## Frehg User Manual

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#### Introduction

Fine Resolution Environmental Hydrodynamic and Groundwater model (Frehg)

#### Existing capabilities:

- Simulate 2D depth-integrated shallow water flow with wetting/drying and complex topography
- Simulate 3D variably-saturated subsurface flow
- Simulate coupled 2D surface and 3D subsurface flow
- Simulate simple advective-diffusive transport of passive scalars

#### Pre-requisite

- **laspack** for solving linear systems (http://www.mgnet.org/mgnet/Codes/laspack/html/node2.html)
- **gcc** or other C-compiler
- mpich for message passing

#### Start a simulation

In the frehg directory:

Create an input folder to put model input data (e.g. ex1\_input)
Create an output folder for saving model outputs (e.g. ex1\_output)
Customize user setting file (named **input** by default), where:

- sim\_id = Simulation ID. User can define case-specific settings in the source code by referring to certain sim\_id
- finput = Directory of input data (e.g. ex1\_input/)
- foutput = Directory of output data (e.g. ex1\_output/)

Compile the code by typing **make** in terminal

Execute simulation by typing ./frehg in terminal

If in parallel mode, execute by typing mpiexec - np N ./frehg (N = total number of subprocesses)

### Surface domain

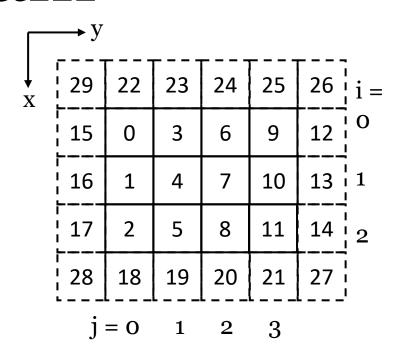
Set sim\_shallowwater = 1 to activate surface flow
Set difuwave = 1 to use the diffusive wave approximation
Surface domain is characterized by:

- NX = number of grids in x direction (i-index)
- **NY** = number of grids in y direction (j-index)
- dx = grid resolution in x direction [m]
- **dy** = grid resolution in y direction [m]

Use the 2D domain on the right side for illustration:

- NX = 3, NY = 4, ghost cells are added along the boundaries
- Variables are stored in allocated 1D arrays
  - Numbers in the cells represent 1D array indices
  - A map is built for conversion between 1D/2D indices (named **smap** in the source code)
  - The map also stores the connections between grid cells

Set bath\_file = 1 to read bathymetry from a **bath** file, otherwise bottom elevation is zero all over the domain



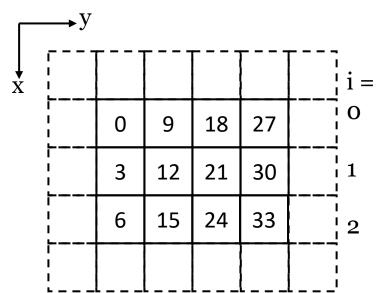
## Subsurface domain

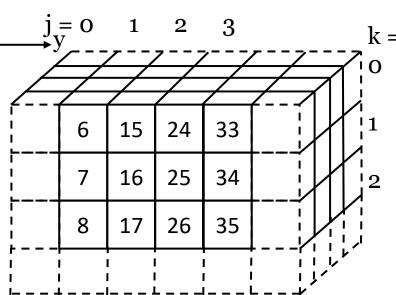
Set sim\_groundwater = 1 to activate subsurface flow Subsurface domain is characterized by:

- botZ = bottom elevation of the domain [m]
- dz = grid resolution in z direction [m]
- dz\_incre = used to create non-uniform z-discretization (not implemented for the current version)

Use the 3D domain on the right side for illustration:

- NX = 3, NY = 4, NZ = 3
- Ghost cells are added (not indexed) along the boundaries
- Variables are stored in allocated 1D arrays
  - Numbers in the cells represent 1D array indices
  - A map is built for conversion between 1D/3D indices (named **gmap** in the source code)
  - The map also stores the connections between grid cells





### Simulation control

Parallelization (set <u>use\_mpi = 1</u>):

- mpi\_nx = number of threads in x direction (must be a factor of NX)
- mpi\_ny = number of threads in y direction (must be a factor of NY)

#### Time control:

- dt = time step size [sec]
- Tend = end time [sec]
- dt\_out = output frequency [sec]

If sim\_groundwater = 1, variable dt is allowed by setting dt\_adjust = 1. Simulation will start from dt and self-adjust between dt\_min and dt\_max:

- dt\_max = maximum dt [sec]
- dt\_min = minimum dt [sec]
- Co\_max = maximum Courant number for subsurface solver

Then dt is adjusted using the water content + Courant number criteria as described in [3]

## Surface domain – IC

Initial conditions for surface flow includes:

- init\_eta = initial surface elevation [m]
- init\_tide = initial tidal elevation at the tidal boundary [m]. This is used when surface elevation at a boundary is a constant.

Spatially-variable initial conditions can be read from file:

- eta\_file = 1 reads file **surf\_ic** from finput folder, which contains cell-by-cell initial surface elevation values in the order of the 1D array
- uv\_file = 1 reads file uu\_ic and vv\_ic from finput folder, which contains cell-by-cell initial velocities in the order of the 1D array
  - If uv\_file = 0, initial velocities are zero
- When restarting a simulation, the user should copy simulated surface elevation and velocities from foutput into finput, rename them to **surf\_ic**, **uu\_ic** and **vv\_ic**, then set eta\_file and **uv\_file** to 1.

## Surface domain – tide

Set tidal boundary condition (or Dirichlet-type BC in general):

- bctype\_SW = type of boundary conditions used for x-minus, x-plus, y-minus and y-plus boundaries
  - e.g. bctype\_SW = 0,0,0,1 indicates Dirichlet BC for y-plus boundary and no flux BC for other boundaries
- n\_tide = total number of tidal boundaries used
- tide\_locX = start, end x-indices of each tidal boundary (when simulating in parallel, this is the global indices)
- tide\_locY = start, end y-indices of each tidal boundary
- tide\_file = 1 reads time-variable tidal elevations from file tideN
   (e.g. tide1), otherwise tidal elevation is fixed at init\_tide
- tide\_dat\_len = number of time-variable tide data points to be read For example, if tidal BC is enforced for cell 10 in the right figure:
- bctype $\_SW = 0.0.01$
- $tide_locX = 1,1$
- tide\_locY = 3.3

29	22	23	24	25	26	i =
15	0	3	6	9	12	0
16	1	4	7	10	13	1
17	2	5	8	11	14	2
l 28	18	19	20	21	27	   

### Surface domain – inflow

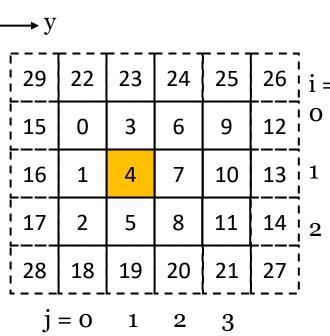
Set inflow boundary condition (or source/sink terms in general):

- inflow\_locX/locY = x-start, x-end, y-start, y-end indices where inflow BC is applied, which is similar to how tide location is defined.
- n\_inflow = total number of inflow BC to be applied
- inflow\_file = 1 if time—variable inflow data is to be read
- init\_inflow = constant inflow rate [m^3/s], which is used when inflow\_file
   0

For example, if inflow BC is enforced for cell 4 in the right figure:

- $inflow_locX = 1,1$
- $Inflow_locY = 1,1$

If inflow\_loc contains N grid cells, inflow rate for each cell is (assume constant) init\_inflow/N



### Surface domain – rainfall

Set evaporation/rainfall boundary conditions:

- evap\_file = 1 if time—variable evaporation data is to be read
- q\_evap = constant evaporation rate [m/s], which is used when evap\_file = o
- rain\_file = 1 if time—variable rainfall data is to be read
- q\_rain = constant rainfall rate [m/s], which is used when rain\_file = 0 Evaporation from the subsurface domain:
- evap\_model = 1 if aerodynamic evaporation model is applied to estimate moisture-dependent evaporation rate on dry surface. Otherwise evaporation only occurs on wet surface.

In the current version, evaporation/rainfall have to be applied to the entire domain. Both evaporation and rainfall rates should be positive here.

## Surface domain – wind

#### Set wind stress over wet surface:

- sim\_wind = 1 if wind effect is modeled
- wind\_file = 1 if time-variable wind speed and direction are read from data files (this function is not implemented yet, so set wind\_file = 0 for now)
- init\_windspd = wind speed [m/s]
- init\_winddir = direction of wind [degrees] measured clockwise from the "north" direction
- north\_angle = direction of "north" direction measured clockwise from the -x direction
- Cw = wind drag coefficient
- CwT = decay rate of wind stress within the thin-layer [1]

## Surface domain – parameters

Set model parameters for the surface domain:

- grav = gravitational constant [m/s^2]
- viscx, viscy = eddy viscosity [m^2/s] (currently version only supports constant eddy viscosity)
- min\_dept = minimum depth below which a grid cell is considered as dry [m]
- manning = Manning's roughness coefficient
- wtfh = minimum depth to trigger the waterfall model [1]. In the current version, the waterfall model is disabled
- hD = depth below which drag coefficient is increased to avoid instability [1]
- rhoa = air density [kg/m<sup>3</sup>]
- $rhow = water density [kg/m^3]$

### Subsurface domain – IC

#### Initial conditions for subsurface flow includes:

- init\_wc = initial water content. If init\_wc is between saturated and residual water content, the domain will be initialized with constant init\_wc
- init\_h = initial pressure head [m]. If init\_wc is out of range and init\_h is not positive, the domain will be initialized with constant init\_h
- init\_wt\_rel = initial water table relative to the topography [m] (must be positive). If neither init\_wc nor init\_h is used, a water table init\_wt\_rel m below topography will be set. Regions below the water table is fully saturated.
- init\_wt\_abs = initial water table [m]. If none of the above 3 settings is invoked, initial water table is located at init\_wt\_abs, which means a non-terrain-following water table is used.
- h\_file = 1 if element-by-element initial head values is to be read from a file named head\_ic.
- wc\_file = 1 if element-by-element initial water content values is to be read from a file named **moisture\_ic**.

### Subsurface domain – BC

Boundary conditions for subsurface flow is set by:

- bctype\_GW = type of boundary conditions used for x-minus, x-plus, y-minus, y-plus, z-minus(bottom), z-plus(top) boundaries, possible values are:
  - o = no flow
  - 1 = constant head (Dirichlet type)
  - 2 = constant flux (Neumann type)
  - 3 = free drainage (only used for bottom boundary)
  - When simulating surface-subsurface exchange, the top boundary cells with positive surface depth will automatically switch to Dirichlet condition.
- qtop = flux at top boundary [m/s]
- qbot = flux at bottom boundary [m/s]
- htop = head at top boundary [m]
- hbot = head at bottom boundary [m]

Note that qtop and qbot are positive if upward, negative otherwise. If  $bctype\_GW[5] = 2$  and net infiltration exists (evaporation+rainfall is downward), infiltration becomes surface ponding and BC is Dirichlet type. If net exfiltration exists, exfiltration rate is used as qtop.

## Subsurface settings

- use\_corrector = 1 activates the explicit corrector step [3], otherwise only the head form of the Richards equation is solved, which is non-conservative in the unsaturated zone
- post\_allocate = 1 activates the post-allocation step [3]
- use\_full3d = 1 activates 3D post-allocation, otherwise post-allocation is only 1D in the vertical direction. For large domain where horizontal mesh size >> vertical mesh size, set use\_full3d = 0 is sufficient.
- use\_mvg = 1 activates the modified Mualem-van Genutchen model [3], which allows larger dt than the original van Genutchen model
  - aev = air entry value when using the MVG model [m]

# Subsurface parameters

- Ksx, Ksy, Ksz = saturated hydraulic conductivities in x, y, z directions [m/s]
- Ss = specific storage [1/m]
- soil\_a = alpha parameter in the van Genutchen model
- soil\_n = n parameter in the van Genutchen model
- wcs = saturated water content
- wcr = residual water content

## Scalar transport

The current version of frehg only simulates advective-diffusive transport of passive scalars.

- n\_scalar = total number of scalars to be modeled
- difux/difuy/difuz = molecular diffusivities of the scalars.
- disp\_lon/disp\_lat = longitudinal/transverse dispersivity in the subsurface domain
- scalar\_surf\_file = 1 if initial surface scalar concentration is to be read from a file named scalar\_surf\_icN, where N represents the index of the scalar.
- init\_s\_surf = initial scalar concentration for the surface domain, which is used if scalar\_surf\_file = o
- scalar\_subs\_file = 1 if initial subsurface scalar concentration is to be read from a file named scalar\_subs\_icN, where N represents the index of the scalar.
- init\_s\_subs = initial scalar concentration for the subsurface domain, which is used if scalar\_subs\_file = 0

## Scalar transport

The current version of frehg only simulates advective-diffusive transport of passive scalars.

- scalar\_tide\_file = 1 if time-variable scalar concentration for tide is to be read from a file named scalarN\_tideM, where N is the index of scalar and M is the index of the tide.
- scalar\_tide\_datlen = number of time-variable scalar data points to be read from the scalarN\_tideM file.
- s\_tide = constant scalar concentration for tide, which is used when scalar\_tide\_file = o
- scalar\_inflow\_file = 1 if time-variable scalar concentration for inflow is to be read from a file named scalarN\_inflowM, where N is the index of scalar and M is the index of the tide.
- scalar\_inflow\_datlen = number of time-variable scalar data points to be read from the scalarN\_inflowM file.
- s\_inflow = constant scalar concentration for tide, which is used when scalar\_inflow\_file = o

#### References

[1] **Li, Z.** and Hodges, B.R., 2019, Model instability and channel connectivity for 2D coastal marsh simulations, *Environ Fluid Mech*, (19): 1309,

https://doi.org/10.1007/s10652-018-9623-7

[2] **Li**, **Z**. and Hodges, B.R., 2019, Modeling subgrid-scale topographic effects on shallow marsh hydrodynamics and salinity transport, Advances in Water Resources, (129) 1-15, <a href="https://doi.org/10.1016/j.advwatres.2019.05.004">https://doi.org/10.1016/j.advwatres.2019.05.004</a>

[3] **Li, Z.,** Ozgen, I. and Maina, F.Z., 2020, A mass-conservative predictor-corrector solution to the 1D Richards equation with adaptive time control, Journal of Hydrology, (592)125809, <a href="https://doi.org/10.1016/j.jhydrol.2020.125809">https://doi.org/10.1016/j.jhydrol.2020.125809</a>