horizontal friction (Section 4.22), turbulence closure (Section 4.21), `HEATFLUX` (Section 4.17) or diagnostics (Section 4.30). The example here is the minimum required to set up a simulation, and many alternative parameterisations or options may be invoked as described in this manual. Note that the parameterisation demonstrated here does not guarantee model stability, and parameters or schemes may require alteration to achieve a stable model run. Describing the process of stability analysis is beyond the scope of this manual. Once a satisfactory parameter file is created, the input file must be re-created so that the specified initial conditions are included:

```
rm gulfs.nc
shoc –g gulfs.prm gulfs.nc
```

It is good practice to view `gulfs.nc` graphically to ensure initial conditions and bathymetry are satisfactory. The resolution of this example is ~9.5 x 12.2 km with maximum depth of ~5400 m resolved by 52 layers.

8. Run the simulation;

```
shoc –p gulfs.prm
```

Any warnings encountered during setup are written to the file `runlog`, model progress is written to `diag.txt` and the model parameterisation as used internally by the model is listed in `setup.txt` (see Section 4.32). It is good practice to view the setup.txt file to ensure the model configuration is as expected. Output may be vied using PLUM, or a similar java based application DIVE (see http://www.emg.cmar.csiro.au/www/en/emg/software/Visualization.html).
The process of stability analysis, sensitivity analysis and calibration may now commence.

15 Sediment Transport

The sediment transport routines may be fully coupled to SHOC by invoking:

```
DO_SEDIMENTS       YES
```

or

```
DO_SEDIMENTS       DO
```

Additionally, a sediment layer structure must be defined for sediments transport to operate, e.g;

```
NSEDLAYERS  4      # The number of sediment layers
0.005              # Depth in the sediment of the 1st layer face
0.020              # Depth in the sediment of the 2nd layer face
0.080              # Depth in the sediment of the 3rd layer face
0.320              # Depth in the sediment of the 4th layer face
```

The tracer list must also include a number of sediment fractions, with corresponding attributes (e.g. particle size, settling velocity etc.) defined. There are also a number of global parameters that must be defined; see the Sediment Transport User Guide for a full explanation. The sediment transport parameters and tracer attributes can be automated, where a set of user defined defaults are used in preference to a fully defined specification in the parameter file. This involves defining the tracer sediment classes that are to be used, the attributes that will be defined for those tracers, and the global parameters used for the sediment transport. The sediment tracer classes are defined using:

```
SED_VARS     <class1> <class2> ... <class_n>
```

Where `<class_n>` is the name of the sediment class the user wishes to be include. These classes are hardwired into the sediment interface module (`sediments/sediments.c`) and can be expanded as desired. Currently, the classes consist of;

```
Gravel
Sand
Mud
FineSed
Dust
```

SHOC will check if the classes defined in `SED_VARS` are included in the list of hardwired names, and if so then will automatically include that tracer in the tracer list. Additionally, a 3D diagnostic tracer named `tss` is automatically generated, and 2D tracers named `ustrcw_skin` and `depth_sed`. Again, these additional tracers are hardwired into `sediments/sediments.c` and can be expanded as desired. The sediment tracer attributes associated with these tracer classes are defined using:

```
SED_VARS_ATTS      <specification_name>
```

Where `<specification_name>` is the name of a default set of attributes the tracers will be assigned to. These default attributes are hardwired to the tracers in `sediments/sediments.c` and can be expanded as desired. Currently the default sets available are:

```
standard    # standard set of attributes
estuary     # Attributes applicable to an estuarine environment
```

If any of the tracer classes are explicitly defined in the tracer list, then any attributes associated with that tracer takes precedence over the defaults defined by SED_VARS_ATTS. Furthermore, and tracer attribute can be defined in the parameter file using:

```
TRACER<m>.attname
or
<name>.attname
```

Where <m> is the tracer number in the list, attname is the tracer attribute name (see the MecoSed Users Guide for a list of attribute names) and <name> is the name of the tracer, e.g.

```
Mud.svel    -0.0001     # Redefine the settling velocity for Mud
```

Various sediment parameters may be spatially varying (e.g. settling velocity). If the settling velocity attribute is the name of a 2D tracer in the tracer list, then the values of that tracer will be used as the settling velocity. In automated mode, if a 2D tracer is found in the tracer list with the name of a sediment tracer class appended with _svel (e.g. Mud_svel, Sand_svel), then that 2D tracer's values will be used as the settling velocity for that sediment tracer class, e.g. Mud may be spatially variable if a 2D tracer exists with the name Mud_svel, or, for example, if a 2D tracer exists with the name settling_mud and the settling velocity attribute for Mud is redefined as;

```
Mud.svel          settling_mud
```

The global sediment transport attributes are defined in automated mode using;

```
SEDFILE           <param_filename>
```

Where <param_filename> may be:

1. The name of a file containing the global parameters,
2. A default name for hardwired parameters. Currently the names standard and estuary are accepted. The initialisation of these parameters exists in model/lib/sediments/sed_init.c and may be expanded as desired,
3. auto, where the parameters may be dynamically prescribed in the routine sed_params_auto() in model/lib/sediments/sed_init.c. Currently this routine is empty.
4. If none of the above are specified, the parameters are assumed to be listed in the main parameter file.

The sediment specification is written in full in the diagnostic file setup.txt (see Section 4.31). If a transport parameter file is generated from a full parameter file using TRANS_DATA (see Section 9) then the sediment specification is also written to this file. Outputting these sediment specifications may be invoked without running the full sediment transport by using;

```
DO_SEDIMENTS      WRITE
```

16 Ecology

The ecology routines may be fully coupled to SHOC by invoking:

```
DO_ECOLOGY  YES
```

or

```
DO_ECOLOGY  DO
```

Additionally, a sediment layer structure must be defined for ecology to operate, (see Section 15).

Ecology also requires a process definition and a parameter specification. These are defined via:

```
processfname      <processes>     # name of ecology processes
```

The name <process> may be one of the following:

```
<filename>
standard
estuary
auto
```

If <filename> is specified, then the BGC processes are defined in a file bearing that name. If defaults is specified, then the processes are hardwired into the module process_defaults.c in the ecology library. Additional process lists may be included in this module, with associated modifications to the calling routines get_eco_processes() in process_defaults.c and read_process_group_from_defaults() in ecology.c. Additionally, there is scope to define processes dynamically using the (currently empty) routine eco_process_auto() in process_defaults.c. This dynamical specification is invoked if auto is specified for <processes>.

The ecological parameters are specified using:

```
biofname          <parameters>    # name of ecology parameters
```

The name <parameters> may be one of the following:

```
<filename>
standard
estuary
auto
```

If <filename> is specified, then the BGC parameters are defined in a file bearing that name. If default is specified, then the processes are hardwired into the module parameter_defaults.c in the ecology library. Additional parameter lists may be included in this module, with associated modifications to the calling routine get_eco_params() in parameter_info.c. Additionally, there is scope to define processes dynamically using the (currently empty) routine eco_params_auto() in parameter_info.c. This dynamical specification is invoked if auto is specified for <parameters>.

Note that the default parameters include hardwiring of the phytoplankton growth rates that have traditionally been specified as netcdf files. It is no longer necessary to supply this netcdf file, just specifying the name '10pplkINP' or '10benINP' is sufficient.

If a tracer list of the tracers required for the ecology processes is not explicitly specified, then these tracers will be automatically generated based on the defined processes. The attributes for these tracers are defined using:

```
ECO_VARS_ATTS     <attributes>      # name of tracer attribute set
```

The name <attributes> may be one of the following:

```
standard
estuary
```

If standard is specified, then the attributes for all possible ecology tracers are hardwired into the routine eco_defaults_standard() in /hd/ecology/ecology.c and can be expanded as desired by creating additional attribute routines and adding them to the calling function eco_set_tracer_defaults() in the same module. Note that a list of all possible ecology tracer names and long names (water column/sediment and benthic) must be maintained in the structures ECONAME3D and ECONAME2D in ecology.c in order for tracer automation to operate correctly.

If any of the tracer classes are explicitly defined in the tracer list, then any attributes associated with that tracer takes precedence over the defaults defined by ECO_VARS_ATTS. Furthermore, any tracer attribute can be defined in the parameter file using:

```
TRACER<m>.attname
or
<name>.attname
```

Where <m> is the tracer number in the list, attname is the tracer attribute name and <name> is the name of the tracer, e.g.

```
PhyL_N.svel -4e-6 # Redefine the settling velocity for large
                  # phytoplankton nitrogen.
```

The ecology specification is written in full in the diagnostic file setup.txt (see Section 4.31). If a transport parameter file is generated from a full parameter file using TRANS_DATA (see Section 9) then the ecology specification is also written to this file. Outputting these ecology specifications may be invoked without running the full sediment transport by using;

```
DO_ECOLOGY  WRITE
```

Ecology requites a LIGHT variables, which historically was a daily mean but with newer versions of the ecology processes can be a copy of short wave radiation (i.e. diurnally variable). This can be input via file:

```
LIGHT             light.nc
LIGHT_INPUT_DT    1 hour
ALBEDO_LIGHT      0.0
```

LIGHT can point to a tracer which reads LIGHT via the reset function, e.g.

```
LIGHT             inlight
LIGHT_INPUT_DT    1 hour
ALBEDO_LIGHT      0.0
```

with

```
TRACER?.name      inlight
TRACER?.name      Light input from swr
```

```
TRACER?.units           W m-2
TRACER?.type            WC2D
TRACER?.fill_value      0.0
TRACER?.valid_range     0.0   2000.0
TRACER?.reset_file      swr.nc
TRACER?.reset_dt        1 hour
```

If `swr` is included in the transport files, then `LIGHT` can be read from this variable along with all other transport variables using;

```
LIGHT             file
```

17 Troubleshooting

Bathymetry altered on successive input file generations :

The bathymetry written to the input file using the –g option is modified from that read in from the parameter file by the BATHYMIN, BATHYMAX and MIN_CELL_THICKNESS parameters. If the input file bathymetry is to be modified (using jvismeco) and used in a successive parameter file, make sure the abovementioned parameters are set to zero, a very large value and zero respectively. Note also that the SMOOTHING option will also have this effect.

Heat flux increasing with time :

Using the HEATFLUX = NET_HEAT with a HEATFLUX_FILE_INPUT_DT > DT (3D time-step) in conjunction with a RADIATION file (SWR_ATTENUATION > 0, SWR_TRANSMISSION > 0) will result in the heatflux increased by the surface short wave contribution during the period HEATFLUX_FILE_INPUT_DT. Set HEATFLUX_FILE_INPUT_DT = DT to overcome this effect.

Model crashes :

Check that momsc = ORDER2. SHOC is a second order model in time and space and 1st order momentum schemes have proved consistently unsuccessful.

Negative variable values inexplicably appear in output :

Set bytespervalue in the output file to 4. Using short representation of output may make very large or small values wrap bits and become negative. Use double representation to avoid this.

Open boundaries appear as OUTSIDE cells :

Each u1 or u2 open boundary should be associated with a FRONT, BACK, LEFT or RIGHT edge. If an open boundary cell location list contains both FRONT and BACK, or LEFT and RIGHT edge cells then they will be masked as OUTSIDE.

Output file does not record further dumps :

Check that the 2.0 Gb limit for output files has not been exceeded.

Reading parameter file difficulties :

Check that no white space, tabs or ^M exists after entries in the parameter file.

River open boundaries aren't advecting tracers :

Make sure there are at least 3 wet cells in the normal direction to the open boundary, or change the boundary condition for tracers from UPSTRM to FILEIN. The UPSTRM condition uses a velocity one cell into the interior of the domain to reflect dynamics occurring in the interior rather than the prescribed boundary dynamics when solving the 1 dimensional advection equation that constitutes the UPSTRM condition. If this interior cell falls on a solid boundary (i.e. only 2 wet cells exist normal to the boundary) then the velocity will be zero and tracer concentration will not change due to the UPSTRM condition.

Segmentation fault using –g option :

(a) Open boundaries in the inside of the domain (i.e. open boundaries not on the edges of the grid) must be adjacent to 'outside' cells. Check that interior open boundaries are adjacent to outside cells using jvismeco.

(b) Solid boundaries on the edge of the grid. SHOC requires a land cell to surround all wet cells, even along the edges of the grid. This is so that there exists a ghost cell location adjacent to each wet cell for setting lateral boundary conditions.

When to re-make an input file using the –g option :

The input netCDF file must be re-generated if changes are made to the bathymetry list, the number of layers or layer spacings used, data used for tracer initialisation, `BATHYMIN`, `BATHYMAX`, `MIN_CELL_THICKNESS`, `SMOOTHING`.

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